Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 11:21 AM EDT

PDB ID	:	3KOX / pdb_00003kox
Title	:	Crystal Structure of ornithine 4,5 aminomutase in complex with 2,4-diaminobutyrate (Anaerobic)
Authors	:	Wolthers, K.R.; Levy, C.W.; Scrutton, N.S.; Leys, D.
Deposited on	:	2009-11-14
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

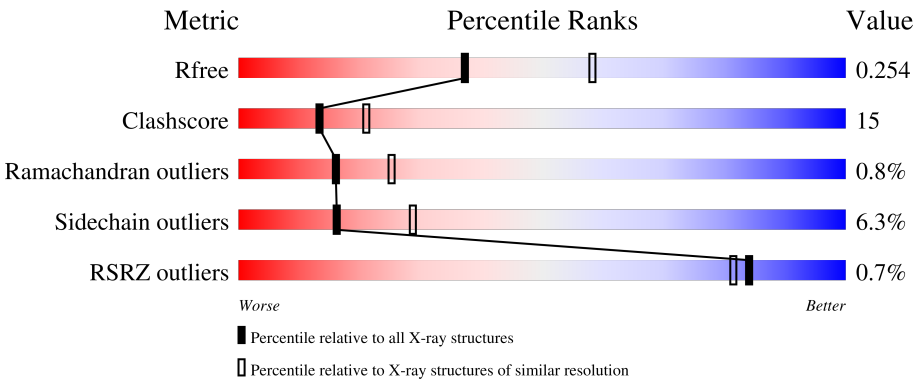
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	763	2%, 70%, 23%, • 5%
1	B	763	71%, 22%, • 5%
1	C	763	68%, 24%, • 5%
1	D	763	71%, 21%, • 5%
2	E	121	69%, 19%, • 10%

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Mol	Chain	Length	Quality of chain
2	F	121	% 64% 26% 10%
2	G	121	66% 22% • 10%
2	H	121	% 74% 15% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	B12	A	1801	X	-	-	-
3	B12	B	1801	X	-	-	-
3	B12	C	1801	X	-	-	-
4	5AD	A	1500	X	-	-	-
4	5AD	D	1500	X	-	-	-
5	Z98	A	767	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 27379 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called D-ornithine aminomutase E component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	728	5651	3561	981	1075	34	0	0	0
1	B	728	5672	3579	984	1075	34	0	0	0
1	C	728	5654	3570	981	1069	34	0	0	0
1	D	728	5664	3575	984	1071	34	0	0	0

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
A	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
A	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
A	744	SER	-	expression tag	UNP Q8VPJ5
A	745	GLU	-	expression tag	UNP Q8VPJ5
A	746	ASP	-	expression tag	UNP Q8VPJ5
A	747	PRO	-	expression tag	UNP Q8VPJ5
A	748	ASN	-	expression tag	UNP Q8VPJ5
A	749	SER	-	expression tag	UNP Q8VPJ5
A	750	SER	-	expression tag	UNP Q8VPJ5
A	751	SER	-	expression tag	UNP Q8VPJ5
A	752	VAL	-	expression tag	UNP Q8VPJ5
A	753	ASP	-	expression tag	UNP Q8VPJ5
A	754	LYS	-	expression tag	UNP Q8VPJ5
A	755	LEU	-	expression tag	UNP Q8VPJ5
A	756	ALA	-	expression tag	UNP Q8VPJ5
A	757	ALA	-	expression tag	UNP Q8VPJ5
A	758	ALA	-	expression tag	UNP Q8VPJ5
A	759	LEU	-	expression tag	UNP Q8VPJ5
A	760	GLU	-	expression tag	UNP Q8VPJ5
A	761	HIS	-	expression tag	UNP Q8VPJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	762	HIS	-	expression tag	UNP Q8VPJ5
A	763	HIS	-	expression tag	UNP Q8VPJ5
A	764	HIS	-	expression tag	UNP Q8VPJ5
A	765	HIS	-	expression tag	UNP Q8VPJ5
A	766	HIS	-	expression tag	UNP Q8VPJ5
B	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
B	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
B	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
B	744	SER	-	expression tag	UNP Q8VPJ5
B	745	GLU	-	expression tag	UNP Q8VPJ5
B	746	ASP	-	expression tag	UNP Q8VPJ5
B	747	PRO	-	expression tag	UNP Q8VPJ5
B	748	ASN	-	expression tag	UNP Q8VPJ5
B	749	SER	-	expression tag	UNP Q8VPJ5
B	750	SER	-	expression tag	UNP Q8VPJ5
B	751	SER	-	expression tag	UNP Q8VPJ5
B	752	VAL	-	expression tag	UNP Q8VPJ5
B	753	ASP	-	expression tag	UNP Q8VPJ5
B	754	LYS	-	expression tag	UNP Q8VPJ5
B	755	LEU	-	expression tag	UNP Q8VPJ5
B	756	ALA	-	expression tag	UNP Q8VPJ5
B	757	ALA	-	expression tag	UNP Q8VPJ5
B	758	ALA	-	expression tag	UNP Q8VPJ5
B	759	LEU	-	expression tag	UNP Q8VPJ5
B	760	GLU	-	expression tag	UNP Q8VPJ5
B	761	HIS	-	expression tag	UNP Q8VPJ5
B	762	HIS	-	expression tag	UNP Q8VPJ5
B	763	HIS	-	expression tag	UNP Q8VPJ5
B	764	HIS	-	expression tag	UNP Q8VPJ5
B	765	HIS	-	expression tag	UNP Q8VPJ5
B	766	HIS	-	expression tag	UNP Q8VPJ5
C	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
C	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
C	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
C	744	SER	-	expression tag	UNP Q8VPJ5
C	745	GLU	-	expression tag	UNP Q8VPJ5
C	746	ASP	-	expression tag	UNP Q8VPJ5
C	747	PRO	-	expression tag	UNP Q8VPJ5
C	748	ASN	-	expression tag	UNP Q8VPJ5
C	749	SER	-	expression tag	UNP Q8VPJ5
C	750	SER	-	expression tag	UNP Q8VPJ5
C	751	SER	-	expression tag	UNP Q8VPJ5

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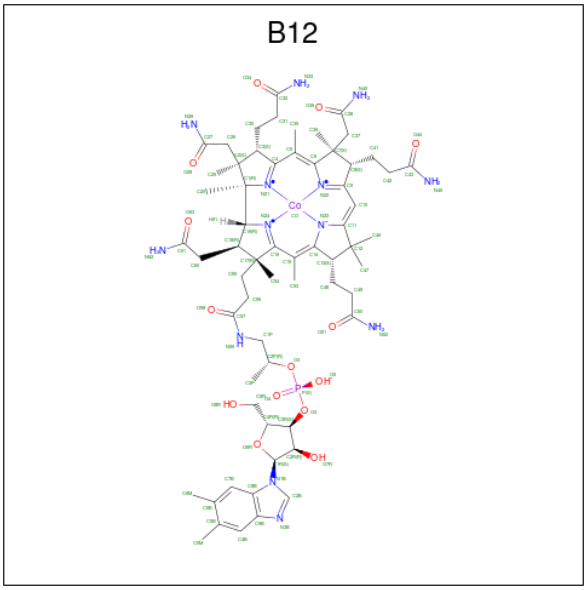
Chain	Residue	Modelled	Actual	Comment	Reference
C	752	VAL	-	expression tag	UNP Q8VPJ5
C	753	ASP	-	expression tag	UNP Q8VPJ5
C	754	LYS	-	expression tag	UNP Q8VPJ5
C	755	LEU	-	expression tag	UNP Q8VPJ5
C	756	ALA	-	expression tag	UNP Q8VPJ5
C	757	ALA	-	expression tag	UNP Q8VPJ5
C	758	ALA	-	expression tag	UNP Q8VPJ5
C	759	LEU	-	expression tag	UNP Q8VPJ5
C	760	GLU	-	expression tag	UNP Q8VPJ5
C	761	HIS	-	expression tag	UNP Q8VPJ5
C	762	HIS	-	expression tag	UNP Q8VPJ5
C	763	HIS	-	expression tag	UNP Q8VPJ5
C	764	HIS	-	expression tag	UNP Q8VPJ5
C	765	HIS	-	expression tag	UNP Q8VPJ5
C	766	HIS	-	expression tag	UNP Q8VPJ5
D	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
D	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
D	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
D	744	SER	-	expression tag	UNP Q8VPJ5
D	745	GLU	-	expression tag	UNP Q8VPJ5
D	746	ASP	-	expression tag	UNP Q8VPJ5
D	747	PRO	-	expression tag	UNP Q8VPJ5
D	748	ASN	-	expression tag	UNP Q8VPJ5
D	749	SER	-	expression tag	UNP Q8VPJ5
D	750	SER	-	expression tag	UNP Q8VPJ5
D	751	SER	-	expression tag	UNP Q8VPJ5
D	752	VAL	-	expression tag	UNP Q8VPJ5
D	753	ASP	-	expression tag	UNP Q8VPJ5
D	754	LYS	-	expression tag	UNP Q8VPJ5
D	755	LEU	-	expression tag	UNP Q8VPJ5
D	756	ALA	-	expression tag	UNP Q8VPJ5
D	757	ALA	-	expression tag	UNP Q8VPJ5
D	758	ALA	-	expression tag	UNP Q8VPJ5
D	759	LEU	-	expression tag	UNP Q8VPJ5
D	760	GLU	-	expression tag	UNP Q8VPJ5
D	761	HIS	-	expression tag	UNP Q8VPJ5
D	762	HIS	-	expression tag	UNP Q8VPJ5
D	763	HIS	-	expression tag	UNP Q8VPJ5
D	764	HIS	-	expression tag	UNP Q8VPJ5
D	765	HIS	-	expression tag	UNP Q8VPJ5
D	766	HIS	-	expression tag	UNP Q8VPJ5

- Molecule 2 is a protein called D-ornithine aminomutase S component.

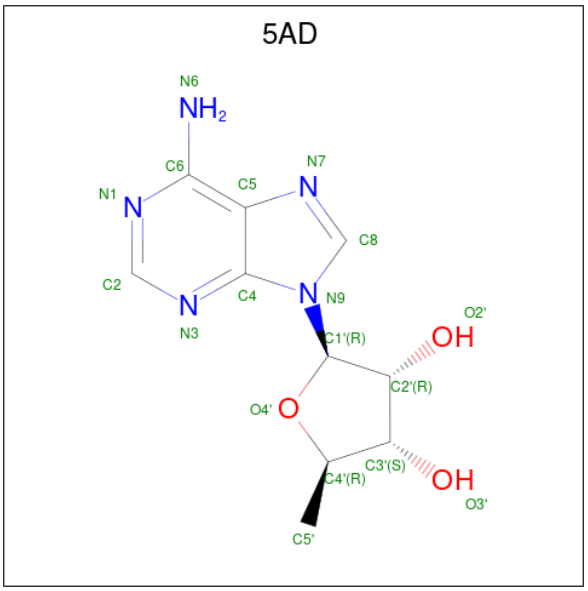
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	109	855	538	152	161	4	0	0	0
			Total	C	N	O	S			
2	F	109	858	539	152	163	4	0	0	0
			Total	C	N	O	S			
2	G	109	855	538	152	161	4	0	0	0
			Total	C	N	O	S			
2	H	109	855	538	152	161	4	0	0	0

- Molecule 3 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



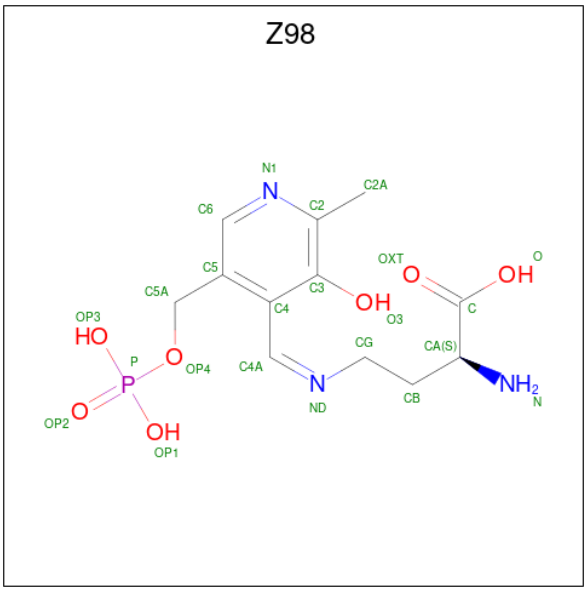
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Co	N	O	P		
3	A	1	91	62	1	13	14	1	0	0
			Total	C	Co	N	O	P		
3	B	1	91	62	1	13	14	1	0	0
			Total	C	Co	N	O	P		
3	C	1	91	62	1	13	14	1	0	0
			Total	C	Co	N	O	P		
3	D	1	91	62	1	13	14	1	0	0

- Molecule 4 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	18	10	5	3	0	0
			Total	C	N	O		
4	B	1	18	10	5	3	0	0
			Total	C	N	O		
4	C	1	18	10	5	3	0	0
			Total	C	N	O		
4	D	1	18	10	5	3	0	0

- Molecule 5 is (2S)-2-amino-4-{[(1Z)-{3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methylidene]amino}butanoic acid (CCD ID: Z98) (formula: $C_{12}H_{18}N_3O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	23	12	3	7	1	0	0
5	B	1	23	12	3	7	1	0	0
5	C	1	23	12	3	7	1	0	0
5	D	1	23	12	3	7	1	0	0

- Molecule 6 is water.

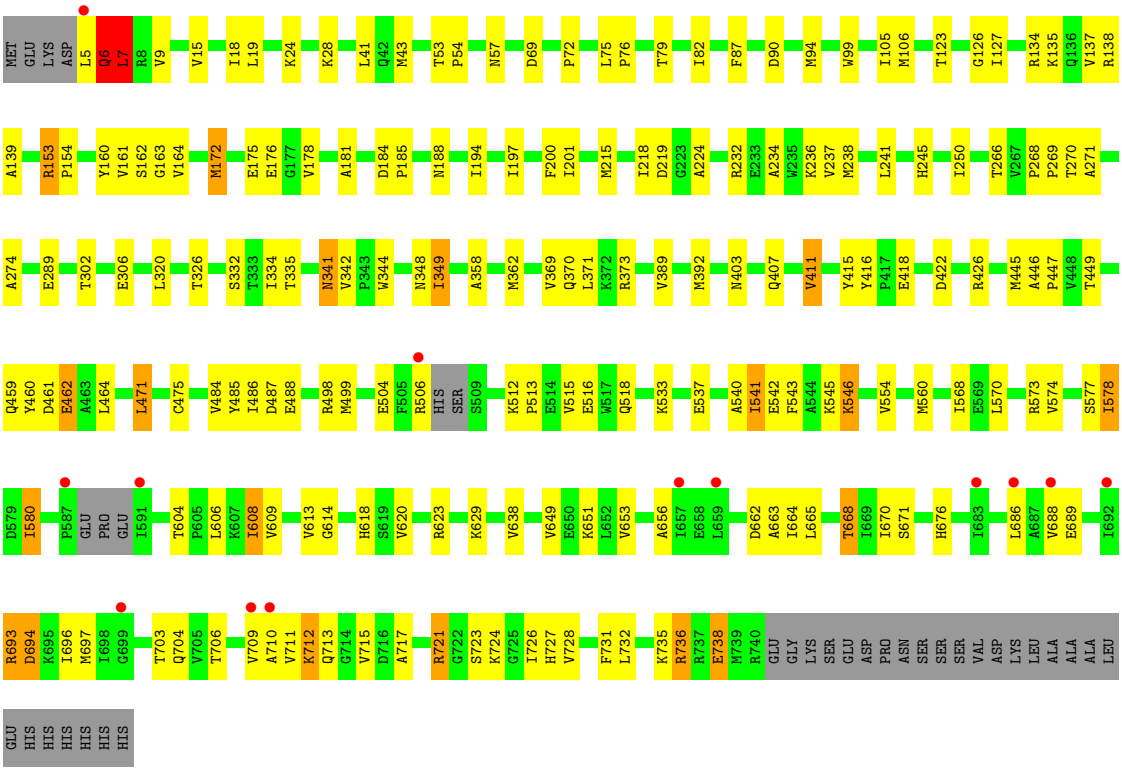
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	144	144	144	0	0
6	E	15	15	15	0	0
6	B	199	199	199	0	0
6	F	33	33	33	0	0
6	C	145	145	145	0	0
6	G	17	17	17	0	0
6	D	217	217	217	0	0
6	H	17	17	17	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

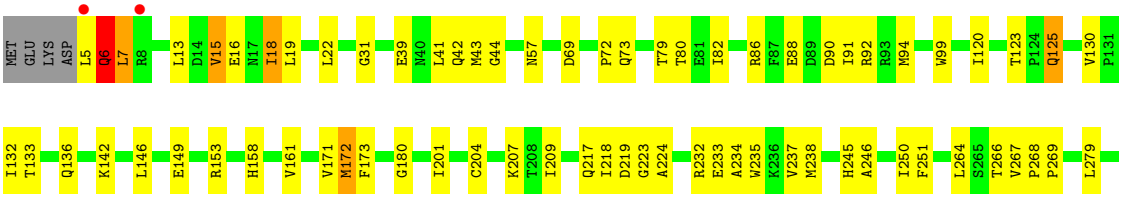
• Molecule 1: D-ornithine aminomutase E component

Chain A: 2% 70% 23% 5%



• Molecule 1: D-ornithine aminomutase E component

Chain B: 71% 22% 5%



P282 Y283 F291 E292 R295 Q299 M300 N301 M305 E306 T315 I322 S332 E338 N341 V342 N348 I349 G364 L365 E374 L377 V381 F391 M392 E393 I396 F410 V411 Y415 Y416 P417 I428 N429 V437 E442 M445 A446

P447 F452 N455 N456 V457 K458 Q459 Y460 L464 L471 E488 N494 R498 M499 E504 F505 R506 HIS SER S509 M510 I511 K512 P513 W517 Q518 G521 T526 M527 F528 A540 I541 V552 E553 V554 R557 Q561 E562 E569 L570 I578 D579 I580

P587 GLU PRO GLU I591 L592 K603 T604 K607 I608 V609 A610 A611 T612 V613 S619 L622 R623 I626 D627 I628 K629 I633 V638 T645 V649 E650 K651 E658 A663 I664 L665 T668 I669 I670 S671 H672 I675 H676 N679 I683 L686 A687

V688 E689 K690 R693 I696 M697 T703 S723 A729 T730 V733 K734 K735 R736 R737 E738 M739 R740 GLU GLY LYS SER GLU ASP PRO ASN SER SER SER VAL ASP LYS LEU ALA ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

- Molecule 1: D-ornithine aminomutase E component

Chain C: 68% 24% • 5%

MET GLU LYS ASP L5 Q6 L7 R8 V9 N10 E11 K12 L13 D14 V15 E16 N17 I18 L19 K20 T26 P27 E39 N40 L41 Q42 M43 I47 V77 I78 T79 I82 D90 I91 R92 R93 M94 R95 M96 H104 I105 M106 R109 S114 H115 G122 T123 I132

K135 Q136 L146 E150 R153 V161 V164 D168 G177 V178 A181 P185 Q186 Y187 N188 V189 I197 F200 I201 D202 A203 K207 M210 A213 D214 M215 A216 Q217 I218 D219 G223 A224 H225 N226 R232 E233 A234 W235 K236 V237 M238 P239 E240 Q244

H245 F251 V255 K259 I262 V267 P268 P269 T270 L279 P282 Y283 M290 N301 Y304 M305 E306 H316 T335 P336 N341 W344 H345 I346 Y347 N348 L359 V369 Q370 R373 L377 K385 E386 R387 A388 V389 M392 E406

F410 V411 D412 S413 G414 Y415 Y416 P417 D422 R426 Q427 I428 D443 Y444 M445 A446 P447 Y460 D461 E462 A463 L464 V465 P468 L471 C475 V479 P480 E481 D487 R498 M499 E500 E504 F505 R506 HIS SER S509 M510 I511 K512 P513 E514 V515 Q518 T522

L525 L529 V535 A536 E537 M547 E551 V554 L570 K571 G572 R573 V574 P575 F576 S577 I578 D579 I580 N581 S582 L583 P587 GLU PRO GLU I591 E594 D595 E596 I597 T604 K607 I608 T612 V613 G614 E615 D616 E617 I626 K629 H630 G631 E634

V640 L643 G644 T645 S646 V647 F648 V649 E650 K651 I657 K660 A663 T668 H676 N679 I683 H684 E685 L686 A687 V688 I692 R693 D694 K695 I696 S723 K724 G725 I726 H727 V728 F731 L732 V733 R736 R740 GLU GLY LYS SER GLU ASP PRO ASN

SER SER SER VAL ASP LYS LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS

- Molecule 1: D-ornithine aminomutase E component

Chain D: 71% 21% • 5%

MET GLU LYS ASP L5 Q6 L7 R8 L13 D14 V15 K24 Y25 T26 P27 K28 E39 N40 L41 Q42 M43 F46 I47 D69 T79 I82 G85 E88 D89 D90 I91 R95 A98 H104 H115 Y116 D117 I120 T123 I127 G128 G129 T133

R138 I147 R153 H158 S159 Y160 V164 M172 F173 E176 P185 Q186 Y187 N188 V189 I194 N195 M196 I197 C204 M210 M215 I218 D219 G223 A224 H225 N226 R232 E233 A234 W235 K236 V237 M238 H245 I250 K258 L264 S265 T266 V267

P268 P269 D280 L281 P282 Y283 A284 M290 M296 Q299 M300 N301 T302 M305 E306 T326 I334 T335 E338 G339 R340 W344 H345 I349 M368 V389 I395 G399 F402 N403 V411 Y416 P417 I424 A425 R426 Q427 I428 N429 I432

V437 M445 A446 P447 V448 T449 F452 Q459 Y460 D461 L464 L471 C475 E478 E491 N494 V495 R498 M499 R506 HIS SER S509 M510 F528 I541 K546 V554 I555 N556 R557 V574 P575 F576 S577 I578 P587 GLU PRO GLU I591 L592 S593

E596 I597 D600 T604 P605 L606 K607 I608 V609 A610 A611 T612 V613 G614 E615 K629 H630 G631 K635 L643 V647 P648 V649 D654 I657 E658 L659 K660 A661 D662 A663 I664 L665 A666 S667 T668 I669 H676 M680 K681 R682 I683 V688 E689 K690 R693 D694

K695 I696 G701 V705 V711 D716 F719 S723 K724 G725 A729 V733 R736 R740 GLU GLY LYS SER GLU ASP PRO ASN SER SER SER VAL ASP LYS LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS

- Molecule 2: D-ornithine aminomutase S component

Chain E:

MET LYS ARG ALA ASP D6 E20 E21 L22 F26 M29 A30 L37 K42 K43 N44 V53 L54 L55 R56 M57 V68 D73 R74 G75 L76 K79 V85 Y86 K87 K92 N93 I94 L103 I113 Q114 ILE PHE LYS GLY GLY VAL LYS

- Molecule 2: D-ornithine aminomutase S component

Chain F:

MET LYS ARG ALA ASP D6 R10 A15 E20 Q23 T24 R25 F26 M29 A30 E31 T45 T46 E50 L54 L55 R56 M57 G58 F59 L62 V68 M72 L76 M77 G82 Y86 A89 K92 S95 E98 L101 A102 L103 K107

D110 Q114 ILE PHE LYS GLY GLY VAL LYS

- Molecule 2: D-ornithine aminomutase S component

Chain G:

MET LYS ARG ALA ASP D6 F7 Q8 Q9 R10 R11 N16 E20 R25 M29 A30 L37 L38 D39 S48 T49 E50 V53 L54 L55 R56 M57 L76 M77 G82 H83 I84 A89 I94 E98 A99 G100 L101 K107 Q114 ILE PHE LYS GLY GLY VAL

LYS

- Molecule 2: D-ornithine aminomutase S component

Chain H:

MET LYS ARG ALA ASP D6 T24 R25 F26 W27 E28 M29 V34 L40 L54 L55 R56 M57 G58 F59 L76 G82 H83 I84 N93 E98 A99 G100 K107 Q114 ILE PHE LYS GLY GLY VAL LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.96Å 231.69Å 123.89Å 90.00° 103.16° 90.00°	Depositor
Resolution (Å)	64.23 – 2.40 64.23 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (64.23-2.40) 99.9 (64.23-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.190 , 0.257 0.191 , 0.254	Depositor DCC
R_{free} test set	7055 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	27379	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5AD, B12, Z98

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.95	4/5756 (0.1%)	1.01	8/7794 (0.1%)
1	B	1.03	3/5777 (0.1%)	1.04	8/7818 (0.1%)
1	C	0.93	2/5759 (0.0%)	0.99	8/7796 (0.1%)
1	D	1.04	5/5769 (0.1%)	1.02	4/7808 (0.1%)
2	E	0.89	0/867	0.95	1/1163 (0.1%)
2	F	1.08	0/870	1.08	0/1167
2	G	0.81	0/867	1.02	0/1163
2	H	0.97	0/867	0.97	1/1163 (0.1%)
All	All	0.98	14/26532 (0.1%)	1.02	30/35872 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	223	GLY	C-O	-8.06	1.18	1.24
1	A	326	THR	CA-C	7.54	1.56	1.52
1	D	194	ILE	CA-CB	-7.37	1.46	1.54
1	B	223	GLY	C-O	-7.24	1.19	1.24
1	D	326	THR	CA-C	6.23	1.55	1.52
1	D	218	ILE	C-O	-6.17	1.16	1.24
1	B	218	ILE	C-O	-5.96	1.17	1.24
1	A	218	ILE	C-O	-5.89	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	284	ALA	CA-CB	-5.79	1.44	1.53
1	A	219	ASP	C-O	-5.74	1.16	1.24
1	D	219	ASP	C-O	-5.62	1.17	1.23
1	A	362	MET	N-CA	-5.55	1.39	1.46
1	B	219	ASP	C-O	-5.33	1.18	1.23
1	C	218	ILE	C-O	-5.01	1.18	1.24

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	647	VAL	CA-C-N	-8.31	111.46	119.85
1	C	647	VAL	C-N-CA	-8.31	111.46	119.85
1	C	683	ILE	CB-CA-C	-7.66	101.98	112.24
1	B	629	LYS	N-CA-C	7.01	119.52	111.11
1	B	342	VAL	N-CA-C	-6.96	102.54	109.02
1	A	620	VAL	N-CA-C	6.89	117.01	110.53
1	D	7	LEU	N-CA-C	6.38	119.88	110.30
1	D	69	ASP	N-CA-C	6.22	120.00	111.54
1	C	626	ILE	CB-CA-C	-6.08	105.63	111.05
1	B	626	ILE	N-CA-C	5.88	116.62	111.56
1	B	374	GLU	N-CA-C	-5.84	99.76	109.46
1	D	657	ILE	CB-CA-C	-5.81	104.43	112.04
1	A	197	ILE	N-CA-C	-5.72	104.77	111.00
1	C	626	ILE	N-CA-C	5.62	116.06	111.62
1	B	626	ILE	CB-CA-C	-5.47	106.24	111.44
1	A	560	MET	N-CA-C	-5.45	104.22	111.24
2	H	26	PHE	N-CA-C	-5.43	105.44	111.36
1	A	163	GLY	N-CA-C	5.36	119.43	111.76
1	B	619	SER	CA-C-N	5.34	127.29	120.56
1	B	619	SER	C-N-CA	5.34	127.29	120.56
1	D	219	ASP	N-CA-C	5.33	118.11	109.79
1	A	693	ARG	N-CA-C	5.28	117.72	111.33
2	E	6	ASP	N-CA-C	5.21	125.59	111.00
1	C	188	ASN	N-CA-C	5.20	117.35	111.11
1	A	268	PRO	CA-C-N	5.16	124.95	119.28
1	A	268	PRO	C-N-CA	5.16	124.95	119.28
1	A	197	ILE	CB-CA-C	-5.10	105.41	112.24
1	C	187	TYR	N-CA-C	-5.10	105.62	111.07
1	C	267	VAL	CB-CA-C	-5.05	105.18	110.53
1	B	31	GLY	N-CA-C	5.03	116.73	111.95

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	6	GLN	Peptide
1	D	6	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5651	0	5584	164	0
1	B	5672	0	5644	185	0
1	C	5654	0	5621	182	0
1	D	5664	0	5636	161	0
2	E	855	0	863	17	0
2	F	858	0	865	24	0
2	G	855	0	863	23	0
2	H	855	0	863	16	0
3	A	91	0	87	17	0
3	B	91	0	87	20	0
3	C	91	0	87	16	0
3	D	91	0	87	14	0
4	A	18	0	11	2	0
4	B	18	0	12	2	0
4	C	18	0	12	3	0
4	D	18	0	12	4	0
5	A	23	0	14	11	0
5	B	23	0	14	8	0
5	C	23	0	14	8	0
5	D	23	0	14	8	0
6	A	144	0	0	8	0
6	B	199	0	0	14	0
6	C	145	0	0	14	0
6	D	217	0	0	20	0
6	E	15	0	0	1	0
6	F	33	0	0	2	0
6	G	17	0	0	2	0
6	H	17	0	0	1	0
All	All	27379	0	26390	782	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (782) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:767:Z98:H4A	1:D:629:LYS:NZ	1.46	1.28
1:B:649:VAL:HG22	1:B:683:ILE:HD11	1.20	1.17
1:A:629:LYS:NZ	5:C:767:Z98:H4A	1.64	1.12
1:B:396:ILE:HD12	2:F:29:MET:HE3	1.26	1.12
2:F:54:LEU:HD23	2:F:57:MET:CE	1.78	1.12
3:C:1801:B12:H362	3:C:1801:B12:H351	1.30	1.11
3:B:1801:B12:H362	3:B:1801:B12:H351	1.29	1.11
1:D:445:MET:HE1	1:D:447:PRO:HB3	1.30	1.11
1:B:649:VAL:CG2	1:B:683:ILE:HD11	1.79	1.10
1:B:629:LYS:NZ	5:D:767:Z98:C4A	2.14	1.10
1:D:41:LEU:HD23	1:D:43:MET:HE2	1.19	1.10
1:A:41:LEU:HD21	1:A:43:MET:HE2	1.29	1.09
1:C:41:LEU:HD23	1:C:43:MET:HE2	1.23	1.09
3:D:1801:B12:H362	3:D:1801:B12:H351	1.27	1.09
1:C:41:LEU:CD2	1:C:43:MET:HE2	1.83	1.09
1:B:649:VAL:HG13	1:B:683:ILE:CD1	1.82	1.09
5:A:767:Z98:H4A	1:C:629:LYS:CE	1.83	1.06
3:A:1801:B12:H362	3:A:1801:B12:H351	1.31	1.06
1:B:649:VAL:CG1	1:B:683:ILE:CD1	2.34	1.05
1:A:41:LEU:CD2	1:A:43:MET:HE2	1.86	1.05
1:C:41:LEU:HD23	1:C:43:MET:CE	1.87	1.04
1:B:445:MET:HE1	1:B:447:PRO:HB3	1.38	1.04
5:B:767:Z98:H4A	1:D:629:LYS:CE	1.86	1.04
1:B:649:VAL:CG1	1:B:683:ILE:HD12	1.88	1.00
5:B:767:Z98:C4A	1:D:629:LYS:NZ	2.26	0.99
1:B:649:VAL:HG22	1:B:683:ILE:CD1	1.93	0.98
1:B:649:VAL:CG2	1:B:683:ILE:CD1	2.42	0.97
2:H:54:LEU:HD23	2:H:57:MET:HE2	1.46	0.97
1:B:153:ARG:HD2	6:B:783:HOH:O	1.63	0.97
3:B:1801:B12:H531	3:B:1801:B12:H552	1.45	0.97
1:A:629:LYS:NZ	5:C:767:Z98:C4A	2.28	0.97
1:B:629:LYS:CE	5:D:767:Z98:H4A	1.95	0.97
1:B:172:MET:C	1:B:172:MET:CE	2.38	0.96
5:A:767:Z98:C4A	1:C:629:LYS:NZ	2.29	0.96
2:F:54:LEU:HD23	2:F:57:MET:HE2	1.44	0.95
5:A:767:Z98:H4A	1:C:629:LYS:NZ	1.83	0.94
1:C:406:GLU:OE2	1:C:428:ILE:HG22	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:VAL:HG12	1:A:686:LEU:HD12	1.48	0.93
1:B:649:VAL:HG11	1:B:683:ILE:HD12	1.50	0.93
1:D:41:LEU:CD2	1:D:43:MET:HE2	1.99	0.93
5:B:767:Z98:H4A	1:D:629:LYS:HZ3	1.33	0.92
1:A:172:MET:HE3	1:A:176:GLU:HG3	1.51	0.92
1:B:445:MET:HE1	1:B:447:PRO:CB	2.00	0.91
1:B:629:LYS:HZ3	5:D:767:Z98:C4A	1.83	0.91
1:B:396:ILE:HD12	2:F:29:MET:CE	2.01	0.91
1:B:172:MET:HE2	1:B:173:PHE:N	1.85	0.90
1:C:445:MET:HE1	1:C:447:PRO:CA	2.00	0.90
1:A:445:MET:HE1	1:A:447:PRO:HB3	1.51	0.90
2:F:54:LEU:HD23	2:F:57:MET:HE1	1.54	0.90
1:C:445:MET:HE1	1:C:447:PRO:HB3	1.54	0.89
1:A:668:THR:HG21	1:A:676:HIS:HA	1.53	0.88
1:B:172:MET:C	1:B:172:MET:HE3	1.98	0.88
1:B:629:LYS:NZ	5:D:767:Z98:H4A	1.88	0.88
1:C:445:MET:HE1	1:C:447:PRO:CB	2.04	0.88
1:B:172:MET:C	1:B:172:MET:HE2	1.98	0.87
5:A:767:Z98:C4A	1:C:629:LYS:HZ1	1.84	0.87
1:C:15:VAL:CG2	1:C:499:MET:HE1	2.05	0.87
1:C:15:VAL:HG23	1:C:499:MET:HE1	1.55	0.87
1:C:240:GLU:OE2	1:C:244:GLN:NE2	2.07	0.87
1:D:445:MET:HE3	1:D:471:LEU:HD23	1.56	0.86
1:D:172:MET:C	1:D:172:MET:CE	2.48	0.86
1:A:15:VAL:HG13	1:A:499:MET:HE1	1.56	0.86
1:A:537:GLU:HG3	1:A:554:VAL:HG21	1.57	0.85
5:B:767:Z98:C4A	1:D:629:LYS:HZ3	1.89	0.85
1:B:15:VAL:HG23	1:B:499:MET:HE1	1.57	0.85
2:H:54:LEU:HD23	2:H:57:MET:CE	2.06	0.85
1:A:606:LEU:HD21	1:A:732:LEU:HD13	1.57	0.85
3:D:1801:B12:H351	3:D:1801:B12:C36	2.07	0.83
1:D:301:ASN:O	1:D:305:MET:CE	2.27	0.83
1:B:629:LYS:HZ1	5:D:767:Z98:C4A	1.88	0.83
5:B:767:Z98:H4A	1:D:629:LYS:HZ1	1.39	0.83
3:B:1801:B12:H362	3:B:1801:B12:C35	2.06	0.82
1:C:406:GLU:CD	1:C:428:ILE:HG22	2.04	0.82
1:D:172:MET:C	1:D:172:MET:HE3	2.04	0.82
1:A:629:LYS:HZ3	5:C:767:Z98:C4A	1.90	0.82
1:B:541:ILE:HD11	1:B:554:VAL:HG23	1.61	0.82
2:G:54:LEU:HD23	2:G:57:MET:CE	2.10	0.82
1:D:668:THR:HG23	1:D:676:HIS:HB2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:679:ASN:O	1:C:683:ILE:HG13	1.80	0.80
1:B:123:THR:O	1:B:498:ARG:NH2	2.12	0.80
3:D:1801:B12:H362	3:D:1801:B12:C35	2.11	0.80
1:D:445:MET:HE1	1:D:447:PRO:CB	2.10	0.80
1:B:668:THR:O	1:B:668:THR:CG2	2.29	0.79
3:B:1801:B12:H351	3:B:1801:B12:C36	2.11	0.79
1:B:86:ARG:NE	1:B:125:GLN:HE22	1.80	0.79
1:D:607:LYS:O	1:D:608:ILE:HD12	1.81	0.79
3:D:1801:B12:H552	3:D:1801:B12:H531	1.65	0.79
1:B:396:ILE:CD1	2:F:29:MET:HE3	2.11	0.79
1:B:649:VAL:CG1	1:B:683:ILE:HD11	2.12	0.79
3:A:1801:B12:H351	3:A:1801:B12:C36	2.10	0.79
1:A:629:LYS:HZ1	5:C:767:Z98:H4A	1.43	0.78
5:A:767:Z98:H4A	1:C:629:LYS:HE2	1.65	0.78
1:D:233:GLU:OE1	1:D:236:LYS:NZ	2.16	0.78
1:B:649:VAL:HG13	1:B:683:ILE:HD11	1.65	0.78
1:B:19:LEU:HD12	1:B:499:MET:HE2	1.66	0.77
1:B:608:ILE:HG13	1:B:663:ALA:HB3	1.66	0.77
1:A:445:MET:HE1	1:A:447:PRO:CB	2.14	0.77
1:C:301:ASN:HD21	1:C:304:TYR:H	1.31	0.77
1:B:172:MET:HE3	1:B:172:MET:O	1.84	0.77
1:B:445:MET:HE1	1:B:447:PRO:CA	2.14	0.76
1:B:668:THR:CG2	1:B:676:HIS:HB2	2.15	0.76
1:A:629:LYS:HZ1	5:C:767:Z98:C4A	1.97	0.75
1:D:41:LEU:HD23	1:D:43:MET:CE	2.10	0.75
3:A:1801:B12:H362	3:A:1801:B12:C35	2.16	0.75
2:F:54:LEU:HA	2:F:57:MET:HE2	1.68	0.75
1:A:629:LYS:CE	5:C:767:Z98:H4A	2.15	0.75
1:D:172:MET:C	1:D:172:MET:HE2	2.12	0.75
2:F:68:VAL:HG12	2:F:72:MET:HE2	1.69	0.74
1:C:537:GLU:HG3	1:C:554:VAL:HG21	1.69	0.74
1:B:649:VAL:HG13	1:B:683:ILE:CG1	2.17	0.74
1:A:403:ASN:O	1:A:407:GLN:HG3	1.87	0.74
1:A:461:ASP:CG	1:A:464:LEU:HD13	2.11	0.74
1:B:649:VAL:CB	1:B:683:ILE:HD11	2.18	0.74
1:D:238:MET:SD	6:D:831:HOH:O	2.46	0.73
1:D:172:MET:HE3	1:D:172:MET:O	1.88	0.73
1:D:668:THR:CG2	1:D:676:HIS:HB2	2.18	0.73
2:G:54:LEU:HA	2:G:57:MET:HE2	1.70	0.73
1:A:302:THR:CG2	1:A:334:ILE:HD12	2.19	0.73
1:A:43:MET:HE1	6:A:803:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:767:Z98:H5A	6:A:919:HOH:O	1.89	0.72
1:D:592:LEU:HD22	6:D:960:HOH:O	1.89	0.72
1:D:158:HIS:CE1	1:D:218:ILE:HD12	2.25	0.72
2:F:54:LEU:CD2	2:F:57:MET:CE	2.64	0.71
1:D:235:TRP:C	6:D:831:HOH:O	2.33	0.71
1:C:47:ILE:HG21	6:C:900:HOH:O	1.89	0.71
1:C:525:LEU:HD21	1:C:547:MET:HE1	1.72	0.71
1:B:738:GLU:O	1:B:738:GLU:HG3	1.91	0.71
1:D:740:ARG:C	6:D:845:HOH:O	2.33	0.71
2:F:57:MET:HE1	2:F:82:GLY:HA2	1.72	0.70
1:C:26:THR:HG22	1:C:27:PRO:HD2	1.74	0.70
1:A:464:LEU:HD22	1:A:471:LEU:CD1	2.21	0.70
1:C:445:MET:CE	1:C:447:PRO:CA	2.70	0.70
1:C:96:MET:HE1	1:C:345:HIS:HB3	1.73	0.70
1:C:445:MET:HE2	1:C:446:ALA:C	2.16	0.70
1:C:649:VAL:HG12	1:C:686:LEU:HD12	1.73	0.70
1:C:479:VAL:HG12	1:C:479:VAL:O	1.92	0.69
1:C:251:PHE:O	1:C:255:VAL:HG23	1.92	0.69
2:G:57:MET:HE1	2:G:82:GLY:HA2	1.74	0.69
1:D:301:ASN:O	1:D:305:MET:HE3	1.91	0.69
3:C:1801:B12:H362	3:C:1801:B12:C35	2.16	0.69
2:F:10:ARG:HD2	6:F:823:HOH:O	1.92	0.68
1:D:711:VAL:HG12	1:D:711:VAL:O	1.93	0.68
3:C:1801:B12:H351	3:C:1801:B12:C36	2.11	0.68
1:B:668:THR:HG21	1:B:676:HIS:HB2	1.75	0.68
1:D:541:ILE:HD11	1:D:554:VAL:HG23	1.76	0.68
1:A:5:LEU:O	1:A:6:GLN:HB2	1.93	0.68
1:A:577:SER:O	1:A:578:ILE:HD12	1.94	0.68
1:A:178:VAL:O	1:A:215:MET:HE3	1.94	0.67
1:B:668:THR:HG23	1:B:676:HIS:CB	2.24	0.67
1:C:305:MET:HE2	6:C:829:HOH:O	1.94	0.67
1:B:668:THR:O	1:B:668:THR:HG23	1.94	0.67
1:D:389:VAL:HG13	2:H:29:MET:HE1	1.77	0.67
2:F:62:LEU:HD23	6:F:429:HOH:O	1.94	0.67
1:D:172:MET:HE1	1:D:173:PHE:HD1	1.60	0.67
1:B:649:VAL:HG13	1:B:683:ILE:HG13	1.77	0.67
1:D:302:THR:HA	1:D:305:MET:HE3	1.76	0.67
1:C:389:VAL:HG13	2:G:29:MET:HE1	1.76	0.66
1:A:5:LEU:O	1:A:5:LEU:HD23	1.96	0.66
1:C:406:GLU:OE2	1:C:428:ILE:CG2	2.43	0.66
1:B:233:GLU:HG2	1:B:235:TRP:CH2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:CB	6:A:911:HOH:O	2.44	0.66
1:A:234:ALA:O	1:A:237:VAL:HG12	1.96	0.66
1:B:629:LYS:HZ3	5:D:767:Z98:C4	2.09	0.66
5:B:767:Z98:H4A	1:D:629:LYS:HE2	1.75	0.66
1:A:703:THR:HG22	1:A:704:GLN:HE21	1.59	0.66
1:C:41:LEU:HD21	1:C:43:MET:HE2	1.76	0.66
1:C:305:MET:CE	6:C:829:HOH:O	2.43	0.66
1:C:608:ILE:HD11	1:C:663:ALA:HB3	1.78	0.66
1:C:597:ILE:CD1	1:C:726:ILE:CD1	2.74	0.65
3:A:1801:B12:N29	3:A:1801:B12:H251	2.09	0.65
1:D:172:MET:CE	1:D:173:PHE:HD1	2.08	0.65
1:B:73:GLN:NE2	1:B:153:ARG:HH22	1.94	0.65
1:A:41:LEU:HD23	1:A:43:MET:HE2	1.76	0.65
1:A:172:MET:HE3	1:A:176:GLU:CG	2.24	0.65
2:F:54:LEU:CD2	2:F:57:MET:HE1	2.26	0.65
1:C:207:LYS:NZ	1:C:217:GLN:HE22	1.95	0.65
1:D:172:MET:HE2	1:D:173:PHE:N	2.11	0.65
1:B:92:ARG:HD2	6:D:841:HOH:O	1.97	0.64
1:B:86:ARG:HE	1:B:125:GLN:NE2	1.95	0.64
1:C:723:SER:O	3:C:1801:B12:O8R	2.16	0.64
1:D:120:ILE:HG13	1:D:133:THR:HG22	1.77	0.64
1:A:445:MET:HE1	1:A:447:PRO:CA	2.27	0.64
1:B:149:GLU:HG2	6:B:795:HOH:O	1.98	0.64
1:D:464:LEU:HD23	1:D:471:LEU:HD13	1.78	0.64
1:B:86:ARG:HE	1:B:125:GLN:HE22	1.46	0.64
1:D:429:ASN:HB3	6:D:873:HOH:O	1.98	0.64
1:C:475:CYS:HB2	2:G:56:ARG:O	1.98	0.64
1:A:568:ILE:HG22	1:A:570:LEU:CD1	2.28	0.64
3:B:1801:B12:N23	4:D:1500:5AD:H4'	2.13	0.64
1:B:171:VAL:HG23	1:B:209:ILE:HD13	1.80	0.63
1:A:153:ARG:HD2	6:A:783:HOH:O	1.97	0.63
1:B:13:LEU:HD13	1:B:91:ILE:HG22	1.80	0.63
1:D:649:VAL:HG23	6:D:943:HOH:O	1.96	0.63
1:B:301:ASN:O	1:B:305:MET:CE	2.46	0.63
1:B:541:ILE:CD1	1:B:554:VAL:HG23	2.27	0.63
2:H:25:ARG:HA	2:H:28:GLU:HG2	1.80	0.63
1:A:697:MET:HE1	1:A:736:ARG:HB2	1.79	0.63
1:B:43:MET:CE	1:B:72:PRO:HB3	2.28	0.63
1:B:88:GLU:OE2	1:B:498:ARG:HD2	1.99	0.63
1:B:172:MET:CE	1:B:173:PHE:N	2.54	0.63
1:B:246:ALA:O	1:B:250:ILE:HG22	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:736:ARG:HD3	6:D:849:HOH:O	1.99	0.63
1:C:335:THR:HG22	1:C:348:ASN:HA	1.81	0.63
1:B:7:LEU:HB2	6:B:940:HOH:O	1.98	0.63
1:C:660:LYS:O	1:C:660:LYS:HG3	1.98	0.62
1:C:238:MET:HE3	1:C:283:TYR:HB2	1.82	0.62
1:C:445:MET:HE1	1:C:447:PRO:HA	1.81	0.62
1:D:668:THR:CG2	1:D:668:THR:O	2.47	0.62
1:B:7:LEU:CD2	1:B:146:LEU:HB3	2.29	0.62
1:B:73:GLN:HE21	1:B:153:ARG:HH22	1.46	0.61
3:A:1801:B12:N22	4:C:1500:5AD:H5'1	2.13	0.61
2:H:54:LEU:HA	2:H:57:MET:HE2	1.81	0.61
1:A:629:LYS:HZ3	5:C:767:Z98:H4A	1.51	0.61
1:A:43:MET:HE1	1:A:72:PRO:HA	1.82	0.61
1:B:86:ARG:NE	1:B:125:GLN:NE2	2.48	0.61
3:B:1801:B12:H492	3:B:1801:B12:C47	2.30	0.61
1:C:13:LEU:HD22	1:C:18:ILE:HD11	1.81	0.61
1:C:597:ILE:CD1	1:C:726:ILE:HD11	2.31	0.61
1:A:464:LEU:CD2	1:A:471:LEU:HD13	2.31	0.61
1:C:79:THR:HG21	1:C:106:MET:HE3	1.82	0.61
1:C:123:THR:O	1:C:498:ARG:NH2	2.32	0.61
1:C:153:ARG:HD2	6:C:791:HOH:O	1.99	0.61
1:C:615:GLU:C	6:C:806:HOH:O	2.43	0.61
2:G:54:LEU:HD23	2:G:57:MET:HE2	1.81	0.61
1:A:568:ILE:HG22	1:A:570:LEU:HD12	1.83	0.61
1:B:19:LEU:CD1	1:B:499:MET:HE2	2.31	0.61
1:C:207:LYS:HZ2	1:C:217:GLN:HE22	1.47	0.61
2:G:94:ILE:HD12	2:G:98:GLU:HB3	1.83	0.61
1:B:511:ILE:CG2	1:B:580:ILE:HD11	2.30	0.60
1:B:511:ILE:HG21	1:B:580:ILE:HD11	1.83	0.60
1:B:623:ARG:HD3	1:D:115:HIS:CE1	2.37	0.60
1:D:574:VAL:HG13	1:D:576:PHE:CE1	2.36	0.60
3:B:1801:B12:H492	3:B:1801:B12:H473	1.83	0.60
1:C:626:ILE:O	1:C:634:GLU:HB2	2.01	0.60
1:D:344:TRP:O	1:D:345:HIS:C	2.41	0.60
1:C:445:MET:HE3	1:C:471:LEU:HD23	1.83	0.60
1:C:616:ASP:N	6:C:806:HOH:O	2.33	0.60
5:B:767:Z98:C4A	1:D:629:LYS:HZ1	2.05	0.60
1:B:80:THR:OG1	1:B:348:ASN:ND2	2.30	0.60
1:C:7:LEU:HD21	1:C:95:ARG:NH2	2.16	0.60
1:A:606:LEU:HD12	1:A:662:ASP:OD2	2.01	0.60
1:B:39:GLU:OE1	1:B:39:GLU:HA	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:MET:HE1	1:B:72:PRO:HA	1.84	0.60
2:H:98:GLU:HG3	6:H:490:HOH:O	2.02	0.60
1:C:668:THR:CG2	1:C:676:HIS:HB2	2.32	0.59
1:B:41:LEU:HD23	1:B:43:MET:HE2	1.85	0.59
1:D:210:MET:HE3	1:D:215:MET:HE2	1.84	0.59
1:A:703:THR:O	1:A:721:ARG:NH1	2.35	0.59
1:B:509:SER:N	6:B:925:HOH:O	2.35	0.59
3:B:1801:B12:H203	3:B:1801:B12:H301	1.84	0.59
1:A:664:ILE:O	1:A:665:LEU:HD23	2.03	0.59
1:B:43:MET:HE1	1:B:72:PRO:HB3	1.85	0.59
1:C:445:MET:CE	1:C:447:PRO:HA	2.32	0.59
1:D:736:ARG:CD	6:D:849:HOH:O	2.50	0.59
1:B:264:LEU:HD21	1:B:291:PHE:CD1	2.37	0.59
1:B:15:VAL:HG22	6:B:913:HOH:O	2.01	0.59
1:C:525:LEU:HB3	1:C:570:LEU:HD12	1.84	0.59
1:A:459:GLN:HG3	1:A:460:TYR:CD2	2.38	0.59
1:D:445:MET:CE	1:D:471:LEU:HD23	2.28	0.59
1:B:513:PRO:O	1:B:521:GLY:HA2	2.03	0.58
3:C:1801:B12:H552	3:C:1801:B12:H531	1.83	0.58
1:D:427:GLN:HG3	6:D:824:HOH:O	2.03	0.58
1:A:79:THR:HB	1:A:332:SER:HA	1.86	0.58
1:B:689:GLU:O	1:B:689:GLU:HG2	2.04	0.58
1:B:738:GLU:O	1:B:738:GLU:CG	2.51	0.58
1:C:202:ASP:OD2	2:G:48:SER:OG	2.16	0.58
1:D:160:TYR:OH	5:D:767:Z98:HB	2.04	0.58
1:A:726:ILE:HG23	1:A:727:HIS:CD2	2.38	0.58
1:C:668:THR:HG23	1:C:676:HIS:CB	2.32	0.58
1:D:607:LYS:C	1:D:608:ILE:HD12	2.28	0.58
1:D:680:MET:HE1	1:D:705:VAL:HG13	1.86	0.58
1:B:18:ILE:O	1:B:142:LYS:NZ	2.33	0.58
1:A:608:ILE:HD13	1:A:638:VAL:CG1	2.34	0.58
1:D:389:VAL:HG13	2:H:29:MET:CE	2.33	0.58
1:C:290:MET:HE2	1:C:385:LYS:HG2	1.86	0.58
1:A:302:THR:HG21	1:A:334:ILE:HD12	1.86	0.57
1:A:580:ILE:CD1	1:C:535:VAL:HG11	2.34	0.57
1:A:546:LYS:HZ2	1:C:578:ILE:HD11	1.69	0.57
1:B:540:ALA:HB1	1:B:570:LEU:HD11	1.85	0.57
1:B:82:ILE:HG22	1:B:90:ASP:HB3	1.85	0.57
1:C:687:ALA:HB3	1:C:693:ARG:HD3	1.85	0.57
1:D:668:THR:HG23	1:D:676:HIS:CB	2.30	0.57
1:A:200:PHE:CD2	2:E:37:LEU:HD13	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:THR:O	1:B:494:ASN:HA	2.05	0.57
1:C:596:GLU:CB	6:C:826:HOH:O	2.52	0.57
1:B:415:TYR:O	1:B:416:TYR:C	2.48	0.57
1:C:445:MET:CE	1:C:447:PRO:N	2.67	0.57
1:D:608:ILE:HG13	1:D:663:ALA:HB3	1.86	0.57
1:A:164:VAL:HG13	1:A:194:ILE:HG12	1.87	0.57
1:A:464:LEU:CD2	1:A:471:LEU:CD1	2.83	0.57
1:B:266:THR:O	1:B:266:THR:HG23	2.03	0.57
1:B:668:THR:O	1:B:668:THR:HG22	2.04	0.57
1:A:41:LEU:CD2	1:A:43:MET:CE	2.74	0.57
4:B:1500:5AD:C4'	3:D:1801:B12:N23	2.67	0.57
1:B:629:LYS:HE2	5:D:767:Z98:H4A	1.81	0.57
1:B:416:TYR:CD1	1:B:417:PRO:HA	2.40	0.56
1:B:445:MET:HA	1:B:455:ASN:OD1	2.05	0.56
1:B:668:THR:CG2	1:B:676:HIS:CB	2.80	0.56
1:C:234:ALA:O	1:C:237:VAL:HG12	2.06	0.56
1:C:537:GLU:CG	1:C:554:VAL:HG21	2.35	0.56
1:C:668:THR:HG23	1:C:676:HIS:HB2	1.87	0.56
1:B:393:GLU:OE2	2:F:25:ARG:NH1	2.32	0.56
1:B:504:GLU:CB	6:B:840:HOH:O	2.52	0.56
1:B:445:MET:CE	1:B:471:LEU:HD23	2.35	0.56
1:C:7:LEU:HD22	1:C:150:GLU:OE2	2.05	0.56
1:C:233:GLU:HG2	1:C:235:TRP:CH2	2.41	0.56
1:A:269:PRO:HB2	1:A:270:THR:HG23	1.89	0.56
1:A:613:VAL:HG21	1:A:649:VAL:CG2	2.36	0.56
1:C:428:ILE:HG21	6:C:778:HOH:O	2.06	0.56
1:D:204:CYS:HB3	1:D:452:PHE:CD2	2.41	0.55
1:B:120:ILE:HG13	1:B:133:THR:HG22	1.87	0.55
1:C:612:THR:HB	1:C:645:THR:HG22	1.89	0.55
1:D:591:ILE:HG23	1:D:591:ILE:O	2.05	0.55
1:C:13:LEU:CD2	1:C:18:ILE:HD11	2.37	0.55
3:B:1801:B12:C35	3:B:1801:B12:C36	2.79	0.55
1:D:509:SER:N	6:D:988:HOH:O	2.40	0.55
1:D:610:ALA:HA	1:D:665:LEU:O	2.06	0.55
3:B:1801:B12:O28	3:B:1801:B12:H3	2.06	0.55
1:C:181:ALA:HB3	1:C:210:MET:HE3	1.88	0.55
2:G:54:LEU:HD23	2:G:57:MET:HE1	1.88	0.55
1:D:445:MET:HE2	1:D:447:PRO:CA	2.36	0.55
1:D:574:VAL:CG1	1:D:576:PHE:CE1	2.90	0.55
1:B:607:LYS:C	1:B:608:ILE:HD12	2.32	0.55
1:C:15:VAL:HG21	1:C:499:MET:HE1	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:605:PRO:O	1:D:736:ARG:NH2	2.39	0.55
3:D:1801:B12:H492	3:D:1801:B12:C47	2.36	0.55
1:A:392:MET:HE2	2:E:26:PHE:CE1	2.42	0.55
1:B:207:LYS:NZ	1:B:217:GLN:NE2	2.55	0.55
1:C:594:GLU:CB	6:C:819:HOH:O	2.55	0.55
1:D:305:MET:HE1	1:D:334:ILE:HG21	1.89	0.55
1:D:445:MET:HE2	1:D:447:PRO:N	2.22	0.55
1:C:161:VAL:HG12	1:C:161:VAL:O	2.06	0.55
1:B:301:ASN:O	1:B:305:MET:HE3	2.06	0.54
3:A:1801:B12:H552	3:A:1801:B12:H531	1.89	0.54
1:D:449:THR:OG1	1:D:478:GLU:OE2	2.16	0.54
1:A:613:VAL:HG21	1:A:649:VAL:HG23	1.89	0.54
4:A:1500:5AD:C4'	3:C:1801:B12:N23	2.70	0.54
1:B:580:ILE:HD13	1:B:580:ILE:N	2.22	0.54
1:A:464:LEU:HD23	1:A:471:LEU:HD13	1.89	0.54
2:E:6:ASP:N	6:E:410:HOH:O	2.40	0.54
1:A:543:PHE:CE1	1:C:578:ILE:HD13	2.42	0.54
1:A:392:MET:CE	2:E:30:ALA:HB2	2.38	0.54
1:B:649:VAL:CB	1:B:683:ILE:CD1	2.83	0.54
1:D:26:THR:HG22	1:D:27:PRO:HD2	1.88	0.54
1:D:510:MET:HE3	1:D:577:SER:HB3	1.90	0.54
2:E:74:ARG:HD2	2:E:113:ILE:HD11	1.88	0.54
1:D:269:PRO:HD2	1:D:280:ASP:CG	2.33	0.54
1:B:668:THR:HG23	1:B:676:HIS:HB3	1.87	0.54
3:B:1801:B12:H531	3:B:1801:B12:C55	2.22	0.53
2:E:53:VAL:O	2:E:57:MET:HG3	2.09	0.53
1:C:445:MET:CE	1:C:471:LEU:HD23	2.39	0.53
1:D:210:MET:HG2	1:D:215:MET:HE2	1.90	0.53
1:A:41:LEU:HD23	1:A:43:MET:CE	2.38	0.53
1:B:238:MET:HE2	1:B:269:PRO:HG2	1.91	0.53
1:A:7:LEU:HB2	6:A:834:HOH:O	2.08	0.53
1:A:53:THR:HG23	1:A:54:PRO:HD2	1.90	0.53
1:B:506:ARG:HH11	1:B:518:GLN:HE22	1.56	0.53
1:B:610:ALA:HB1	1:B:622:LEU:HD21	1.91	0.53
1:C:82:ILE:HG22	1:C:90:ASP:HB3	1.90	0.53
2:G:7:PHE:CZ	2:G:11:ARG:HD2	2.43	0.53
1:A:369:VAL:CG1	1:C:369:VAL:CG1	2.87	0.53
1:A:728:VAL:HG21	3:A:1801:B12:HM62	1.91	0.53
1:C:7:LEU:CD2	1:C:95:ARG:NH2	2.72	0.53
1:A:5:LEU:O	1:A:6:GLN:CB	2.56	0.53
1:A:713:GLN:HA	1:A:713:GLN:HE21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:607:LYS:NZ	6:C:815:HOH:O	2.31	0.53
1:D:606:LEU:HD11	1:D:608:ILE:HD11	1.91	0.53
1:B:364:GLY:O	1:B:365:LEU:C	2.49	0.53
1:B:629:LYS:NZ	1:D:226:ASN:OD1	2.40	0.53
1:D:445:MET:CE	1:D:447:PRO:CA	2.87	0.53
1:C:6:GLN:HG2	1:C:7:LEU:N	2.24	0.53
1:D:399:GLY:HA3	1:D:403:ASN:HD22	1.73	0.53
1:D:669:ILE:N	1:D:669:ILE:HD13	2.24	0.53
1:C:232:ARG:HA	1:C:232:ARG:HH11	1.74	0.52
1:A:126:GLY:O	1:A:127:ILE:HD13	2.10	0.52
2:F:86:TYR:O	2:F:89:ALA:HB3	2.09	0.52
1:A:123:THR:O	1:A:498:ARG:NH2	2.42	0.52
1:C:415:TYR:O	1:C:416:TYR:C	2.53	0.52
1:A:370:GLN:NE2	1:C:370:GLN:OE1	2.40	0.52
1:B:149:GLU:CG	6:B:795:HOH:O	2.56	0.52
1:D:596:GLU:CB	6:D:960:HOH:O	2.56	0.52
1:A:392:MET:HE1	2:E:30:ALA:HB2	1.92	0.52
1:C:392:MET:HE1	2:G:30:ALA:HB2	1.92	0.52
3:A:1801:B12:C6	4:C:1500:5AD:H5'1	2.39	0.52
1:A:134:ARG:NH1	1:A:175:GLU:OE2	2.34	0.52
1:A:623:ARG:HD3	1:C:115:HIS:CE1	2.44	0.52
1:C:7:LEU:HD12	1:C:146:LEU:HB3	1.91	0.52
1:D:123:THR:O	1:D:498:ARG:NH2	2.42	0.52
1:A:162:SER:OG	5:A:767:Z98:N1	2.37	0.52
1:B:267:VAL:HG22	1:B:299:GLN:HB3	1.91	0.52
4:B:1500:5AD:H4'	3:D:1801:B12:N23	2.25	0.52
1:A:709:VAL:O	1:A:712:LYS:HB3	2.09	0.52
1:B:43:MET:HE1	1:B:72:PRO:CA	2.40	0.52
1:A:710:ALA:O	1:A:715:VAL:HG23	2.10	0.51
1:B:234:ALA:O	1:B:237:VAL:HG12	2.10	0.51
1:C:392:MET:CE	2:G:30:ALA:HB2	2.39	0.51
2:G:20:GLU:HB3	6:G:725:HOH:O	2.10	0.51
2:E:92:LYS:HB2	2:E:94:ILE:HG12	1.92	0.51
1:D:172:MET:HE1	1:D:173:PHE:CD1	2.44	0.51
1:A:57:ASN:HB3	1:A:99:TRP:CH2	2.45	0.51
1:B:628:ILE:HD12	1:D:424:ILE:HD11	1.92	0.51
1:C:445:MET:HE3	1:C:471:LEU:CD2	2.39	0.51
1:C:580:ILE:HG22	1:C:580:ILE:O	2.11	0.51
5:A:767:Z98:H4A	1:C:629:LYS:HZ1	1.57	0.51
1:D:340:ARG:HG2	1:D:555:ILE:HD12	1.93	0.51
1:A:201:ILE:HD13	2:E:44:ASN:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:LYS:NZ	1:B:217:GLN:HE22	2.09	0.51
1:C:608:ILE:CD1	1:C:663:ALA:HB3	2.39	0.51
4:A:1500:5AD:H4'	3:C:1801:B12:N23	2.24	0.51
1:A:200:PHE:CE2	2:E:37:LEU:HD13	2.45	0.51
2:E:85:VAL:HG22	2:E:103:LEU:HD12	1.93	0.51
2:F:55:LEU:HD23	2:F:59:PHE:O	2.11	0.51
1:C:207:LYS:NZ	1:C:217:GLN:NE2	2.59	0.51
1:B:541:ILE:HD12	1:B:552:VAL:HG12	1.93	0.51
2:F:103:LEU:HD23	2:F:107:LYS:O	2.11	0.51
1:C:660:LYS:O	1:C:660:LYS:CG	2.59	0.51
1:A:94:MET:HE2	1:A:105:ILE:HG21	1.93	0.51
1:A:694:ASP:OD1	1:A:694:ASP:C	2.54	0.51
1:D:266:THR:O	1:D:266:THR:HG23	2.10	0.51
3:A:1801:B12:N23	4:C:1500:5AD:H4'	2.26	0.50
2:E:20:GLU:H	2:E:20:GLU:CD	2.18	0.50
2:F:45:THR:OG1	2:F:46:THR:N	2.43	0.50
1:C:506:ARG:HH11	1:C:518:GLN:HE22	1.60	0.50
1:A:87:PHE:HE1	1:A:139:ALA:CB	2.23	0.50
1:A:172:MET:C	1:A:172:MET:HE2	2.36	0.50
2:G:114:GLN:C	6:G:125:HOH:O	2.54	0.50
1:D:541:ILE:CD1	1:D:554:VAL:HG23	2.41	0.50
1:B:43:MET:HE1	1:B:72:PRO:CB	2.41	0.50
1:C:123:THR:HG23	1:C:135:LYS:HD3	1.93	0.50
1:B:445:MET:HE1	1:B:447:PRO:HA	1.93	0.50
1:C:41:LEU:HD23	1:C:43:MET:HE3	1.89	0.50
1:B:668:THR:HG23	1:B:676:HIS:HB2	1.85	0.50
3:D:1801:B12:H252	3:D:1801:B12:H601	1.93	0.50
1:A:289:GLU:CD	1:A:373:ARG:HH21	2.19	0.50
1:A:512:LYS:HB2	1:A:513:PRO:CD	2.42	0.50
1:B:295:ARG:HD3	6:B:898:HOH:O	2.11	0.50
1:D:88:GLU:OE2	1:D:498:ARG:HD2	2.12	0.50
1:A:540:ALA:HB1	1:A:570:LEU:HD11	1.93	0.49
1:B:42:GLN:NE2	1:B:44:GLY:O	2.45	0.49
1:B:132:ILE:HA	1:B:136:GLN:OE1	2.12	0.49
1:D:416:TYR:CG	1:D:417:PRO:HA	2.46	0.49
2:F:95:SER:OG	2:F:98:GLU:HG3	2.12	0.49
1:C:161:VAL:O	1:C:161:VAL:CG1	2.60	0.49
1:C:581:ASN:C	1:C:583:LEU:H	2.20	0.49
1:D:611:ALA:HB1	1:D:647:VAL:HG21	1.94	0.49
1:A:138:ARG:O	1:A:139:ALA:C	2.54	0.49
1:B:233:GLU:HG2	1:B:235:TRP:CZ2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:512:LYS:HB2	1:C:513:PRO:HD2	1.94	0.49
1:B:130:VAL:HG13	6:B:774:HOH:O	2.13	0.49
1:D:723:SER:O	3:D:1801:B12:H5R1	2.12	0.49
1:A:710:ALA:O	1:A:715:VAL:CG2	2.61	0.49
1:B:445:MET:CE	1:B:447:PRO:CA	2.90	0.49
1:C:346:ILE:HG23	6:C:891:HOH:O	2.11	0.49
1:D:123:THR:O	1:D:494:ASN:HA	2.12	0.49
3:D:1801:B12:C36	3:D:1801:B12:C35	2.80	0.49
1:A:543:PHE:CZ	1:C:578:ILE:HD13	2.47	0.49
1:B:445:MET:HE2	1:B:446:ALA:C	2.37	0.49
1:D:264:LEU:N	1:D:264:LEU:HD12	2.28	0.49
1:C:213:ALA:HB3	1:C:215:MET:HG3	1.94	0.49
1:D:729:ALA:O	1:D:733:VAL:HG22	2.12	0.49
3:D:1801:B12:C47	3:D:1801:B12:C49	2.91	0.49
1:A:629:LYS:HE2	5:C:767:Z98:H4A	1.94	0.49
1:A:546:LYS:NZ	1:C:578:ILE:HD11	2.28	0.48
1:C:207:LYS:HZ2	1:C:217:GLN:NE2	2.10	0.48
1:B:161:VAL:HG12	1:B:161:VAL:O	2.12	0.48
2:F:110:ASP:O	2:F:114:GLN:HB2	2.13	0.48
1:D:654:ASP:HA	1:D:657:ILE:HD12	1.94	0.48
1:B:250:ILE:O	1:B:251:PHE:C	2.54	0.48
1:B:445:MET:HE3	1:B:471:LEU:CD2	2.44	0.48
1:C:224:ALA:HB3	1:C:245:HIS:CE1	2.48	0.48
1:D:631:GLY:O	1:D:725:GLY:HA3	2.13	0.48
1:A:389:VAL:HG21	2:E:22:LEU:HD11	1.95	0.48
1:D:592:LEU:CD2	6:D:960:HOH:O	2.56	0.48
1:D:654:ASP:OD1	1:D:690:LYS:NZ	2.47	0.48
3:D:1801:B12:H492	3:D:1801:B12:H473	1.95	0.48
1:A:19:LEU:CD1	1:A:499:MET:HE2	2.44	0.48
1:B:204:CYS:HB3	1:B:452:PHE:CD2	2.49	0.48
1:B:506:ARG:HH11	1:B:518:GLN:NE2	2.12	0.48
3:C:1801:B12:O7R	3:C:1801:B12:H2B	2.14	0.48
1:B:224:ALA:HB3	1:B:245:HIS:CE1	2.49	0.48
1:C:616:ASP:HA	6:C:806:HOH:O	2.13	0.48
1:C:649:VAL:CG1	1:C:686:LEU:HD12	2.43	0.48
1:D:13:LEU:HD13	1:D:91:ILE:HG22	1.95	0.48
1:A:238:MET:HA	1:A:241:LEU:HD12	1.95	0.48
1:A:369:VAL:HG13	1:C:369:VAL:CG1	2.44	0.48
1:A:513:PRO:HA	1:C:529:LEU:HD23	1.95	0.48
1:A:608:ILE:HD13	1:A:638:VAL:HG11	1.96	0.48
1:B:526:THR:HG23	1:B:569:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:ILE:HD12	1:B:638:VAL:HG11	1.96	0.48
1:D:445:MET:HE2	1:D:446:ALA:C	2.38	0.48
1:D:668:THR:C	1:D:669:ILE:HD13	2.38	0.48
1:A:79:THR:HG21	1:A:106:MET:HE3	1.95	0.48
1:C:132:ILE:HA	1:C:136:GLN:OE1	2.14	0.48
1:A:461:ASP:O	1:A:462:GLU:C	2.56	0.47
1:A:161:VAL:O	1:A:161:VAL:HG12	2.15	0.47
2:F:50:GLU:HG3	2:F:77:MET:HE1	1.96	0.47
1:D:117:ASP:HA	1:D:164:VAL:HG23	1.95	0.47
1:D:711:VAL:O	1:D:711:VAL:CG1	2.59	0.47
1:A:426:ARG:HA	6:A:871:HOH:O	2.13	0.47
1:C:522:THR:HA	1:C:572:GLY:O	2.15	0.47
1:C:616:ASP:CA	6:C:806:HOH:O	2.62	0.47
1:B:377:LEU:O	1:B:381:VAL:HG23	2.15	0.47
1:B:670:ILE:HG23	3:B:1801:B12:O34	2.14	0.47
1:D:79:THR:HA	1:D:104:HIS:HB3	1.97	0.47
1:A:82:ILE:HG22	1:A:90:ASP:HB3	1.96	0.47
1:B:201:ILE:HD13	1:B:437:VAL:HG13	1.97	0.47
2:F:23:GLN:O	2:F:26:PHE:HB3	2.15	0.47
1:C:93:ARG:HA	1:C:96:MET:HE2	1.95	0.47
1:C:94:MET:HE2	1:C:105:ILE:CG2	2.45	0.47
1:C:612:THR:HG22	1:C:616:ASP:HB3	1.96	0.47
1:C:684:HIS:O	1:C:688:VAL:HG23	2.14	0.47
1:D:224:ALA:CB	1:D:245:HIS:CE1	2.98	0.47
2:H:54:LEU:CD2	2:H:57:MET:CE	2.87	0.47
1:A:475:CYS:HB2	2:E:56:ARG:O	2.15	0.47
1:B:391:PHE:HA	1:B:416:TYR:CZ	2.50	0.47
1:B:649:VAL:HG12	1:B:686:LEU:CD1	2.45	0.47
1:C:373:ARG:HA	1:C:377:LEU:HD23	1.97	0.47
1:D:172:MET:CE	1:D:173:PHE:N	2.74	0.47
1:D:269:PRO:HD2	1:D:280:ASP:OD1	2.15	0.47
1:D:290:MET:HE3	2:H:26:PHE:CG	2.49	0.47
1:B:80:THR:HG1	1:B:348:ASN:HD22	1.57	0.47
1:C:26:THR:HG22	1:C:27:PRO:CD	2.43	0.47
1:C:200:PHE:CE2	2:G:37:LEU:HD13	2.50	0.47
1:A:668:THR:HG21	1:A:676:HIS:CA	2.36	0.47
1:C:479:VAL:O	1:C:481:GLU:N	2.48	0.47
1:A:415:TYR:O	1:A:416:TYR:C	2.58	0.46
1:A:485:TYR:C	1:A:486:ILE:HD12	2.40	0.46
1:C:445:MET:HE1	1:C:447:PRO:N	2.29	0.46
1:C:525:LEU:HD21	1:C:547:MET:CE	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:THR:HG22	1:A:348:ASN:HA	1.97	0.46
1:B:233:GLU:CG	1:B:235:TRP:CH2	2.98	0.46
1:B:416:TYR:CG	1:B:417:PRO:HA	2.50	0.46
1:A:459:GLN:HG3	1:A:460:TYR:CE2	2.51	0.46
1:B:428:ILE:CG2	1:B:429:ASN:N	2.78	0.46
1:D:15:VAL:CG2	1:D:499:MET:HE1	2.45	0.46
6:A:768:HOH:O	2:E:87:LYS:CB	2.64	0.46
3:B:1801:B12:C47	3:B:1801:B12:C49	2.90	0.46
1:B:43:MET:HE3	1:B:72:PRO:HB3	1.97	0.46
1:B:528:PHE:C	1:B:528:PHE:CD2	2.93	0.46
1:C:7:LEU:HD21	1:C:95:ARG:CZ	2.45	0.46
1:C:387:ARG:NH1	1:C:416:TYR:O	2.43	0.46
1:D:123:THR:OG1	1:D:495:VAL:HG12	2.16	0.46
1:B:410:PHE:C	1:B:411:VAL:HG23	2.40	0.46
1:B:672:HIS:O	1:B:675:ILE:HG22	2.15	0.46
1:C:189:VAL:HG12	1:C:426:ARG:HG3	1.98	0.46
1:C:416:TYR:CG	1:C:417:PRO:HA	2.51	0.46
1:D:600:ASP:OD2	1:D:736:ARG:NH1	2.49	0.46
2:H:59:PHE:CE1	2:H:100:GLY:HA3	2.51	0.46
1:A:341:ASN:ND2	1:A:342:VAL:O	2.43	0.46
1:B:57:ASN:HB3	1:B:99:TRP:CH2	2.51	0.46
1:C:282:PRO:HG3	1:C:377:LEU:HD12	1.97	0.46
1:C:410:PHE:C	1:C:411:VAL:HG23	2.39	0.46
1:B:158:HIS:HA	1:B:180:GLY:O	2.16	0.46
1:C:444:TYR:CD2	1:C:444:TYR:C	2.93	0.46
1:A:236:LYS:HG2	1:A:415:TYR:HB2	1.98	0.46
1:A:426:ARG:NH1	1:C:634:GLU:OE2	2.31	0.46
1:B:7:LEU:HD23	1:B:146:LEU:HB3	1.96	0.46
1:C:77:VAL:CG1	1:C:104:HIS:HB2	2.46	0.46
3:A:1801:B12:N29	3:A:1801:B12:C25	2.76	0.46
1:B:445:MET:HE3	1:B:471:LEU:HD23	1.97	0.46
1:B:649:VAL:HG21	1:B:683:ILE:CD1	2.39	0.46
1:C:728:VAL:HG21	3:C:1801:B12:HM62	1.98	0.46
3:C:1801:B12:H251	3:C:1801:B12:N29	2.31	0.46
1:D:85:GLY:HA2	1:D:129:GLY:O	2.16	0.45
1:D:649:VAL:HG13	1:D:683:ILE:HG13	1.97	0.45
1:D:606:LEU:CD1	1:D:608:ILE:CD1	2.94	0.45
1:B:607:LYS:O	1:B:608:ILE:HD12	2.17	0.45
1:C:15:VAL:HG23	1:C:16:GLU:N	2.30	0.45
1:D:5:LEU:HD23	1:D:5:LEU:C	2.42	0.45
1:A:344:TRP:CD1	1:A:515:VAL:HB	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:LYS:NZ	1:C:226:ASN:OD1	2.49	0.45
1:B:268:PRO:HA	1:B:269:PRO:HD3	1.81	0.45
1:C:468:PRO:O	1:C:471:LEU:HB2	2.15	0.45
1:D:267:VAL:HG22	1:D:299:GLN:HB3	1.98	0.45
1:A:75:LEU:N	1:A:76:PRO:CD	2.80	0.45
1:A:649:VAL:O	1:A:653:VAL:HG23	2.16	0.45
1:B:315:THR:HB	6:B:852:HOH:O	2.15	0.45
1:C:305:MET:HE1	1:C:316:HIS:NE2	2.32	0.45
1:D:302:THR:HG23	6:D:973:HOH:O	2.17	0.45
1:A:271:ALA:O	1:A:274:ALA:HB3	2.17	0.45
1:A:504:GLU:HA	6:A:868:HOH:O	2.17	0.45
1:A:723:SER:O	3:A:1801:B12:O8R	2.29	0.45
1:B:90:ASP:O	1:B:94:MET:HG3	2.17	0.45
2:G:53:VAL:O	2:G:57:MET:HG3	2.17	0.45
1:D:82:ILE:HG22	1:D:90:ASP:HB3	1.98	0.45
1:D:593:SER:O	1:D:597:ILE:HG13	2.17	0.45
1:A:138:ARG:HE	1:A:176:GLU:CD	2.25	0.45
1:A:671:SER:HB2	1:A:676:HIS:ND1	2.32	0.45
2:E:54:LEU:HD12	2:E:68:VAL:HG23	1.99	0.45
1:C:8:ARG:HD3	1:C:11:GLU:CD	2.42	0.45
3:C:1801:B12:H252	3:C:1801:B12:H601	1.98	0.45
2:G:50:GLU:HG3	2:G:77:MET:HE1	1.99	0.45
1:D:210:MET:HG2	1:D:215:MET:CE	2.46	0.45
1:D:416:TYR:CD1	1:D:417:PRO:HA	2.52	0.45
2:H:54:LEU:HD23	2:H:57:MET:HE1	1.95	0.45
3:C:1801:B12:C35	3:C:1801:B12:C36	2.84	0.45
2:G:25:ARG:HG2	2:G:29:MET:HE2	1.98	0.45
1:B:729:ALA:O	1:B:733:VAL:HG13	2.17	0.45
1:C:679:ASN:O	1:C:683:ILE:CG1	2.58	0.45
1:D:224:ALA:HB3	1:D:245:HIS:CE1	2.52	0.45
1:D:445:MET:CE	1:D:447:PRO:CB	2.88	0.45
3:A:1801:B12:H2B	3:A:1801:B12:O7R	2.17	0.44
1:B:207:LYS:HZ3	1:B:217:GLN:NE2	2.13	0.44
1:B:224:ALA:CB	1:B:245:HIS:CE1	3.00	0.44
2:F:50:GLU:CG	2:F:77:MET:HE1	2.47	0.44
1:C:615:GLU:O	1:C:646:SER:OG	2.34	0.44
1:A:609:VAL:HG21	1:A:656:ALA:HB2	1.99	0.44
1:D:459:GLN:HE22	2:H:83:HIS:CE1	2.35	0.44
1:A:542:GLU:HG3	1:C:583:LEU:CD2	2.47	0.44
1:B:541:ILE:HD13	1:B:570:LEU:CD2	2.47	0.44
1:A:608:ILE:HG13	1:A:663:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1801:B12:O7R	3:A:1801:B12:C2B	2.65	0.44
1:B:561:GLN:O	1:B:562:GLU:C	2.60	0.44
1:C:94:MET:HE2	1:C:105:ILE:HG21	1.99	0.44
1:D:197:ILE:HG22	1:D:437:VAL:HG21	1.99	0.44
1:D:5:LEU:HD12	6:D:987:HOH:O	2.17	0.44
1:D:13:LEU:HD11	1:D:147:ILE:HD11	2.00	0.44
3:B:1801:B12:N23	4:D:1500:5AD:C4'	2.75	0.44
1:D:701:GLY:HA2	1:D:719:PHE:O	2.18	0.44
1:A:735:LYS:O	1:A:738:GLU:N	2.49	0.44
1:B:688:VAL:C	1:B:690:LYS:H	2.26	0.44
3:B:1801:B12:H261	4:D:1500:5AD:H5'3	2.00	0.44
3:C:1801:B12:H253	3:C:1801:B12:H301	1.81	0.44
2:H:57:MET:HE1	2:H:82:GLY:HA2	2.00	0.44
1:A:153:ARG:HA	1:A:154:PRO:HD3	1.90	0.44
1:A:613:VAL:HG22	1:A:614:GLY:H	1.82	0.44
1:A:668:THR:HB	1:A:676:HIS:HB2	1.99	0.44
5:A:767:Z98:H4A	1:C:629:LYS:HE3	1.87	0.44
1:C:13:LEU:HD22	1:C:18:ILE:CD1	2.47	0.44
1:D:600:ASP:OD2	1:D:600:ASP:C	2.61	0.44
2:H:40:LEU:HA	2:H:40:LEU:HD23	1.72	0.44
1:A:320:LEU:HD13	1:A:358:ALA:HB3	1.99	0.44
1:A:606:LEU:CD2	1:A:732:LEU:HD13	2.39	0.44
1:B:292:GLU:HG3	6:B:944:HOH:O	2.18	0.44
3:B:1801:B12:H473	3:B:1801:B12:C49	2.33	0.44
1:D:668:THR:HG23	1:D:668:THR:O	2.17	0.44
3:D:1801:B12:H203	3:D:1801:B12:H301	2.00	0.44
1:A:568:ILE:CG2	1:A:570:LEU:HD11	2.48	0.43
1:C:177:GLY:O	1:C:178:VAL:C	2.61	0.43
1:C:597:ILE:HD13	1:C:726:ILE:CD1	2.47	0.43
1:D:611:ALA:HB2	1:D:643:LEU:HB2	2.00	0.43
1:C:413:SER:OG	1:C:422:ASP:OD2	2.32	0.43
1:C:460:TYR:O	1:C:461:ASP:HB2	2.17	0.43
1:D:667:SER:OG	1:D:669:ILE:HD11	2.18	0.43
1:B:377:LEU:HB2	1:D:368:MET:HG2	2.00	0.43
1:D:648:PRO:O	1:D:649:VAL:C	2.60	0.43
1:B:79:THR:HB	1:B:332:SER:HA	2.00	0.43
1:C:13:LEU:CD1	1:C:91:ILE:HG22	2.48	0.43
1:A:369:VAL:CG1	1:C:369:VAL:HG13	2.48	0.43
1:A:542:GLU:HG3	1:C:583:LEU:HD23	2.01	0.43
1:B:687:ALA:HB3	1:B:693:ARG:HD3	2.00	0.43
1:D:196:MET:SD	1:D:402:PHE:CD1	3.11	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:ARG:CZ	1:D:432:ILE:HD12	2.49	0.43
1:C:268:PRO:HA	1:C:269:PRO:HD3	1.83	0.43
1:D:428:ILE:HB	6:D:882:HOH:O	2.18	0.43
1:A:160:TYR:CE1	5:A:767:Z98:HG	2.53	0.43
1:A:484:VAL:HG12	1:A:486:ILE:CD1	2.49	0.43
3:B:1801:B12:C6	4:D:1500:5AD:H5'1	2.48	0.43
1:C:574:VAL:HG13	1:C:576:PHE:CE1	2.54	0.43
1:A:713:GLN:HA	1:A:713:GLN:NE2	2.34	0.43
1:A:184:ASP:HA	1:A:185:PRO:HD2	1.90	0.43
1:A:188:ASN:HB3	1:A:194:ILE:HB	2.01	0.43
1:B:658:GLU:HG2	6:B:966:HOH:O	2.17	0.43
1:C:270:THR:HG21	1:C:279:LEU:HD13	2.01	0.43
1:D:250:ILE:HG23	2:H:34:VAL:HG21	2.01	0.43
1:A:135:LYS:NZ	1:A:488:GLU:OE2	2.30	0.43
1:A:580:ILE:HD12	1:C:535:VAL:HG11	2.00	0.43
1:B:730:THR:HG22	1:B:734:LYS:HD2	2.01	0.43
1:D:116:TYR:HE2	1:D:120:ILE:HD13	1.84	0.43
1:D:281:LEU:HB3	1:D:282:PRO:HD3	2.00	0.43
1:D:528:PHE:CD2	1:D:528:PHE:C	2.96	0.43
1:A:422:ASP:OD1	1:A:422:ASP:N	2.51	0.42
1:B:161:VAL:O	1:B:161:VAL:CG1	2.67	0.42
1:C:631:GLY:O	1:C:725:GLY:HA3	2.19	0.42
1:A:344:TRP:CG	1:A:515:VAL:HB	2.54	0.42
1:B:301:ASN:O	1:B:305:MET:HE1	2.18	0.42
1:A:512:LYS:HB2	1:A:513:PRO:HD2	2.00	0.42
1:A:717:ALA:HB2	1:A:731:PHE:CE1	2.54	0.42
3:A:1801:B12:C36	3:A:1801:B12:C35	2.84	0.42
1:B:172:MET:HE1	1:B:173:PHE:HD1	1.84	0.42
1:B:322:ILE:HD13	1:B:322:ILE:HA	1.87	0.42
1:D:172:MET:HE2	1:D:173:PHE:HD1	1.84	0.42
1:A:7:LEU:HD23	1:A:7:LEU:HA	1.75	0.42
1:B:587:PRO:C	6:B:848:HOH:O	2.61	0.42
1:C:5:LEU:O	1:C:5:LEU:HD23	2.19	0.42
1:C:668:THR:CG2	1:C:668:THR:O	2.68	0.42
1:D:680:MET:HE1	1:D:705:VAL:CG1	2.50	0.42
1:B:604:THR:O	1:B:736:ARG:NH2	2.37	0.42
1:C:551:GLU:CD	1:C:573:ARG:HE	2.28	0.42
2:G:89:ALA:HB2	2:G:99:ALA:HB2	2.01	0.42
1:D:424:ILE:HG21	1:D:426:ARG:CZ	2.50	0.42
1:A:445:MET:CE	1:A:447:PRO:CA	2.96	0.42
3:A:1801:B12:H473	3:A:1801:B12:H481	0.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:VAL:CG1	1:B:686:LEU:HD12	2.50	0.42
1:C:359:LEU:HD23	1:C:359:LEU:HA	1.98	0.42
3:C:1801:B12:H473	3:C:1801:B12:H481	1.52	0.42
1:D:210:MET:HE3	1:D:215:MET:CE	2.49	0.42
1:D:649:VAL:CG1	1:D:683:ILE:HG13	2.49	0.42
1:A:541:ILE:O	1:A:545:LYS:HG2	2.20	0.42
1:B:517:TRP:O	1:B:518:GLN:C	2.60	0.42
1:C:79:THR:HB	6:C:790:HOH:O	2.19	0.42
1:C:626:ILE:HD13	1:C:640:VAL:HG11	2.00	0.42
2:F:25:ARG:O	2:F:29:MET:HG2	2.20	0.42
1:A:711:VAL:HA	1:A:715:VAL:O	2.20	0.42
5:A:767:Z98:C4A	1:C:629:LYS:HZ3	2.23	0.42
1:B:22:LEU:HB2	6:B:864:HOH:O	2.18	0.42
1:C:6:GLN:CG	1:C:7:LEU:N	2.80	0.42
1:D:268:PRO:HA	1:D:269:PRO:HD3	1.74	0.42
1:A:19:LEU:HD11	1:A:499:MET:HE2	2.02	0.42
3:A:1801:B12:H252	3:A:1801:B12:H601	2.02	0.42
1:C:504:GLU:C	1:C:506:ARG:H	2.27	0.42
1:D:95:ARG:O	1:D:98:ALA:HB3	2.20	0.42
1:D:475:CYS:HB2	2:H:56:ARG:O	2.20	0.42
1:D:668:THR:O	1:D:668:THR:HG22	2.18	0.42
3:D:1801:B12:H492	3:D:1801:B12:H471	2.01	0.42
1:A:515:VAL:HG23	1:A:516:GLU:HG2	2.02	0.41
1:A:688:VAL:HG22	1:A:693:ARG:HG2	2.02	0.41
1:B:282:PRO:HG3	1:B:377:LEU:CD1	2.50	0.41
1:B:513:PRO:O	1:B:521:GLY:CA	2.68	0.41
3:B:1801:B12:HM51	3:B:1801:B12:HM63	1.87	0.41
1:C:443:ASP:O	2:G:83:HIS:CE1	2.73	0.41
1:D:264:LEU:HD13	1:D:296:MET:HE2	2.01	0.41
1:D:266:THR:HG23	6:D:777:HOH:O	2.20	0.41
1:A:123:THR:HG23	1:A:135:LYS:HD3	2.03	0.41
1:A:724:LYS:HB2	1:A:726:ILE:HG22	2.01	0.41
1:C:109:ARG:NH2	1:C:114:SER:OG	2.54	0.41
1:C:577:SER:O	1:C:578:ILE:HD12	2.20	0.41
1:D:606:LEU:HD12	1:D:608:ILE:CD1	2.50	0.41
1:A:161:VAL:HG23	1:A:181:ALA:HB1	2.02	0.41
1:D:335:THR:O	1:D:338:GLU:HB2	2.21	0.41
1:D:578:ILE:HD13	1:D:578:ILE:HA	1.78	0.41
1:A:137:VAL:HG11	1:A:172:MET:HE1	2.01	0.41
1:B:5:LEU:HD23	1:B:5:LEU:C	2.44	0.41
1:B:123:THR:OG1	1:B:488:GLU:OE2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:612:THR:HB	1:B:645:THR:HG22	2.03	0.41
1:C:185:PRO:HB3	1:C:203:ALA:HB2	2.02	0.41
1:C:200:PHE:CD2	2:G:37:LEU:HD13	2.55	0.41
3:C:1801:B12:O7R	3:C:1801:B12:C2B	2.68	0.41
1:D:301:ASN:HB2	6:D:926:HOH:O	2.19	0.41
1:A:445:MET:HE2	1:A:446:ALA:C	2.46	0.41
1:C:122:GLY:HA2	1:C:487:ASP:O	2.20	0.41
1:C:617:GLU:HB2	3:C:1801:B12:C43	2.51	0.41
1:C:657:ILE:CG1	1:C:692:ILE:HD13	2.51	0.41
1:D:736:ARG:HD2	6:D:849:HOH:O	2.17	0.41
1:A:568:ILE:HG22	1:A:570:LEU:HD11	2.00	0.41
1:B:458:LYS:C	1:B:460:TYR:N	2.77	0.41
3:B:1801:B12:H492	3:B:1801:B12:H471	2.01	0.41
1:C:82:ILE:CG2	1:C:90:ASP:HB3	2.51	0.41
1:C:344:TRP:CD1	1:C:515:VAL:HB	2.56	0.41
1:C:445:MET:HE2	1:C:447:PRO:N	2.30	0.41
2:G:76:LEU:HB3	2:G:84:ILE:HD11	2.02	0.41
1:A:164:VAL:CG1	1:A:194:ILE:HG12	2.50	0.41
1:A:608:ILE:HD13	1:A:638:VAL:HG13	2.03	0.41
1:B:279:LEU:HD11	1:D:46:PHE:CE1	2.55	0.41
1:B:663:ALA:HA	1:B:697:MET:O	2.21	0.41
2:G:16:ASN:HD22	2:G:16:ASN:HA	1.73	0.41
1:D:233:GLU:HG2	1:D:235:TRP:CH2	2.56	0.41
1:A:349:ILE:N	1:A:349:ILE:CD1	2.84	0.41
1:A:371:LEU:HD23	1:C:369:VAL:HG22	2.03	0.41
1:A:389:VAL:HG13	2:E:29:MET:HE1	2.03	0.41
1:B:201:ILE:HD13	1:B:437:VAL:CG1	2.51	0.41
1:B:679:ASN:O	1:B:683:ILE:HD13	2.20	0.41
1:D:26:THR:HG22	1:D:27:PRO:CD	2.49	0.41
1:D:428:ILE:HG23	6:D:873:HOH:O	2.21	0.41
1:B:610:ALA:HA	1:B:665:LEU:O	2.21	0.40
1:A:618:HIS:CD2	3:A:1801:B12:H482	2.57	0.40
3:B:1801:B12:H473	3:B:1801:B12:H481	1.86	0.40
1:C:197:ILE:HG22	1:C:201:ILE:HD11	2.03	0.40
1:C:335:THR:HA	1:C:336:PRO:HD3	1.91	0.40
1:D:608:ILE:CG1	1:D:663:ALA:HB3	2.50	0.40
1:D:693:ARG:HH22	1:D:716:ASP:CG	2.29	0.40
1:D:495:VAL:O	1:D:499:MET:HG2	2.21	0.40
1:A:266:THR:HG23	1:A:266:THR:O	2.22	0.40
1:A:613:VAL:CG2	1:A:649:VAL:HG23	2.51	0.40
1:B:552:VAL:CG1	1:B:570:LEU:HD23	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:688:VAL:HG12	1:B:689:GLU:N	2.35	0.40
1:D:186:GLN:O	1:D:187:TYR:C	2.64	0.40
1:A:224:ALA:HB3	1:A:245:HIS:CE1	2.57	0.40
1:B:238:MET:SD	1:B:283:TYR:HB2	2.62	0.40
1:C:259:LYS:HA	1:C:262:ILE:HD12	2.02	0.40
1:D:138:ARG:HE	1:D:176:GLU:CD	2.30	0.40
1:D:185:PRO:O	1:D:189:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	722/763 (95%)	674 (93%)	42 (6%)	6 (1%)	16	25
1	B	722/763 (95%)	683 (95%)	32 (4%)	7 (1%)	12	20
1	C	722/763 (95%)	691 (96%)	22 (3%)	9 (1%)	10	16
1	D	722/763 (95%)	690 (96%)	30 (4%)	2 (0%)	36	50
2	E	107/121 (88%)	101 (94%)	5 (5%)	1 (1%)	14	22
2	F	107/121 (88%)	103 (96%)	3 (3%)	1 (1%)	14	22
2	G	107/121 (88%)	105 (98%)	2 (2%)	0	100	100
2	H	107/121 (88%)	106 (99%)	1 (1%)	0	100	100
All	All	3316/3536 (94%)	3153 (95%)	137 (4%)	26 (1%)	16	25

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	462	GLU
1	B	7	LEU

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Mol	Chain	Res	Type
1	B	739	MET
1	C	6	GLN
1	C	505	PHE
2	E	93	ASN
1	B	6	GLN
1	B	689	GLU
1	C	461	ASP
1	B	69	ASP
1	C	582	SER
1	A	487	ASP
1	A	736	ARG
1	C	480	PRO
1	C	487	ASP
1	A	7	LEU
2	F	15	ALA
1	C	7	LEU
1	B	16	GLU
1	C	688	VAL
1	D	461	ASP
1	B	411	VAL
1	C	411	VAL
1	D	411	VAL
1	A	411	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	598/644 (93%)	559 (94%)	39 (6%)	15 27
1	B	604/644 (94%)	574 (95%)	30 (5%)	22 38
1	C	600/644 (93%)	565 (94%)	35 (6%)	18 32
1	D	602/644 (94%)	556 (92%)	46 (8%)	12 21
2	E	89/100 (89%)	82 (92%)	7 (8%)	11 19
2	F	90/100 (90%)	85 (94%)	5 (6%)	19 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	89/100 (89%)	82 (92%)	7 (8%)	11	19
2	H	89/100 (89%)	84 (94%)	5 (6%)	19	33
All	All	2761/2976 (93%)	2587 (94%)	174 (6%)	16	29

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	7	LEU
1	A	9	VAL
1	A	18	ILE
1	A	24	LYS
1	A	28	LYS
1	A	69	ASP
1	A	153	ARG
1	A	172	MET
1	A	232	ARG
1	A	250	ILE
1	A	306	GLU
1	A	341	ASN
1	A	349	ILE
1	A	411	VAL
1	A	418	GLU
1	A	449	THR
1	A	471	LEU
1	A	506	ARG
1	A	518	GLN
1	A	533	LYS
1	A	541	ILE
1	A	546	LYS
1	A	573	ARG
1	A	574	VAL
1	A	578	ILE
1	A	580	ILE
1	A	604	THR
1	A	608	ILE
1	A	651	LYS
1	A	668	THR
1	A	670	ILE
1	A	689	GLU
1	A	694	ASP

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Mol	Chain	Res	Type
1	A	696	ILE
1	A	706	THR
1	A	712	LYS
1	A	721	ARG
1	A	738	GLU
2	E	20	GLU
2	E	42	LYS
2	E	73	ASP
2	E	76	LEU
2	E	79	LYS
2	E	93	ASN
2	E	114	GLN
1	B	6	GLN
1	B	15	VAL
1	B	18	ILE
1	B	125	GLN
1	B	172	MET
1	B	232	ARG
1	B	292	GLU
1	B	306	GLU
1	B	338	GLU
1	B	341	ASN
1	B	349	ILE
1	B	411	VAL
1	B	428	ILE
1	B	442	GLU
1	B	457	VAL
1	B	464	LEU
1	B	471	LEU
1	B	557	ARG
1	B	578	ILE
1	B	580	ILE
1	B	592	LEU
1	B	603	LYS
1	B	608	ILE
1	B	613	VAL
1	B	651	LYS
1	B	668	THR
1	B	696	ILE
1	B	703	THR
1	B	723	SER
1	B	736	ARG

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Mol	Chain	Res	Type
2	F	20	GLU
2	F	31	GLU
2	F	76	LEU
2	F	92	LYS
2	F	101	LEU
1	C	7	LEU
1	C	9	VAL
1	C	13	LEU
1	C	20	LYS
1	C	26	THR
1	C	39	GLU
1	C	79	THR
1	C	164	VAL
1	C	168	ASP
1	C	232	ARG
1	C	301	ASN
1	C	306	GLU
1	C	341	ASN
1	C	411	VAL
1	C	428	ILE
1	C	462	GLU
1	C	464	LEU
1	C	465	VAL
1	C	471	LEU
1	C	500	GLU
1	C	570	LEU
1	C	576	PHE
1	C	578	ILE
1	C	604	THR
1	C	608	ILE
1	C	613	VAL
1	C	643	LEU
1	C	651	LYS
1	C	668	THR
1	C	683	ILE
1	C	694	ASP
1	C	696	ILE
1	C	731	PHE
1	C	733	VAL
1	C	736	ARG
2	G	8	GLN
2	G	9	GLN

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Mol	Chain	Res	Type
2	G	39	ASP
2	G	76	LEU
2	G	84	ILE
2	G	101	LEU
2	G	107	LYS
1	D	5	LEU
1	D	6	GLN
1	D	8	ARG
1	D	15	VAL
1	D	24	LYS
1	D	26	THR
1	D	28	LYS
1	D	39	GLU
1	D	47	ILE
1	D	127	ILE
1	D	153	ARG
1	D	172	MET
1	D	232	ARG
1	D	258	LYS
1	D	306	GLU
1	D	338	GLU
1	D	349	ILE
1	D	395	ILE
1	D	411	VAL
1	D	427	GLN
1	D	449	THR
1	D	471	LEU
1	D	491	GLU
1	D	546	LYS
1	D	557	ARG
1	D	577	SER
1	D	578	ILE
1	D	591	ILE
1	D	597	ILE
1	D	604	THR
1	D	606	LEU
1	D	608	ILE
1	D	613	VAL
1	D	615	GLU
1	D	635	LYS
1	D	657	ILE
1	D	659	LEU

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Mol	Chain	Res	Type
1	D	660	LYS
1	D	662	ASP
1	D	668	THR
1	D	669	ILE
1	D	682	ARG
1	D	683	ILE
1	D	694	ASP
1	D	696	ILE
1	D	736	ARG
2	H	24	THR
2	H	76	LEU
2	H	84	ILE
2	H	93	ASN
2	H	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	319	ASN
1	A	331	GLN
1	A	348	ASN
1	A	370	GLN
1	A	407	GLN
1	A	704	GLN
1	A	713	GLN
2	E	8	GLN
2	E	16	ASN
2	E	114	GLN
1	B	36	GLN
1	B	73	GLN
1	B	125	GLN
1	B	217	GLN
1	B	319	ASN
1	B	348	ASN
1	B	370	GLN
1	B	420	ASN
1	B	518	GLN
2	F	8	GLN
1	C	6	GLN
1	C	36	GLN
1	C	217	GLN

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Mol	Chain	Res	Type
1	C	301	ASN
1	C	357	GLN
1	C	370	GLN
1	C	518	GLN
2	G	8	GLN
2	G	16	ASN
2	G	93	ASN
1	D	6	GLN
1	D	36	GLN
1	D	228	ASN
1	D	319	ASN
1	D	341	ASN
1	D	370	GLN
1	D	403	ASN
2	H	16	ASN
2	H	83	HIS
2	H	93	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	B12	D	1801	1	94,101,101	1.48	12 (12%)	149,166,166	2.39	36 (24%)
4	5AD	D	1500	-	20,20,20	1.72	4 (20%)	28,30,30	3.14	13 (46%)
5	Z98	A	767	-	22,23,23	1.96	8 (36%)	27,32,32	2.32	5 (18%)
5	Z98	B	767	-	22,23,23	1.55	6 (27%)	27,32,32	1.82	7 (25%)
4	5AD	C	1500	-	20,20,20	1.74	3 (15%)	28,30,30	2.75	13 (46%)
5	Z98	C	767	-	22,23,23	1.55	2 (9%)	27,32,32	1.73	6 (22%)
3	B12	B	1801	1	94,101,101	1.77	11 (11%)	149,166,166	2.41	34 (22%)
4	5AD	A	1500	-	20,20,20	1.80	5 (25%)	28,30,30	2.85	15 (53%)
3	B12	C	1801	1	94,101,101	1.75	13 (13%)	149,166,166	2.56	37 (24%)
5	Z98	D	767	-	22,23,23	1.53	3 (13%)	27,32,32	1.61	4 (14%)
4	5AD	B	1500	-	20,20,20	1.73	4 (20%)	28,30,30	2.55	12 (42%)
3	B12	A	1801	1	94,101,101	1.47	11 (11%)	149,166,166	2.49	39 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	B12	D	1801	1	-	6/56/223/223	0/3/11/11
4	5AD	D	1500	-	1/1/4/4	0/4/20/20	0/3/3/3
5	Z98	A	767	-	-	10/17/17/17	0/1/1/1
5	Z98	B	767	-	-	7/17/17/17	0/1/1/1
4	5AD	C	1500	-	-	0/4/20/20	0/3/3/3
5	Z98	C	767	-	-	7/17/17/17	0/1/1/1
3	B12	B	1801	1	1/1/36/38	7/56/223/223	0/3/11/11
4	5AD	A	1500	-	1/1/4/4	0/4/20/20	0/3/3/3
3	B12	C	1801	1	1/1/36/38	10/56/223/223	0/3/11/11
5	Z98	D	767	-	-	8/17/17/17	0/1/1/1
4	5AD	B	1500	-	-	0/4/20/20	0/3/3/3
3	B12	A	1801	1	1/1/36/38	18/56/223/223	0/3/11/11

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1801	B12	C19-N24	-9.96	1.36	1.49
3	B	1801	B12	C19-N24	-9.45	1.37	1.49
3	B	1801	B12	C14-N23	6.99	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1801	B12	C14-N23	6.71	1.44	1.35
3	A	1801	B12	C14-N23	5.93	1.43	1.35
3	D	1801	B12	C14-N23	5.90	1.42	1.35
3	B	1801	B12	C8B-C9B	5.86	1.49	1.40
3	A	1801	B12	C19-N24	-5.84	1.41	1.49
4	C	1500	5AD	C5-C4	5.29	1.48	1.39
3	D	1801	B12	C8B-C9B	5.18	1.48	1.40
3	D	1801	B12	C19-N24	-5.08	1.42	1.49
4	A	1500	5AD	C5-C4	4.90	1.47	1.39
4	B	1500	5AD	C5-C4	4.85	1.47	1.39
4	D	1500	5AD	C5-C4	4.37	1.46	1.39
3	C	1801	B12	C9-N22	4.17	1.40	1.30
5	C	767	Z98	P-OP2	4.11	1.63	1.50
3	A	1801	B12	C8B-C9B	4.09	1.47	1.40
3	B	1801	B12	C9-N22	4.08	1.40	1.30
5	A	767	Z98	P-OP2	3.78	1.62	1.50
5	A	767	Z98	OP4-C5A	-3.73	1.31	1.44
4	D	1500	5AD	C5-C6	3.71	1.51	1.41
3	C	1801	B12	C8B-C9B	3.59	1.46	1.40
5	A	767	Z98	C2A-C2	3.57	1.56	1.50
3	D	1801	B12	C11-N23	3.47	1.43	1.36
3	D	1801	B12	C9-N22	3.46	1.39	1.30
3	C	1801	B12	C16-C15	-3.46	1.34	1.44
3	B	1801	B12	C16-C15	-3.44	1.34	1.44
3	D	1801	B12	C16-C15	-3.34	1.35	1.44
3	A	1801	B12	C8B-N1B	-3.32	1.32	1.39
3	D	1801	B12	C6B-C5B	3.30	1.48	1.40
4	C	1500	5AD	C5-C6	3.27	1.50	1.41
3	A	1801	B12	C6B-C5B	3.27	1.48	1.40
3	A	1801	B12	C16-C15	-3.19	1.35	1.44
3	A	1801	B12	C11-N23	3.15	1.42	1.36
3	A	1801	B12	C10-C9	3.14	1.48	1.39
3	B	1801	B12	C6B-C5B	3.14	1.48	1.40
5	A	767	Z98	C4-C4A	-3.14	1.40	1.46
3	B	1801	B12	C9B-N3B	-3.10	1.34	1.39
3	A	1801	B12	C9B-N3B	-3.06	1.34	1.39
3	A	1801	B12	C9-N22	3.04	1.38	1.30
4	B	1500	5AD	C5-C6	3.00	1.49	1.41
3	D	1801	B12	C10-C9	2.97	1.47	1.39
3	C	1801	B12	C11-N23	2.97	1.42	1.36
5	B	767	Z98	P-OP2	2.93	1.59	1.50
4	C	1500	5AD	C8-N7	2.93	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	767	Z98	C2A-C2	2.92	1.55	1.50
3	B	1801	B12	C2B-N3B	2.91	1.37	1.31
4	A	1500	5AD	C8-N7	2.90	1.37	1.31
3	C	1801	B12	C14-C15	2.82	1.50	1.38
3	D	1801	B12	C8B-N1B	-2.81	1.33	1.39
4	A	1500	5AD	C5-C6	2.75	1.48	1.41
3	D	1801	B12	C14-C15	2.74	1.50	1.38
5	B	767	Z98	C4-C4A	-2.73	1.40	1.46
3	C	1801	B12	C9B-N3B	-2.71	1.34	1.39
5	B	767	Z98	C3-C2	-2.71	1.38	1.41
5	B	767	Z98	C4A-ND	2.65	1.36	1.27
4	D	1500	5AD	C8-N7	2.64	1.36	1.31
3	A	1801	B12	C14-C15	2.59	1.49	1.38
5	A	767	Z98	P-OP3	2.57	1.64	1.54
3	B	1801	B12	C14-C15	2.48	1.49	1.38
5	D	767	Z98	C4A-ND	2.47	1.35	1.27
4	B	1500	5AD	C8-N7	2.45	1.36	1.31
3	C	1801	B12	C2B-N3B	2.42	1.36	1.31
3	B	1801	B12	C8B-N1B	-2.39	1.34	1.39
3	C	1801	B12	C12-C11	-2.39	1.48	1.52
4	A	1500	5AD	C5-N7	-2.38	1.34	1.39
3	B	1801	B12	C11-N23	2.38	1.41	1.36
3	D	1801	B12	C9B-N3B	-2.35	1.35	1.39
4	A	1500	5AD	C3'-C2'	-2.35	1.47	1.53
5	C	767	Z98	C4A-ND	2.31	1.34	1.27
3	C	1801	B12	C6B-C5B	2.31	1.46	1.40
5	B	767	Z98	C2A-C2	2.30	1.54	1.50
3	C	1801	B12	C10-C11	-2.28	1.30	1.37
5	A	767	Z98	P-OP1	-2.22	1.46	1.54
5	D	767	Z98	C4-C4A	-2.18	1.42	1.46
3	C	1801	B12	C2B-N1B	-2.11	1.34	1.37
4	B	1500	5AD	C4-N3	2.09	1.38	1.34
4	D	1500	5AD	O4'-C1'	2.08	1.46	1.42
5	A	767	Z98	C4-C5	-2.07	1.39	1.42
5	B	767	Z98	O-C	-2.05	1.24	1.30
3	D	1801	B12	C1-C2	-2.02	1.54	1.58
5	A	767	Z98	C4A-ND	2.01	1.33	1.27

All (221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1801	B12	C20-C1-C19	-11.59	98.19	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1801	B12	C20-C1-C19	-10.08	99.64	109.35
3	A	1801	B12	C1-C19-N24	9.38	116.69	106.25
3	C	1801	B12	C20-C1-C19	-9.37	100.33	109.35
3	C	1801	B12	C12-C11-C10	-9.11	111.66	123.40
3	D	1801	B12	C1-C19-N24	9.07	116.34	106.25
3	A	1801	B12	C13-C12-C11	-8.91	91.01	100.97
3	D	1801	B12	C13-C12-C11	-8.25	91.75	100.97
3	C	1801	B12	C19-C1-N21	8.13	110.52	102.14
3	C	1801	B12	C47-C12-C46	8.10	122.83	109.41
3	C	1801	B12	C13-C12-C11	-8.04	91.98	100.97
3	D	1801	B12	C20-C1-C19	-7.93	101.72	109.35
3	B	1801	B12	C1-C19-N24	7.44	114.52	106.25
5	A	767	Z98	OP3-P-OP4	-7.32	87.60	106.67
3	A	1801	B12	C1-C19-C18	7.31	133.76	121.90
3	B	1801	B12	C19-C1-N21	7.29	109.65	102.14
3	D	1801	B12	C19-C1-N21	7.25	109.61	102.14
3	C	1801	B12	C1-C19-N24	7.22	114.28	106.25
4	D	1500	5AD	C5-C4-N3	-7.07	116.98	126.72
3	B	1801	B12	C13-C12-C11	-7.01	93.13	100.97
3	D	1801	B12	C12-C11-C10	-6.94	114.45	123.40
3	C	1801	B12	C18-C19-N24	6.90	112.70	102.33
5	A	767	Z98	OP1-P-OP4	6.77	124.33	106.67
3	B	1801	B12	C18-C19-N24	6.67	112.36	102.33
3	D	1801	B12	C46-C12-C13	-6.65	85.78	112.74
3	A	1801	B12	C19-C1-N21	6.52	108.86	102.14
3	B	1801	B12	C12-C11-C10	-6.52	114.99	123.40
3	A	1801	B12	C47-C12-C46	6.50	120.18	109.41
3	D	1801	B12	C1-C19-C18	6.46	132.38	121.90
3	A	1801	B12	C46-C12-C13	-6.45	86.59	112.74
4	D	1500	5AD	O2'-C2'-C1'	6.25	131.62	110.10
3	C	1801	B12	C20-C1-N21	-6.23	99.96	110.26
4	A	1500	5AD	C5-C4-N3	-6.23	118.14	126.72
4	C	1500	5AD	C5-C4-N3	-6.18	118.20	126.72
3	D	1801	B12	C47-C12-C46	6.15	119.59	109.41
4	B	1500	5AD	C5-C4-N3	-6.12	118.29	126.72
5	C	767	Z98	CG-ND-C4A	6.07	138.15	118.72
3	C	1801	B12	C12-C11-N23	5.81	119.84	111.83
3	B	1801	B12	C2-C1-C19	5.79	127.62	118.61
3	B	1801	B12	C1-C19-C18	5.60	130.98	121.90
3	C	1801	B12	C46-C12-C13	-5.55	90.25	112.74
3	C	1801	B12	C1-C19-C18	5.55	130.90	121.90
4	D	1500	5AD	C2-N3-C4	5.37	124.95	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1801	B12	C47-C12-C13	-5.37	90.97	112.74
3	B	1801	B12	C46-C12-C13	-5.33	91.13	112.74
3	A	1801	B12	C12-C11-C10	-5.32	116.55	123.40
4	B	1500	5AD	N3-C4-N9	5.31	136.19	127.17
3	D	1801	B12	C19-N24-C16	5.19	112.97	107.29
4	D	1500	5AD	C3'-C2'-C1'	5.18	111.25	101.46
3	B	1801	B12	C47-C12-C46	5.13	117.89	109.41
3	A	1801	B12	C9B-C8B-N1B	5.10	107.56	105.30
5	B	767	Z98	CG-ND-C4A	5.08	134.98	118.72
4	C	1500	5AD	N3-C4-N9	5.07	135.78	127.17
3	A	1801	B12	C12-C11-N23	5.05	118.78	111.83
4	A	1500	5AD	C3'-C2'-C1'	5.04	111.00	101.46
3	D	1801	B12	C12-C11-N23	5.03	118.75	111.83
3	A	1801	B12	C26-C2-C1	5.00	117.73	110.00
3	B	1801	B12	C12-C11-N23	4.91	118.59	111.83
4	A	1500	5AD	O2'-C2'-C1'	4.90	126.98	110.10
3	D	1801	B12	C25-C2-C1	-4.90	106.43	113.75
4	A	1500	5AD	N3-C4-N9	4.89	135.49	127.17
3	B	1801	B12	C9B-C8B-N1B	4.86	107.46	105.30
3	A	1801	B12	C2-C1-N21	4.75	108.38	101.78
4	D	1500	5AD	N3-C4-N9	4.75	135.24	127.17
4	D	1500	5AD	C4-C5-N7	-4.69	105.22	110.58
4	D	1500	5AD	N3-C2-N1	-4.66	121.53	128.58
3	C	1801	B12	C9-C10-C11	-4.64	119.34	125.97
3	A	1801	B12	C2-C1-C19	4.57	125.72	118.61
3	A	1801	B12	C20-C1-N21	-4.55	102.73	110.26
3	C	1801	B12	C2-C1-C19	4.44	125.52	118.61
4	C	1500	5AD	C2-N3-C4	4.38	122.53	111.83
3	A	1801	B12	C19-N24-C16	4.37	112.07	107.29
3	C	1801	B12	C9B-C8B-N1B	4.28	107.20	105.30
4	B	1500	5AD	N3-C2-N1	-4.26	122.13	128.58
4	B	1500	5AD	C2-N3-C4	4.23	122.16	111.83
3	C	1801	B12	C17-C16-C15	4.19	132.89	126.26
4	A	1500	5AD	C2-N3-C4	4.18	122.03	111.83
3	C	1801	B12	C8B-C9B-N3B	-4.17	105.49	110.00
3	D	1801	B12	C8B-C9B-N3B	-4.13	105.54	110.00
4	A	1500	5AD	N3-C2-N1	-4.12	122.34	128.58
3	D	1801	B12	C18-C19-N24	4.10	108.50	102.33
3	D	1801	B12	C9B-C8B-N1B	4.10	107.12	105.30
4	C	1500	5AD	C3'-C2'-C1'	4.08	109.17	101.46
3	D	1801	B12	C2-C1-N21	4.07	107.44	101.78
4	C	1500	5AD	N3-C2-N1	-4.04	122.47	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	767	Z98	OP1-P-OP4	4.02	117.16	106.67
3	B	1801	B12	C47-C12-C11	4.00	124.38	110.08
4	C	1500	5AD	O2'-C2'-C1'	3.98	123.82	110.10
3	C	1801	B12	C7B-C8B-C9B	-3.98	117.71	122.47
3	D	1801	B12	C17-C16-C15	3.97	132.54	126.26
3	B	1801	B12	C47-C12-C13	-3.94	96.75	112.74
3	B	1801	B12	C8B-C9B-N3B	-3.91	105.77	110.00
3	D	1801	B12	C47-C12-C13	-3.90	96.91	112.74
3	B	1801	B12	C9-C10-C11	-3.88	120.42	125.97
3	A	1801	B12	C8B-C9B-N3B	-3.87	105.82	110.00
3	A	1801	B12	C17-C16-C15	3.86	132.37	126.26
5	D	767	Z98	OP4-C5A-C5	3.82	116.52	109.36
3	B	1801	B12	C20-C1-C2	-3.80	107.01	113.28
4	C	1500	5AD	O2'-C2'-C3'	3.73	123.76	111.82
3	C	1801	B12	C9B-N3B-C2B	3.68	108.91	104.40
4	B	1500	5AD	O4'-C1'-N9	3.67	115.14	108.09
4	A	1500	5AD	O2'-C2'-C3'	-3.66	100.09	111.82
3	C	1801	B12	C47-C12-C13	-3.65	97.96	112.74
4	A	1500	5AD	C4-C5-N7	-3.64	106.42	110.58
4	D	1500	5AD	C5-N7-C8	3.59	109.10	103.45
3	A	1801	B12	C15-C14-N23	-3.59	121.94	126.26
3	C	1801	B12	C47-C12-C11	3.55	122.75	110.08
3	D	1801	B12	C20-C1-C2	-3.52	107.48	113.28
3	D	1801	B12	C12-C13-C14	3.51	108.03	102.26
3	A	1801	B12	C18-C19-N24	3.51	107.60	102.33
4	C	1500	5AD	C4-C5-N7	-3.50	106.58	110.58
3	B	1801	B12	C18-C17-C16	3.49	104.90	100.69
3	C	1801	B12	C15-C16-N24	-3.48	117.46	122.42
3	B	1801	B12	C17-C16-C15	3.44	131.70	126.26
3	D	1801	B12	C18-C17-C16	3.41	104.81	100.69
4	D	1500	5AD	C6-C5-N7	3.40	138.64	132.09
3	C	1801	B12	C12-C13-C14	3.39	107.83	102.26
3	D	1801	B12	C10-C9-N22	-3.33	121.95	125.74
3	C	1801	B12	C19-N24-C16	3.31	110.91	107.29
5	A	767	Z98	CG-ND-C4A	3.30	129.30	118.72
4	A	1500	5AD	C5-N7-C8	3.23	108.53	103.45
3	B	1801	B12	C54-C17-C18	-3.22	108.37	112.99
4	B	1500	5AD	C4-C5-N7	-3.22	106.91	110.58
4	B	1500	5AD	C4-N9-C8	3.19	109.09	105.74
3	A	1801	B12	C47-C12-C11	3.18	121.44	110.08
3	D	1801	B12	C9B-N3B-C2B	3.16	108.28	104.40
4	C	1500	5AD	C4-N9-C8	3.16	109.05	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1801	B12	C2-C1-C19	3.14	123.50	118.61
3	A	1801	B12	C54-C17-C18	-3.12	108.51	112.99
3	C	1801	B12	C18-C17-C16	3.11	104.44	100.69
3	A	1801	B12	C18-C17-C16	3.06	104.38	100.69
3	B	1801	B12	C19-N24-C16	3.03	110.60	107.29
4	B	1500	5AD	C5-N7-C8	2.99	108.16	103.45
3	A	1801	B12	C9B-N3B-C2B	2.99	108.07	104.40
3	C	1801	B12	C2-C1-N21	2.99	105.93	101.78
3	D	1801	B12	C4B-C9B-N3B	2.96	135.49	130.51
3	C	1801	B12	O6R-C4R-C5R	2.95	115.46	109.22
3	D	1801	B12	C47-C12-C11	2.94	120.58	110.08
4	C	1500	5AD	C5-N7-C8	2.94	108.06	103.45
5	C	767	Z98	C4-C4A-ND	-2.90	110.66	124.04
3	B	1801	B12	C15-C16-N24	-2.88	118.33	122.42
3	C	1801	B12	C5R-C4R-C3R	-2.84	105.89	114.84
4	C	1500	5AD	C5'-C4'-C3'	-2.83	112.72	115.70
3	A	1801	B12	C12-C13-C14	2.83	106.91	102.26
3	B	1801	B12	C9B-N3B-C2B	2.81	107.84	104.40
3	B	1801	B12	C15-C14-N23	-2.80	122.88	126.26
3	C	1801	B12	C26-C2-C1	2.79	114.32	110.00
4	D	1500	5AD	N9-C8-N7	-2.77	110.01	113.94
3	D	1801	B12	C20-C1-N21	-2.76	105.70	110.26
3	B	1801	B12	C7B-C8B-C9B	-2.74	119.19	122.47
5	B	767	Z98	OP3-P-OP2	-2.72	100.23	110.83
3	C	1801	B12	C3-C4-N21	-2.67	108.66	111.98
3	D	1801	B12	C46-C12-C11	2.67	119.63	110.08
5	D	767	Z98	CG-ND-C4A	2.66	127.25	118.72
3	A	1801	B12	C20-C1-C2	-2.62	108.96	113.28
3	D	1801	B12	C15-C16-N24	-2.61	118.70	122.42
3	A	1801	B12	O6R-C1R-N1B	2.60	113.08	108.09
4	A	1500	5AD	O3'-C3'-C4'	2.57	116.77	110.47
3	D	1801	B12	C8B-N1B-C1R	-2.57	121.06	125.41
3	B	1801	B12	C53-C15-C16	-2.57	116.01	120.36
4	C	1500	5AD	N9-C8-N7	-2.56	110.30	113.94
3	B	1801	B12	C48-C13-C12	2.54	123.80	116.52
3	D	1801	B12	C9-C10-C11	-2.54	122.34	125.97
3	B	1801	B12	C7-C6-C5	-2.54	124.10	128.07
4	B	1500	5AD	N9-C8-N7	-2.54	110.33	113.94
5	A	767	Z98	CB-CG-ND	2.53	117.50	110.82
3	C	1801	B12	O2-P-O4	-2.51	101.79	109.81
5	B	767	Z98	C3-C4-C4A	-2.49	115.91	120.40
4	C	1500	5AD	C6-C5-N7	2.48	136.87	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1801	B12	C7-C6-C5	-2.47	124.21	128.07
3	B	1801	B12	O3-C2P-C1P	2.47	111.83	106.94
4	A	1500	5AD	N9-C8-N7	-2.46	110.45	113.94
3	A	1801	B12	C25-C2-C1	-2.43	110.13	113.75
5	A	767	Z98	C2A-C2-C3	2.42	123.63	120.80
3	B	1801	B12	C36-C7-C37	2.42	114.85	110.74
4	D	1500	5AD	O4'-C1'-C2'	-2.41	101.45	106.62
3	D	1801	B12	C54-C17-C18	-2.41	109.53	112.99
4	D	1500	5AD	C5'-C4'-C3'	-2.40	113.18	115.70
4	B	1500	5AD	C6-C5-N7	2.36	136.64	132.09
4	A	1500	5AD	C6-C5-N7	2.36	136.63	132.09
4	A	1500	5AD	C4-N9-C8	2.35	108.21	105.74
3	B	1801	B12	C60-C18-C19	2.35	120.69	114.59
3	A	1801	B12	C15-C16-N24	-2.35	119.08	122.42
3	B	1801	B12	C2-C1-N21	2.34	105.03	101.78
3	D	1801	B12	C17-C16-N24	-2.33	107.61	111.17
4	A	1500	5AD	C5'-C4'-C3'	-2.33	113.26	115.70
3	A	1801	B12	C46-C12-C11	2.32	118.37	110.08
3	D	1801	B12	C15-C14-N23	-2.31	123.48	126.26
3	C	1801	B12	C2P-C1P-N59	-2.29	109.55	112.92
5	B	767	Z98	C4-C4A-ND	2.28	134.57	124.04
3	D	1801	B12	C7-C6-C5	-2.26	124.54	128.07
3	B	1801	B12	C12-C13-C14	2.25	105.96	102.26
3	A	1801	B12	C7-C6-N22	2.24	112.02	107.94
5	C	767	Z98	CB-CG-ND	-2.23	104.94	110.82
4	A	1500	5AD	C2'-C1'-N9	-2.22	107.78	113.30
3	B	1801	B12	C3-C4-N21	-2.22	109.22	111.98
4	B	1500	5AD	C2'-C1'-N9	-2.20	107.83	113.30
4	B	1500	5AD	C3'-C2'-C1'	2.20	105.62	101.46
3	D	1801	B12	C3R-C2R-C1R	2.19	104.70	99.89
3	C	1801	B12	N1B-C2B-N3B	-2.17	110.85	113.94
5	B	767	Z98	C2A-C2-N1	2.17	121.73	117.64
5	C	767	Z98	C2A-C2-C3	-2.16	118.27	120.80
3	A	1801	B12	C10-C9-N22	-2.14	123.30	125.74
3	D	1801	B12	C2P-C1P-N59	-2.14	109.78	112.92
5	C	767	Z98	C2A-C2-N1	2.12	121.64	117.64
5	D	767	Z98	C2A-C2-N1	2.12	121.63	117.64
3	C	1801	B12	C4B-C9B-N3B	2.11	134.06	130.51
5	C	767	Z98	CG-CB-CA	2.10	117.98	112.72
3	A	1801	B12	C37-C7-C8	2.08	113.86	108.37
5	B	767	Z98	C5-C4-C4A	2.08	124.68	121.47
3	A	1801	B12	C56-C55-C17	2.08	119.59	115.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1801	B12	C7B-C8B-C9B	-2.06	120.00	122.47
3	C	1801	B12	C10-C11-N23	2.05	127.88	124.42
3	C	1801	B12	C15-C14-N23	-2.03	123.81	126.26
3	A	1801	B12	C9-N22-C6	-2.03	102.83	105.28
3	C	1801	B12	O2-P-O3	2.03	108.54	102.87
4	D	1500	5AD	C4-N9-C8	2.03	107.87	105.74
3	A	1801	B12	C9-C10-C11	-2.02	123.08	125.97
5	B	767	Z98	C5A-C5-C6	-2.01	116.08	119.36
3	C	1801	B12	C3R-C2R-C1R	2.00	104.30	99.89
3	A	1801	B12	C26-C2-C3	-2.00	103.92	107.42

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1801	B12	C19
3	B	1801	B12	C19
3	C	1801	B12	C19
4	A	1500	5AD	C2'
4	D	1500	5AD	C2'

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1801	B12	C16-C17-C55-C56
3	A	1801	B12	C2R-C1R-N1B-C2B
5	A	767	Z98	C5A-OP4-P-OP1
5	A	767	Z98	C5A-OP4-P-OP2
5	A	767	Z98	C5A-OP4-P-OP3
5	A	767	Z98	N-CA-CB-CG
5	A	767	Z98	CA-CB-CG-ND
5	A	767	Z98	C4-C4A-ND-CG
5	B	767	Z98	N-CA-CB-CG
5	B	767	Z98	CA-CB-CG-ND
5	B	767	Z98	C4-C4A-ND-CG
5	C	767	Z98	C5-C4-C4A-ND
5	C	767	Z98	CA-CB-CG-ND
5	D	767	Z98	CA-CB-CG-ND
5	D	767	Z98	C4-C4A-ND-CG
3	C	1801	B12	C3R-C4R-C5R-O8R
3	C	1801	B12	C4-C3-C30-C31
3	C	1801	B12	O6R-C4R-C5R-O8R
3	B	1801	B12	C2R-C1R-N1B-C2B

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Mol	Chain	Res	Type	Atoms
3	A	1801	B12	C18-C17-C55-C56
3	D	1801	B12	C18-C17-C55-C56
3	B	1801	B12	C16-C17-C55-C56
3	D	1801	B12	C16-C17-C55-C56
3	B	1801	B12	C2R-C1R-N1B-C8B
5	A	767	Z98	C5-C4-C4A-ND
3	A	1801	B12	N59-C1P-C2P-O3
3	C	1801	B12	C2R-C1R-N1B-C2B
5	A	767	Z98	C3-C4-C4A-ND
5	B	767	Z98	C3-C4-C4A-ND
3	C	1801	B12	C2-C3-C30-C31
3	A	1801	B12	O6R-C4R-C5R-O8R
3	A	1801	B12	C2-C3-C30-C31
5	C	767	Z98	C3-C4-C4A-ND
3	A	1801	B12	N59-C1P-C2P-C3P
3	A	1801	B12	C2R-C1R-N1B-C8B
3	C	1801	B12	C2R-C1R-N1B-C8B
5	B	767	Z98	C5-C4-C4A-ND
3	B	1801	B12	C18-C17-C55-C56
3	D	1801	B12	C2R-C1R-N1B-C2B
5	B	767	Z98	OXT-C-CA-CB
3	A	1801	B12	C4-C3-C30-C31
3	B	1801	B12	O6R-C1R-N1B-C8B
3	C	1801	B12	O6R-C1R-N1B-C8B
5	C	767	Z98	C-CA-CB-CG
5	B	767	Z98	O-C-CA-CB
5	D	767	Z98	C3-C4-C4A-ND
5	D	767	Z98	N-CA-CB-CG
3	A	1801	B12	C42-C41-C8-C7
3	A	1801	B12	C3R-C4R-C5R-O8R
5	C	767	Z98	CB-CG-ND-C4A
3	A	1801	B12	C14-C13-C48-C49
3	A	1801	B12	C48-C49-C50-O51
3	A	1801	B12	O6R-C1R-N1B-C8B
3	D	1801	B12	C2R-C1R-N1B-C8B
3	D	1801	B12	O6R-C1R-N1B-C8B
5	A	767	Z98	O-C-CA-CB
5	A	767	Z98	OXT-C-CA-CB
5	C	767	Z98	OXT-C-CA-CB
5	C	767	Z98	O-C-CA-CB
5	D	767	Z98	O-C-CA-CB
5	D	767	Z98	OXT-C-CA-CB

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Mol	Chain	Res	Type	Atoms
3	A	1801	B12	C13-C48-C49-C50
3	D	1801	B12	O6R-C1R-N1B-C2B
3	A	1801	B12	C12-C13-C48-C49
5	D	767	Z98	C5-C4-C4A-ND
3	A	1801	B12	C2R-C3R-O2-P
3	B	1801	B12	C2P-O3-P-O5
3	C	1801	B12	O6R-C1R-N1B-C2B
3	A	1801	B12	C42-C41-C8-C9
3	C	1801	B12	C55-C56-C57-O58
3	C	1801	B12	C55-C56-C57-N59
3	B	1801	B12	O6R-C1R-N1B-C2B
5	D	767	Z98	O-C-CA-N

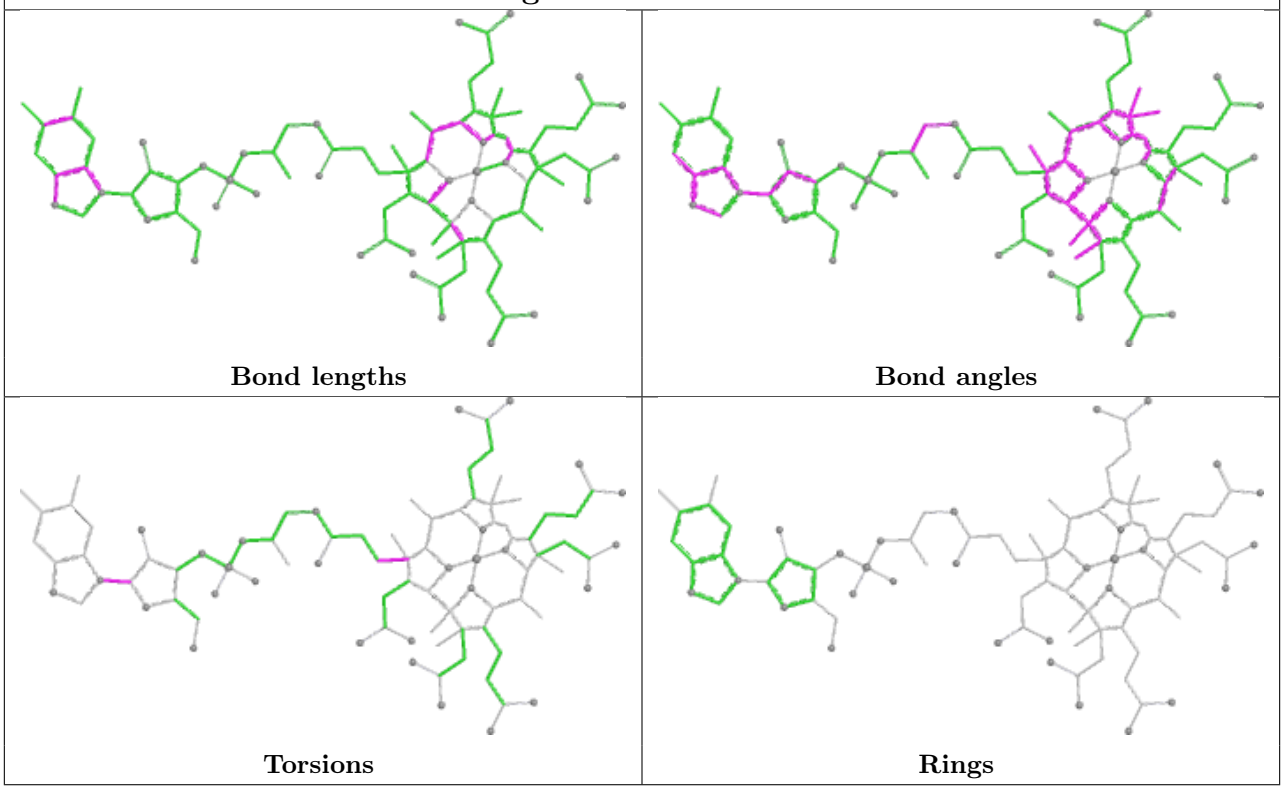
There are no ring outliers.

12 monomers are involved in 102 short contacts:

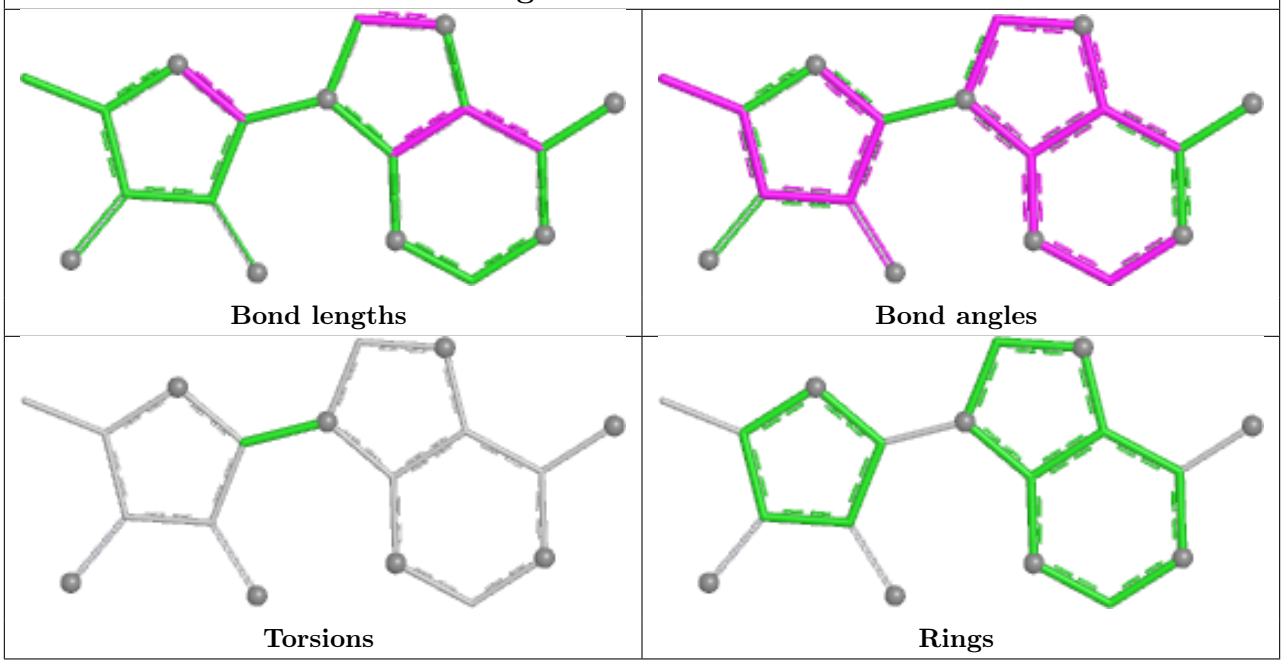
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1801	B12	14	0
4	D	1500	5AD	4	0
5	A	767	Z98	11	0
5	B	767	Z98	8	0
4	C	1500	5AD	3	0
5	C	767	Z98	8	0
3	B	1801	B12	20	0
4	A	1500	5AD	2	0
3	C	1801	B12	16	0
5	D	767	Z98	8	0
4	B	1500	5AD	2	0
3	A	1801	B12	17	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

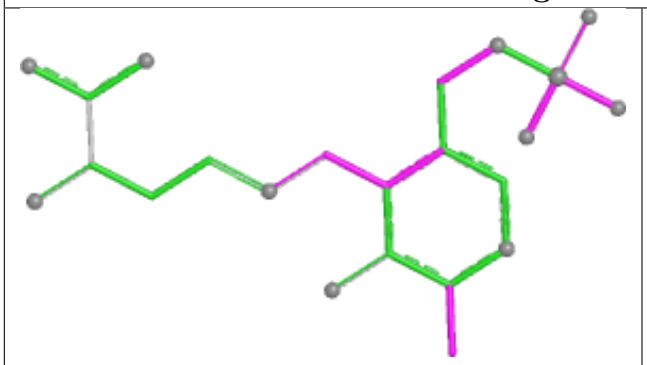
Ligand B12 D 1801



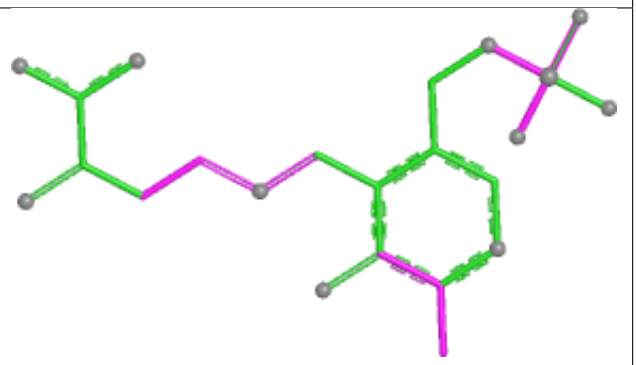
Ligand 5AD D 1500



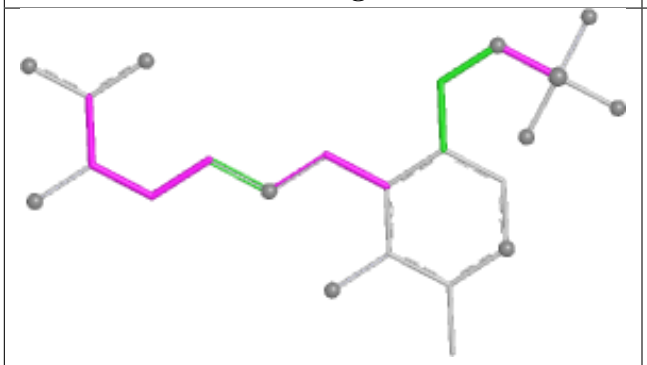
Ligand Z98 A 767



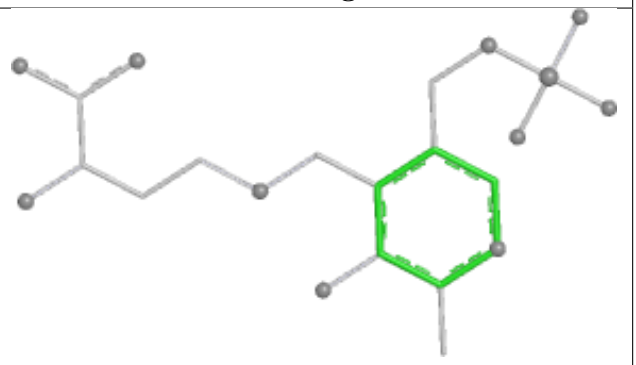
Bond lengths



Bond angles

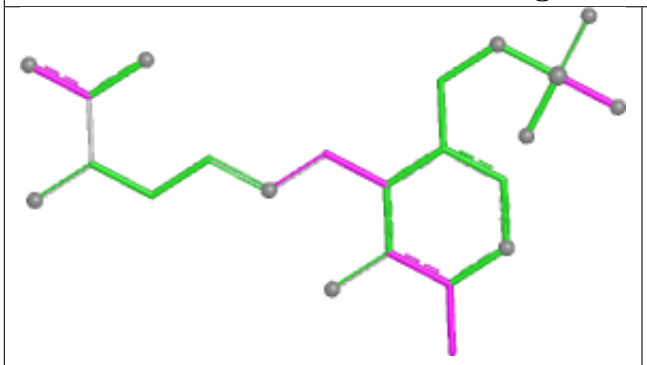


Torsions



Rings

Ligand Z98 B 767



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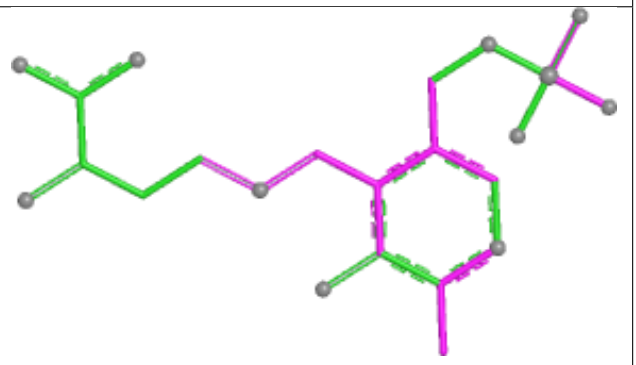
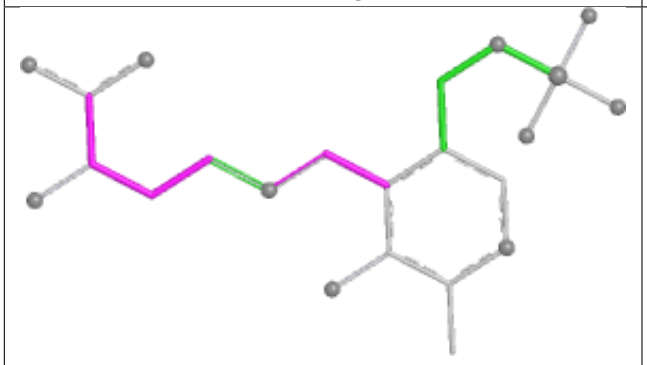


Bond angles



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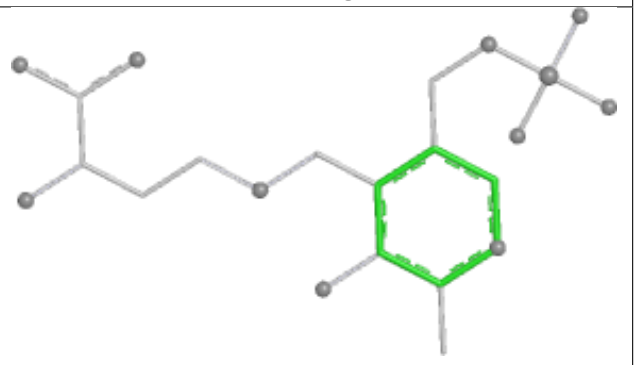
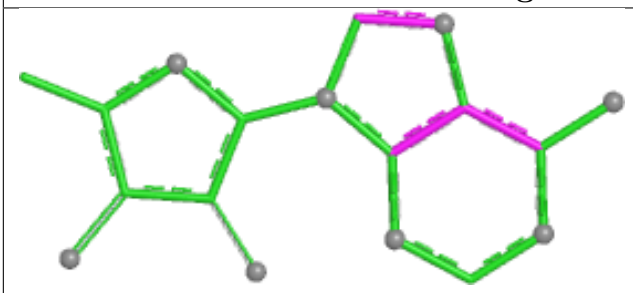
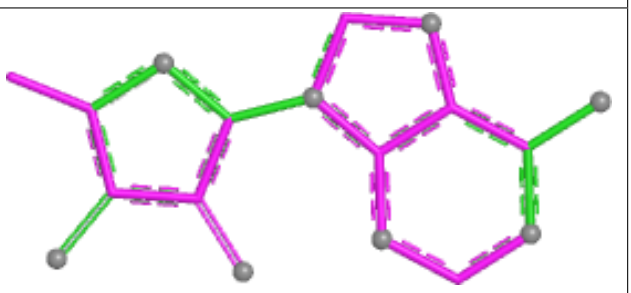


Rings

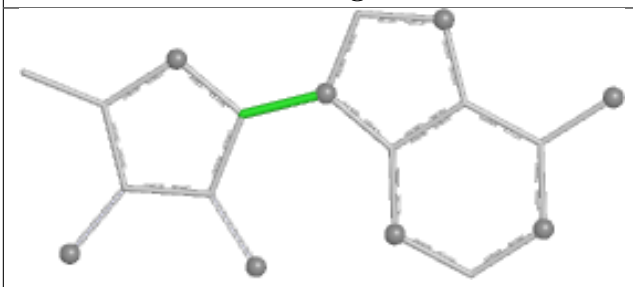
Ligand 5AD C 1500



Bond lengths



Bond angles



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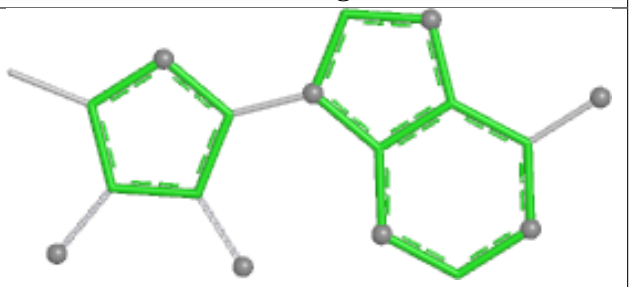
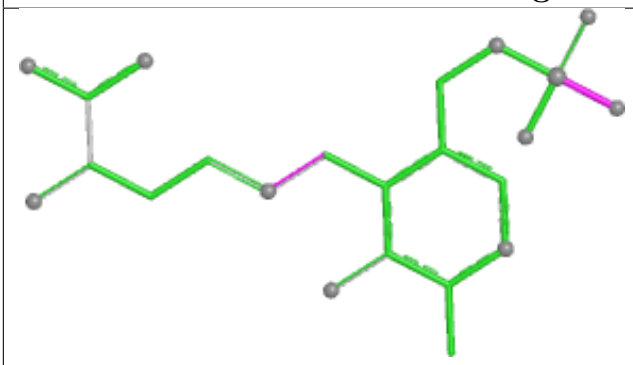
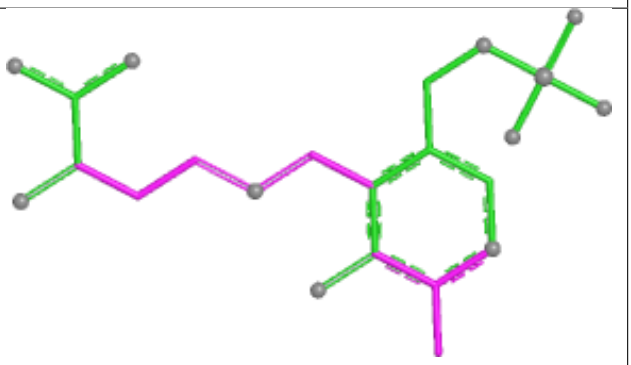


Rings

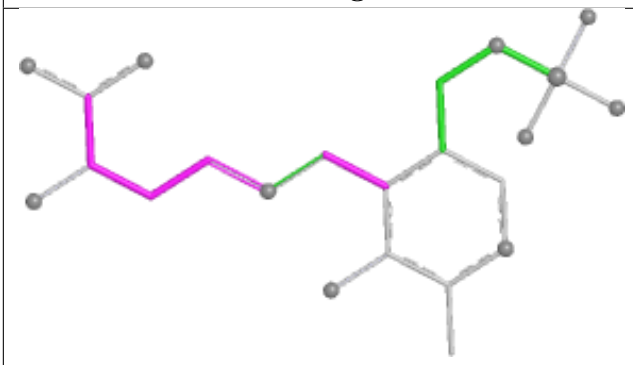
Ligand Z98 C 767



Bond lengths



Bond angles



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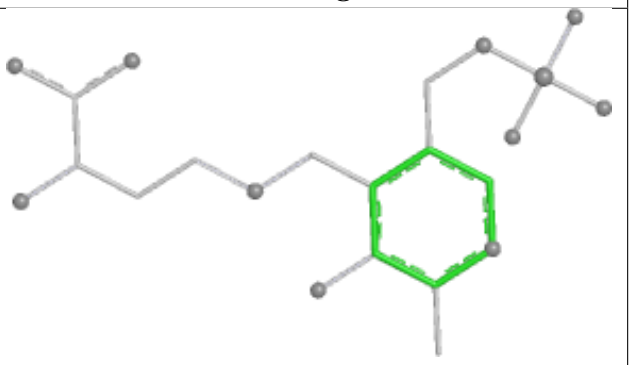
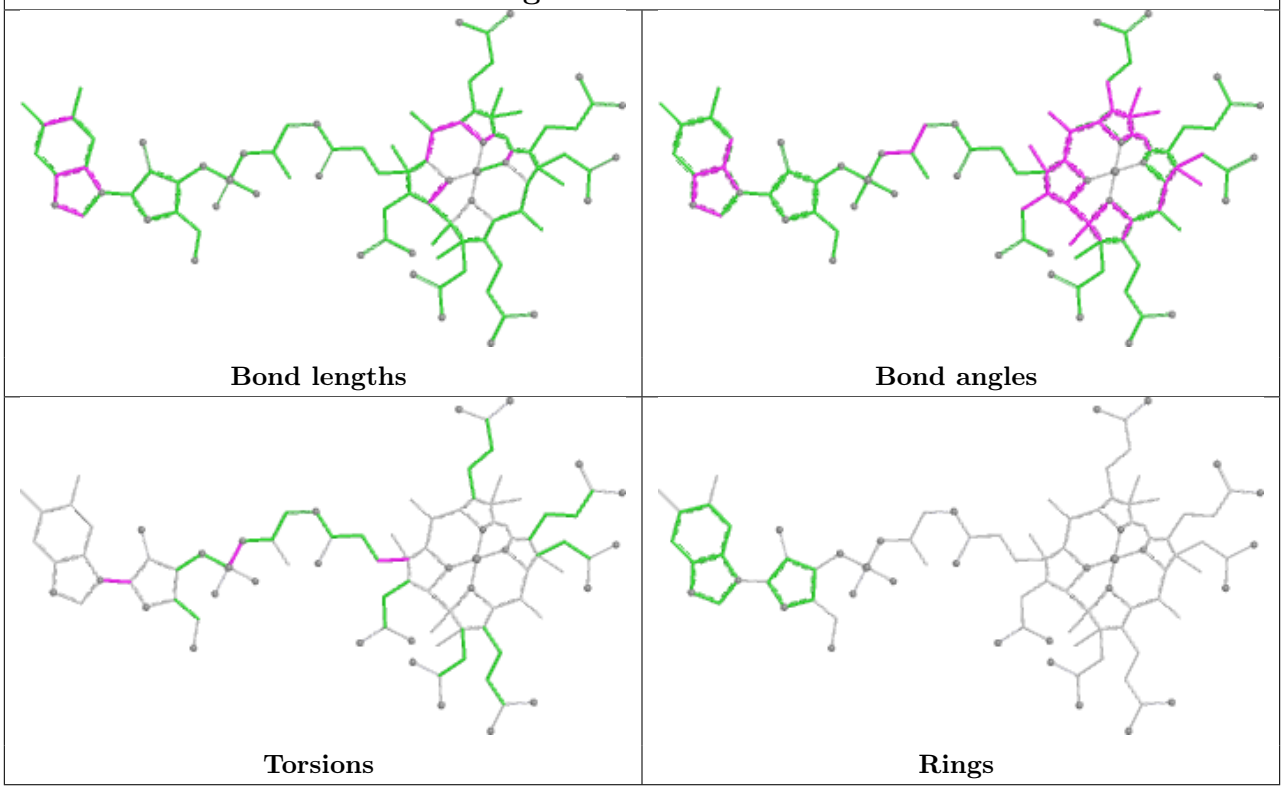
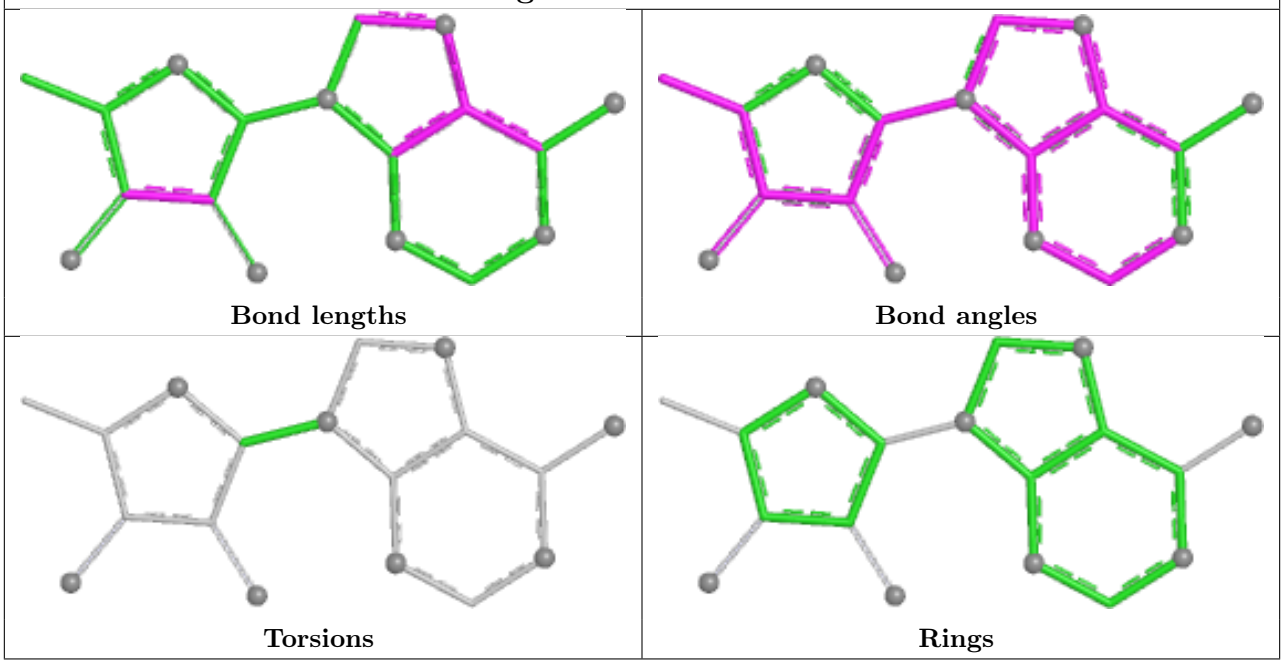


Rings

Ligand B12 B 1801



Ligand 5AD A 1500



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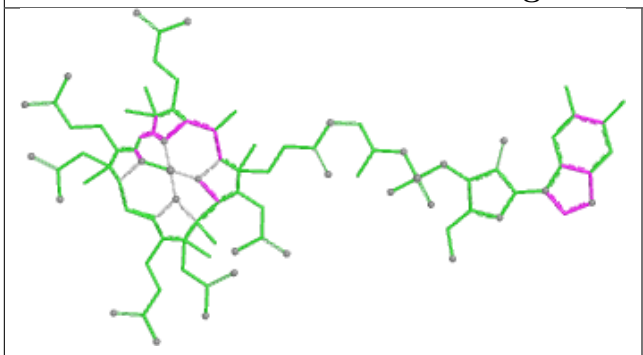
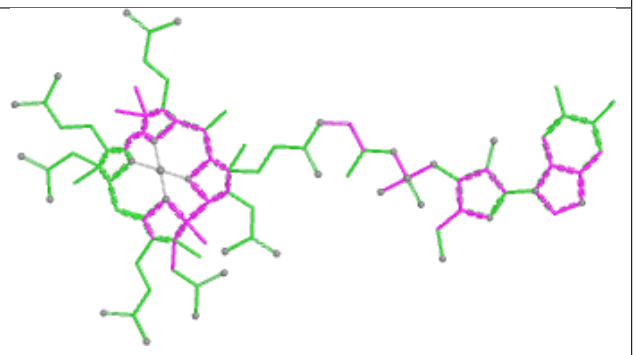
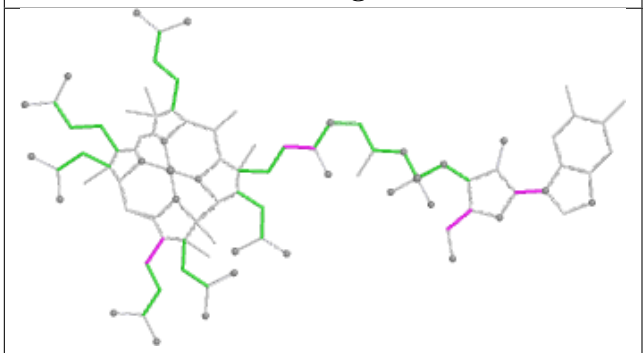


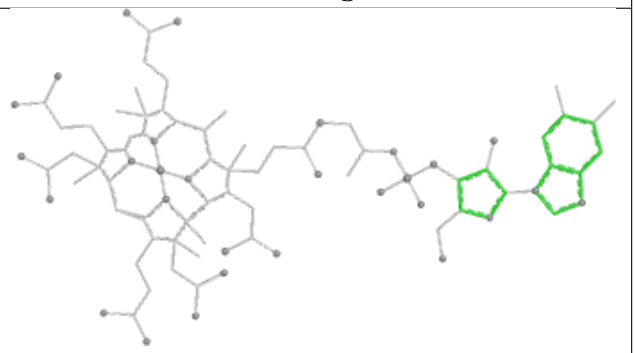
Bond lengths



Bond angles

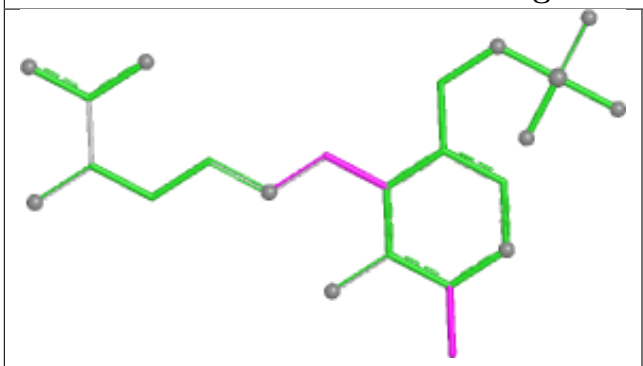


Torsions

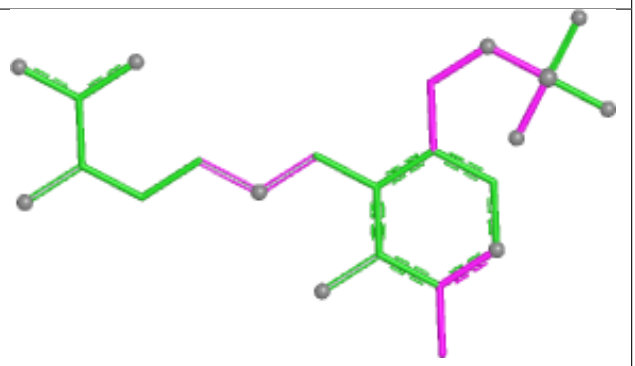


Rings

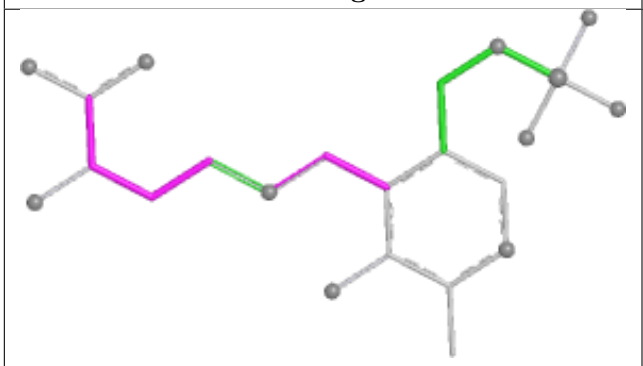
Ligand Z98 D 767



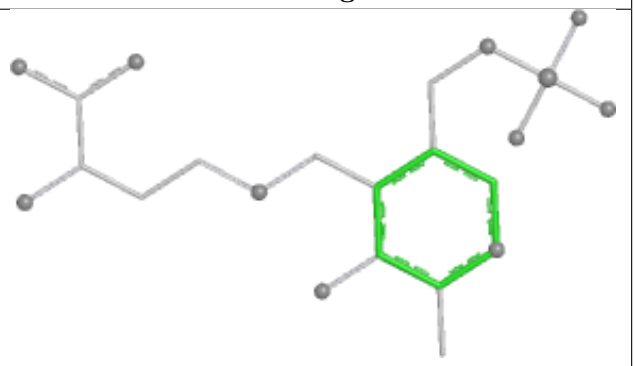
Bond lengths



Bond angles

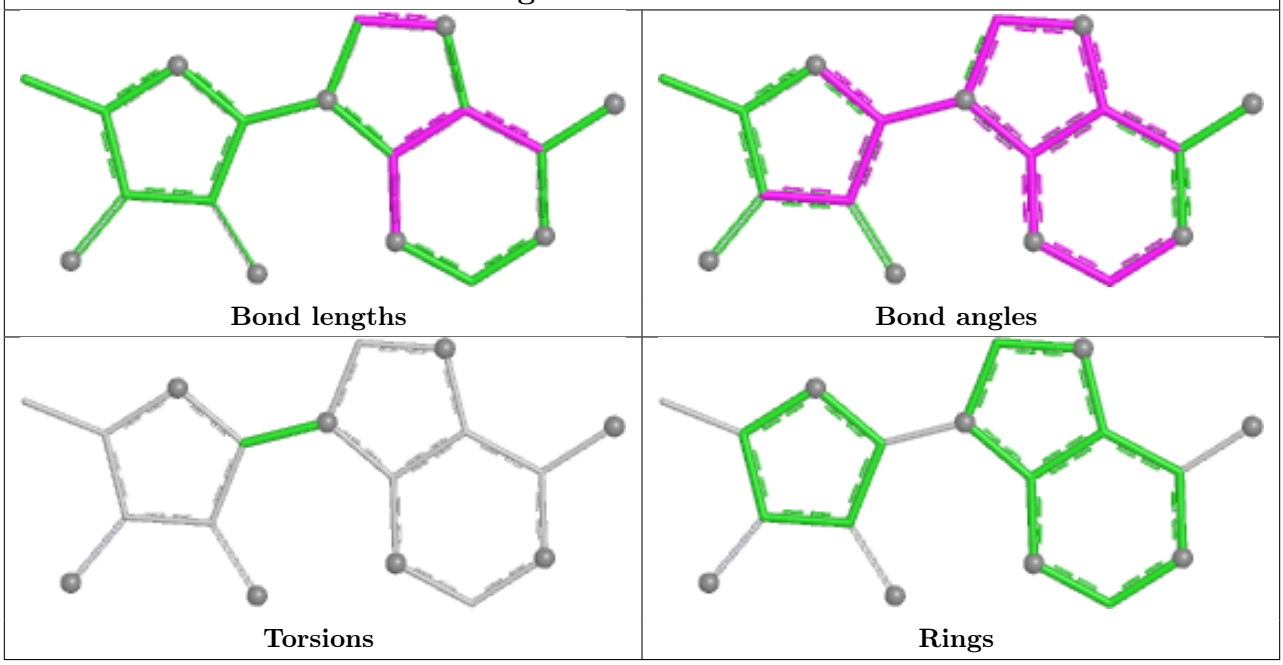


Torsions

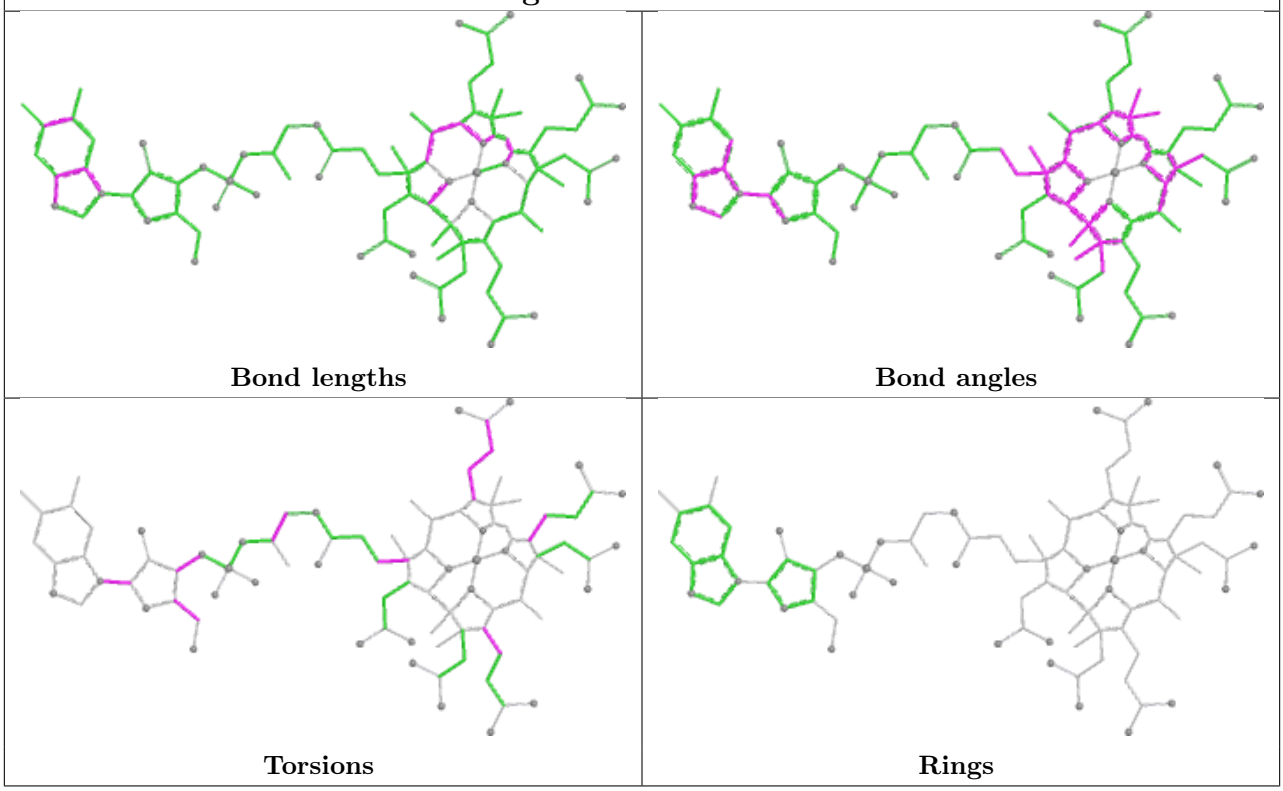


Rings

Ligand 5AD B 1500



Ligand B12 A 1801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	728/763 (95%)	-0.11	13 (1%)	67	63	13, 27, 68, 84	0
1	B	728/763 (95%)	-0.46	2 (0%)	90	88	10, 22, 42, 56	0
1	C	728/763 (95%)	-0.30	3 (0%)	88	86	12, 28, 49, 66	0
1	D	728/763 (95%)	-0.37	3 (0%)	88	86	10, 23, 50, 65	0
2	E	109/121 (90%)	-0.17	0	100	100	17, 32, 46, 50	0
2	F	109/121 (90%)	-0.34	1 (0%)	81	78	15, 24, 37, 45	0
2	G	109/121 (90%)	-0.11	0	100	100	24, 35, 50, 55	0
2	H	109/121 (90%)	-0.20	1 (0%)	81	78	15, 27, 45, 61	0
All	All	3348/3536 (94%)	-0.30	23 (0%)	84	81	10, 26, 54, 84	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	591	ILE	3.9
1	A	683	ILE	3.2
1	B	5	LEU	3.0
1	A	692	ILE	2.7
1	A	688	VAL	2.7
1	C	5	LEU	2.5
1	A	5	LEU	2.5
1	A	709	VAL	2.5
1	C	587	PRO	2.4
1	C	511	ILE	2.4
1	D	6	GLN	2.4
1	A	659	LEU	2.4
1	A	506	ARG	2.3
1	A	587	PRO	2.3
1	A	699	GLY	2.3
1	D	688	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	8	ARG	2.3
1	A	710	ALA	2.2
1	A	686	LEU	2.2
1	D	591	ILE	2.1
2	F	6	ASP	2.1
1	A	657	ILE	2.1
2	H	6	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

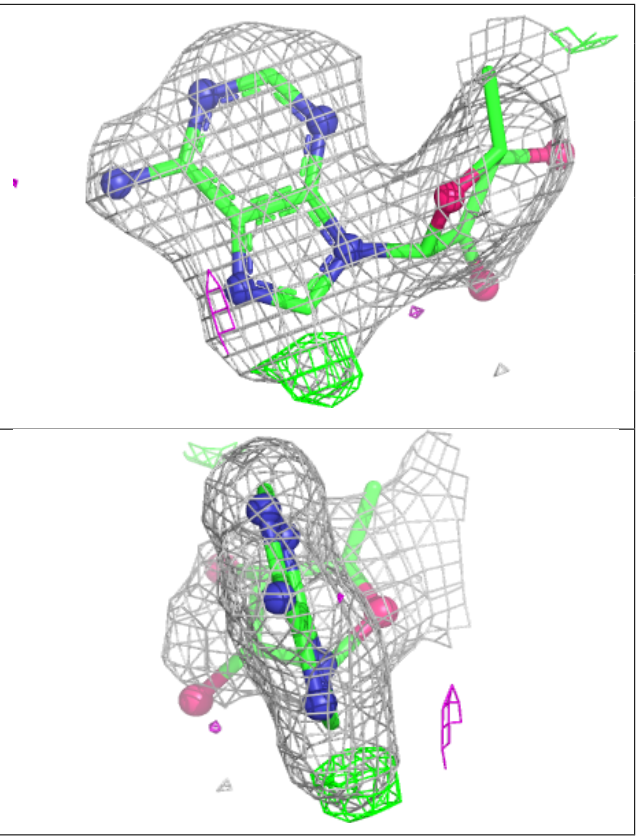
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	5AD	C	1500	18/18	0.80	0.13	53,54,55,57	0
4	5AD	D	1500	18/18	0.84	0.13	38,40,45,45	0
4	5AD	A	1500	18/18	0.86	0.13	39,43,47,47	0
4	5AD	B	1500	18/18	0.89	0.09	25,38,42,42	0
3	B12	A	1801	91/91	0.94	0.09	27,43,50,54	0
3	B12	D	1801	91/91	0.95	0.08	19,29,40,43	0
5	Z98	C	767	23/23	0.95	0.09	26,34,43,44	0
5	Z98	B	767	23/23	0.96	0.08	18,23,33,34	0
5	Z98	A	767	23/23	0.96	0.09	21,32,42,43	0
3	B12	B	1801	91/91	0.97	0.06	14,21,29,35	0
3	B12	C	1801	91/91	0.97	0.06	12,23,31,34	0
5	Z98	D	767	23/23	0.97	0.08	19,24,46,46	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

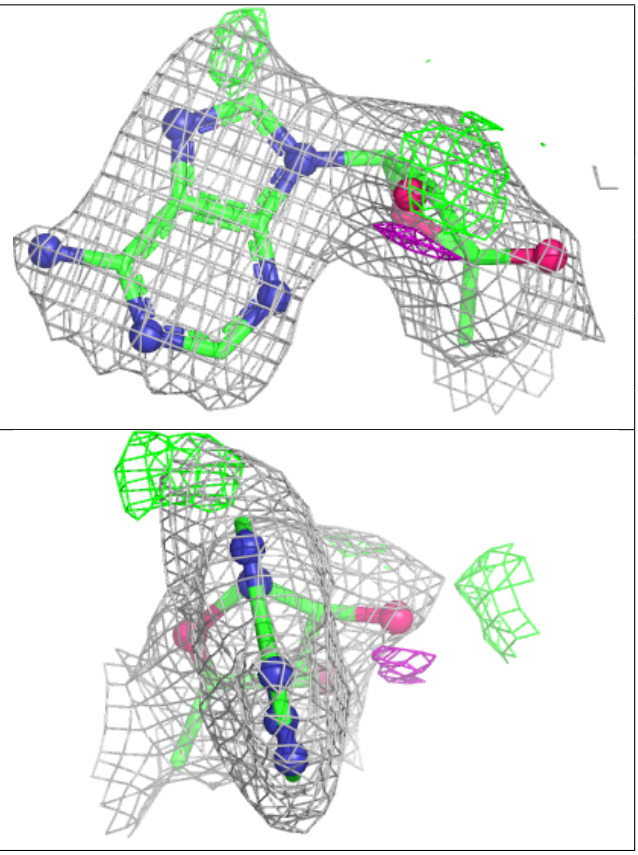
Electron density around 5AD C 1500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



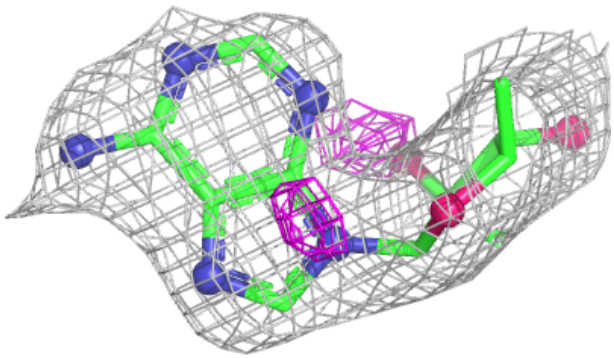
Electron density around 5AD D 1500:

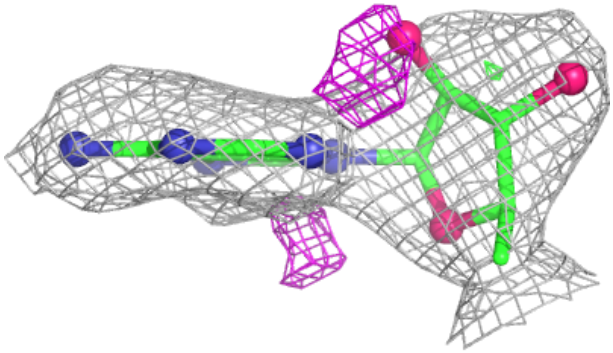
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

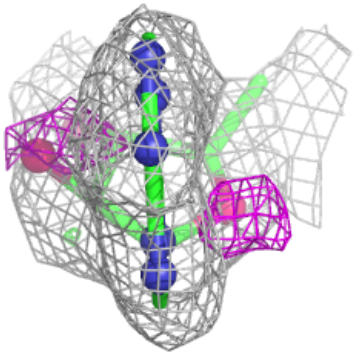


Electron density around 5AD A 1500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

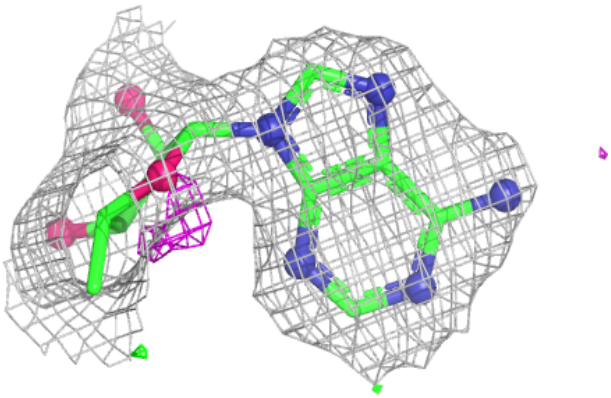


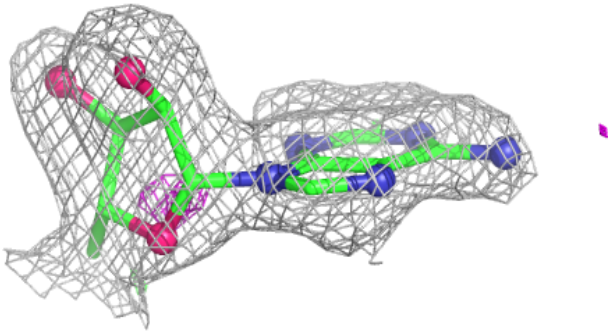


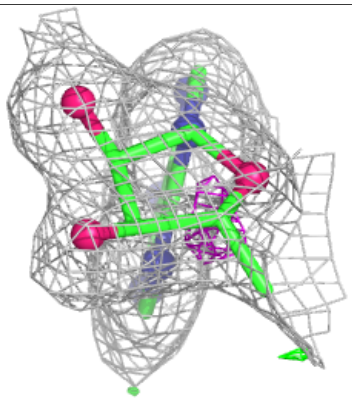


Electron density around 5AD B 1500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

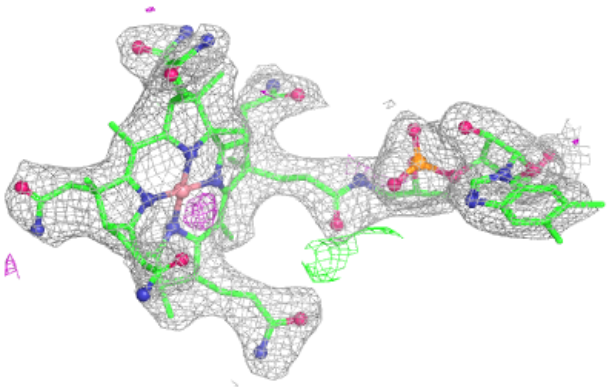


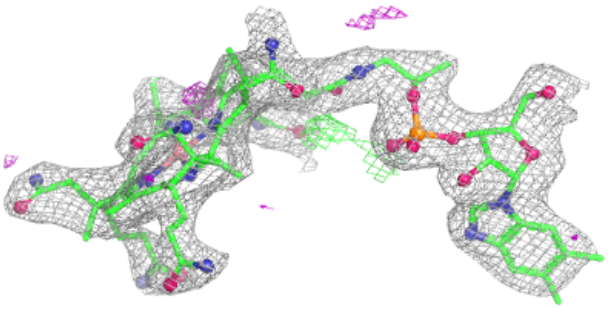


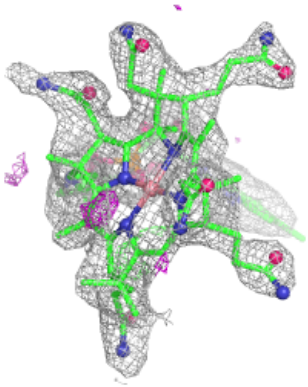


Electron density around B12 A 1801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around B12 D 1801:

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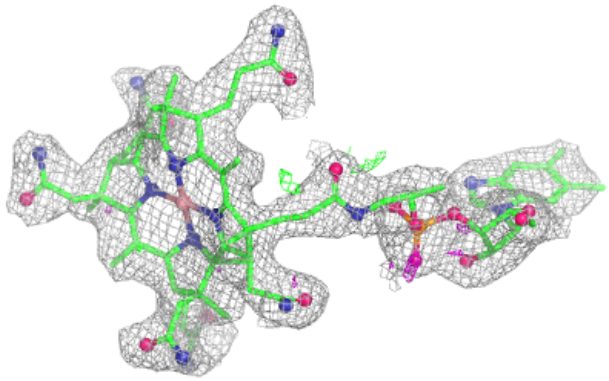
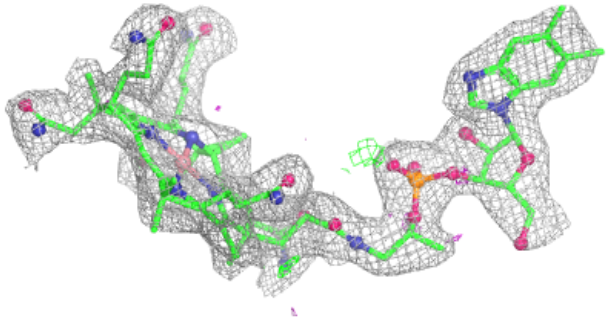
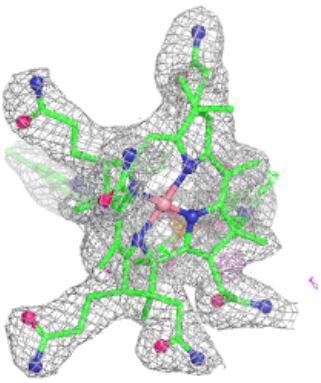
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

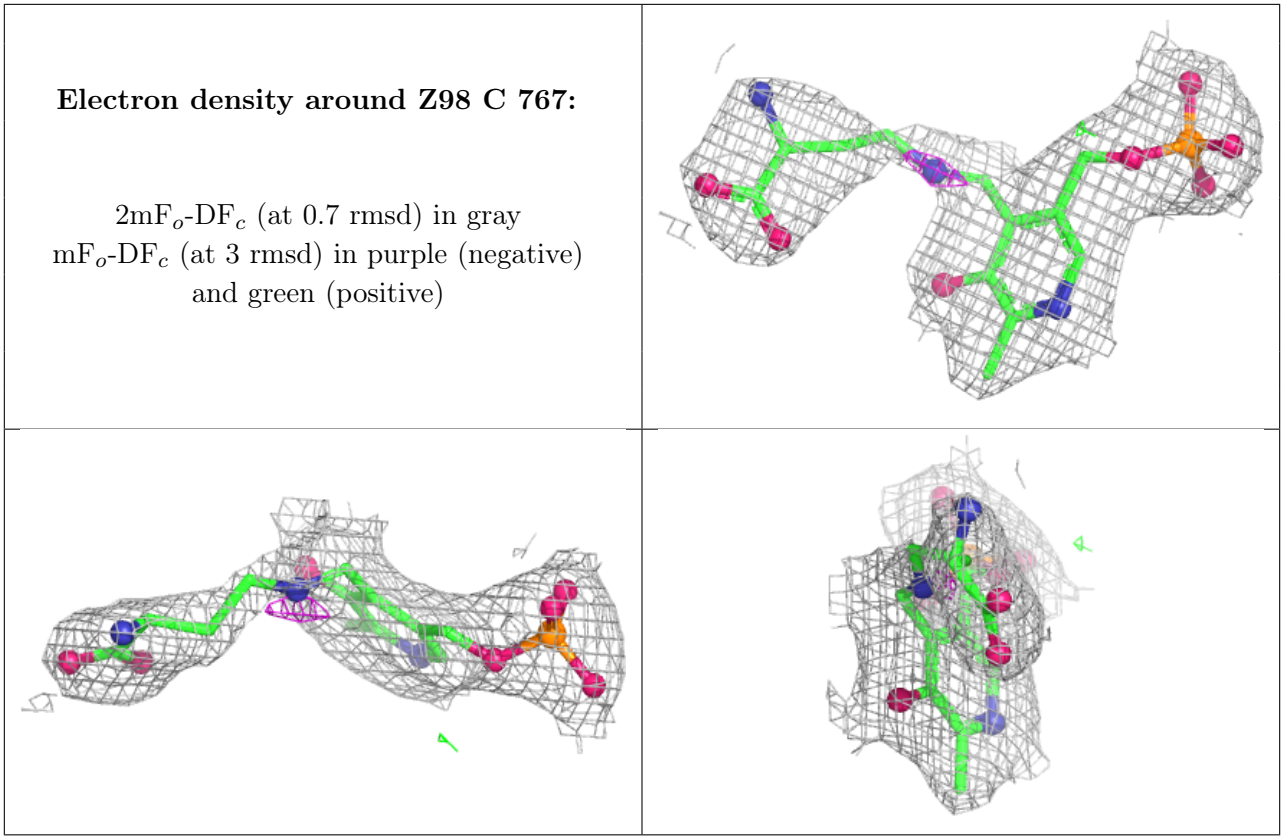






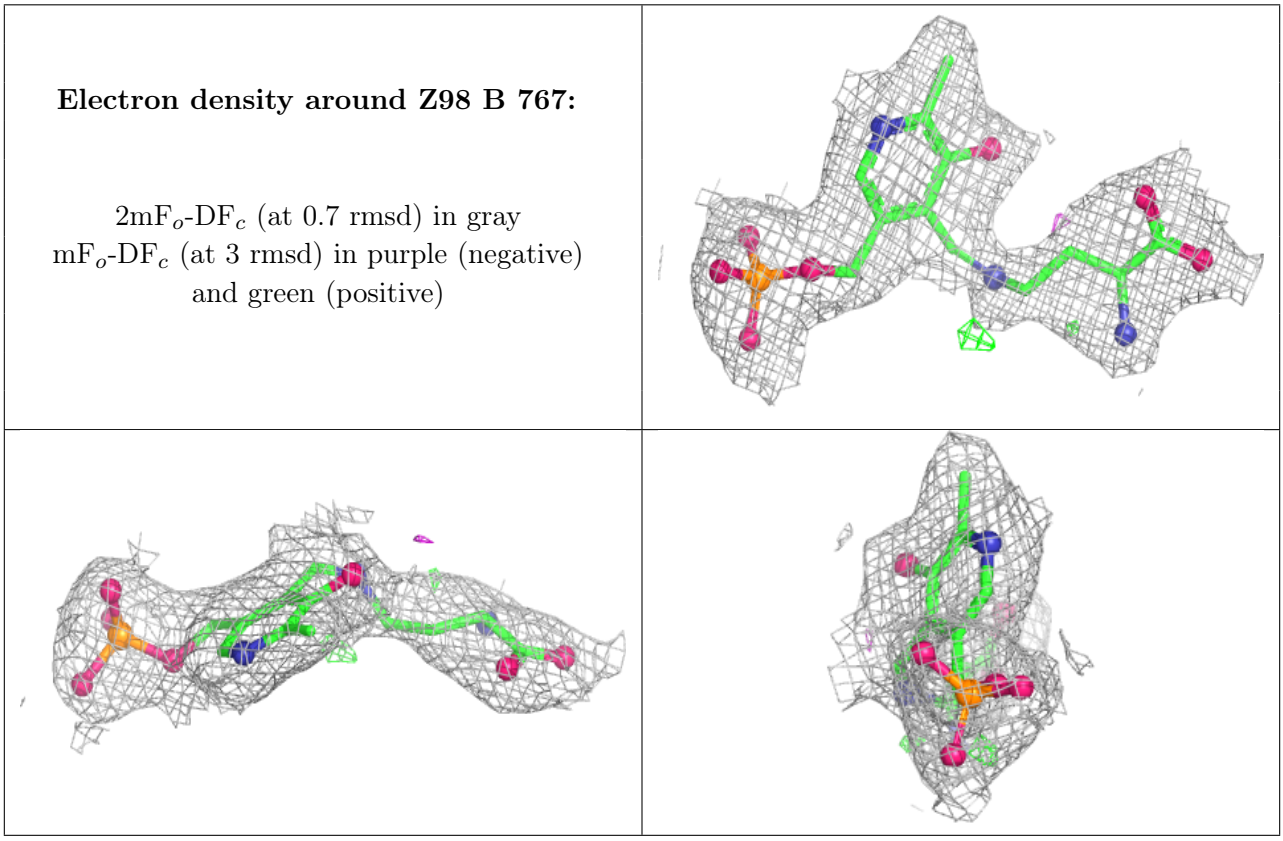
Electron density around Z98 C 767:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



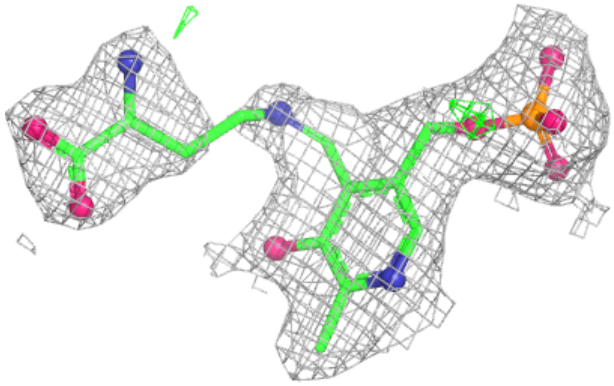
Electron density around Z98 B 767:

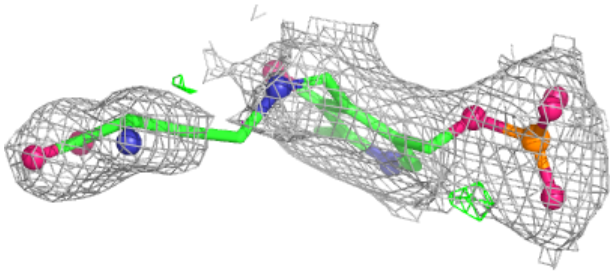
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

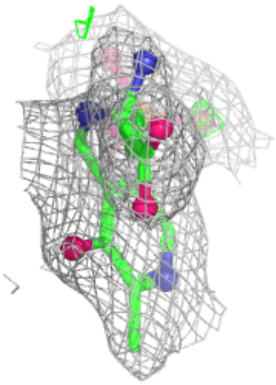


Electron density around Z98 A 767:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

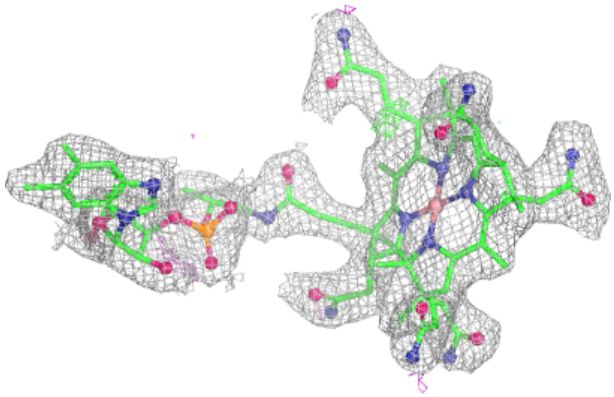


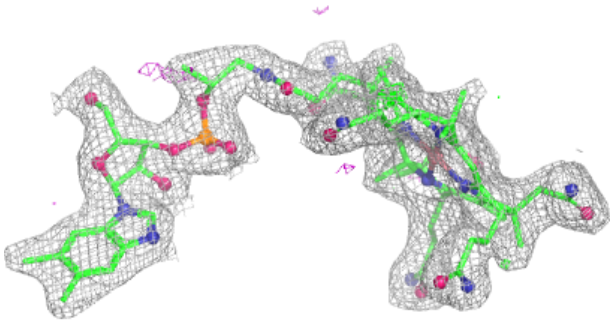


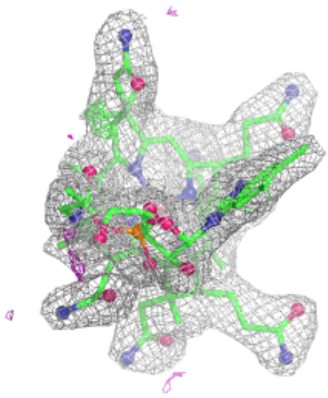


Electron density around B12 B 1801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around B12 C 1801:

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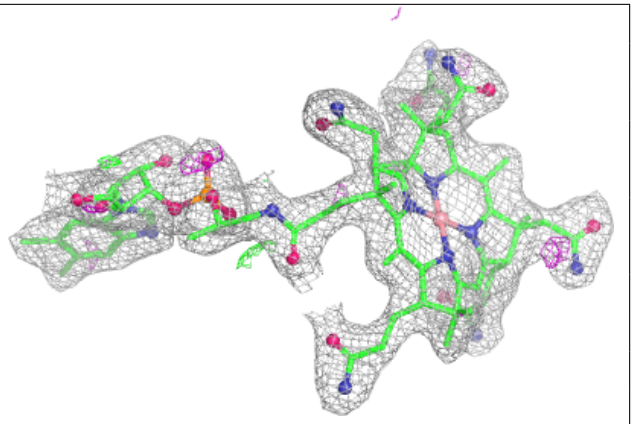
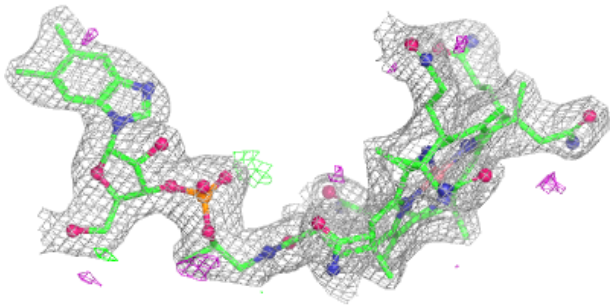
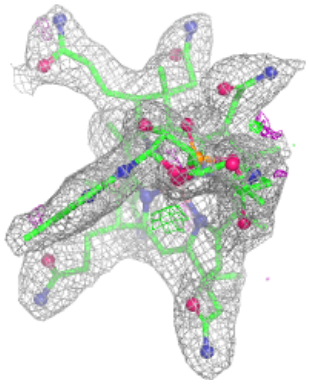
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

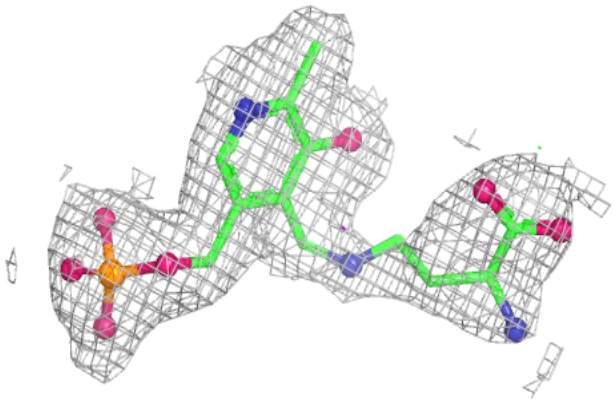


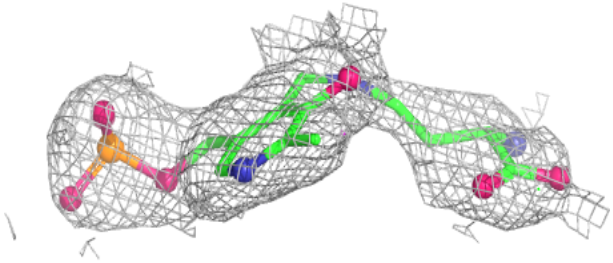


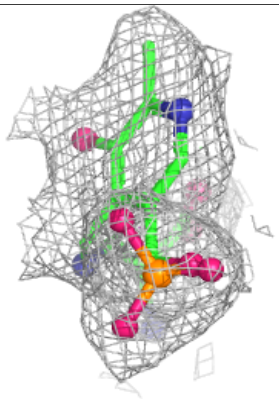


Electron density around Z98 D 767:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.