Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:59 PM UTC

PDB ID	:	7TGL / pdb_00007tgl
Title	:	Crystal structure of AMP+PPi bound DesD, the desferrioxamine synthetase from the Streptomyces griseoflavus ferrimycin biosynthetic pathway
Authors	:	Patel, K.D.; Gulick, A.M.
Deposited on	:	2022-01-07
Resolution	:	2.89 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 ⓘ 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 ⓘ) were used in the production of this report:

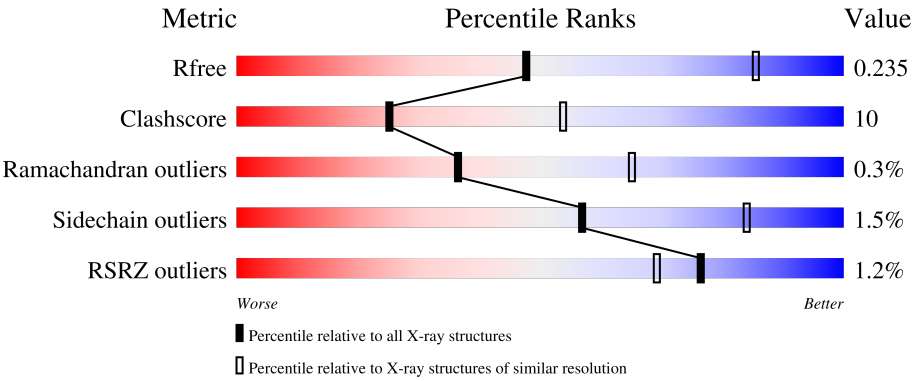
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	612	75% 19%
1	B	612	78% 17%
1	C	612	76% 21%
1	D	612	79% 17%
1	E	612	66% 30%

2 Entry composition

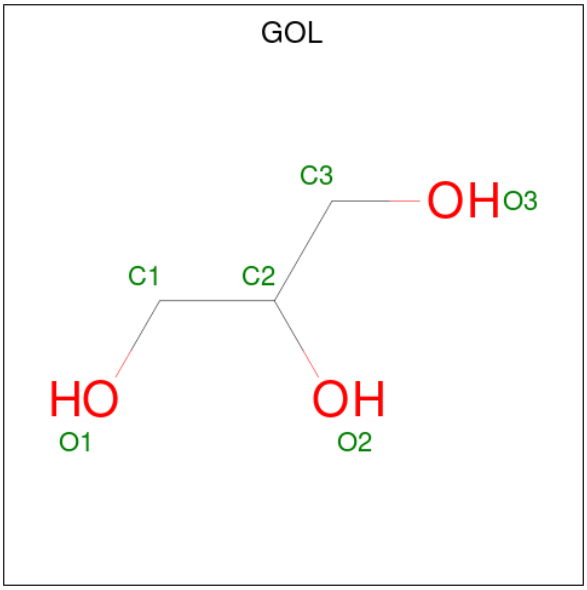
There are 7 unique types of molecules in this entry. The entry contains 23630 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Desferrioxamine synthetase DesD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	0	0
			4675	2973	814	873	15			
1	B	592	Total	C	N	O	S	0	0	0
			4670	2970	815	870	15			
1	C	591	Total	C	N	O	S	0	0	0
			4658	2964	811	868	15			
1	D	591	Total	C	N	O	S	0	0	0
			4660	2966	811	868	15			
1	E	591	Total	C	N	O	S	0	0	0
			4668	2970	813	870	15			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



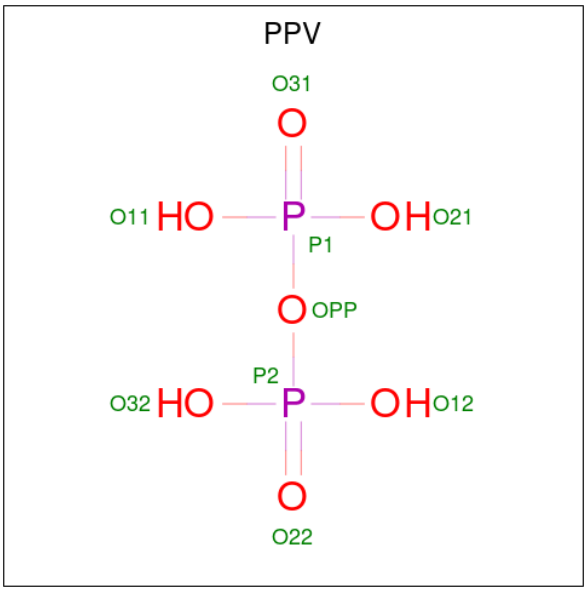
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			6	3	3			

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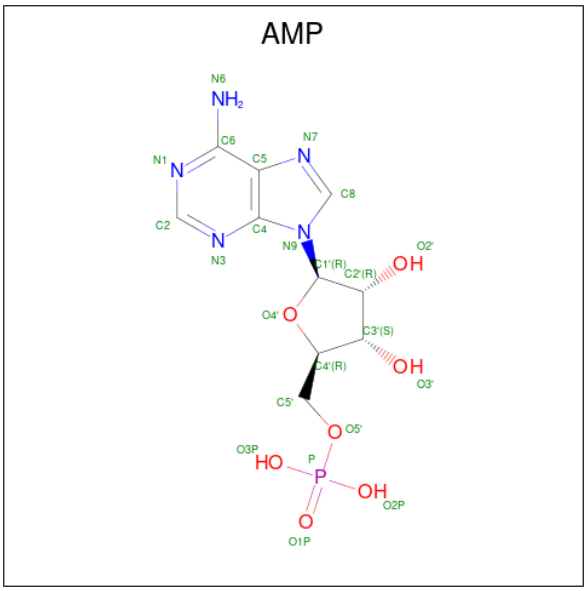
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	C	1	Total 6	C 3	O 3	0	0
2	C	1	Total 6	C 3	O 3	0	0
2	D	1	Total 6	C 3	O 3	0	0
2	D	1	Total 6	C 3	O 3	0	0
2	E	1	Total 6	C 3	O 3	0	0
2	E	1	Total 6	C 3	O 3	0	0
2	E	1	Total 6	C 3	O 3	0	0

- Molecule 3 is PYROPHOSPHATE (CCD ID: PPV) (formula: $H_4O_7P_2$) (labeled as "Ligand of Interest" by depositor).



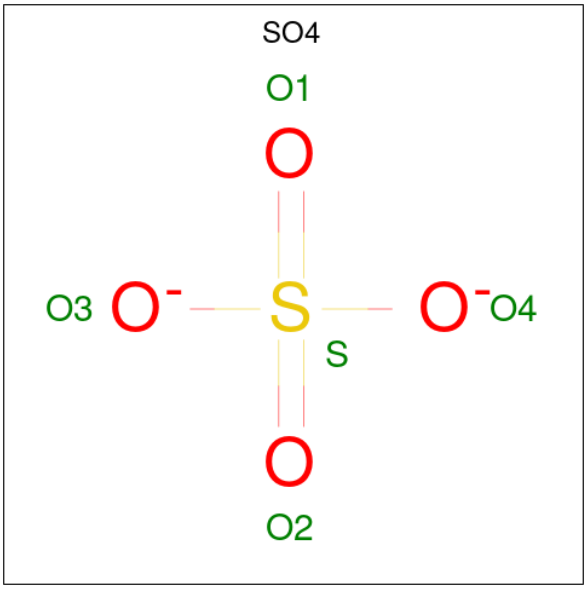
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 9 7 2	0	0
3	B	1	Total O P 9 7 2	0	0
3	C	1	Total O P 9 7 2	0	0
3	D	1	Total O P 9 7 2	0	0
3	E	1	Total O P 9 7 2	0	0

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Mg 2 2	0	0
6	B	2	Total Mg 2 2	0	0
6	C	2	Total Mg 2 2	0	0
6	D	2	Total Mg 2 2	0	0
6	E	2	Total Mg 2 2	0	0

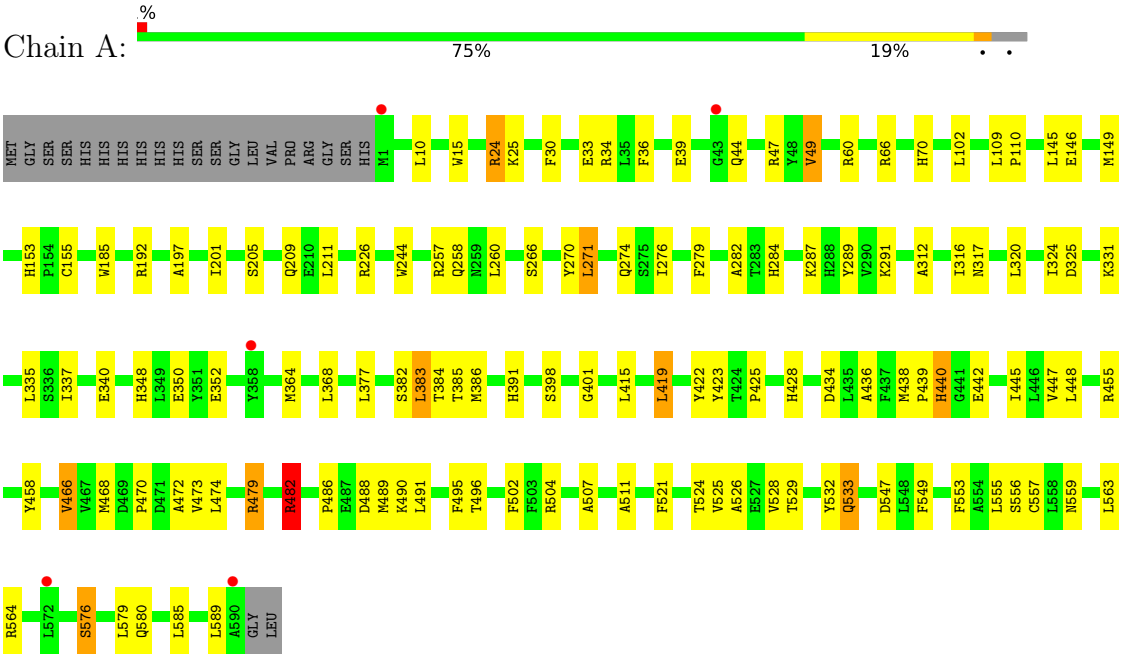
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 1 1	0	0
7	C	1	Total O 1 1	0	0
7	D	3	Total O 3 3	0	0

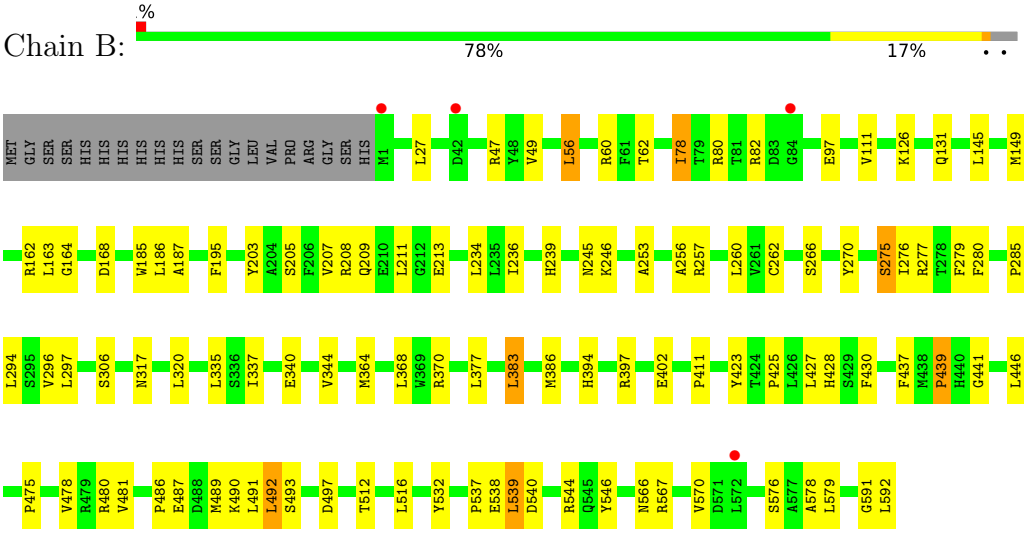
3 Residue-property plots (i)

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: Desferrioxamine synthetase DesD

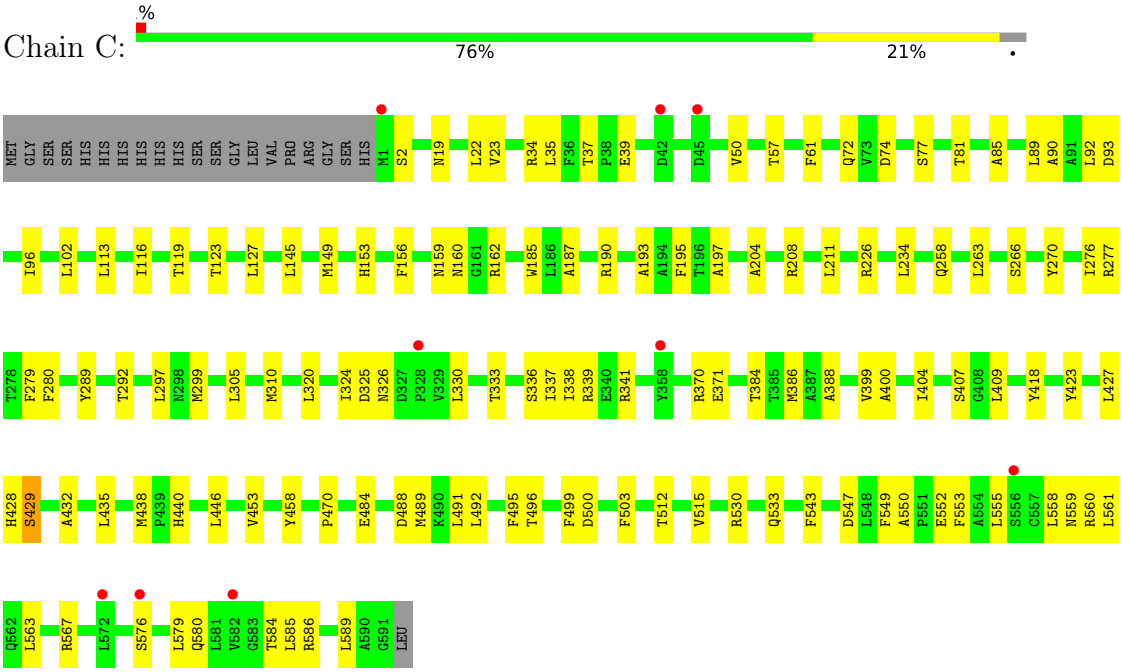


• Molecule 1: Desferrioxamine synthetase DesD



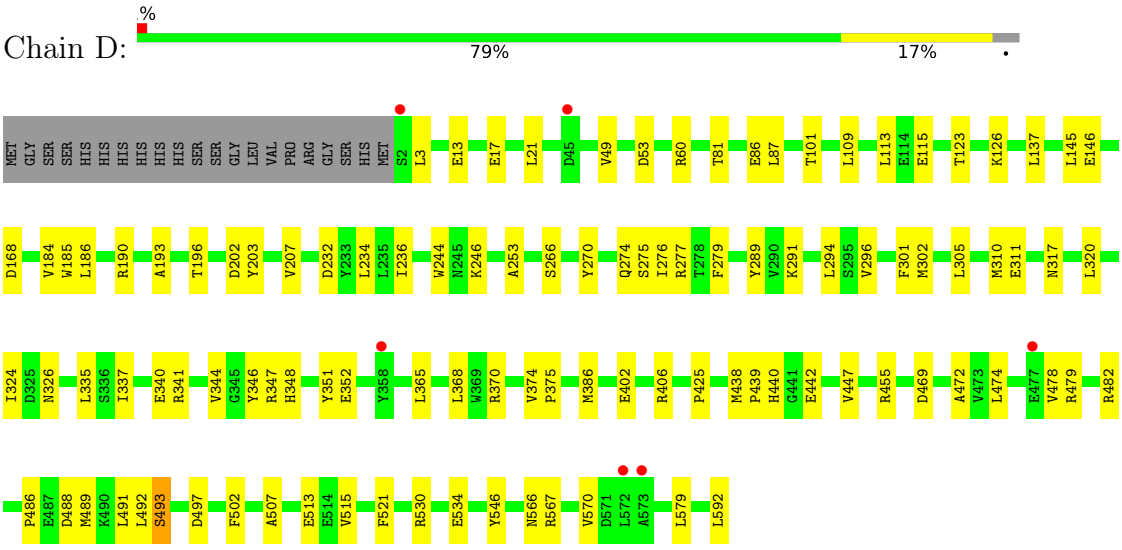
• Molecule 1: Desferrioxamine synthetase DesD

Chain C:



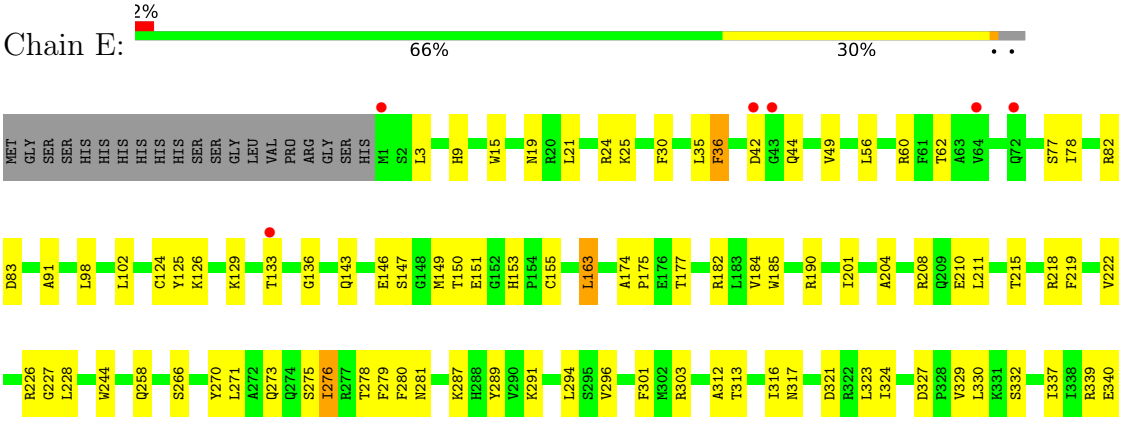
• Molecule 1: Desferrioxamine synthetase DesD

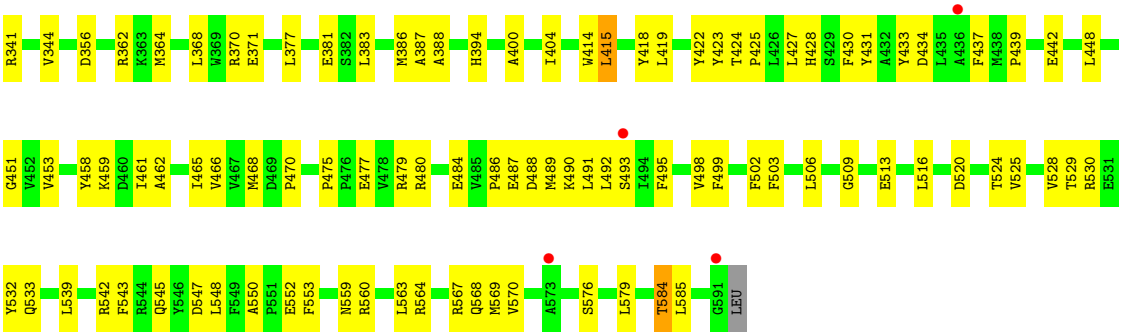
Chain D:



• Molecule 1: Desferrioxamine synthetase DesD

Chain E:




R341 V344 D356 R362 K363 M364 L368 W369 R370 E371 L377 E381 S382 L383 M386 A387 A388 H394 A400 I404 W414 L415 Y418 L419 Y422 Y423 T424 P425 L426 L427 H428 S429 F430 Y431 A432 Y433 D434 L435 A436 F437 M438 P439 E442 L448
G451 V452 V453 Y458 K459 D460 I461 A462 I465 V466 V467 M468 D469 P470 P475 P476 E477 V478 R479 R480 E484 V485 P486 E487 D488 M489 K490 L491 L492 S493 I494 F495 V498 F499 F502 F503 L506 G509 E513 L516 D520 T524 V525 V528 T529 R530 E531
Y532 Q533 L539 R542 F543 R544 Q545 Y546 D547 L548 F549 A550 P551 E552 F553 N559 R560 L563 R564 R567 Q568 M569 V570 A573 S576 L579 T584 L585 G591 LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	126.50Å 236.75Å 330.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.46 – 2.89 39.46 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.46-2.89) 92.6 (39.46-2.89)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.189 , 0.235 0.194 , 0.235	Depositor DCC
R_{free} test set	1988 reflections (1.80%)	wwPDB-VP
Wilson B-factor (Å^2)	73.0	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	23630	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PPV, AMP, GOL, SO4

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	0.45	1/4789 (0.0%)	0.67	4/6521 (0.1%)
1	B	0.45	1/4783 (0.0%)	0.65	3/6512 (0.0%)
1	C	0.37	0/4772	0.58	0/6499
1	D	0.40	0/4774	0.59	0/6501
1	E	0.35	0/4782	0.56	0/6512
All	All	0.41	2/23900 (0.0%)	0.61	7/32545 (0.0%)

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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	475	PRO	CA-C	-6.21	1.48	1.51
1	A	479	ARG	NE-CZ	-5.13	1.27	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	482	ARG	CB-CG-CD	-6.86	95.53	111.30
1	A	533	GLN	CA-CB-CG	6.13	126.35	114.10
1	B	475	PRO	O-C-N	-5.95	118.58	121.31
1	A	482	ARG	CA-CB-CG	5.90	125.90	114.10
1	B	245	ASN	CA-C-N	-5.42	115.08	121.90
1	B	245	ASN	C-N-CA	-5.42	115.08	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	289	TYR	CA-CB-CG	5.04	122.97	113.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	482	ARG	Sidechain

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	4675	0	4554	90	0
1	B	4670	0	4549	74	1
1	C	4658	0	4522	84	0
1	D	4660	0	4529	71	0
1	E	4668	0	4543	140	1
2	A	12	0	16	0	0
2	B	30	0	40	0	0
2	C	12	0	16	0	0
2	D	12	0	16	3	0
2	E	18	0	24	3	0
3	A	9	0	0	1	0
3	B	9	0	0	0	0
3	C	9	0	0	1	0
3	D	9	0	0	0	0
3	E	9	0	0	2	0
4	A	23	0	12	1	0
4	B	23	0	12	0	0
4	C	23	0	12	1	0
4	D	23	0	12	0	0
4	E	23	0	12	0	0
5	A	5	0	0	0	0
5	B	15	0	0	1	0
5	D	15	0	0	0	0
5	E	5	0	0	0	0
6	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	D	3	0	0	0	0
All	All	23630	0	22869	449	1

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 10.

All (449) 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)
1:A:149:MET:HE1	1:A:391:HIS:HB2	1.48	0.94
1:C:226:ARG:HE	1:C:258:GLN:HE21	1.05	0.93
1:A:470:PRO:O	1:A:482:ARG:NH1	2.08	0.88
1:C:429:SER:HB3	1:C:435:LEU:HD23	1.54	0.86
1:D:185:TRP:HE1	1:D:266:SER:HB3	1.41	0.86
1:E:185:TRP:HE1	1:E:266:SER:HB3	1.43	0.84
1:E:418:TYR:HB2	1:E:453:VAL:HG21	1.61	0.82
1:B:538:GLU:HG2	1:B:539:LEU:HD13	1.61	0.80
1:E:564:ARG:HH21	2:E:603:GOL:H31	1.44	0.80
1:A:474:LEU:HD12	1:A:479:ARG:HD2	1.65	0.78
1:D:17:GLU:HG3	1:D:21:LEU:HD11	1.66	0.78
1:E:442:GLU:O	1:E:459:LYS:NZ	2.16	0.77
1:A:496:THR:HG21	1:A:556:SER:HB3	1.67	0.77
1:A:489:MET:HE1	1:A:576:SER:HB3	1.67	0.76
1:A:472:ALA:O	1:A:479:ARG:NH2	2.20	0.75
1:E:539:LEU:HB2	1:E:543:PHE:CE1	2.22	0.75
1:C:491:LEU:HD23	1:C:495:PHE:CE2	2.21	0.75
1:C:555:LEU:HD13	1:C:585:LEU:HD11	1.71	0.71
1:E:487:GLU:OE2	1:E:545:GLN:NE2	2.23	0.71
1:A:386:MET:HE3	1:A:502:PHE:CE2	2.26	0.70
1:E:434:ASP:OD1	1:E:542:ARG:NH2	2.25	0.70
1:C:552:GLU:HB3	1:C:584:THR:CG2	2.21	0.69
1:E:133:THR:HG23	1:E:136:GLY:H	1.57	0.69
1:E:419:LEU:HD13	1:E:528:VAL:HG11	1.73	0.69
1:B:236:ILE:HG12	1:B:344:VAL:HG21	1.75	0.69
1:E:539:LEU:HB2	1:E:543:PHE:HE1	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:PRO:HG2	1:A:489:MET:HE2	1.75	0.69
1:C:489:MET:HG2	1:C:492:LEU:HD11	1.75	0.69
1:D:276:ILE:HD12	1:D:276:ILE:H	1.58	0.68
1:D:302:MET:HE1	1:D:567:ARG:HH11	1.59	0.68
1:B:570:VAL:HG12	1:B:578:ALA:HB3	1.76	0.67
1:E:386:MET:HE2	1:E:502:PHE:CE2	2.29	0.67
1:A:473:VAL:HA	1:A:479:ARG:HH12	1.59	0.66
1:E:430:PHE:HE2	1:E:491:LEU:HD13	1.58	0.66
1:E:143:GLN:HE21	1:E:271:LEU:HD23	1.60	0.66
1:A:488:ASP:N	1:A:488:ASP:OD1	2.29	0.66
1:C:19:ASN:O	1:C:23:VAL:HG23	1.96	0.65
1:C:119:THR:HG23	1:C:160:ASN:HB2	1.78	0.65
1:A:10:LEU:HB3	1:B:256:ALA:HB2	1.79	0.65
1:E:386:MET:HE1	1:E:422:TYR:CZ	2.31	0.65
1:A:337:ILE:HG22	1:A:458:TYR:HB2	1.79	0.65
1:A:325:ASP:HA	1:A:331:LYS:HE3	1.80	0.64
1:B:317:ASN:ND2	1:B:340:GLU:HB2	2.12	0.64
1:A:468:MET:O	1:A:490:LYS:NZ	2.31	0.64
1:A:419:LEU:HB3	1:A:423:TYR:HB3	1.80	0.64
1:D:474:LEU:HD13	1:D:478:VAL:HG12	1.79	0.64
1:D:493:SER:O	1:D:497:ASP:HB2	1.98	0.63
1:B:208:ARG:HG3	1:B:208:ARG:HH11	1.62	0.63
1:C:547:ASP:OD1	1:C:550:ALA:N	2.30	0.63
1:A:415:LEU:O	1:A:419:LEU:HD12	1.99	0.63
1:A:70:HIS:HD2	1:A:504:ARG:HG2	1.63	0.63
1:A:470:PRO:HA	1:A:482:ARG:HD2	1.79	0.63
1:E:430:PHE:CE2	1:E:491:LEU:HD13	2.33	0.63
1:B:377:LEU:HD11	1:B:383:LEU:HD22	1.81	0.63
1:C:159:ASN:HB2	1:C:299:MET:HE2	1.81	0.63
1:E:146:GLU:HG2	1:E:273:GLN:OE1	1.99	0.63
1:D:479:ARG:HB3	1:D:482:ARG:HH21	1.65	0.62
1:C:561:LEU:HD21	1:C:579:LEU:HA	1.81	0.62
1:D:301:PHE:HZ	1:D:570:VAL:HG22	1.65	0.61
1:C:491:LEU:HD23	1:C:495:PHE:CZ	2.36	0.61
1:D:335:LEU:HD22	1:D:425:PRO:HB3	1.82	0.61
1:D:305:LEU:HG	1:D:310:MET:HE3	1.81	0.61
1:E:427:LEU:H	1:E:427:LEU:HD12	1.65	0.61
1:B:80:ARG:NH2	1:B:97:GLU:OE2	2.34	0.61
1:E:24:ARG:HB3	1:E:78:ILE:HD11	1.83	0.60
1:E:149:MET:HE1	1:E:388:ALA:HA	1.82	0.60
1:C:187:ALA:HB2	1:C:263:LEU:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:337:ILE:HG22	1:E:458:TYR:HB2	1.83	0.60
1:B:289:TYR:HB2	1:B:370:ARG:HB3	1.83	0.60
1:A:386:MET:HE1	1:A:422:TYR:CZ	2.36	0.60
1:C:22:LEU:HD21	1:C:116:ILE:HD12	1.83	0.60
1:E:129:LYS:NZ	1:E:147:SER:O	2.35	0.60
1:D:3:LEU:HD21	1:E:184:VAL:HG22	1.84	0.59
1:A:320:LEU:O	1:A:324:ILE:HG13	2.03	0.59
1:D:17:GLU:O	1:D:21:LEU:HD12	2.03	0.59
1:E:185:TRP:NE1	1:E:266:SER:HB3	2.16	0.59
1:A:153:HIS:CE1	1:A:155:CYS:HB2	2.37	0.59
1:A:559:ASN:O	1:A:563:LEU:HD12	2.02	0.59
1:C:305:LEU:HG	1:C:310:MET:HE3	1.84	0.59
1:E:226:ARG:HE	1:E:258:GLN:HE21	1.49	0.59
1:E:564:ARG:NH2	2:E:603:GOL:H31	2.18	0.59
1:A:525:VAL:O	1:A:529:THR:OG1	2.18	0.58
1:D:236:ILE:HG12	1:D:344:VAL:HG21	1.85	0.58
1:E:489:MET:HE1	1:E:576:SER:HB2	1.84	0.58
1:E:149:MET:HE1	1:E:388:ALA:CA	2.32	0.58
1:E:525:VAL:O	1:E:529:THR:HG23	2.02	0.58
1:B:208:ARG:HD3	1:B:213:GLU:HG2	1.85	0.58
1:D:469:ASP:HB3	1:D:472:ALA:HB2	1.86	0.58
1:A:205:SER:O	1:A:209:GLN:HG3	2.03	0.58
1:C:226:ARG:NE	1:C:258:GLN:HE21	1.90	0.58
1:C:337:ILE:HG22	1:C:458:TYR:HB2	1.85	0.57
1:C:226:ARG:HE	1:C:258:GLN:NE2	1.88	0.57
1:D:491:LEU:HD22	1:D:546:TYR:HB3	1.86	0.57
1:E:400:ALA:O	1:E:404:ILE:HG13	2.04	0.57
1:C:552:GLU:HB3	1:C:584:THR:HG21	1.86	0.57
1:E:210:GLU:HA	1:E:287:LYS:HE2	1.85	0.57
1:B:537:PRO:HA	1:B:540:ASP:OD1	2.05	0.57
1:C:92:LEU:O	1:C:96:ILE:HG13	2.05	0.57
1:A:70:HIS:HD2	1:A:504:ARG:CG	2.17	0.57
1:C:326:ASN:HD21	1:E:190:ARG:NH1	2.02	0.57
1:E:468:MET:O	1:E:490:LYS:NZ	2.38	0.57
1:E:533:GLN:HA	1:E:543:PHE:HE2	1.70	0.57
1:B:185:TRP:HE1	1:B:266:SER:HB3	1.70	0.56
1:E:468:MET:HE2	1:E:490:LYS:HG2	1.85	0.56
1:E:280:PHE:HB2	1:E:289:TYR:HE1	1.69	0.56
1:A:49:VAL:HG23	1:A:60:ARG:HG2	1.88	0.56
1:D:246:LYS:HD2	2:D:601:GOL:H12	1.87	0.56
1:C:297:LEU:HD22	1:C:567:ARG:NH1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:475:PRO:O	1:E:479:ARG:HG3	2.05	0.56
1:A:153:HIS:HE1	1:A:155:CYS:HB2	1.70	0.56
1:C:400:ALA:O	1:C:404:ILE:HG13	2.06	0.56
1:A:102:LEU:HB3	1:A:563:LEU:CD2	2.35	0.55
1:D:146:GLU:OE1	1:D:274:GLN:HG3	2.06	0.55
1:B:489:MET:HA	1:B:492:LEU:HD23	1.89	0.55
1:C:547:ASP:OD1	1:C:549:PHE:N	2.40	0.55
1:E:291:LYS:NZ	3:E:604:PPV:OPP	2.36	0.55
1:C:423:TYR:CE1	1:C:427:LEU:HD21	2.42	0.55
1:C:576:SER:HA	1:C:579:LEU:HD11	1.87	0.55
1:D:386:MET:HE3	1:D:502:PHE:CE2	2.41	0.55
1:C:185:TRP:CE2	1:C:211:LEU:HD21	2.43	0.54
1:B:203:TYR:O	1:B:207:VAL:HG22	2.06	0.54
1:D:196:THR:HG21	1:D:311:GLU:O	2.07	0.54
1:E:552:GLU:HB3	1:E:584:THR:OG1	2.07	0.54
1:E:339:ARG:HH21	1:E:341:ARG:CZ	2.20	0.54
1:E:149:MET:HE1	1:E:388:ALA:N	2.22	0.54
1:A:576:SER:HA	1:A:579:LEU:HD23	1.90	0.54
1:E:470:PRO:HG3	1:E:484:GLU:HG2	1.90	0.54
1:C:270:TYR:HB3	1:C:279:PHE:HB3	1.89	0.53
1:D:479:ARG:HB3	1:D:482:ARG:NH2	2.23	0.53
1:B:487:GLU:OE2	1:B:546:TYR:OH	2.22	0.53
1:D:347:ARG:HD2	1:D:352:GLU:OE2	2.09	0.53
1:D:438:MET:HE3	1:D:440:HIS:HD2	1.74	0.53
1:A:70:HIS:CD2	1:A:504:ARG:HG2	2.44	0.53
1:A:383:LEU:HD12	1:A:445:ILE:CG2	2.38	0.53
1:D:275:SER:O	1:D:277:ARG:N	2.40	0.53
1:C:388:ALA:O	1:C:399:VAL:HB	2.08	0.53
1:E:424:THR:HA	1:E:427:LEU:CD1	2.39	0.53
1:C:297:LEU:HD22	1:C:567:ARG:HH12	1.73	0.53
1:E:477:GLU:HA	1:E:480:ARG:HH21	1.73	0.53
1:E:542:ARG:HA	1:E:545:GLN:HB3	1.91	0.53
1:A:145:LEU:HD13	1:A:384:THR:HB	1.91	0.52
1:A:472:ALA:O	1:A:479:ARG:CZ	2.57	0.52
1:B:145:LEU:O	1:B:149:MET:HG2	2.09	0.52
1:A:317:ASN:ND2	1:A:340:GLU:HB2	2.24	0.52
1:A:377:LEU:HD11	1:A:383:LEU:HD23	1.91	0.52
1:E:270:TYR:HB3	1:E:279:PHE:HB3	1.91	0.52
1:A:428:HIS:HA	1:A:532:TYR:OH	2.09	0.52
1:A:270:TYR:HB3	1:A:279:PHE:HB3	1.92	0.52
1:D:440:HIS:CE1	1:D:442:GLU:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:ARG:HG2	1:B:567:ARG:HH11	1.73	0.52
1:D:137:LEU:HB3	1:D:145:LEU:CD2	2.40	0.52
1:D:185:TRP:NE1	1:D:266:SER:HB3	2.18	0.52
1:C:320:LEU:HD23	1:C:337:ILE:HD13	1.92	0.52
1:D:447:VAL:HG21	1:D:455:ARG:CZ	2.40	0.52
1:E:386:MET:HE3	1:E:418:TYR:OH	2.09	0.51
1:E:415:LEU:HD22	1:E:419:LEU:HD11	1.92	0.51
1:E:547:ASP:OD1	1:E:550:ALA:N	2.44	0.51
1:E:486:PRO:O	1:E:490:LYS:HG3	2.10	0.51
1:E:414:TRP:NE1	1:E:451:GLY:O	2.37	0.51
1:A:39:GLU:HG3	1:A:49:VAL:HG12	1.93	0.51
1:B:411:PRO:HB2	1:B:516:LEU:HD13	1.92	0.51
1:E:21:LEU:O	1:E:24:ARG:HG3	2.10	0.51
1:B:486:PRO:O	1:B:490:LYS:HG3	2.11	0.51
1:D:530:ARG:NH2	1:D:592:LEU:OXT	2.44	0.51
1:B:111:VAL:HG12	1:B:566:ASN:HD21	1.75	0.50
1:C:428:HIS:CD2	1:C:432:ALA:HB3	2.45	0.50
1:E:62:THR:HG23	1:E:77:SER:HB2	1.93	0.50
1:E:491:LEU:HG	1:E:495:PHE:CE1	2.47	0.50
1:D:489:MET:HE3	1:D:579:LEU:HD12	1.92	0.50
1:C:579:LEU:HD12	1:C:579:LEU:H	1.76	0.50
1:A:507:ALA:HB2	1:A:521:PHE:CD2	2.47	0.50
1:C:320:LEU:O	1:C:324:ILE:HG13	2.11	0.50
1:E:424:THR:HA	1:E:427:LEU:HD13	1.94	0.50
1:C:193:ALA:HB1	1:C:234:LEU:HD11	1.92	0.50
1:C:339:ARG:NH2	1:C:371:GLU:OE2	2.42	0.50
1:C:488:ASP:O	1:C:489:MET:HB2	2.10	0.50
1:E:576:SER:HA	1:E:579:LEU:CD1	2.42	0.50
1:D:513:GLU:HB3	1:D:515:VAL:HG23	1.94	0.50
1:D:440:HIS:HE1	1:D:442:GLU:HB3	1.77	0.49
1:C:74:ASP:HB3	1:C:77:SER:HB3	1.93	0.49
1:C:496:THR:HA	1:C:500:ASP:HB3	1.94	0.49
1:D:530:ARG:O	1:D:534:GLU:HG2	2.13	0.49
1:E:386:MET:HE1	1:E:422:TYR:CE2	2.47	0.49
1:A:398:SER:HG	1:A:401:GLY:H	1.58	0.49
1:B:320:LEU:HD23	1:B:337:ILE:HG21	1.94	0.49
1:E:419:LEU:HB3	1:E:423:TYR:HB3	1.94	0.49
1:C:90:ALA:HB3	1:C:93:ASP:HB2	1.95	0.49
1:A:192:ARG:HH22	1:A:257:ARG:HH22	1.59	0.49
1:E:182:ARG:HG2	1:E:266:SER:O	2.13	0.49
1:E:423:TYR:HE2	1:E:529:THR:HG22	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:THR:O	1:A:533:GLN:HG2	2.12	0.49
1:C:549:PHE:CD1	1:C:589:LEU:HB3	2.47	0.49
1:E:488:ASP:N	1:E:488:ASP:OD1	2.45	0.49
1:A:473:VAL:HA	1:A:479:ARG:NH1	2.26	0.49
1:D:190:ARG:HG3	1:D:232:ASP:O	2.12	0.49
1:E:324:ILE:HA	1:E:330:LEU:HD12	1.95	0.49
1:A:185:TRP:HE1	1:A:266:SER:HB3	1.78	0.48
1:A:524:THR:O	1:A:528:VAL:HG22	2.13	0.48
1:B:591:GLY:C	1:B:592:LEU:HD23	2.38	0.48
1:B:335:LEU:HD22	1:B:425:PRO:HB3	1.95	0.48
1:A:325:ASP:HA	1:A:331:LYS:CE	2.42	0.48
1:E:339:ARG:HG3	1:E:371:GLU:OE1	2.14	0.48
1:E:431:TYR:OH	1:E:548:LEU:HD11	2.13	0.48
1:A:30:PHE:HB2	1:A:36:PHE:CZ	2.49	0.48
1:A:185:TRP:CZ2	1:A:211:LEU:HD21	2.48	0.48
1:B:208:ARG:HG3	1:B:208:ARG:NH1	2.28	0.48
1:B:386:MET:HE2	1:B:441:GLY:HA2	1.96	0.48
1:A:434:ASP:O	1:A:468:MET:HG3	2.13	0.48
1:E:461:ILE:O	1:E:465:ILE:HG23	2.13	0.48
1:B:49:VAL:HG23	1:B:60:ARG:HG2	1.95	0.48
1:B:153:HIS:CE1	1:B:155:CYS:HB2	2.49	0.48
1:C:123:THR:O	1:C:127:LEU:HG	2.14	0.48
1:B:195:PHE:HB2	1:B:234:LEU:HD22	1.96	0.48
1:B:386:MET:HG3	1:B:446:LEU:HD11	1.96	0.47
1:B:185:TRP:CE2	1:B:211:LEU:HD21	2.49	0.47
1:B:478:VAL:O	1:B:481:VAL:HG22	2.14	0.47
1:E:488:ASP:O	1:E:489:MET:HB2	2.13	0.47
1:B:164:GLY:HA3	1:B:296:VAL:HG23	1.96	0.47
1:E:323:LEU:HD21	1:E:433:TYR:CZ	2.49	0.47
1:A:146:GLU:OE2	1:A:274:GLN:HG3	2.14	0.47
1:C:559:ASN:O	1:C:563:LEU:HD13	2.15	0.47
1:E:126:LYS:NZ	1:E:150:THR:O	2.45	0.47
1:E:312:ALA:HB1	1:E:316:ILE:HD11	1.96	0.47
1:E:428:HIS:HA	1:E:532:TYR:OH	2.14	0.47
1:D:497:ASP:OD1	2:D:602:GOL:H11	2.13	0.47
1:C:423:TYR:CZ	1:C:427:LEU:HD21	2.50	0.47
1:A:553:PHE:HE1	1:A:585:LEU:HD12	1.79	0.47
1:B:489:MET:HE1	1:B:576:SER:HB2	1.97	0.47
1:C:438:MET:HE2	1:C:440:HIS:HD2	1.80	0.47
1:E:289:TYR:HB2	1:E:370:ARG:HB3	1.96	0.47
1:C:92:LEU:HD22	1:C:113:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:428:HIS:HD2	1:C:432:ALA:HB3	1.80	0.47
1:C:330:LEU:O	1:C:333:THR:OG1	2.30	0.46
1:C:470:PRO:HG3	1:C:484:GLU:HB2	1.96	0.46
1:E:153:HIS:CE1	1:E:155:CYS:HB2	2.51	0.46
1:E:275:SER:C	1:E:276:ILE:HG13	2.40	0.46
1:E:516:LEU:HD23	1:E:520:ASP:HB2	1.96	0.46
1:D:60:ARG:HH12	1:D:81:THR:HG21	1.79	0.46
1:A:109:LEU:HB3	1:A:110:PRO:HD3	1.96	0.46
1:A:386:MET:HE3	1:A:502:PHE:CD2	2.50	0.46
1:B:126:LYS:HD2	1:B:150:THR:HG22	1.98	0.46
1:A:291:LYS:HB3	1:A:368:LEU:HG	1.97	0.46
1:B:291:LYS:HB3	1:B:368:LEU:HG	1.96	0.46
1:D:123:THR:HA	1:D:126:LYS:HE3	1.97	0.46
1:D:185:TRP:O	1:D:186:LEU:HD23	2.15	0.46
1:E:125:TYR:CE2	1:E:177:THR:HG22	2.50	0.46
1:A:197:ALA:HB1	1:A:201:ILE:HB	1.98	0.46
1:B:236:ILE:HG12	1:B:344:VAL:CG2	2.45	0.46
1:E:49:VAL:HG23	1:E:60:ARG:HG2	1.98	0.46
1:E:437:PHE:C	1:E:439:PRO:HD3	2.41	0.46
1:B:185:TRP:NE1	1:B:266:SER:HB3	2.30	0.46
1:D:109:LEU:O	1:D:113:LEU:HG	2.14	0.46
1:E:82:ARG:HG2	1:E:83:ASP:OD1	2.15	0.46
1:E:317:ASN:ND2	1:E:340:GLU:HB2	2.31	0.46
1:E:301:PHE:CE2	1:E:569:MET:HE3	2.50	0.46
1:A:291:LYS:NZ	3:A:603:PPV:O32	2.40	0.46
1:A:312:ALA:O	1:A:316:ILE:HG13	2.16	0.46
1:C:39:GLU:OE2	1:C:39:GLU:N	2.48	0.46
1:E:278:THR:OG1	3:E:604:PPV:O22	2.20	0.46
1:E:567:ARG:HE	1:E:567:ARG:HB3	1.56	0.46
1:D:294:LEU:HG	1:D:296:VAL:HG13	1.98	0.46
1:E:30:PHE:HB2	1:E:36:PHE:CZ	2.51	0.46
1:E:323:LEU:HD21	1:E:433:TYR:CE1	2.51	0.46
1:A:377:LEU:HD21	1:A:383:LEU:HD22	1.98	0.45
1:C:277:ARG:NH2	3:C:603:PPV:O22	2.43	0.45
1:C:338:ILE:HG13	1:C:370:ARG:HD3	1.98	0.45
1:D:137:LEU:HB3	1:D:145:LEU:HD23	1.99	0.45
1:A:271:LEU:CD1	1:A:282:ALA:HB2	2.47	0.45
1:C:34:ARG:HH12	1:C:584:THR:H	1.63	0.45
1:D:3:LEU:HD13	1:E:244:TRP:CZ2	2.50	0.45
1:E:98:LEU:HA	1:E:98:LEU:HD23	1.70	0.45
1:E:227:GLY:C	1:E:228:LEU:HD23	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:524:THR:O	1:E:528:VAL:HG12	2.16	0.45
1:E:530:ARG:HA	1:E:533:GLN:HB2	1.98	0.45
1:A:33:GLU:OE1	1:A:557:CYS:HB3	2.16	0.45
1:A:466:VAL:HG13	1:A:468:MET:HG2	1.99	0.45
1:B:447:VAL:HG21	1:B:455:ARG:CZ	2.46	0.45
1:C:145:LEU:O	1:C:149:MET:HG2	2.16	0.45
1:D:489:MET:HA	1:D:492:LEU:HG	1.97	0.45
1:E:579:LEU:HD12	1:E:579:LEU:H	1.81	0.45
1:A:419:LEU:HD12	1:A:419:LEU:H	1.81	0.45
1:B:186:LEU:HD23	1:B:262:CYS:HA	1.97	0.45
1:B:253:ALA:O	1:B:257:ARG:HG3	2.16	0.45
1:E:303:ARG:HA	1:E:303:ARG:HD3	1.84	0.45
1:E:492:LEU:HD23	1:E:495:PHE:HB2	1.99	0.45
1:A:340:GLU:HG2	1:A:368:LEU:HD13	1.99	0.45
1:D:244:TRP:CZ2	1:E:3:LEU:HD23	2.52	0.45
1:D:341:ARG:HH11	1:D:341:ARG:HG3	1.81	0.45
1:E:329:VAL:O	1:E:332:SER:OG	2.29	0.45
1:E:559:ASN:O	1:E:563:LEU:HG	2.17	0.45
1:A:555:LEU:HD13	1:A:585:LEU:HD11	1.98	0.45
1:B:205:SER:O	1:B:209:GLN:HG3	2.16	0.45
1:C:560:ARG:HB3	1:C:580:GLN:OE1	2.17	0.45
1:E:312:ALA:O	1:E:316:ILE:HD12	2.16	0.45
1:E:313:THR:HG23	1:E:462:ALA:HB3	1.97	0.45
1:A:415:LEU:HG	1:A:419:LEU:HD11	1.99	0.45
1:B:540:ASP:O	1:B:544:ARG:HG3	2.16	0.45
1:C:153:HIS:HB2	1:C:299:MET:HE1	1.97	0.45
1:D:115:GLU:OE1	1:D:566:ASN:ND2	2.48	0.45
1:C:72:GLN:NE2	1:C:512:THR:OG1	2.45	0.44
1:D:184:VAL:HG22	1:E:3:LEU:HD11	1.98	0.44
1:E:201:ILE:HD11	1:E:341:ARG:CZ	2.47	0.44
1:E:9:HIS:O	1:E:124:CYS:HB3	2.17	0.44
1:E:149:MET:HE1	1:E:387:ALA:C	2.42	0.44
1:E:516:LEU:CD2	1:E:520:ASP:HB2	2.47	0.44
1:D:402:GLU:O	1:D:406:ARG:HG3	2.17	0.44
1:A:44:GLN:HB3	1:A:47:ARG:HB3	1.99	0.44
1:B:280:PHE:HZ	1:B:285:PRO:HB3	1.82	0.44
1:E:102:LEU:HB3	1:E:563:LEU:HD13	1.98	0.44
1:E:321:ASP:HA	1:E:324:ILE:HD12	2.00	0.44
1:A:438:MET:HE3	1:A:440:HIS:CD2	2.52	0.44
1:B:340:GLU:HG2	1:B:368:LEU:HD13	1.99	0.44
1:B:47:ARG:HD2	1:B:62:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:ALA:O	1:E:208:ARG:NH1	2.51	0.44
1:E:226:ARG:NE	1:E:258:GLN:HE21	2.15	0.44
1:C:543:PHE:HD1	1:C:543:PHE:N	2.16	0.44
1:D:253:ALA:HA	1:E:15:TRP:CZ2	2.53	0.44
1:D:270:TYR:HB3	1:D:279:PHE:HB3	1.99	0.43
1:E:56:LEU:O	1:E:82:ARG:HG3	2.18	0.43
1:E:163:LEU:HD23	1:E:163:LEU:HA	1.63	0.43
1:C:185:TRP:HE1	1:C:266:SER:HB3	1.83	0.43
1:D:168:ASP:HB3	1:E:244:TRP:CZ3	2.53	0.43
1:E:533:GLN:HA	1:E:543:PHE:CE2	2.49	0.43
1:C:543:PHE:N	1:C:543:PHE:CD1	2.85	0.43
1:C:488:ASP:N	1:C:488:ASP:OD1	2.52	0.43
1:C:495:PHE:O	1:C:499:PHE:HB2	2.18	0.43
1:A:66:ARG:HH21	1:A:511:ALA:HB1	1.84	0.43
1:B:187:ALA:O	1:B:260:LEU:HA	2.19	0.43
1:B:397:ARG:NH1	1:B:402:GLU:OE2	2.52	0.43
1:D:13:GLU:H	1:D:13:GLU:CD	2.27	0.43
1:D:203:TYR:O	1:D:207:VAL:HG22	2.19	0.43
1:E:381:GLU:HA	1:E:448:LEU:O	2.18	0.43
1:E:533:GLN:CD	1:E:543:PHE:HD2	2.26	0.43
1:E:509:GLY:O	1:E:513:GLU:HB2	2.19	0.43
1:B:27:LEU:HD12	1:B:78:ILE:HD13	2.01	0.43
1:C:492:LEU:HD22	1:C:496:THR:HG21	2.00	0.43
1:C:530:ARG:HA	1:C:533:GLN:HB2	2.01	0.43
1:E:560:ARG:HH11	2:E:603:GOL:H11	1.84	0.43
1:B:480:ARG:H	1:B:480:ARG:HG2	1.65	0.43
1:D:291:LYS:HB3	1:D:368:LEU:HG	2.01	0.43
1:B:493:SER:O	1:B:497:ASP:HB2	2.18	0.43
1:E:553:PHE:CE1	1:E:585:LEU:HD12	2.53	0.43
1:E:175:PRO:HB3	1:E:273:GLN:O	2.19	0.42
1:E:219:PHE:O	1:E:222:VAL:HG22	2.19	0.42
1:A:244:TRP:CZ3	1:B:168:ASP:HB3	2.54	0.42
1:B:246:LYS:HD2	1:B:364:MET:HE1	2.00	0.42
1:B:430:PHE:CZ	1:B:491:LEU:HD13	2.53	0.42
1:B:489:MET:HA	1:B:492:LEU:CD2	2.49	0.42
1:E:153:HIS:HE1	1:E:155:CYS:HB2	1.84	0.42
1:D:276:ILE:H	1:D:276:ILE:CD1	2.28	0.42
1:D:491:LEU:HD12	1:D:491:LEU:HA	1.85	0.42
1:E:291:LYS:HB3	1:E:368:LEU:HG	2.00	0.42
1:A:438:MET:HE3	1:A:440:HIS:HD2	1.84	0.42
1:E:210:GLU:O	1:E:211:LEU:HD23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:TRP:CZ2	1:B:253:ALA:HA	2.54	0.42
1:D:86:GLU:C	1:D:87:LEU:HD23	2.44	0.42
1:E:25:LYS:HD2	1:E:151:GLU:OE2	2.18	0.42
1:E:539:LEU:O	1:E:542:ARG:N	2.49	0.42
1:B:270:TYR:HB3	1:B:279:PHE:HB3	2.01	0.42
1:B:280:PHE:CZ	1:B:285:PRO:HB3	2.54	0.42
1:C:35:LEU:HD13	1:C:102:LEU:HD22	2.02	0.42
1:C:50:VAL:HG23	1:C:61:PHE:HE1	1.84	0.42
1:C:341:ARG:HG2	1:C:371:GLU:HG3	2.00	0.42
1:D:289:TYR:HB2	1:D:370:ARG:HB3	2.00	0.42
1:D:320:LEU:HD23	1:D:337:ILE:HG21	2.02	0.42
1:E:377:LEU:HD11	1:E:383:LEU:CD2	2.49	0.42
1:B:428:HIS:HA	1:B:532:TYR:OH	2.18	0.42
1:C:386:MET:HG3	1:C:446:LEU:HD11	2.00	0.42
1:A:364:MET:HE2	1:A:364:MET:HB3	1.87	0.42
1:B:423:TYR:CZ	1:B:427:LEU:HD21	2.53	0.42
1:B:56:LEU:HB2	1:B:82:ARG:HH21	1.84	0.42
1:C:145:LEU:HD13	1:C:384:THR:OG1	2.19	0.42
1:D:507:ALA:HB2	1:D:521:PHE:CD1	2.54	0.42
1:E:294:LEU:O	1:E:296:VAL:N	2.53	0.42
1:E:19:ASN:OD1	1:E:91:ALA:N	2.39	0.42
1:E:356:ASP:O	1:E:362:ARG:NE	2.53	0.42
1:A:383:LEU:HD13	1:A:383:LEU:HA	1.82	0.41
1:B:162:ARG:HD2	1:B:162:ARG:N	2.35	0.41
1:B:209:GLN:HE21	1:B:209:GLN:HB3	1.66	0.41
1:B:364:MET:HE2	1:B:364:MET:HB3	1.91	0.41
1:D:317:ASN:OD1	1:D:340:GLU:N	2.49	0.41
1:D:320:LEU:O	1:D:324:ILE:HG13	2.21	0.41
1:E:215:THR:HG23	1:E:218:ARG:NH2	2.34	0.41
1:E:488:ASP:C	1:E:490:LYS:H	2.28	0.41
1:A:553:PHE:CD1	1:A:553:PHE:C	2.98	0.41
1:E:503:PHE:O	1:E:506:LEU:N	2.52	0.41
1:A:226:ARG:HE	1:A:258:GLN:HE21	1.66	0.41
1:B:246:LYS:HE3	5:B:608:SO4:O3	2.19	0.41
1:A:350:GLU:OE1	1:A:350:GLU:N	2.46	0.41
1:D:348:HIS:CE1	1:D:351:TYR:CD2	3.08	0.41
1:D:488:ASP:O	1:D:489:MET:HB2	2.21	0.41
1:A:226:ARG:HH21	1:A:258:GLN:HE21	1.69	0.41
1:B:131:GLN:HB3	1:B:394:HIS:CE1	2.55	0.41
1:D:145:LEU:HD23	1:D:145:LEU:HA	1.81	0.41
1:E:174:ALA:HB3	1:E:177:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LEU:HD22	1:A:425:PRO:HB3	2.03	0.41
1:A:382:SER:OG	1:A:448:LEU:HB2	2.21	0.41
1:B:185:TRP:CZ2	1:B:211:LEU:HD21	2.55	0.41
1:C:280:PHE:HD1	1:C:289:TYR:CE1	2.38	0.41
1:C:299:MET:O	1:C:299:MET:HG2	2.20	0.41
1:D:497:ASP:OD2	2:D:602:GOL:H32	2.21	0.41
1:E:394:HIS:ND1	1:E:394:HIS:N	2.65	0.41
1:E:498:VAL:HG12	1:E:499:PHE:CD1	2.55	0.41
1:B:437:PHE:C	1:B:439:PRO:HD3	2.46	0.41
1:C:418:TYR:HB2	1:C:453:VAL:HG11	2.02	0.41
1:C:499:PHE:HD1	1:C:503:PHE:HD1	1.68	0.41
1:C:81:THR:HA	1:C:85:ALA:O	2.20	0.41
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.85	0.41
1:A:284:HIS:HB2	1:A:287:LYS:HD2	2.03	0.41
1:A:348:HIS:O	1:A:352:GLU:HG3	2.21	0.41
1:A:436:ALA:HB3	1:A:466:VAL:HG12	2.01	0.41
1:A:447:VAL:HG21	1:A:455:ARG:CZ	2.51	0.41
1:A:526:ALA:HB2	1:A:589:LEU:HD22	2.03	0.41
1:B:56:LEU:HB3	1:B:82:ARG:HE	1.85	0.41
1:B:163:LEU:HD23	1:B:163:LEU:HA	1.93	0.41
1:C:195:PHE:HE2	1:C:197:ALA:HB2	1.85	0.41
1:C:553:PHE:O	1:C:584:THR:HG23	2.21	0.41
1:D:49:VAL:HG23	1:D:60:ARG:HG2	2.02	0.41
1:D:374:VAL:N	1:D:375:PRO:HD2	2.35	0.41
1:E:327:ASP:OD2	1:E:428:HIS:NE2	2.53	0.41
1:E:423:TYR:CE2	1:E:529:THR:HG22	2.55	0.41
1:B:163:LEU:HB2	1:B:297:LEU:HB3	2.02	0.41
1:D:346:TYR:CG	1:D:365:LEU:HD23	2.56	0.41
1:E:364:MET:HE2	1:E:364:MET:HB3	1.83	0.41
1:E:568:GLN:HG3	1:E:570:VAL:O	2.21	0.41
1:A:491:LEU:HD23	1:A:495:PHE:CE2	2.56	0.40
1:B:49:VAL:HG23	1:B:60:ARG:CG	2.50	0.40
1:C:277:ARG:HB2	1:C:292:THR:O	2.20	0.40
1:E:271:LEU:O	1:E:273:GLN:NE2	2.53	0.40
1:E:424:THR:OG1	1:E:425:PRO:HD3	2.22	0.40
1:A:24:ARG:HG3	1:A:25:LYS:N	2.36	0.40
1:A:547:ASP:OD1	1:A:549:PHE:N	2.48	0.40
1:C:162:ARG:HE	1:C:276:ILE:HD11	1.85	0.40
1:D:486:PRO:O	1:D:488:ASP:O	2.39	0.40
1:A:442:GLU:OE1	4:A:604:AMP:H5'2	2.21	0.40
1:A:564:ARG:HD3	1:A:580:GLN:NE2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:HIS:CG	1:B:294:LEU:HD13	2.56	0.40
1:C:89:LEU:HA	1:C:89:LEU:HD23	1.64	0.40
1:C:204:ALA:O	1:C:208:ARG:HD2	2.22	0.40
1:C:299:MET:HE3	4:C:604:AMP:O2'	2.21	0.40
1:D:193:ALA:HB1	1:D:234:LEU:HD11	2.03	0.40
1:C:156:PHE:CE2	1:C:558:LEU:HD13	2.56	0.40
1:C:190:ARG:HG2	1:C:234:LEU:HD23	2.04	0.40
1:D:53:ASP:OD1	1:D:101:THR:OG1	2.39	0.40
1:E:281:ASN:ND2	1:E:287:LYS:HD3	2.36	0.40
1:B:275:SER:C	1:B:277:ARG:H	2.29	0.40
1:B:489:MET:HE3	1:B:579:LEU:HD12	2.04	0.40
1:C:407:SER:O	1:C:409:LEU:HD12	2.21	0.40
1:E:492:LEU:HD23	1:E:492:LEU:HA	1.94	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:ARG:NH1	1:E:42:ASP:O[5_555]	2.18	0.02

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	588/612 (96%)	557 (95%)	29 (5%)	2 (0%)	36	65
1	B	590/612 (96%)	564 (96%)	24 (4%)	2 (0%)	36	65
1	C	589/612 (96%)	554 (94%)	34 (6%)	1 (0%)	43	72
1	D	589/612 (96%)	563 (96%)	25 (4%)	1 (0%)	43	72
1	E	589/612 (96%)	545 (92%)	42 (7%)	2 (0%)	36	65
All	All	2945/3060 (96%)	2783 (94%)	154 (5%)	8 (0%)	36	65

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	ILE
1	E	44	GLN
1	D	439	PRO
1	B	276	ILE
1	B	439	PRO
1	A	439	PRO
1	C	515	VAL
1	E	276	ILE

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	484/504 (96%)	474 (98%)	10 (2%)	47 77
1	B	481/504 (95%)	472 (98%)	9 (2%)	50 79
1	C	478/504 (95%)	471 (98%)	7 (2%)	57 84
1	D	479/504 (95%)	476 (99%)	3 (1%)	78 93
1	E	481/504 (95%)	473 (98%)	8 (2%)	53 82
All	All	2403/2520 (95%)	2366 (98%)	37 (2%)	57 84

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	34	ARG
1	A	49	VAL
1	A	271	LEU
1	A	383	LEU
1	A	385	THR
1	A	419	LEU
1	A	440	HIS
1	A	466	VAL
1	A	576	SER

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Mol	Chain	Res	Type
1	B	56	LEU
1	B	78	ILE
1	B	275	SER
1	B	306	SER
1	B	383	LEU
1	B	466	VAL
1	B	492	LEU
1	B	512	THR
1	B	539	LEU
1	C	2	SER
1	C	37	THR
1	C	57	THR
1	C	325	ASP
1	C	336	SER
1	C	429	SER
1	C	586	ARG
1	D	202	ASP
1	D	326	ASN
1	D	493	SER
1	E	35	LEU
1	E	36	PHE
1	E	163	LEU
1	E	344	VAL
1	E	415	LEU
1	E	466	VAL
1	E	493	SER
1	E	584	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	258	GLN
1	A	273	GLN
1	A	317	ASN
1	B	143	GLN
1	B	209	GLN
1	B	258	GLN
1	B	273	GLN
1	C	143	GLN
1	C	258	GLN
1	C	273	GLN

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Mol	Chain	Res	Type
1	C	326	ASN
1	D	100	HIS
1	D	160	ASN
1	D	284	HIS
1	D	454	GLN
1	E	100	HIS
1	E	131	GLN
1	E	143	GLN
1	E	160	ASN
1	E	209	GLN
1	E	258	GLN
1	E	284	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 42 ligands modelled in this entry, 10 are monoatomic - leaving 32 for Mogul analysis.

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	$\#\|Z\| > 2$
4	AMP	C	604	6	25,25,25	1.44	4 (16%)	37,38,38	2.14	7 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	E	601	-	5,5,5	1.70	2 (40%)	5,5,5	0.96	0
5	SO4	E	606	-	4,4,4	0.44	0	6,6,6	0.35	0
5	SO4	D	605	-	4,4,4	0.49	0	6,6,6	0.35	0
4	AMP	B	607	6	25,25,25	1.38	3 (12%)	37,38,38	2.16	7 (18%)
5	SO4	D	607	-	4,4,4	0.30	0	6,6,6	0.13	0
3	PPV	C	603	6	6,8,8	0.81	0	12,13,13	0.82	0
2	GOL	C	602	-	5,5,5	0.93	0	5,5,5	0.95	0
4	AMP	D	604	6	25,25,25	1.36	3 (12%)	37,38,38	1.93	7 (18%)
2	GOL	B	602	-	5,5,5	1.82	1 (20%)	5,5,5	0.94	0
2	GOL	B	604	-	5,5,5	1.60	2 (40%)	5,5,5	1.05	0
4	AMP	A	604	6	25,25,25	1.32	3 (12%)	37,38,38	2.05	11 (29%)
2	GOL	D	602	-	5,5,5	1.11	0	5,5,5	1.32	1 (20%)
3	PPV	B	606	6	6,8,8	1.21	0	12,13,13	0.86	0
2	GOL	D	601	-	5,5,5	0.88	0	5,5,5	1.20	1 (20%)
2	GOL	B	601	-	5,5,5	1.94	2 (40%)	5,5,5	1.16	0
2	GOL	C	601	-	5,5,5	1.01	0	5,5,5	1.13	1 (20%)
2	GOL	A	601	-	5,5,5	1.35	1 (20%)	5,5,5	0.84	0
5	SO4	A	605	-	4,4,4	0.50	0	6,6,6	0.52	0
5	SO4	B	608	-	4,4,4	0.39	0	6,6,6	0.63	0
2	GOL	B	605	-	5,5,5	1.22	1 (20%)	5,5,5	0.87	0
2	GOL	E	602	-	5,5,5	0.92	0	5,5,5	1.34	1 (20%)
5	SO4	B	610	-	4,4,4	0.50	0	6,6,6	0.52	0
3	PPV	E	604	6	6,8,8	0.73	0	12,13,13	0.79	0
5	SO4	D	606	-	4,4,4	0.38	0	6,6,6	0.11	0
3	PPV	A	603	6	6,8,8	0.82	0	12,13,13	0.69	0
4	AMP	E	605	6	25,25,25	1.53	4 (16%)	37,38,38	2.09	9 (24%)
5	SO4	B	609	-	4,4,4	0.50	0	6,6,6	0.55	0
2	GOL	B	603	-	5,5,5	1.26	1 (20%)	5,5,5	1.16	0
2	GOL	E	603	-	5,5,5	1.36	1 (20%)	5,5,5	0.80	0
2	GOL	A	602	-	5,5,5	0.69	0	5,5,5	1.33	0
3	PPV	D	603	6	6,8,8	0.80	0	12,13,13	0.78	0

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
4	AMP	C	604	6	-	3/10/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	E	601	-	-	2/4/4/4	-
4	AMP	B	607	6	-	3/10/26/26	0/3/3/3
3	PPV	C	603	6	-	0/6/6/6	-
2	GOL	C	602	-	-	2/4/4/4	-
4	AMP	D	604	6	-	4/10/26/26	0/3/3/3
2	GOL	B	602	-	-	0/4/4/4	-
2	GOL	B	604	-	-	2/4/4/4	-
4	AMP	A	604	6	-	3/10/26/26	0/3/3/3
2	GOL	D	602	-	-	1/4/4/4	-
3	PPV	B	606	6	-	0/6/6/6	-
2	GOL	D	601	-	-	2/4/4/4	-
2	GOL	B	601	-	-	0/4/4/4	-
2	GOL	C	601	-	-	0/4/4/4	-
2	GOL	A	601	-	-	4/4/4/4	-
2	GOL	B	605	-	-	4/4/4/4	-
2	GOL	E	602	-	-	2/4/4/4	-
3	PPV	E	604	6	-	0/6/6/6	-
3	PPV	A	603	6	-	0/6/6/6	-
4	AMP	E	605	6	-	5/10/26/26	0/3/3/3
2	GOL	B	603	-	-	2/4/4/4	-
2	GOL	E	603	-	-	0/4/4/4	-
2	GOL	A	602	-	-	2/4/4/4	-
3	PPV	D	603	6	-	0/6/6/6	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	605	AMP	C5-C4	5.58	1.49	1.39
4	C	604	AMP	C5-C4	4.83	1.47	1.39
4	A	604	AMP	C5-C4	4.68	1.47	1.39
4	D	604	AMP	C5-C4	4.58	1.47	1.39
4	B	607	AMP	C5-C4	4.33	1.46	1.39
2	B	601	GOL	C3-C2	3.67	1.65	1.51
2	B	602	GOL	C3-C2	3.33	1.64	1.51
4	B	607	AMP	C5-C6	3.28	1.50	1.41
4	C	604	AMP	C5-C6	3.02	1.49	1.41
2	E	601	GOL	C3-C2	2.75	1.62	1.51
2	B	604	GOL	C3-C2	2.67	1.62	1.51
4	A	604	AMP	C5-C6	2.61	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	604	AMP	C5-C6	2.60	1.48	1.41
2	E	601	GOL	C1-C2	2.59	1.61	1.51
2	B	603	GOL	C1-C2	2.57	1.61	1.51
4	E	605	AMP	C5-C6	2.56	1.48	1.41
4	E	605	AMP	C8-N7	2.46	1.36	1.31
4	D	604	AMP	C5-N7	-2.42	1.34	1.39
4	C	604	AMP	C8-N7	2.33	1.36	1.31
2	A	601	GOL	C3-C2	2.30	1.60	1.51
4	B	607	AMP	C5-N7	-2.28	1.34	1.39
2	B	601	GOL	C1-C2	2.26	1.60	1.51
2	B	604	GOL	C1-C2	2.22	1.60	1.51
4	C	604	AMP	C5-N7	-2.13	1.35	1.39
4	A	604	AMP	C5-N7	-2.10	1.35	1.39
4	E	605	AMP	C5-N7	-2.03	1.35	1.39
2	B	605	GOL	C1-C2	2.03	1.59	1.51
2	E	603	GOL	C3-C2	2.01	1.59	1.51

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	604	AMP	C5-C4-N3	-7.15	116.88	126.72
4	B	607	AMP	C5-C4-N3	-6.96	117.13	126.72
4	E	605	AMP	C5-C4-N3	-6.81	117.34	126.72
4	D	604	AMP	C5-C4-N3	-6.60	117.63	126.72
4	E	605	AMP	N3-C4-N9	5.69	136.84	127.17
4	C	604	AMP	N3-C4-N9	5.58	136.66	127.17
4	A	604	AMP	C5-C4-N3	-5.55	119.08	126.72
4	B	607	AMP	N3-C4-N9	5.42	136.38	127.17
4	A	604	AMP	N3-C4-N9	5.15	135.93	127.17
4	D	604	AMP	N3-C4-N9	5.14	135.91	127.17
4	B	607	AMP	C2-N3-C4	4.38	122.52	111.83
4	C	604	AMP	C2-N3-C4	4.16	121.99	111.83
4	E	605	AMP	C2-N3-C4	4.00	121.61	111.83
4	D	604	AMP	C2-N3-C4	3.87	121.29	111.83
4	B	607	AMP	C4-C5-N7	-3.77	106.27	110.58
4	A	604	AMP	C2-N3-C4	3.55	120.50	111.83
4	A	604	AMP	O5'-P-O1P	-3.55	96.86	106.44
4	E	605	AMP	N3-C2-N1	-3.52	123.26	128.58
4	C	604	AMP	C4-C5-N7	-3.46	106.62	110.58
4	B	607	AMP	N3-C2-N1	-3.44	123.38	128.58
4	A	604	AMP	N3-C2-N1	-3.26	123.65	128.58
4	B	607	AMP	O5'-P-O1P	-3.17	97.88	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	604	AMP	O3P-P-O5'	-3.16	98.43	106.67
4	A	604	AMP	C4-N9-C8	3.02	108.90	105.74
4	C	604	AMP	N3-C2-N1	-2.96	124.10	128.58
4	B	607	AMP	C5-N7-C8	2.96	108.10	103.45
4	D	604	AMP	C4-C5-N7	-2.96	107.20	110.58
4	D	604	AMP	N3-C2-N1	-2.80	124.34	128.58
4	E	605	AMP	C4-C5-N7	-2.73	107.46	110.58
4	E	605	AMP	O5'-P-O1P	-2.67	99.23	106.44
4	A	604	AMP	C4-C5-N7	-2.64	107.56	110.58
4	C	604	AMP	C5-N7-C8	2.53	107.43	103.45
4	A	604	AMP	O3P-P-O2P	2.47	117.07	107.80
4	A	604	AMP	O2P-P-O5'	-2.43	100.32	106.67
4	A	604	AMP	C5-N7-C8	2.37	107.17	103.45
4	E	605	AMP	N6-C6-N1	2.36	123.64	118.38
4	E	605	AMP	O3P-P-O2P	2.23	116.16	107.80
2	D	602	GOL	C3-C2-C1	-2.16	103.86	111.80
2	E	602	GOL	C3-C2-C1	-2.11	104.07	111.80
4	E	605	AMP	C2-N1-C6	2.09	122.16	118.73
4	D	604	AMP	C5-N7-C8	2.06	106.69	103.45
4	A	604	AMP	C2-N1-C6	2.03	122.07	118.73
4	D	604	AMP	O5'-P-O1P	-2.03	100.97	106.44
2	D	601	GOL	C3-C2-C1	-2.02	104.38	111.80
2	C	601	GOL	C3-C2-C1	-2.00	104.45	111.80

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	O1-C1-C2-C3
2	A	601	GOL	C1-C2-C3-O3
2	A	602	GOL	O1-C1-C2-O2
2	A	602	GOL	O1-C1-C2-C3
2	B	603	GOL	C1-C2-C3-O3
2	B	604	GOL	O1-C1-C2-O2
2	B	604	GOL	O1-C1-C2-C3
2	B	605	GOL	C1-C2-C3-O3
2	E	601	GOL	C1-C2-C3-O3
2	E	602	GOL	O1-C1-C2-C3
4	B	607	AMP	C5'-O5'-P-O1P
4	B	607	AMP	C5'-O5'-P-O2P
4	B	607	AMP	C5'-O5'-P-O3P
4	C	604	AMP	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
4	C	604	AMP	C5'-O5'-P-O3P
4	D	604	AMP	C5'-O5'-P-O1P
4	D	604	AMP	C5'-O5'-P-O2P
4	D	604	AMP	C5'-O5'-P-O3P
4	E	605	AMP	C5'-O5'-P-O2P
4	E	605	AMP	C5'-O5'-P-O3P
2	B	605	GOL	O1-C1-C2-C3
2	D	601	GOL	O1-C1-C2-C3
2	A	601	GOL	O1-C1-C2-O2
2	B	605	GOL	O2-C2-C3-O3
2	E	601	GOL	O2-C2-C3-O3
2	E	602	GOL	O1-C1-C2-O2
2	A	601	GOL	O2-C2-C3-O3
2	B	603	GOL	O2-C2-C3-O3
2	B	605	GOL	O1-C1-C2-O2
2	D	601	GOL	O1-C1-C2-O2
4	C	604	AMP	C5'-O5'-P-O1P
4	E	605	AMP	C5'-O5'-P-O1P
2	D	602	GOL	O2-C2-C3-O3
2	C	602	GOL	C1-C2-C3-O3
2	C	602	GOL	O2-C2-C3-O3
4	A	604	AMP	O4'-C4'-C5'-O5'
4	E	605	AMP	O4'-C4'-C5'-O5'
4	A	604	AMP	C5'-O5'-P-O3P
4	E	605	AMP	O4'-C1'-N9-C8
4	D	604	AMP	O4'-C4'-C5'-O5'
4	A	604	AMP	C3'-C4'-C5'-O5'

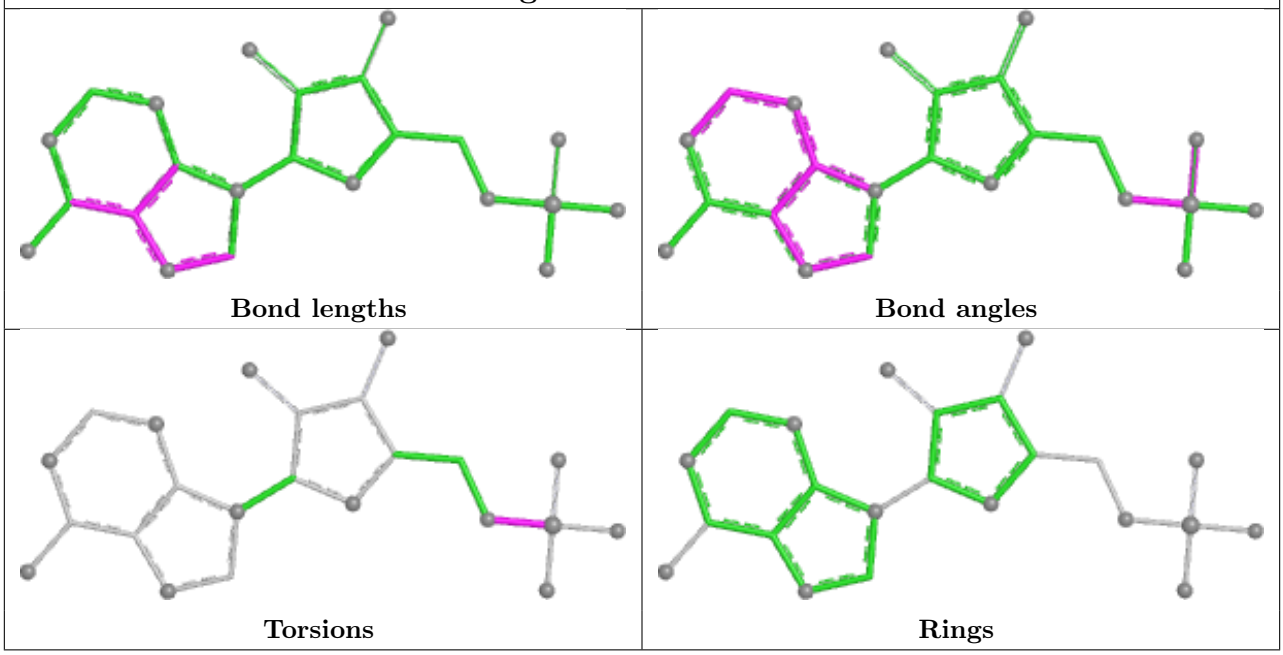
There are no ring outliers.

9 monomers are involved in 13 short contacts:

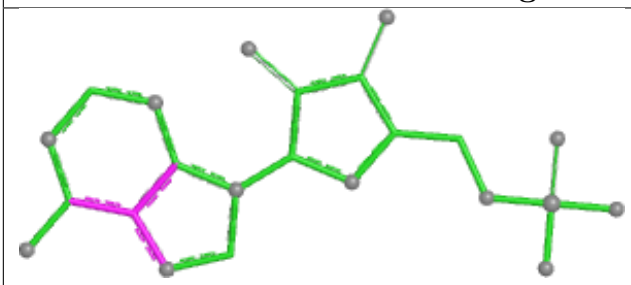
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	604	AMP	1	0
3	C	603	PPV	1	0
4	A	604	AMP	1	0
2	D	602	GOL	2	0
2	D	601	GOL	1	0
5	B	608	SO4	1	0
3	E	604	PPV	2	0
3	A	603	PPV	1	0
2	E	603	GOL	3	0

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.

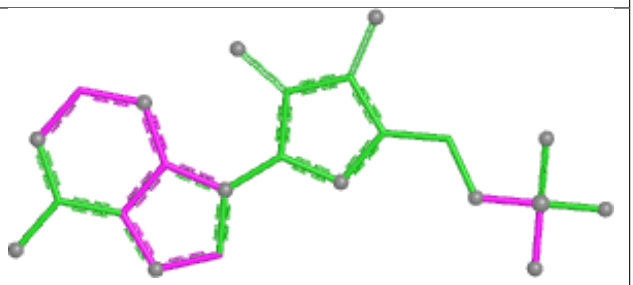
Ligand AMP C 604



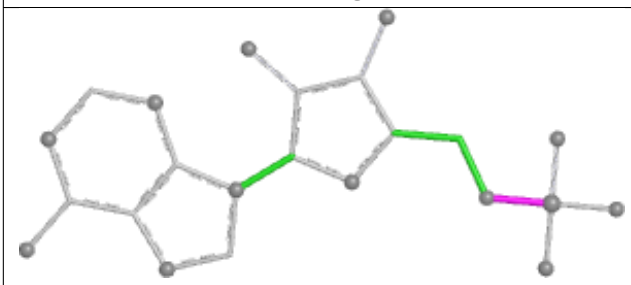
Ligand AMP B 607



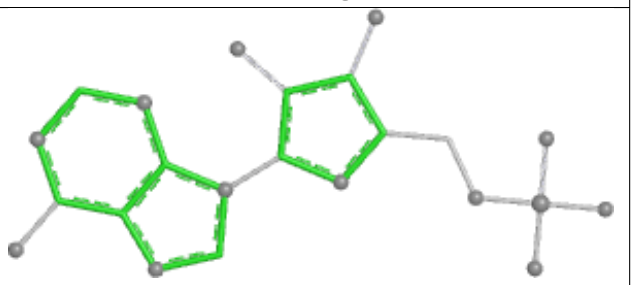
Bond lengths



Bond angles

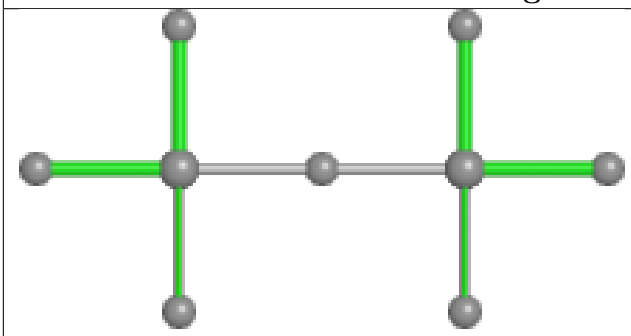


Torsions

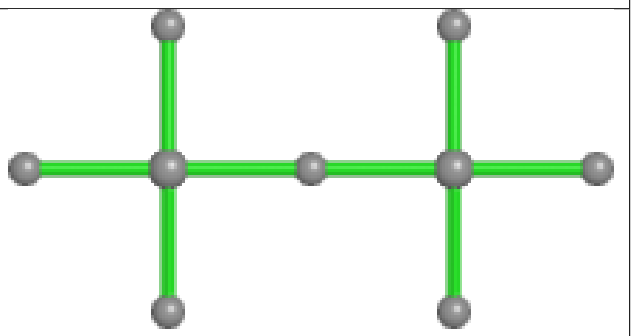


Rings

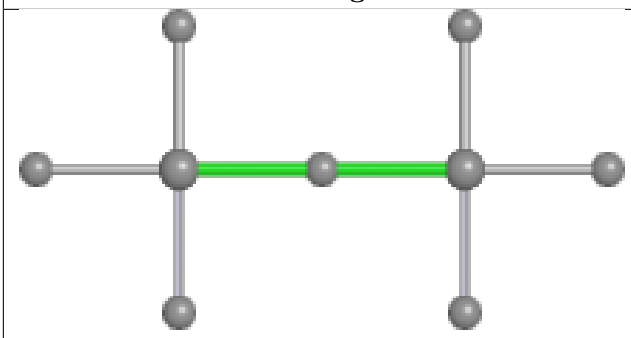
Ligand PPV C 603



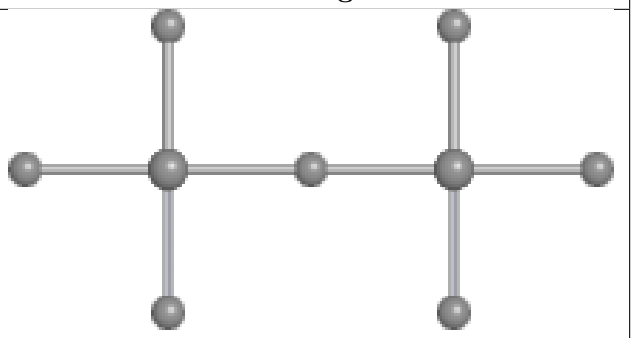
Bond lengths



Bond angles

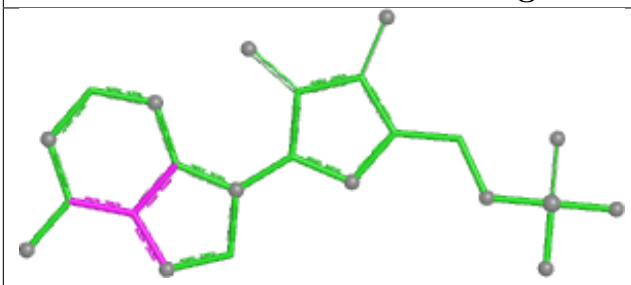


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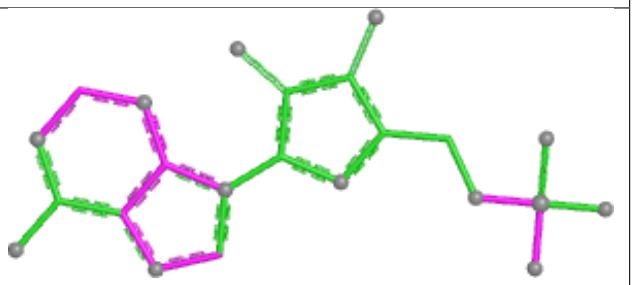


Rings

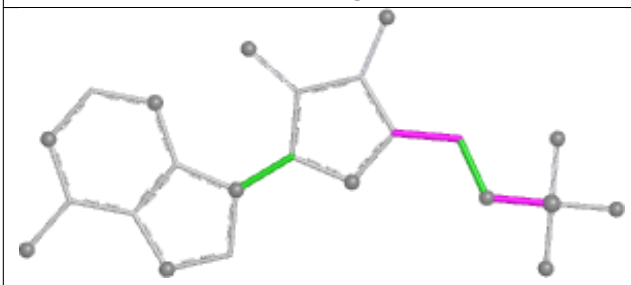
Ligand AMP D 604



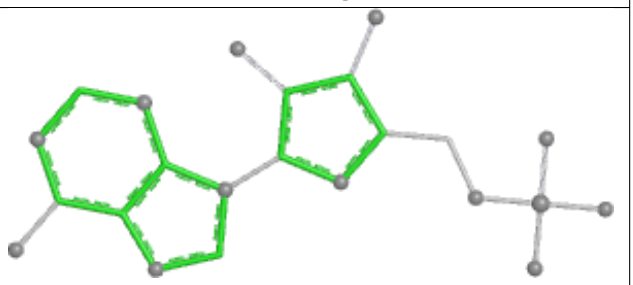
Bond lengths



Bond angles

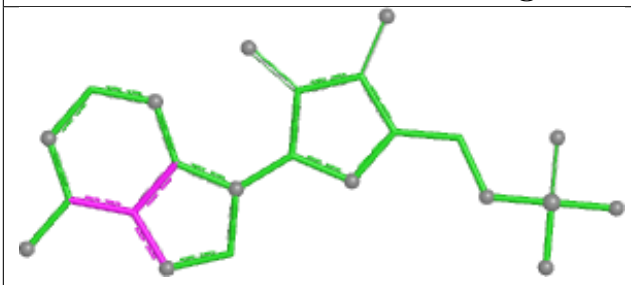


Torsions

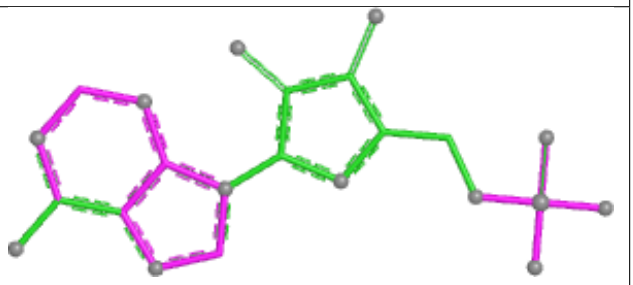


Rings

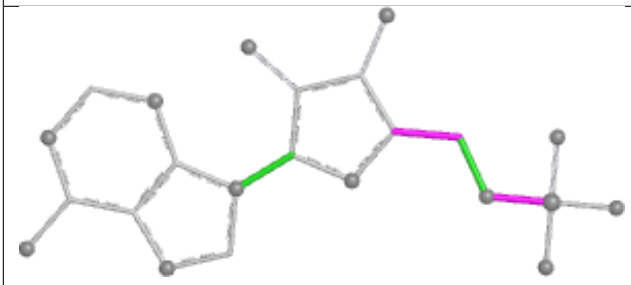
Ligand AMP A 604



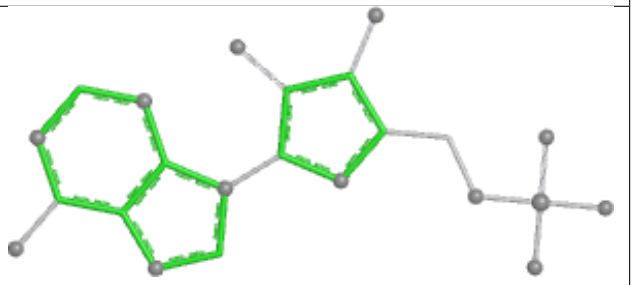
Bond lengths



Bond angles

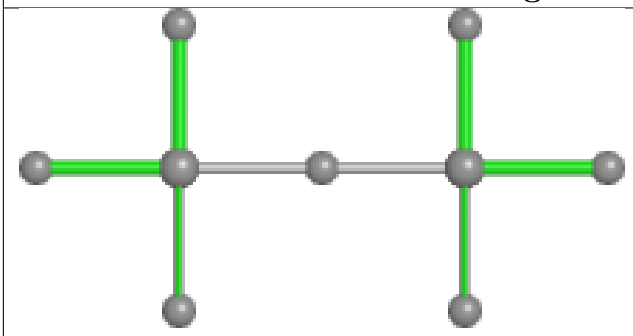


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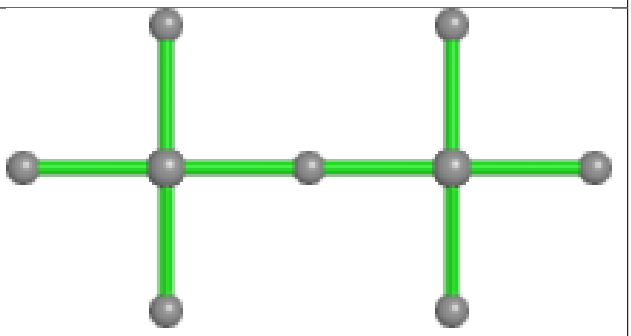


Rings

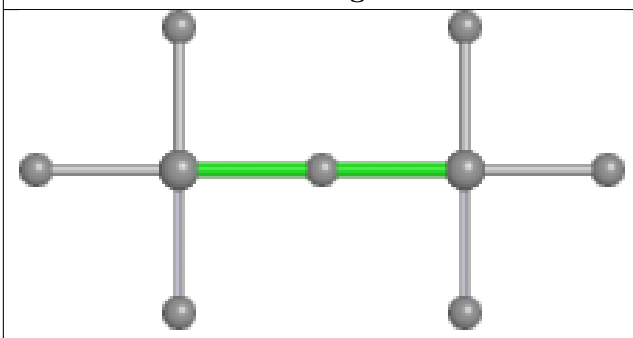
Ligand PPV B 606



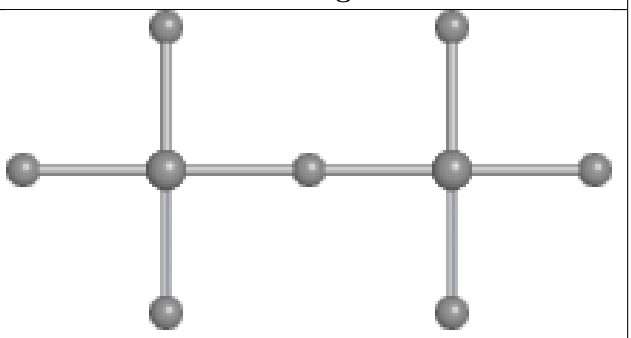
Bond lengths



Bond angles

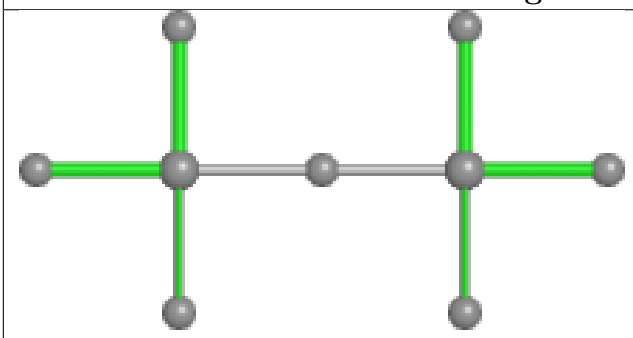


Torsions

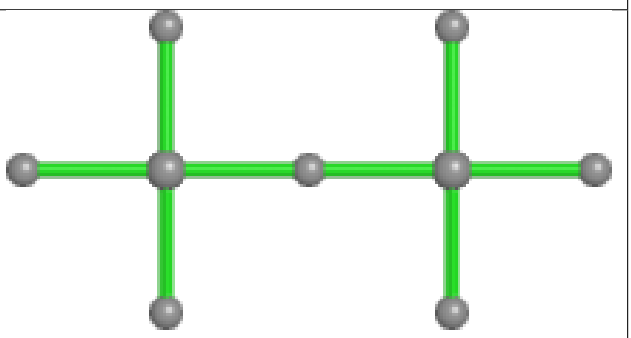


Rings

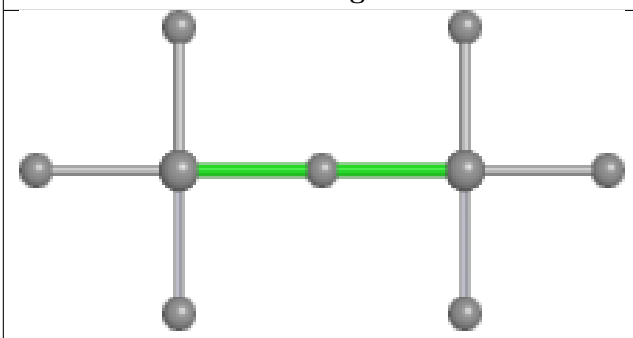
Ligand PPV E 604



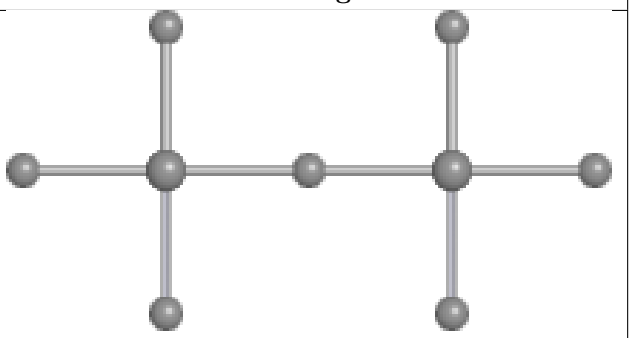
Bond lengths



Bond angles

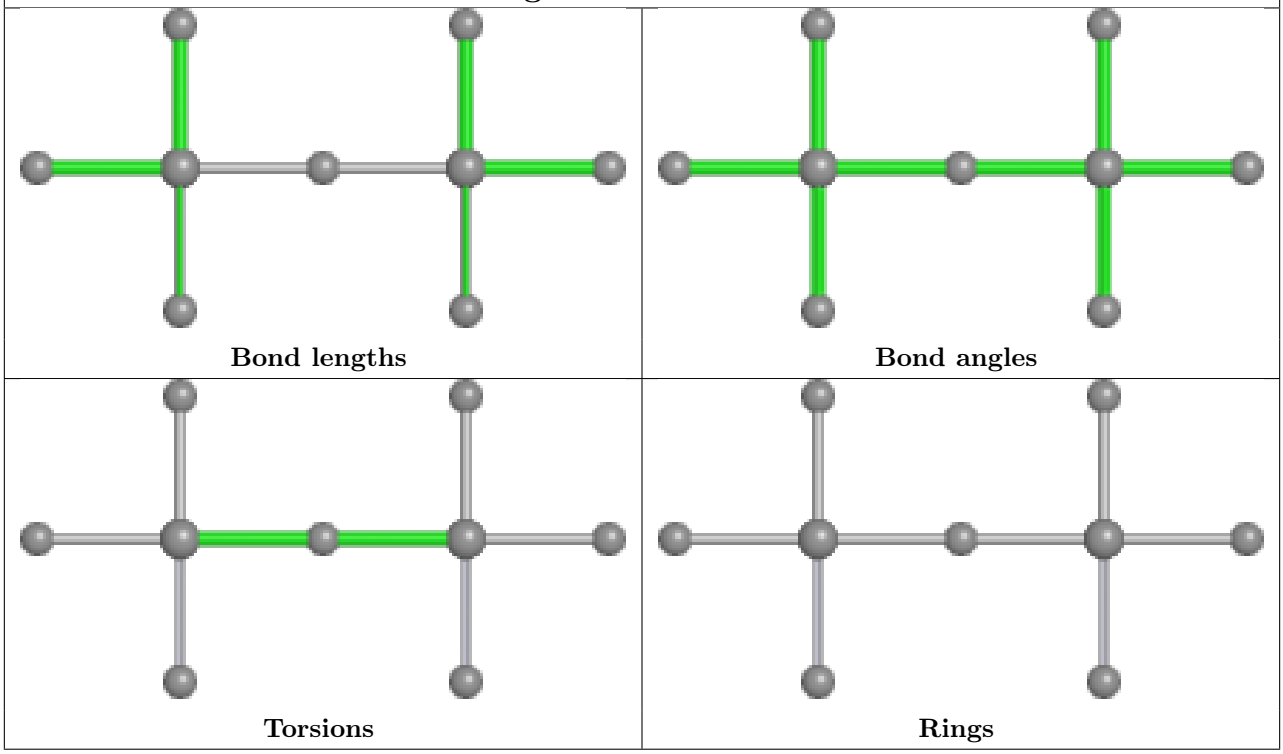


Torsions

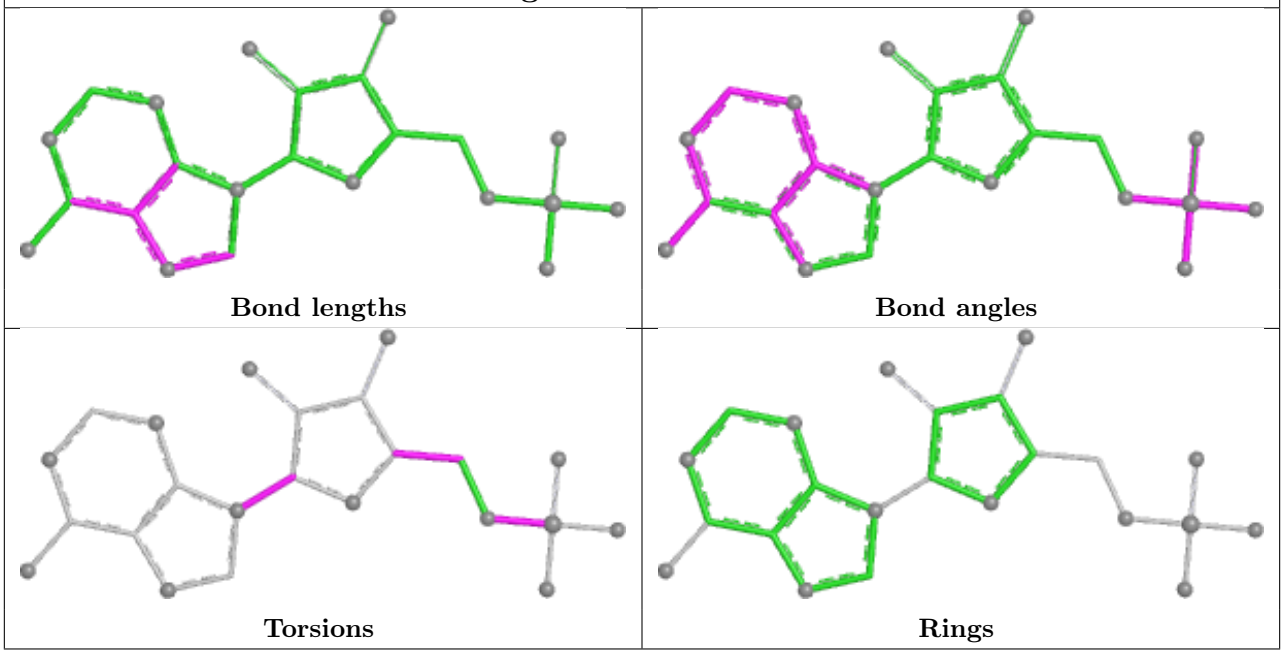


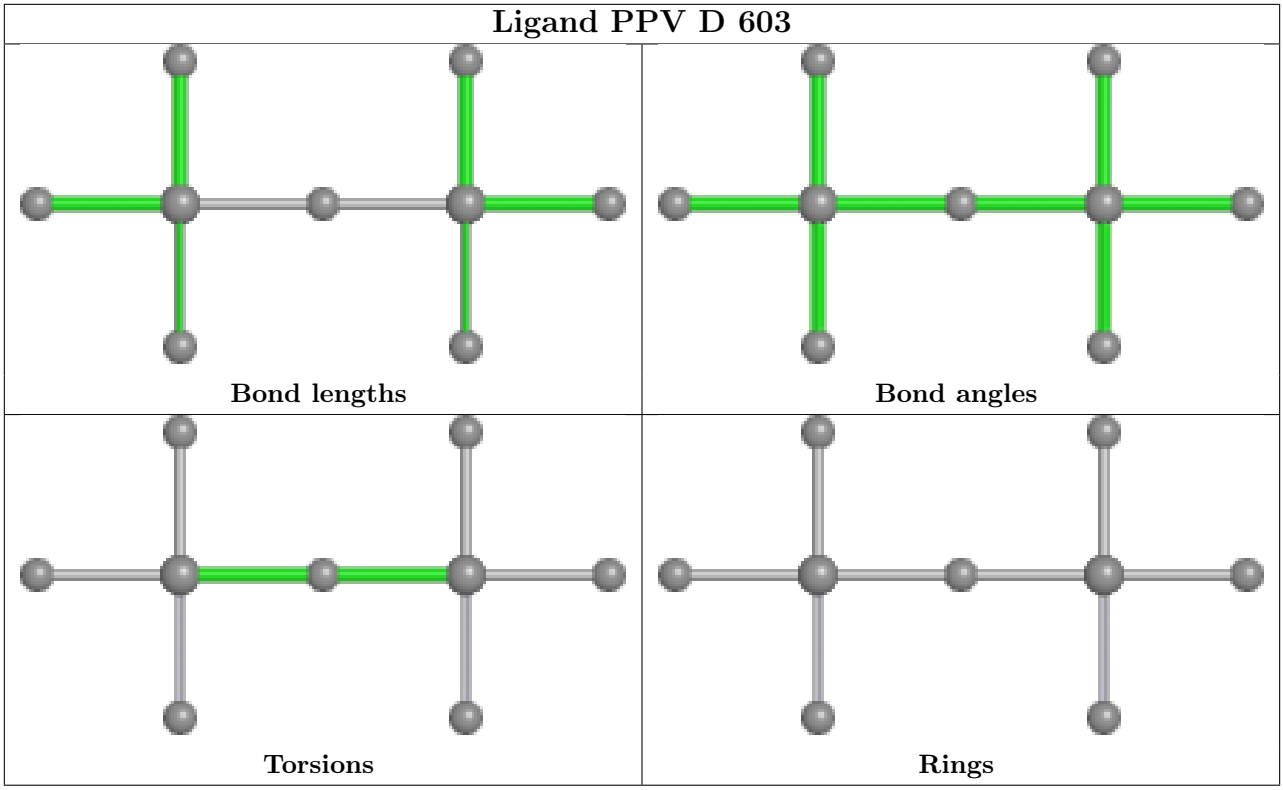
Rings

Ligand PPV A 603



Ligand AMP E 605





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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	590/612 (96%)	-0.28	5 (0%)	82	77	52, 76, 116, 180	0
1	B	592/612 (96%)	-0.40	4 (0%)	84	79	50, 68, 100, 147	0
1	C	591/612 (96%)	-0.06	9 (1%)	72	64	60, 92, 137, 153	0
1	D	591/612 (96%)	-0.31	6 (1%)	79	73	60, 75, 103, 150	0
1	E	591/612 (96%)	0.11	10 (1%)	69	61	59, 99, 141, 171	0
All	All	2955/3060 (96%)	-0.19	34 (1%)	76	69	50, 79, 130, 180	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	GLY	4.4
1	D	358	TYR	3.7
1	B	42	ASP	3.4
1	C	45	ASP	3.3
1	A	358	TYR	3.3
1	A	590	ALA	3.3
1	E	42	ASP	3.2
1	D	572	LEU	3.2
1	E	573	ALA	3.0
1	D	45	ASP	3.0
1	E	591	GLY	2.9
1	A	1	MET	2.9
1	C	358	TYR	2.9
1	E	436	ALA	2.7
1	D	477	GLU	2.7
1	C	1	MET	2.7
1	C	572	LEU	2.7
1	E	493	SER	2.6
1	B	1	MET	2.5
1	E	43	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	582	VAL	2.4
1	B	572	LEU	2.3
1	C	42	ASP	2.3
1	C	576	SER	2.3
1	A	572	LEU	2.3
1	C	556	SER	2.3
1	D	2	SER	2.3
1	B	84	GLY	2.2
1	E	1	MET	2.1
1	E	133	THR	2.1
1	D	573	ALA	2.1
1	E	72	GLN	2.1
1	E	64	VAL	2.0
1	C	328	PRO	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, 95^{th} 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
5	SO4	D	606	5/5	0.66	0.14	112,116,121,134	0
2	GOL	E	601	6/6	0.81	0.17	81,83,87,89	0
2	GOL	B	605	6/6	0.81	0.20	82,89,91,92	0
5	SO4	D	607	5/5	0.81	0.18	112,112,123,129	0
2	GOL	B	604	6/6	0.82	0.21	81,85,89,91	0
2	GOL	B	602	6/6	0.84	0.13	72,77,81,82	0
2	GOL	A	601	6/6	0.85	0.14	61,74,79,80	0
5	SO4	A	605	5/5	0.86	0.28	90,90,95,105	0
5	SO4	B	610	5/5	0.86	0.24	91,95,100,114	0

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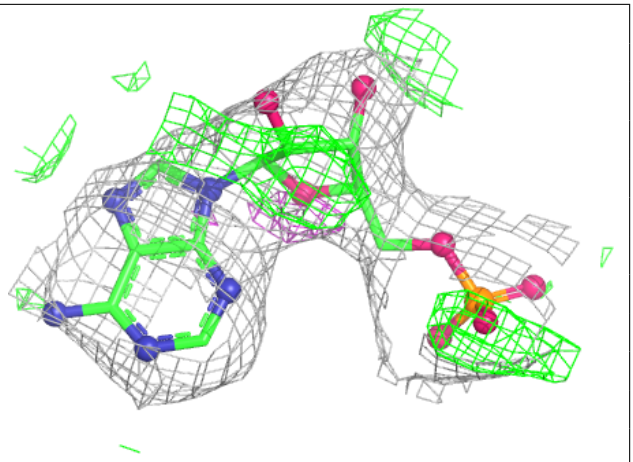
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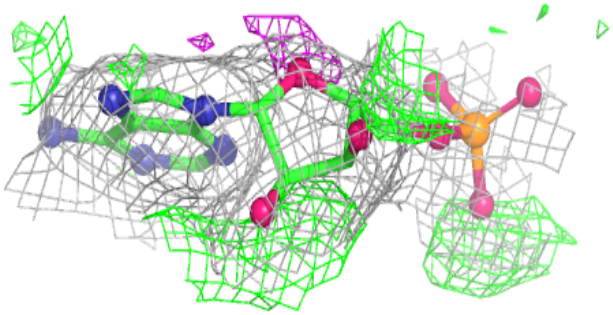
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	B	609	5/5	0.87	0.24	79,84,88,106	0
4	AMP	E	605	23/23	0.87	0.12	84,92,96,99	0
5	SO4	D	605	5/5	0.88	0.28	101,104,104,116	0
2	GOL	D	602	6/6	0.89	0.15	77,80,81,82	0
2	GOL	B	601	6/6	0.90	0.14	64,68,74,76	0
2	GOL	C	601	6/6	0.90	0.13	66,71,78,78	0
5	SO4	B	608	5/5	0.90	0.21	77,79,102,105	0
2	GOL	E	603	6/6	0.90	0.15	84,91,93,94	0
2	GOL	D	601	6/6	0.91	0.15	64,70,76,77	0
2	GOL	B	603	6/6	0.91	0.16	68,72,75,79	0
2	GOL	A	602	6/6	0.91	0.14	71,72,75,79	0
5	SO4	E	606	5/5	0.91	0.23	103,104,106,123	0
4	AMP	A	604	23/23	0.93	0.09	64,74,77,77	0
4	AMP	C	604	23/23	0.94	0.08	77,81,86,89	0
2	GOL	C	602	6/6	0.94	0.16	81,82,87,88	0
3	PPV	E	604	9/9	0.95	0.06	84,90,93,93	0
2	GOL	E	602	6/6	0.95	0.11	77,79,81,87	0
6	MG	B	611	1/1	0.95	0.14	61,61,61,61	0
4	AMP	B	607	23/23	0.96	0.07	61,65,69,70	0
4	AMP	D	604	23/23	0.96	0.08	66,70,75,78	0
3	PPV	B	606	9/9	0.97	0.05	56,62,68,86	0
6	MG	A	606	1/1	0.97	0.15	54,54,54,54	0
3	PPV	A	603	9/9	0.97	0.06	60,67,75,84	0
6	MG	C	606	1/1	0.97	0.11	71,71,71,71	0
6	MG	D	608	1/1	0.97	0.10	62,62,62,62	0
3	PPV	D	603	9/9	0.98	0.05	63,67,70,73	0
3	PPV	C	603	9/9	0.98	0.04	70,79,80,82	0
6	MG	A	607	1/1	0.98	0.06	61,61,61,61	0
6	MG	C	605	1/1	0.99	0.02	79,79,79,79	0
6	MG	D	609	1/1	0.99	0.03	61,61,61,61	0
6	MG	E	607	1/1	0.99	0.09	77,77,77,77	0
6	MG	E	608	1/1	0.99	0.08	85,85,85,85	0
6	MG	B	612	1/1	1.00	0.02	65,65,65,65	0

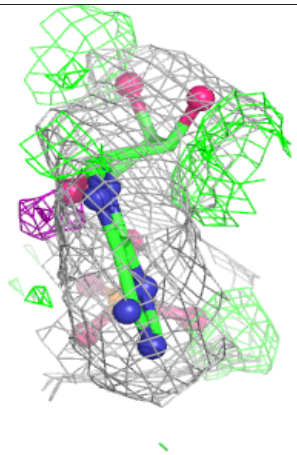
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP E 605:

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

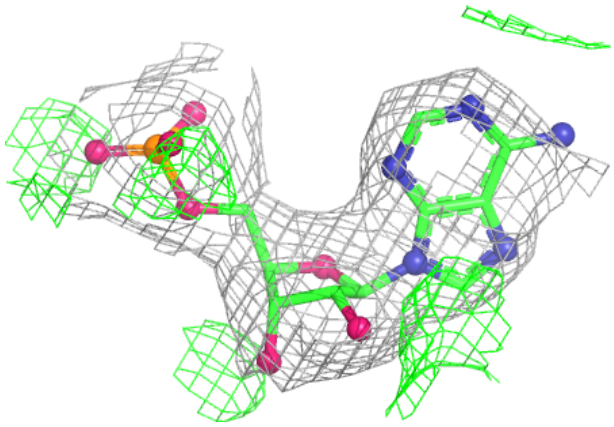


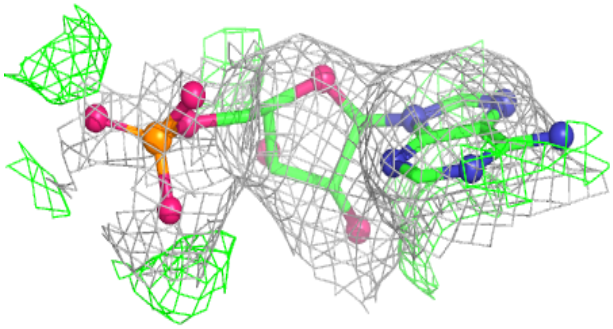


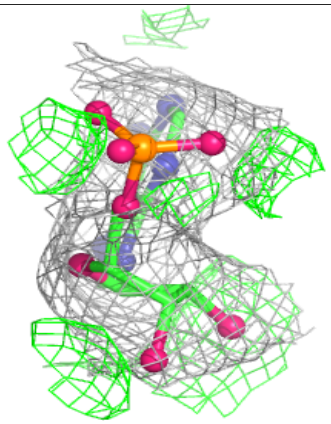


Electron density around AMP A 604:

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

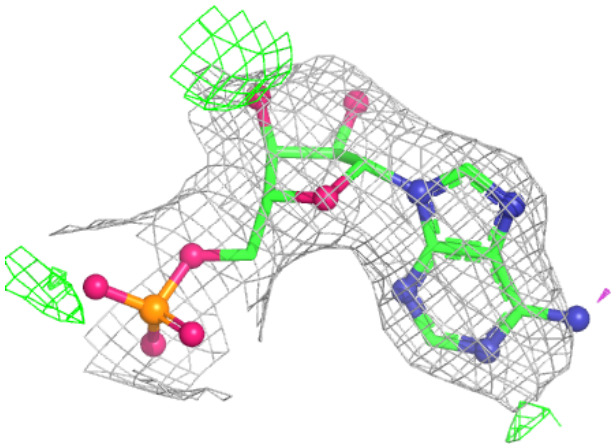


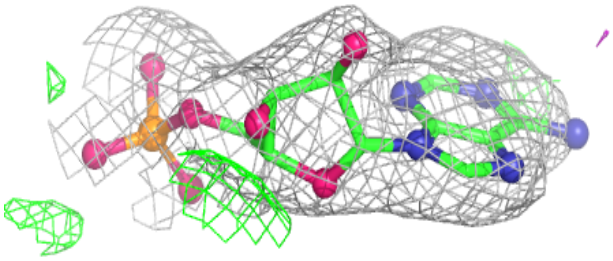


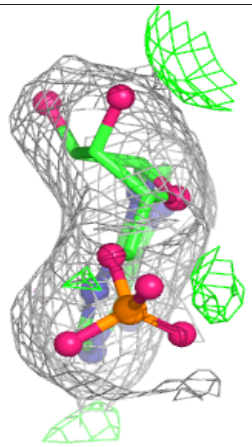


Electron density around AMP C 604:

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

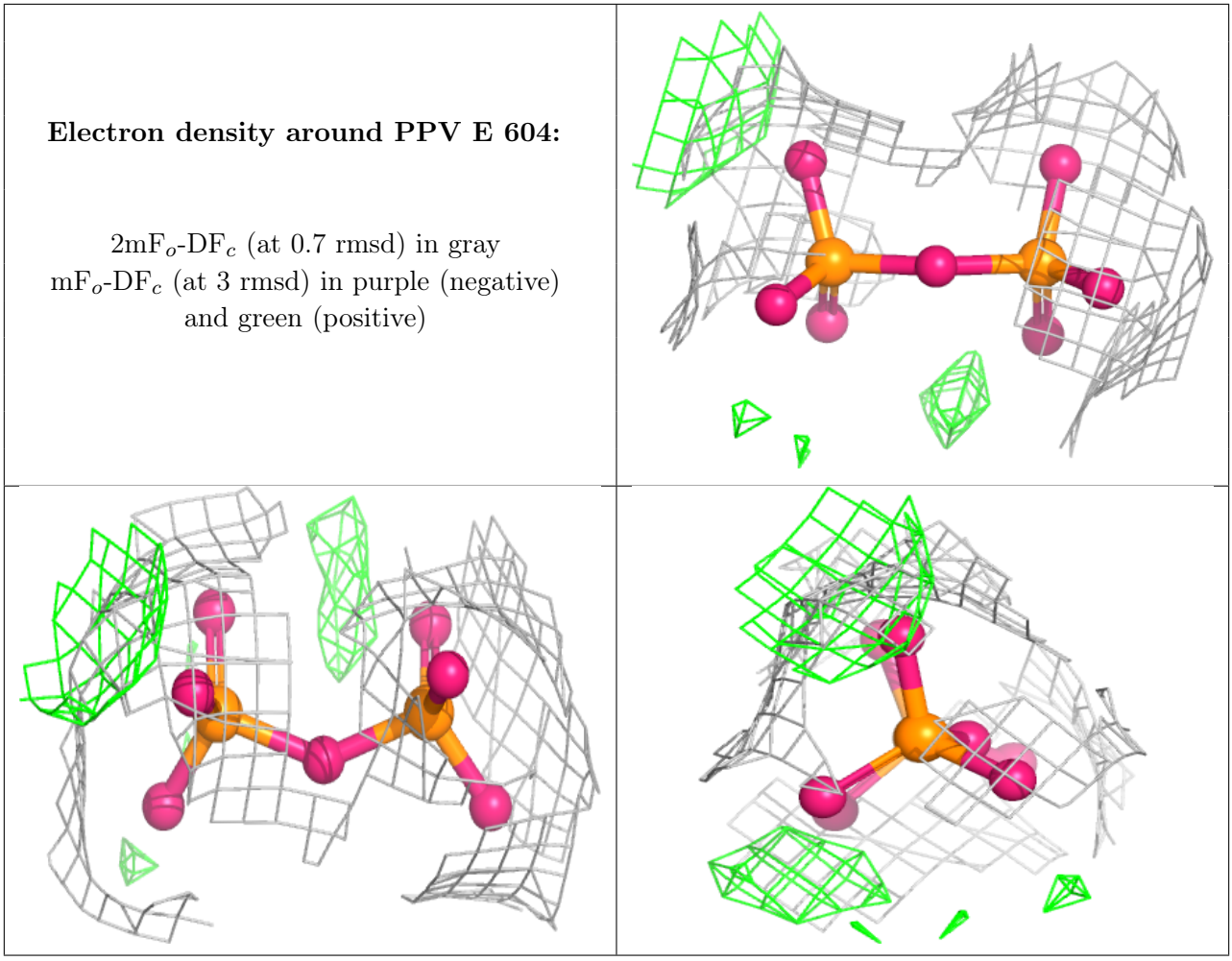






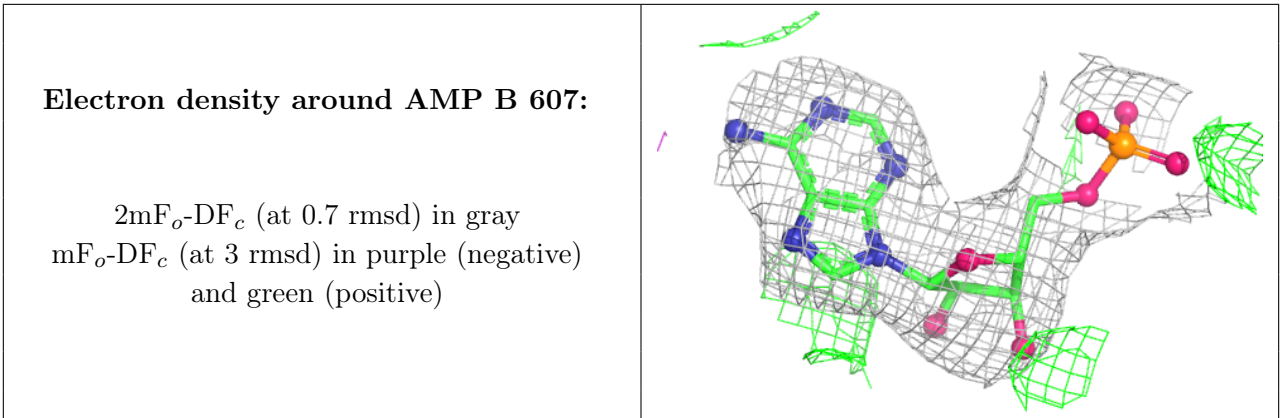
Electron density around PPV E 604:

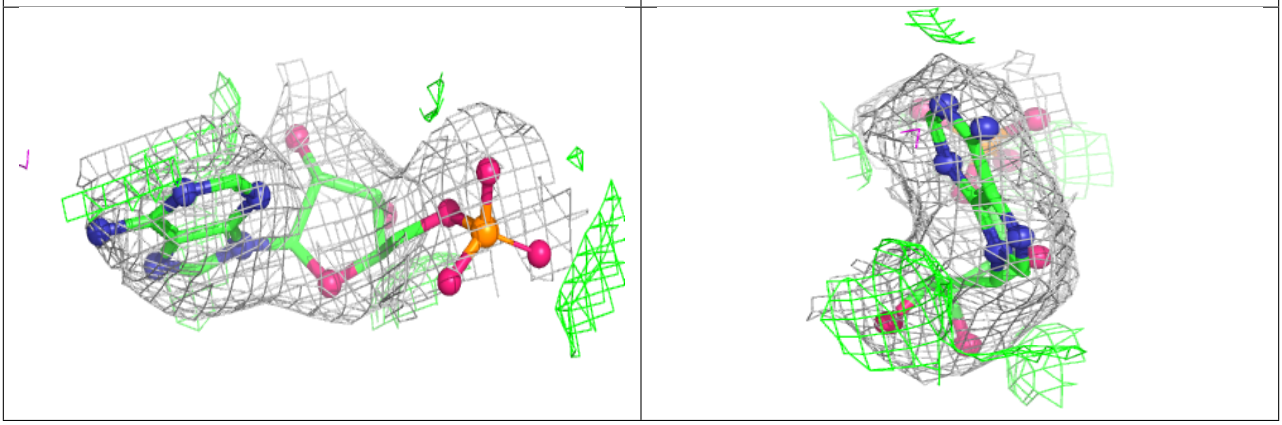
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around AMP B 607:

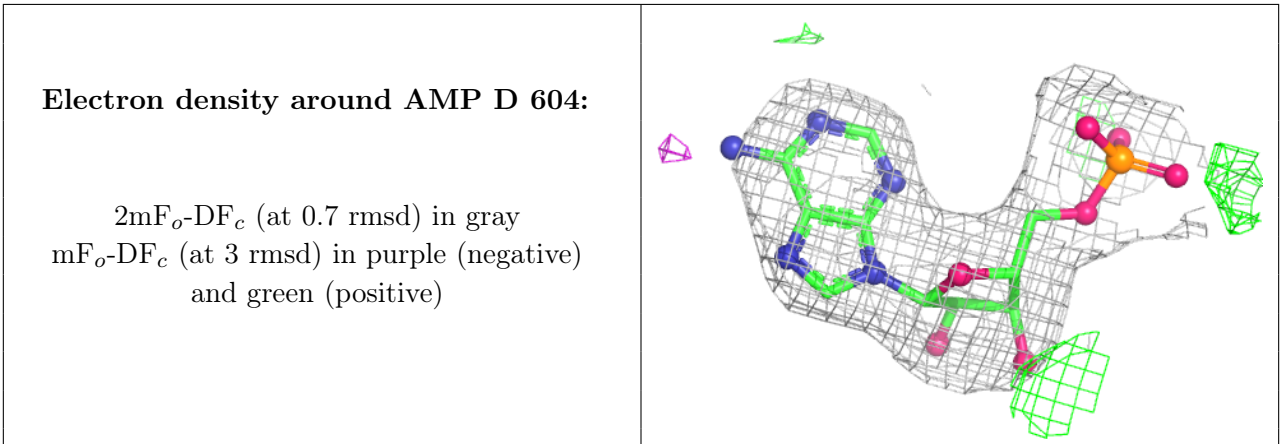
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

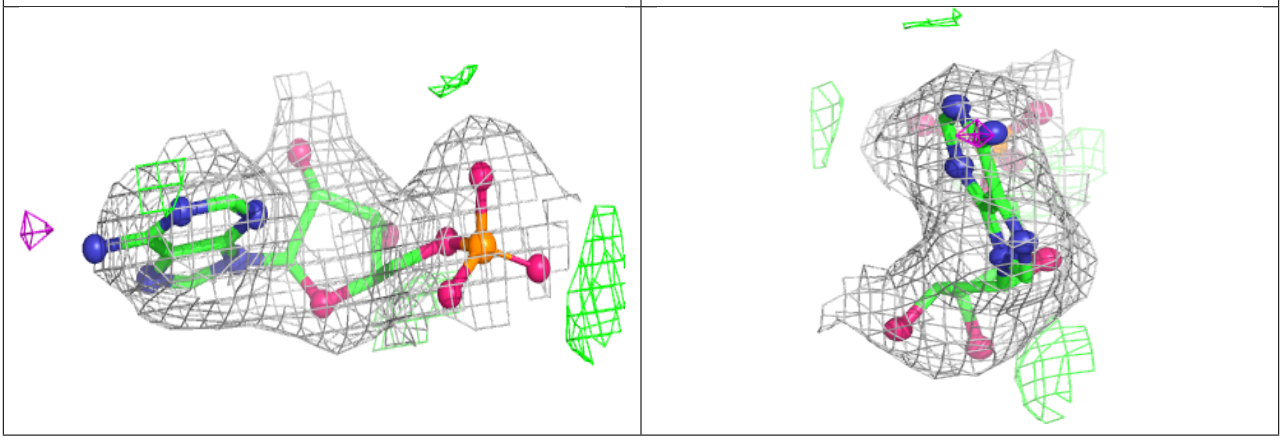




Electron density around AMP D 604:

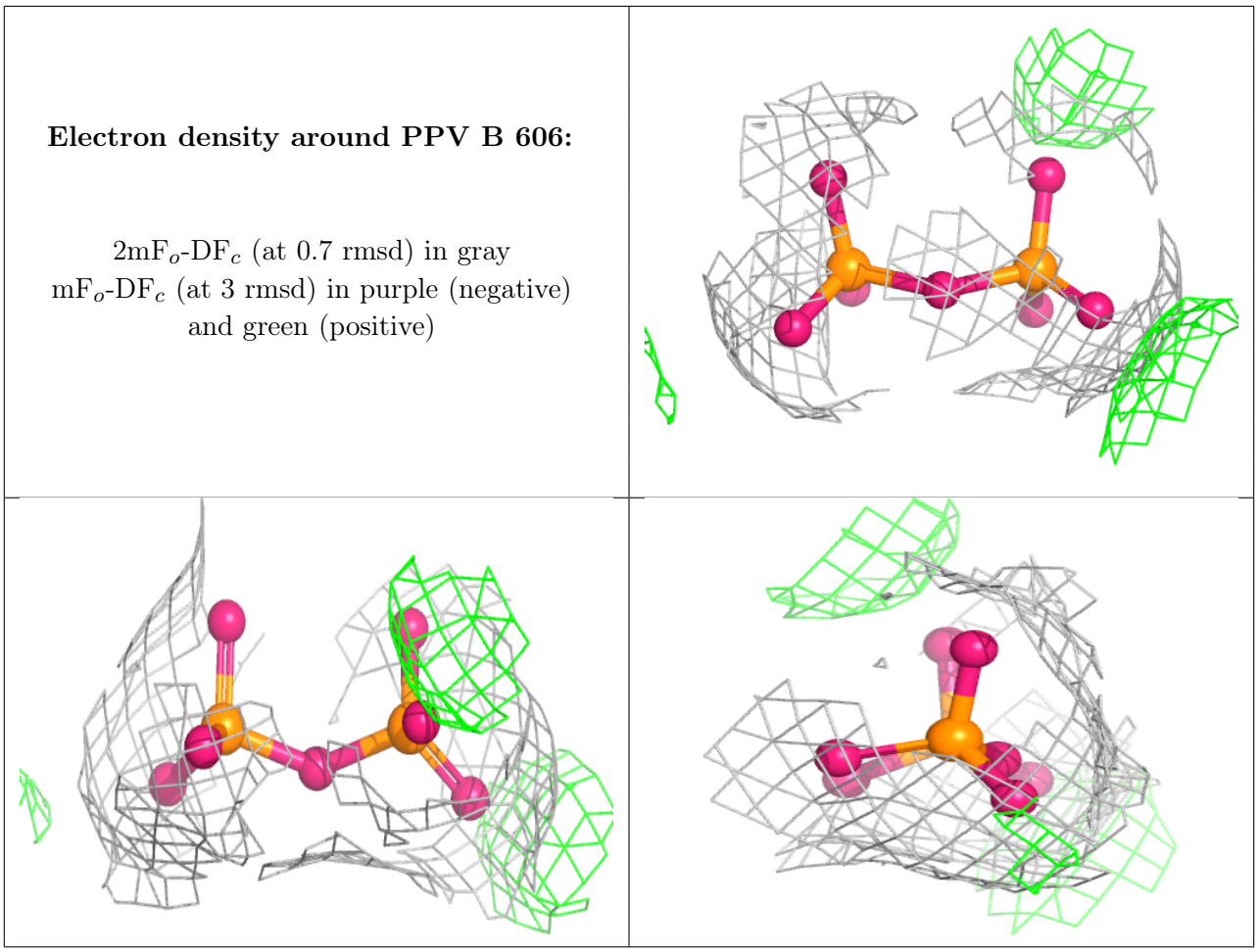
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





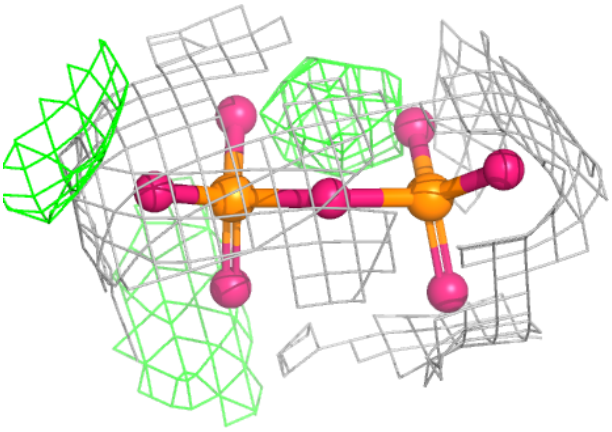
Electron density around PPV B 606:

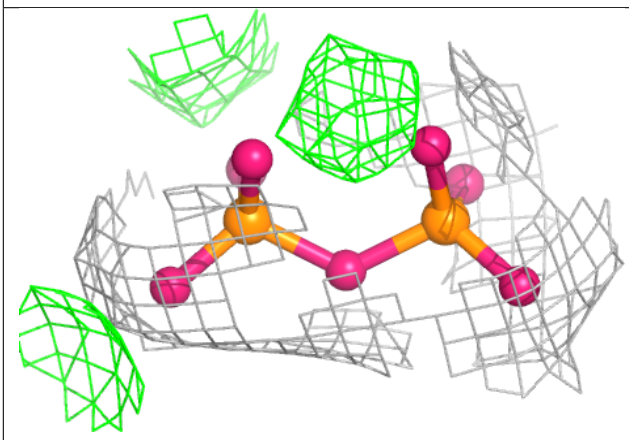
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

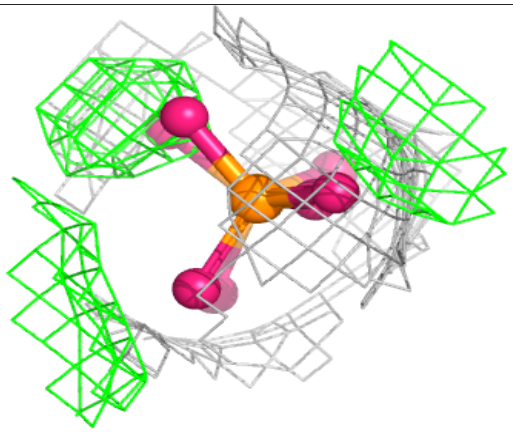


Electron density around PPV A 603:

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

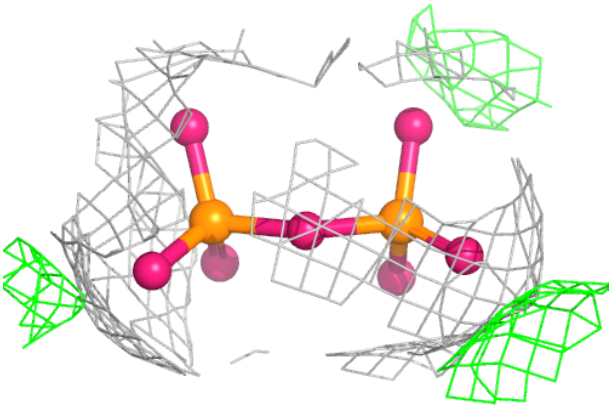


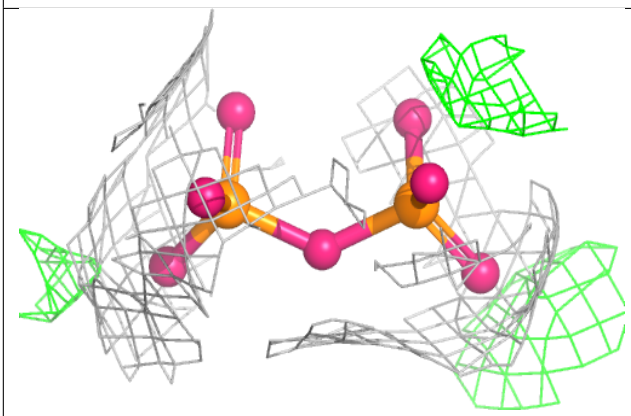


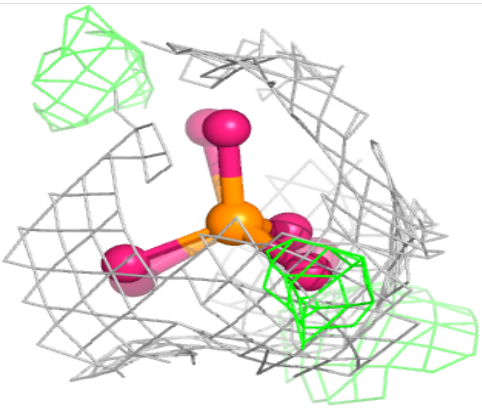


Electron density around PPV D 603:

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

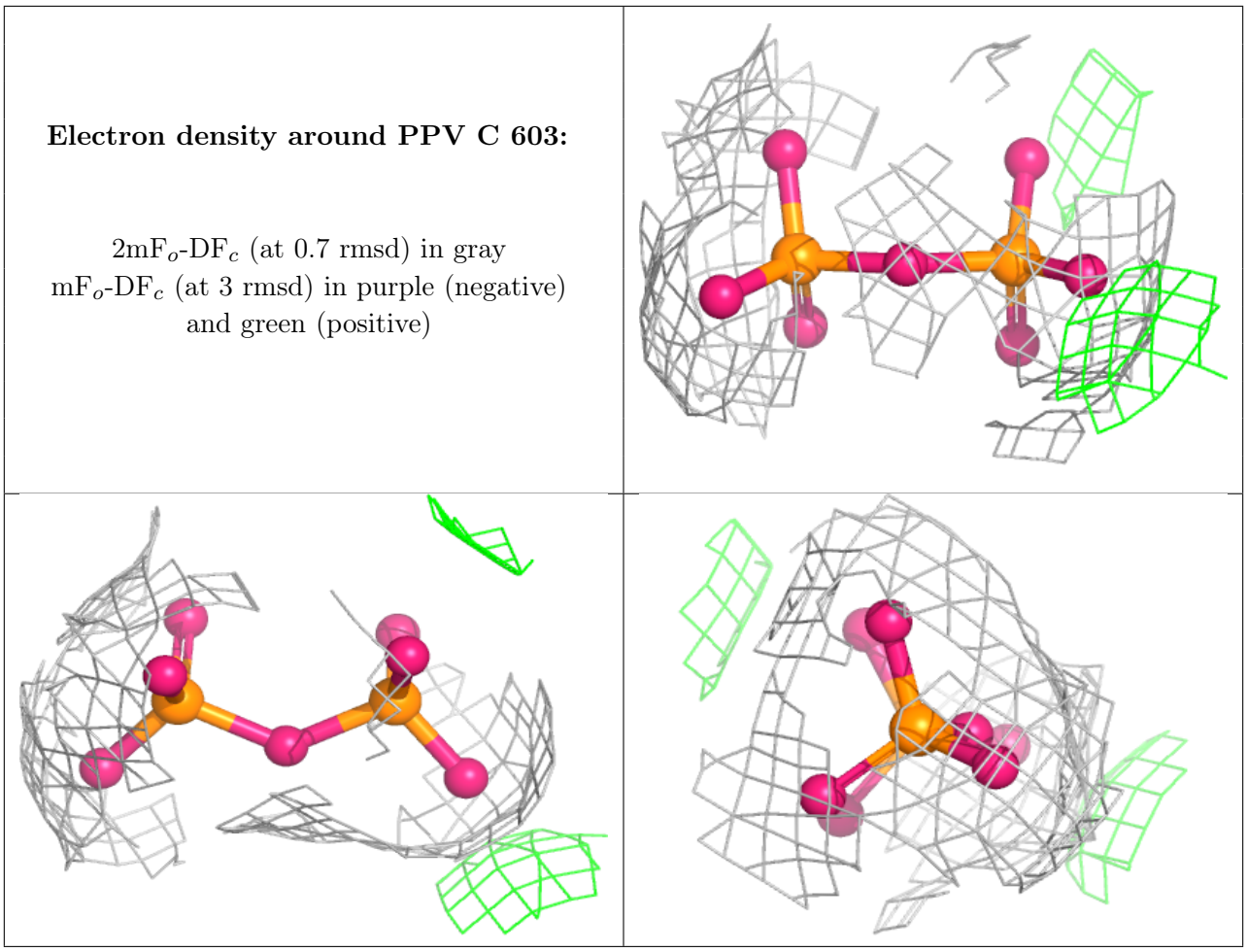






Electron density around PPV C 603:

$2mF_o$-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

There are no such residues in this entry.