Full wwPDB X-ray Structure Validation Report (i)

Aug 13, 2026 – 09:19 PM JST

PDB ID	:	9VI2 / pdb_00009vi2
Title	:	Crystal structure of fused glycerol dehydratase
Authors	:	Park, R.Y.; Seo, M.D.
Deposited on	:	2025-06-17
Resolution	:	2.91 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:

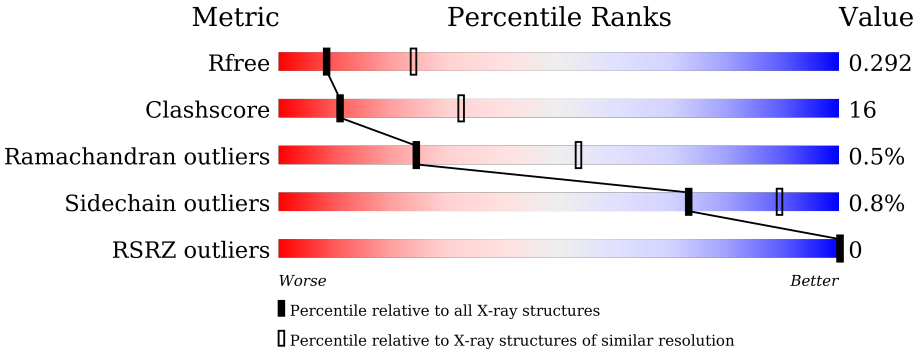
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	754	66% 31% •
1	B	754	69% 29% •
1	E	754	66% 31% • •
1	F	754	69% 29% •
2	C	141	63% 34% • •
2	D	141	65% 33% •

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Mol	Chain	Length	Quality of chain
2	G	141	60% 38%
2	H	141	72% 23%

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	B	2601	-	-	X	-
3	B12	E	2601	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27220 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 Glycerol dehydrase alpha subunit,Glycerol dehydrase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	737	5583	3486	976	1088	33	0	0	0
			Total	C	N	O	S			
1	B	736	5627	3513	986	1095	33	0	0	0
			Total	C	N	O	S			
1	E	737	5599	3495	978	1093	33	0	0	0
			Total	C	N	O	S			
1	F	739	5635	3517	987	1097	34	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	556	GLN	-	linker	UNP Q59476
A	557	GLY	-	linker	UNP Q59476
A	558	GLY	-	linker	UNP Q59476
A	559	ILE	-	linker	UNP Q59476
A	560	PRO	-	linker	UNP Q59476
A	561	VAL	-	linker	UNP Q59476
B	556	GLN	-	linker	UNP Q59476
B	557	GLY	-	linker	UNP Q59476
B	558	GLY	-	linker	UNP Q59476
B	559	ILE	-	linker	UNP Q59476
B	560	PRO	-	linker	UNP Q59476
B	561	VAL	-	linker	UNP Q59476
E	556	GLN	-	linker	UNP Q59476
E	557	GLY	-	linker	UNP Q59476
E	558	GLY	-	linker	UNP Q59476
E	559	ILE	-	linker	UNP Q59476
E	560	PRO	-	linker	UNP Q59476
E	561	VAL	-	linker	UNP Q59476
F	556	GLN	-	linker	UNP Q59476
F	557	GLY	-	linker	UNP Q59476

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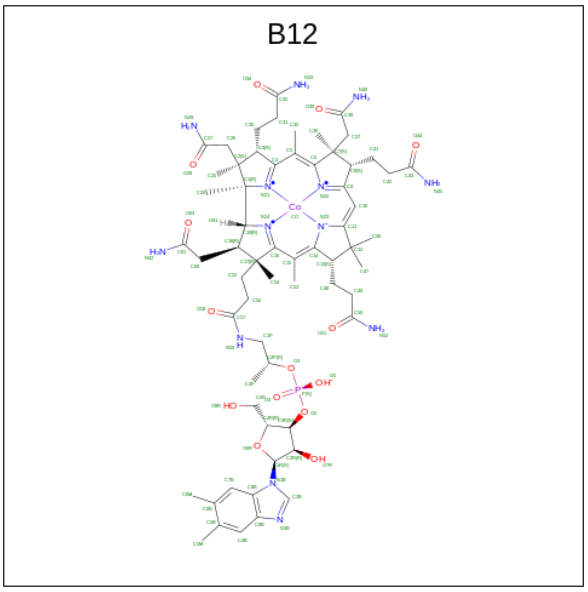
Chain	Residue	Modelled	Actual	Comment	Reference
F	558	GLY	-	linker	UNP Q59476
F	559	ILE	-	linker	UNP Q59476
F	560	PRO	-	linker	UNP Q59476
F	561	VAL	-	linker	UNP Q59476

- Molecule 2 is a protein called Glycerol dehydrase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	139	1106	691	209	203	3	0	0	0
			Total	C	N	O	S			
2	D	138	1112	695	209	205	3	0	0	0
			Total	C	N	O	S			
2	G	137	1093	684	204	202	3	0	0	0
			Total	C	N	O	S			
2	H	138	1101	690	205	203	3	0	0	0

- Molecule 3 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$) (labeled as "Ligand of Interest" by depositor).



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	E	1	91	62	1	13	14	1	0	0

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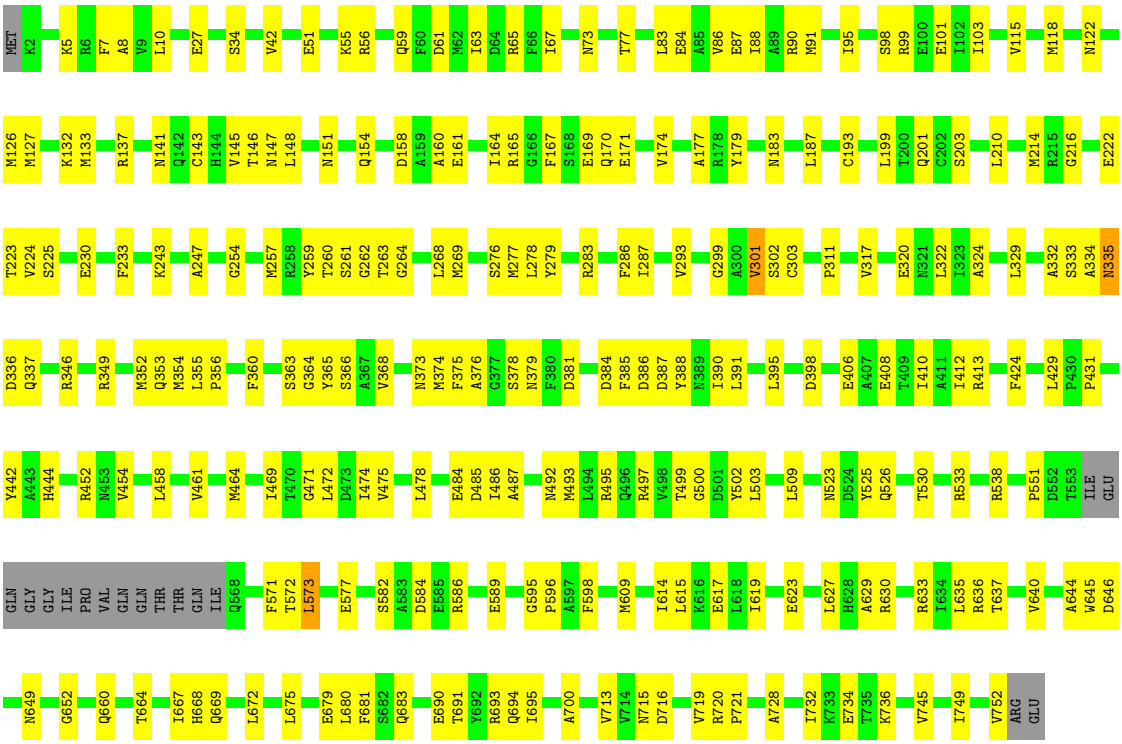
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Co	N	O	P		
3	E	1	91	62	1	13	14	1	0	0

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.

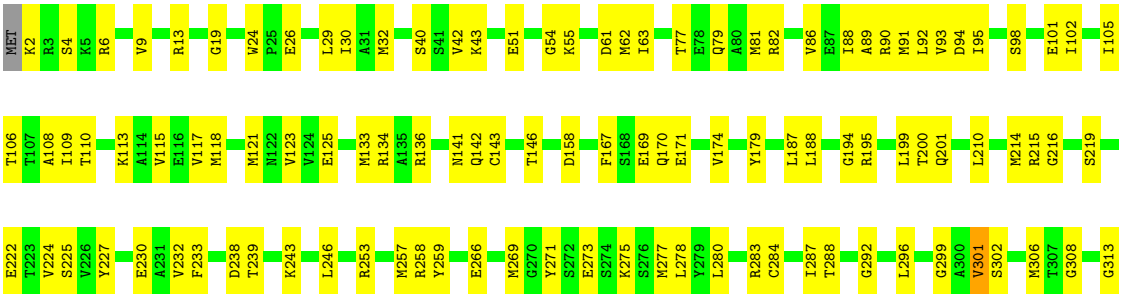
• Molecule 1: Glycerol dehydrase alpha subunit,Glycerol dehydrase beta subunit

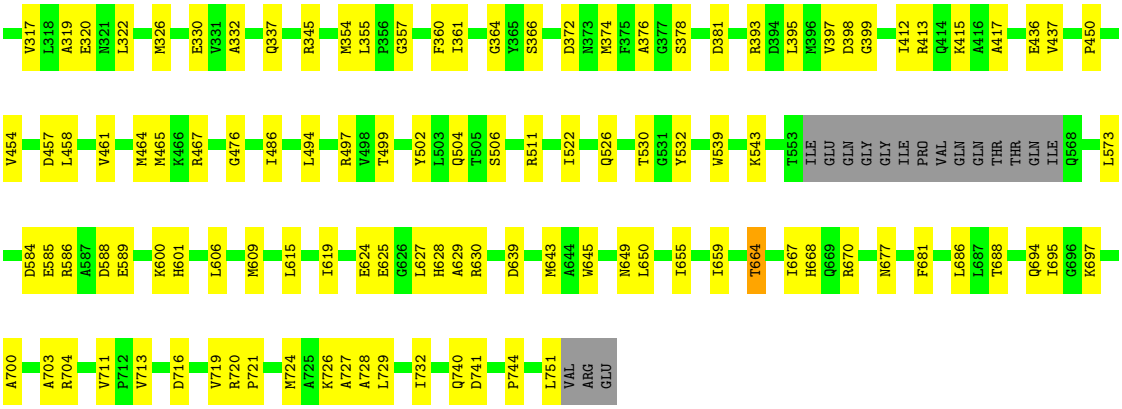
Chain A:



• Molecule 1: Glycerol dehydrase alpha subunit,Glycerol dehydrase beta subunit

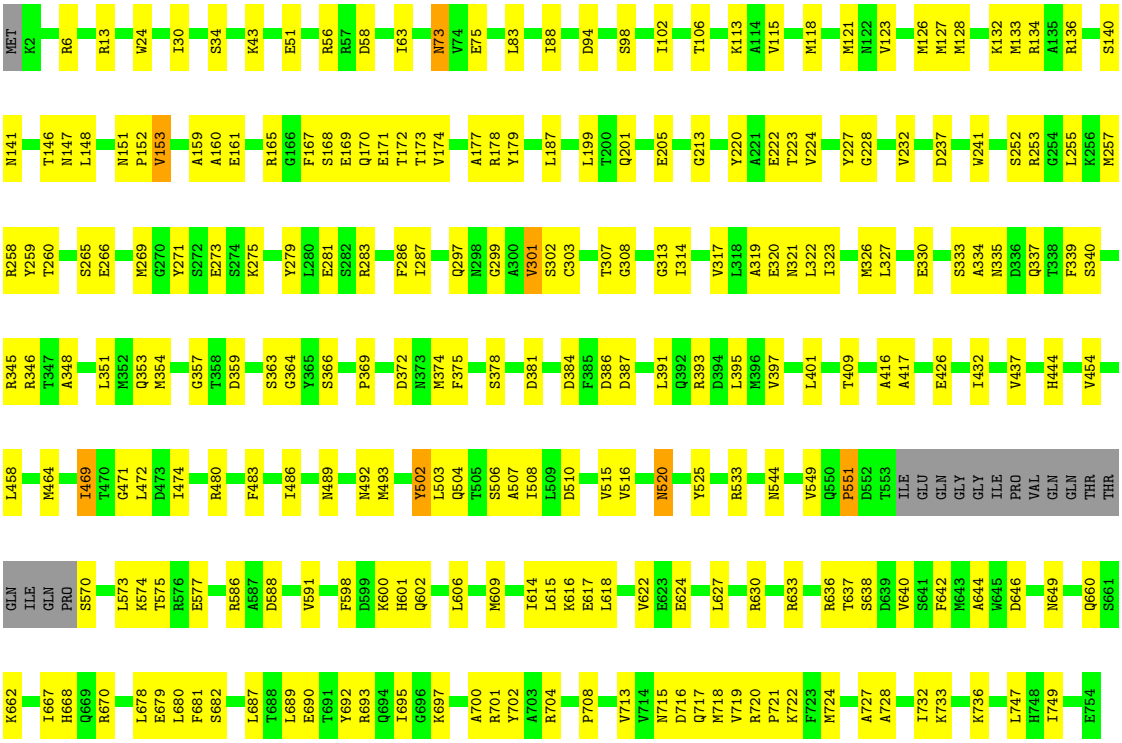
Chain B:





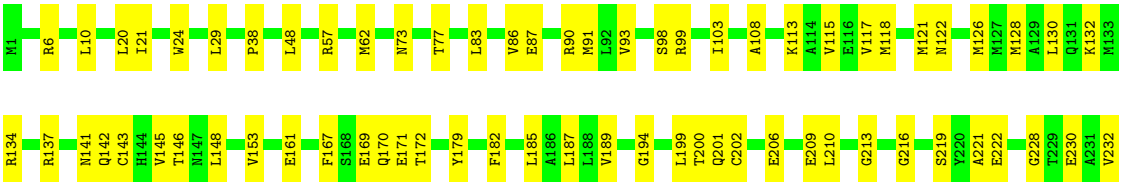
• Molecule 1: Glycerol dehydrase alpha subunit,Glycerol dehydrase beta subunit

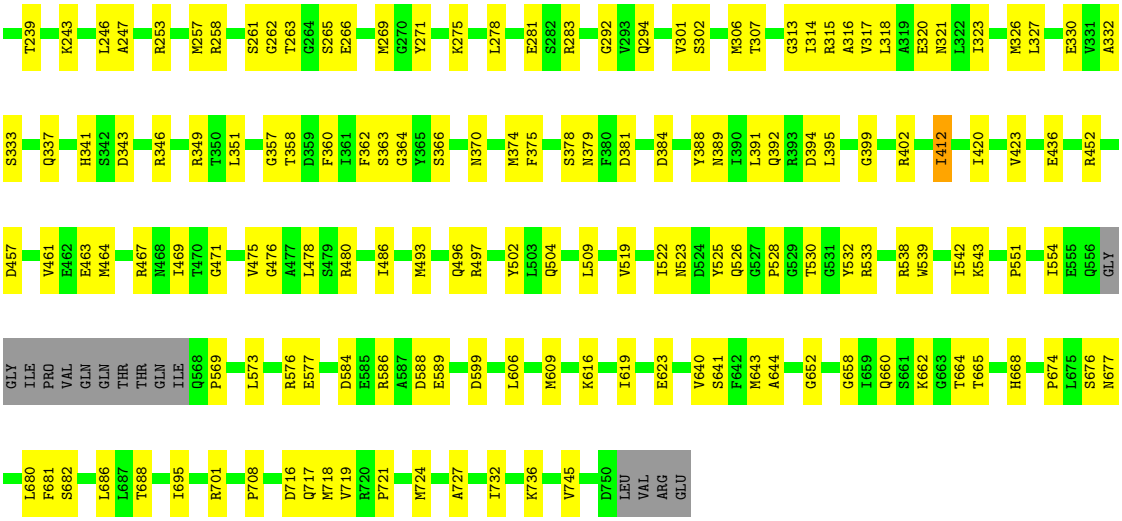
Chain E:



• Molecule 1: Glycerol dehydrase alpha subunit,Glycerol dehydrase beta subunit

Chain F:



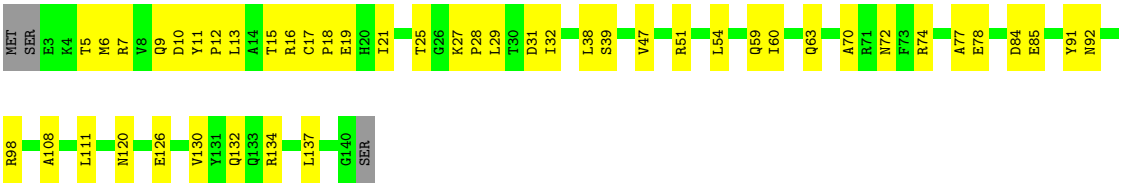


- Molecule 2: Glycerol dehydrase gamma subunit

Chain C:

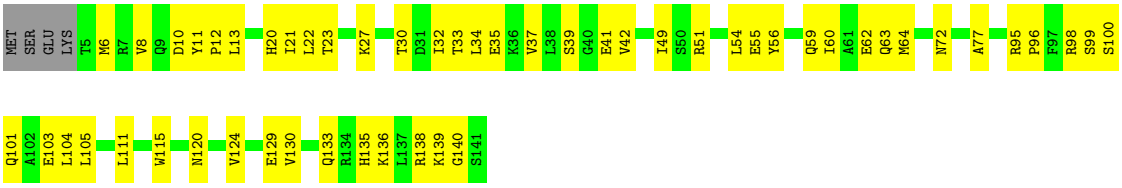
- Molecule 2: Glycerol dehydrase gamma subunit

Chain D:



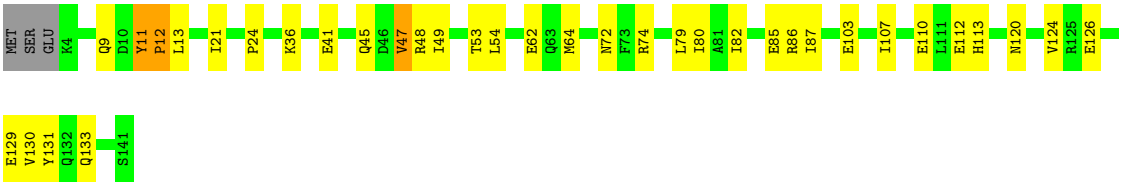
- Molecule 2: Glycerol dehydrase gamma subunit

Chain G:



- Molecule 2: Glycerol dehydrase gamma subunit

Chain H:


MET
SER
GLU
K4
Q9
D10
Y11
P12
L13
I21
P24
K36
E41
Q45
D46
V47
R48
I49
T53
L54
E62
Q63
M64
N72
F73
R74
L79
I80
A81
I82
E85
R86
I87
E103
I107
E110
L111
E112
H113
N120
V124
R125
E126
E129
V130
Y131
Q132
Q133
S141

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	152.04Å 153.29Å 377.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.76 – 2.91 29.76 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.76-2.91) 97.2 (29.76-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.66 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.238 , 0.291 0.238 , 0.292	Depositor DCC
R_{free} test set	4801 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 3.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.269 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	27220	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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: B12

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	0.46	0/5674	0.57	2/7696 (0.0%)
1	B	0.42	0/5717	0.49	0/7743
1	E	0.43	0/5688	0.49	0/7707
1	F	0.35	0/5725	0.49	0/7756
2	C	0.69	1/1126 (0.1%)	0.59	3/1525 (0.2%)
2	D	0.30	0/1132	0.40	0/1533
2	G	0.38	0/1113	0.46	0/1509
2	H	0.45	0/1121	0.54	0/1516
All	All	0.43	1/27296 (0.0%)	0.51	5/36985 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	18	PRO	N-CD	-18.46	1.21	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	335	ASN	N-CA-C	-8.55	102.43	112.86
1	A	485	ASP	N-CA-C	-7.48	102.49	111.69
2	C	17	CYS	CA-C-N	-6.13	113.50	119.87
2	C	17	CYS	C-N-CA	-6.13	113.50	119.87
2	C	18	PRO	N-CD-CG	5.23	111.04	103.20

There are no chirality outliers.

There are no planarity outliers.

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	5583	0	5485	189	0
1	B	5627	0	5582	185	0
1	E	5599	0	5526	197	0
1	F	5635	0	5588	182	0
2	C	1106	0	1107	40	0
2	D	1112	0	1121	38	0
2	G	1093	0	1096	41	0
2	H	1101	0	1107	33	0
3	A	91	0	87	16	0
3	B	91	0	88	31	0
3	E	182	0	174	49	0
All	All	27220	0	26961	893	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 16.

All (893) 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:B:210:LEU:CD2	1:B:214:MET:HE3	1.75	1.17
1:B:511:ARG:HB3	1:B:511:ARG:NH1	1.59	1.16
1:E:375:PHE:HA	3:E:2601:B12:H602	1.27	1.16
1:B:210:LEU:HD21	1:B:214:MET:HE3	1.18	1.15
1:E:302:SER:HB3	3:E:2601:B12:H532	1.20	1.13
1:A:374:MET:O	3:B:2601:B12:N62	1.87	1.06
2:H:112:GLU:OE2	2:H:113:HIS:NE2	1.88	1.06
1:F:519:VAL:HG13	2:H:64:MET:HE2	1.07	1.04
1:E:649:ASN:OD1	1:E:670:ARG:HG3	1.58	1.03
1:F:247:ALA:HA	1:F:257:MET:HE3	1.37	1.03
1:F:519:VAL:CG1	2:H:64:MET:HE2	1.94	0.98
1:F:599:ASP:OD1	1:F:599:ASP:O	1.82	0.97
1:B:210:LEU:HD21	1:B:214:MET:CE	1.97	0.95
2:D:51:ARG:HG2	2:D:77:ALA:HB1	1.50	0.91
1:B:511:ARG:HB3	1:B:511:ARG:HH11	1.30	0.91
1:B:511:ARG:HH11	1:B:511:ARG:CB	1.85	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:2601:B12:H451	3:E:2601:B12:C10	1.85	0.90
1:F:519:VAL:HG13	2:H:64:MET:CE	2.01	0.89
1:E:232:VAL:HG23	1:E:271:TYR:HB2	1.55	0.88
1:B:606:LEU:HD22	1:B:726:LYS:HG2	1.55	0.88
1:A:474:ILE:O	1:A:478:LEU:HD12	1.73	0.88
1:A:199:LEU:HD23	1:A:493:MET:HE2	1.56	0.86
3:A:2601:B12:C30	3:A:2601:B12:H203	2.06	0.86
1:B:188:LEU:HD12	1:B:188:LEU:O	1.76	0.85
1:B:98:SER:OG	1:B:101:GLU:HG3	1.76	0.85
1:E:165:ARG:O	1:E:401:LEU:HD13	1.78	0.84
1:E:141:ASN:HD22	1:E:401:LEU:HD23	1.41	0.82
1:F:573:LEU:HD13	1:F:616:LYS:HG3	1.62	0.82
3:B:2601:B12:H492	3:B:2601:B12:C2B	2.10	0.82
1:B:210:LEU:CD2	1:B:214:MET:CE	2.57	0.81
1:E:720:ARG:HG3	1:E:724:MET:HE3	1.63	0.81
1:E:269:MET:HE3	3:E:2601:B12:H522	1.46	0.80
1:B:625:GLU:HG2	1:B:697:LYS:HG3	1.63	0.80
3:A:2601:B12:H203	3:A:2601:B12:H301	1.62	0.80
1:A:410:ILE:HD11	1:B:4:SER:HB2	1.64	0.79
1:A:247:ALA:HA	1:A:257:MET:HE3	1.64	0.78
1:F:210:LEU:HD22	1:F:246:LEU:CD1	2.13	0.78
3:A:2601:B12:H201	3:A:2601:B12:H621	1.47	0.77
2:C:6:MET:H	2:C:59:GLN:NE2	1.84	0.76
1:B:511:ARG:HB3	1:B:511:ARG:CZ	2.17	0.75
1:F:584:ASP:OD1	1:F:652:GLY:HA2	1.87	0.75
1:E:269:MET:CE	3:E:2601:B12:H522	2.00	0.75
2:C:8:VAL:HG21	2:C:64:MET:HE3	1.69	0.74
1:F:247:ALA:CA	1:F:257:MET:HE3	2.15	0.74
1:A:675:LEU:HD13	3:A:2601:B12:H361	1.69	0.74
1:A:493:MET:HE1	1:A:509:LEU:CD1	2.17	0.73
1:A:471:GLY:O	1:A:475:VAL:HG23	1.87	0.73
1:F:686:LEU:HD21	1:F:719:VAL:CG2	2.19	0.73
3:A:2601:B12:H531	3:A:2601:B12:H561	1.71	0.73
1:E:174:VAL:O	3:E:2601:B12:H251	1.90	0.72
1:E:375:PHE:HA	3:E:2601:B12:C60	2.16	0.72
1:B:522:ILE:HD12	1:B:522:ILE:H	1.55	0.71
1:F:463:GLU:O	1:F:467:ARG:HG3	1.89	0.71
1:B:79:GLN:HG3	1:B:82:ARG:NH2	2.05	0.71
2:C:8:VAL:CG2	2:C:64:MET:HE3	2.21	0.71
1:E:618:LEU:O	1:E:622:VAL:HG23	1.91	0.70
1:E:98:SER:O	1:E:102:ILE:HD12	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:292:GLY:HA3	2:H:72:ASN:HB2	1.74	0.70
1:F:522:ILE:H	1:F:522:ILE:HD12	1.55	0.70
2:H:126:GLU:O	2:H:130:VAL:HG23	1.91	0.70
1:B:210:LEU:HD23	1:B:214:MET:HE3	1.73	0.70
3:E:2601:B12:H491	3:E:2601:B12:H2B	1.73	0.70
1:B:284:CYS:HA	1:B:287:ILE:HD12	1.74	0.69
3:B:2601:B12:C11	3:B:2601:B12:H491	2.21	0.69
1:E:126:MET:HE1	1:E:319:ALA:HB2	1.73	0.69
1:B:79:GLN:HG3	1:B:82:ARG:HH21	1.54	0.69
1:B:457:ASP:O	1:B:461:VAL:HG12	1.93	0.69
1:B:627:LEU:HD13	1:B:700:ALA:HB1	1.75	0.69
3:B:2601:B12:H561	3:B:2601:B12:C53	2.24	0.68
2:H:36:LYS:NZ	2:H:41:GLU:CD	2.51	0.68
1:A:680:LEU:HD12	1:A:681:PHE:N	2.08	0.68
1:F:586:ARG:HH21	1:F:588:ASP:CG	2.01	0.68
1:F:115:VAL:CG1	1:F:278:LEU:HG	2.24	0.68
1:E:680:LEU:HD21	3:E:2602:B12:H203	1.76	0.68
1:F:228:GLY:O	1:F:283:ARG:NH1	2.27	0.68
1:F:115:VAL:HG12	1:F:278:LEU:HG	1.74	0.68
3:B:2601:B12:H531	3:B:2601:B12:H543	1.76	0.67
1:F:201:GLN:HG3	1:F:221:ALA:HA	1.75	0.67
3:B:2601:B12:H2B	3:B:2601:B12:C14	2.25	0.67
1:B:504:GLN:HG3	2:D:11:TYR:HE1	1.59	0.67
1:A:675:LEU:HB3	3:A:2601:B12:H361	1.77	0.67
2:G:13:LEU:HB3	2:G:21:ILE:HD11	1.75	0.67
2:C:103:GLU:O	2:C:107:ILE:HG13	1.95	0.67
1:E:649:ASN:OD1	1:E:670:ARG:CG	2.41	0.67
1:A:716:ASP:HB3	1:A:719:VAL:HG23	1.77	0.66
1:E:302:SER:HA	1:E:337:GLN:HG3	1.78	0.66
1:B:366:SER:HB2	1:B:378:SER:HB3	1.78	0.66
1:B:625:GLU:CG	1:B:697:LYS:HG3	2.25	0.66
1:B:118:MET:HG3	1:B:319:ALA:HB1	1.78	0.66
3:B:2601:B12:H492	3:B:2601:B12:H2B	1.76	0.66
1:E:624:GLU:HB3	1:E:697:LYS:NZ	2.11	0.66
1:B:615:LEU:O	1:B:619:ILE:HG13	1.95	0.66
1:A:302:SER:HA	1:A:337:GLN:HG3	1.78	0.66
3:A:2601:B12:H482	1:B:269:MET:HE2	1.77	0.65
1:E:56:ARG:HD2	1:E:58:ASP:OD1	1.96	0.65
3:E:2601:B12:H2B	3:E:2601:B12:C49	2.26	0.65
2:G:100:SER:HB3	2:G:138:ARG:HH21	1.62	0.65
2:C:9:GLN:H	2:C:9:GLN:CD	2.05	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:200:THR:H	1:F:219:SER:HB2	1.62	0.65
1:A:261:SER:OG	1:A:262:GLY:N	2.29	0.65
1:A:269:MET:HE3	3:B:2601:B12:N52	2.11	0.65
1:B:238:ASP:OD2	1:B:243:LYS:NZ	2.29	0.65
2:D:13:LEU:HB3	2:D:21:ILE:HD11	1.79	0.65
3:E:2601:B12:H1P1	1:F:682:SER:O	1.97	0.65
3:E:2602:B12:H351	3:E:2602:B12:H372	1.76	0.65
1:A:269:MET:HE1	3:B:2601:B12:N45	2.11	0.65
1:A:617:GLU:OE1	1:A:693:ARG:HD2	1.97	0.65
1:F:366:SER:HB2	1:F:378:SER:HB3	1.79	0.64
1:A:95:ILE:O	1:A:526:GLN:NE2	2.30	0.64
1:A:299:GLY:C	1:A:301:VAL:H	2.05	0.64
1:E:308:GLY:O	1:E:345:ARG:NH2	2.30	0.64
1:A:573:LEU:HD21	1:A:749:ILE:HD12	1.79	0.64
1:E:351:LEU:HD12	1:F:351:LEU:HD12	1.80	0.64
1:B:142:GLN:HB2	1:B:169:GLU:HB2	1.79	0.64
1:E:303:CYS:HA	1:F:724:MET:HE1	1.80	0.64
2:C:13:LEU:HB3	2:C:21:ILE:HD11	1.79	0.63
1:A:84:GLU:O	1:A:88:ILE:HD12	1.98	0.63
1:E:13:ARG:NH2	1:F:384:ASP:OD1	2.30	0.63
1:B:700:ALA:O	1:B:704:ARG:HG3	1.98	0.63
1:E:167:PHE:CE1	1:E:401:LEU:HD21	2.32	0.63
1:E:617:GLU:HG3	1:E:689:LEU:HB3	1.80	0.63
3:E:2602:B12:H91	3:E:2602:B12:O28	1.99	0.63
1:A:551:PRO:HG3	1:B:24:TRP:HB2	1.81	0.63
1:B:465:MET:HE2	1:B:465:MET:HA	1.80	0.63
1:E:640:VAL:HB	1:E:660:GLN:HG3	1.80	0.63
1:F:332:ALA:HA	1:F:360:PHE:HB2	1.79	0.63
1:B:288:THR:HG21	1:B:296:LEU:HB2	1.81	0.63
1:A:584:ASP:OD1	1:A:652:GLY:HA2	1.98	0.62
1:E:161:GLU:HG3	1:E:409:THR:HG23	1.81	0.62
1:F:586:ARG:HB2	1:F:589:GLU:HB3	1.81	0.62
1:F:716:ASP:HB3	1:F:719:VAL:HG23	1.80	0.62
1:A:464:MET:HG3	1:A:469:ILE:HD12	1.80	0.62
1:B:627:LEU:HD11	1:B:704:ARG:HD3	1.82	0.62
2:C:120:ASN:O	2:C:124:VAL:HG23	1.99	0.62
1:E:314:ILE:HG13	1:F:394:ASP:HB3	1.81	0.62
1:A:199:LEU:CD2	1:A:493:MET:HE2	2.28	0.62
1:B:650:LEU:HD11	1:B:744:PRO:HG2	1.81	0.62
3:E:2601:B12:H491	3:E:2601:B12:C2B	2.30	0.62
3:B:2601:B12:H561	3:B:2601:B12:H531	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:LEU:HD22	1:F:246:LEU:HD12	1.80	0.61
1:A:499:THR:HG21	2:C:14:ALA:HB2	1.82	0.61
1:F:528:PRO:HA	1:F:533:ARG:HH21	1.65	0.61
1:A:493:MET:HE1	1:A:509:LEU:HD12	1.81	0.61
2:C:7:ARG:HB2	2:C:9:GLN:OE1	2.00	0.61
3:E:2601:B12:H451	3:E:2601:B12:H10	1.62	0.61
2:G:96:PRO:O	2:G:98:ARG:NH1	2.33	0.61
1:F:302:SER:HA	1:F:337:GLN:HG3	1.83	0.61
1:B:171:GLU:HA	1:B:201:GLN:HG3	1.83	0.61
2:H:120:ASN:O	2:H:124:VAL:HG23	2.01	0.61
1:A:86:VAL:O	1:A:90:ARG:HG3	2.01	0.61
1:B:302:SER:HA	1:B:337:GLN:HG3	1.82	0.61
2:C:6:MET:H	2:C:59:GLN:HE22	1.47	0.61
2:C:51:ARG:HD2	2:C:77:ALA:HB1	1.81	0.61
1:A:174:VAL:HG12	1:A:183:ASN:HD22	1.65	0.61
1:A:458:LEU:HA	1:A:461:VAL:HG12	1.83	0.61
1:E:728:ALA:O	1:E:732:ILE:HG13	2.00	0.61
1:B:366:SER:HB3	1:B:381:ASP:HA	1.83	0.60
1:A:199:LEU:HD23	1:A:493:MET:CE	2.29	0.60
3:A:2601:B12:H301	3:A:2601:B12:C20	2.29	0.60
1:B:187:LEU:HD23	1:B:200:THR:HG23	1.82	0.60
1:B:106:THR:C	1:B:108:ALA:H	2.10	0.60
3:B:2601:B12:C11	3:B:2601:B12:C49	2.79	0.60
1:E:94:ASP:O	1:E:132:LYS:NZ	2.33	0.60
1:F:48:LEU:HD21	1:F:57:ARG:NE	2.16	0.60
1:F:478:LEU:HD22	1:F:486:ILE:HD11	1.82	0.60
1:A:337:GLN:HE22	1:A:375:PHE:HB3	1.66	0.60
1:A:366:SER:HB3	1:A:381:ASP:HA	1.82	0.60
1:B:511:ARG:NH1	1:B:511:ARG:CB	2.42	0.60
2:C:11:TYR:C	2:C:13:LEU:N	2.58	0.60
1:E:178:ARG:HD2	1:E:458:LEU:HD13	1.83	0.60
1:F:121:MET:O	1:F:315:ARG:NH1	2.34	0.60
1:F:346:ARG:HB2	1:F:379:ASN:OD1	2.01	0.60
1:B:210:LEU:O	1:B:214:MET:HG3	2.01	0.60
1:F:619:ILE:O	1:F:623:GLU:HG3	2.02	0.60
1:B:118:MET:CE	1:B:121:MET:HE1	2.32	0.60
1:A:586:ARG:O	1:A:652:GLY:HA3	2.02	0.60
1:B:630:ARG:NH2	1:B:650:LEU:O	2.34	0.60
2:D:19:GLU:H	2:D:19:GLU:CD	2.06	0.60
1:B:728:ALA:O	1:B:732:ILE:HG13	2.02	0.59
3:B:2601:B12:H362	3:B:2601:B12:H351	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:515:VAL:O	1:E:520:ASN:ND2	2.30	0.59
1:E:472:LEU:HD22	2:G:37:VAL:HG11	1.84	0.59
1:F:137:ARG:HG3	1:F:523:ASN:HA	1.84	0.59
1:E:682:SER:CB	3:E:2602:B12:H201	2.32	0.59
1:A:88:ILE:HD12	1:A:88:ILE:H	1.68	0.59
1:A:264:GLY:H	1:A:277:MET:HG2	1.68	0.59
2:H:112:GLU:OE2	2:H:113:HIS:CD2	2.54	0.59
1:B:24:TRP:HD1	1:B:26:GLU:OE1	1.85	0.59
1:B:436:GLU:HG2	1:B:450:PRO:HG2	1.84	0.59
1:A:51:GLU:HG2	1:A:55:LYS:O	2.02	0.59
1:A:147:ASN:HD21	1:A:151:ASN:N	2.01	0.59
1:B:169:GLU:HG2	1:B:199:LEU:HD12	1.85	0.59
1:B:201:GLN:NE2	1:B:222:GLU:OE1	2.31	0.59
1:E:471:GLY:HA2	1:E:474:ILE:HG12	1.84	0.59
1:A:660:GLN:HG3	1:A:664:THR:HB	1.83	0.58
1:B:200:THR:H	1:B:219:SER:HB2	1.66	0.58
1:E:102:ILE:HD12	1:E:102:ILE:H	1.67	0.58
1:E:627:LEU:HD13	1:E:700:ALA:HB1	1.85	0.58
1:A:264:GLY:N	1:A:277:MET:HG2	2.17	0.58
3:E:2602:B12:C2B	3:E:2602:B12:H492	2.34	0.58
1:A:354:MET:HE3	1:A:388:TYR:CE1	2.37	0.58
1:B:258:ARG:NE	1:B:330:GLU:OE2	2.34	0.58
3:E:2601:B12:H332	1:F:677:ASN:HD21	1.52	0.58
2:G:120:ASN:O	2:G:124:VAL:HG23	2.02	0.58
1:B:115:VAL:HG12	1:B:278:LEU:HG	1.84	0.58
2:G:32:ILE:HA	2:G:42:VAL:HG21	1.85	0.58
2:H:36:LYS:NZ	2:H:41:GLU:OE1	2.35	0.58
1:A:366:SER:HB2	1:A:378:SER:HB3	1.85	0.58
2:H:36:LYS:HZ2	2:H:41:GLU:CD	2.10	0.58
1:A:87:GLU:O	1:A:91:MET:HG3	2.02	0.58
1:A:732:ILE:HG23	1:A:736:LYS:HE3	1.86	0.58
1:E:720:ARG:HD3	1:E:724:MET:HE1	1.86	0.58
1:A:424:PHE:HA	1:A:429:LEU:HD12	1.85	0.58
1:B:106:THR:HG21	1:B:326:MET:HE3	1.85	0.58
1:E:369:PRO:HD3	1:F:6:ARG:HH21	1.69	0.58
2:G:33:THR:O	2:G:37:VAL:HG23	2.04	0.58
1:E:720:ARG:CG	1:E:724:MET:HE3	2.32	0.58
3:E:2601:B12:O8R	1:F:662:LYS:NZ	2.23	0.58
1:A:174:VAL:HG12	1:A:183:ASN:ND2	2.19	0.57
1:A:493:MET:HE1	1:A:509:LEU:HD11	1.85	0.57
1:A:572:THR:O	1:A:752:VAL:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:678:LEU:HD13	1:E:702:TYR:CE1	2.39	0.57
3:E:2601:B12:H203	1:F:680:LEU:HD21	1.85	0.57
1:F:87:GLU:O	1:F:91:MET:HG3	2.04	0.57
1:A:63:ILE:HG12	1:A:287:ILE:HD11	1.85	0.57
1:A:472:LEU:HA	1:A:475:VAL:HG23	1.86	0.57
1:B:522:ILE:HD12	1:B:522:ILE:N	2.19	0.57
1:F:38:PRO:HD3	1:F:275:LYS:HE2	1.86	0.57
1:E:598:PHE:O	1:E:633:ARG:NH1	2.37	0.57
3:E:2601:B12:N33	1:F:677:ASN:OD1	2.37	0.57
1:A:615:LEU:O	1:A:619:ILE:HG13	2.05	0.57
2:C:55:GLU:O	2:C:59:GLN:HG3	2.04	0.57
1:E:314:ILE:CG1	1:F:394:ASP:HB3	2.34	0.57
3:B:2601:B12:H491	3:B:2601:B12:H473	1.86	0.57
1:E:169:GLU:HB3	1:E:220:TYR:OH	2.04	0.57
3:A:2601:B12:N29	3:A:2601:B12:C19	2.68	0.57
1:E:508:ILE:HG13	1:E:516:VAL:HG13	1.87	0.57
1:F:640:VAL:HA	1:F:643:MET:HE3	1.85	0.57
1:A:627:LEU:HD13	1:A:700:ALA:HB1	1.86	0.57
1:A:596:PRO:HB3	1:A:635:LEU:HD23	1.87	0.56
2:C:126:GLU:O	2:C:130:VAL:HG23	2.05	0.56
1:A:61:ASP:HB2	1:A:230:GLU:OE2	2.05	0.56
1:E:681:PHE:HB3	1:E:687:LEU:HD21	1.88	0.56
1:F:77:THR:HA	1:F:108:ALA:HB1	1.86	0.56
1:F:366:SER:HB3	1:F:381:ASP:HA	1.87	0.56
1:F:239:THR:HG21	2:H:131:TYR:CE1	2.41	0.56
2:D:7:ARG:HA	2:D:63:GLN:HE21	1.70	0.56
2:D:19:GLU:OE1	2:D:19:GLU:N	2.27	0.56
1:E:307:THR:O	1:E:313:GLY:HA3	2.06	0.56
1:E:337:GLN:HE22	1:E:375:PHE:HB3	1.70	0.56
1:F:732:ILE:HG23	1:F:736:LYS:HE3	1.87	0.56
1:B:415:LYS:NZ	1:B:486:ILE:HD11	2.20	0.56
3:E:2601:B12:H531	3:E:2601:B12:H543	1.87	0.56
1:A:174:VAL:HG21	1:A:177:ALA:HA	1.86	0.56
1:A:303:CYS:HA	1:B:724:MET:HE1	1.88	0.56
1:E:602:GLN:NE2	1:E:733:LYS:HB2	2.21	0.56
1:E:366:SER:HB2	1:E:378:SER:HB3	1.87	0.56
1:A:683:GLN:HE22	1:A:715:ASN:ND2	2.04	0.56
1:A:636:ARG:HG3	1:A:637:THR:HG22	1.87	0.55
1:A:332:ALA:HA	1:A:360:PHE:HB2	1.88	0.55
1:B:62:MET:HE1	1:B:239:THR:CG2	2.35	0.55
1:B:332:ALA:HA	1:B:360:PHE:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:LEU:HD11	1:B:727:ALA:HB2	1.87	0.55
1:B:681:PHE:CZ	1:B:695:ILE:HG12	2.41	0.55
3:E:2601:B12:HM53	3:E:2601:B12:H353	1.88	0.55
1:F:519:VAL:HA	2:H:64:MET:CE	2.36	0.55
1:A:115:VAL:HG12	1:A:278:LEU:HG	1.88	0.55
1:B:322:LEU:O	1:B:326:MET:HG2	2.07	0.55
1:B:458:LEU:HA	1:B:461:VAL:HG12	1.87	0.55
2:C:6:MET:HE1	2:C:17:CYS:SG	2.47	0.55
1:E:179:TYR:HE2	1:E:454:VAL:HG13	1.72	0.55
1:E:302:SER:CB	3:E:2601:B12:H532	2.13	0.55
1:A:595:GLY:HA3	1:A:734:GLU:OE2	2.05	0.55
3:E:2601:B12:H451	3:E:2601:B12:C9	2.20	0.55
1:E:172:THR:HB	1:E:187:LEU:HD22	1.88	0.55
1:F:528:PRO:HA	1:F:533:ARG:NH2	2.21	0.55
1:E:132:LYS:HB2	1:E:525:TYR:HD2	1.72	0.55
1:E:667:ILE:HD12	1:E:679:GLU:HB2	1.89	0.55
1:F:539:TRP:CE2	1:F:543:LYS:HD3	2.42	0.55
1:B:232:VAL:HG23	1:B:271:TYR:HB2	1.88	0.55
1:F:476:GLY:O	1:F:480:ARG:HG3	2.07	0.55
1:B:624:GLU:O	1:B:624:GLU:HG3	2.05	0.55
1:E:489:ASN:O	1:E:493:MET:HG2	2.07	0.55
1:E:681:PHE:CZ	1:E:695:ILE:HG12	2.42	0.55
1:E:297:GLN:NE2	1:E:363:SER:OG	2.37	0.54
1:A:225:SER:O	1:A:243:LYS:NZ	2.34	0.54
1:B:458:LEU:HA	1:B:461:VAL:CG1	2.37	0.54
1:F:216:GLY:HA2	1:F:497:ARG:NH2	2.23	0.54
1:A:503:LEU:HB3	2:C:73:PHE:CZ	2.42	0.54
1:E:375:PHE:C	3:E:2601:B12:H541	2.33	0.54
1:E:606:LEU:HD21	1:E:727:ALA:HA	1.88	0.54
1:E:638:SER:O	1:E:660:GLN:NE2	2.28	0.54
1:F:317:VAL:HG11	1:F:349:ARG:HH21	1.71	0.54
2:G:55:GLU:OE2	2:G:59:GLN:NE2	2.40	0.54
1:E:627:LEU:HD11	1:E:704:ARG:HG2	1.89	0.54
1:A:158:ASP:OD1	1:A:413:ARG:NH1	2.31	0.54
2:C:131:TYR:HB3	2:C:137:LEU:HD12	1.89	0.54
2:D:25:THR:OG1	2:D:27:LYS:HD2	2.08	0.54
1:A:122:ASN:O	1:A:126:MET:HG3	2.07	0.54
1:A:406:GLU:O	1:A:410:ILE:HG12	2.07	0.54
2:C:99:SER:HB3	2:C:103:GLU:HB2	1.89	0.54
2:G:49:ILE:HG12	2:G:54:LEU:HG	1.89	0.54
2:D:11:TYR:O	2:D:13:LEU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:ASN:C	1:E:73:ASN:HD22	2.15	0.54
3:E:2602:B12:H91	3:E:2602:B12:C27	2.36	0.54
1:A:222:GLU:O	1:A:260:THR:OG1	2.23	0.54
2:G:11:TYR:HA	2:G:60:ILE:HD13	1.89	0.54
1:B:179:TYR:HE2	1:B:454:VAL:HG13	1.72	0.54
1:B:275:LYS:HB2	1:B:280:LEU:HD21	1.89	0.54
1:B:686:LEU:HD21	1:B:719:VAL:CG2	2.38	0.54
2:D:70:ALA:O	2:D:74:ARG:HG3	2.08	0.54
1:B:62:MET:HE1	1:B:239:THR:HG22	1.89	0.53
2:D:126:GLU:O	2:D:130:VAL:HG23	2.08	0.53
1:B:29:LEU:HD22	1:B:306:MET:HE1	1.91	0.53
1:A:199:LEU:CD2	1:A:493:MET:CE	2.87	0.53
1:E:322:LEU:O	1:E:326:MET:HG2	2.07	0.53
1:A:551:PRO:HB2	1:B:24:TRP:CE3	2.42	0.53
1:F:294:GLN:NE2	1:F:330:GLU:OE1	2.41	0.53
1:F:686:LEU:HD21	1:F:719:VAL:HG21	1.88	0.53
1:A:584:ASP:CG	1:A:652:GLY:HA2	2.33	0.53
1:B:143:CYS:SG	1:B:170:GLN:HG2	2.48	0.53
1:B:210:LEU:HD23	1:B:214:MET:CE	2.35	0.53
2:G:111:LEU:HA	2:G:115:TRP:HD1	1.73	0.53
1:E:136:ARG:NH1	1:E:506:SER:O	2.39	0.53
1:E:173:THR:OG1	3:E:2601:B12:H262	2.08	0.53
1:A:27:GLU:HB3	1:B:732:ILE:HD13	1.91	0.53
1:A:598:PHE:O	1:A:633:ARG:NH1	2.33	0.53
1:A:680:LEU:HD12	1:A:681:PHE:H	1.72	0.53
1:B:639:ASP:O	1:B:643:MET:HG3	2.08	0.53
1:E:115:VAL:HG11	1:E:279:TYR:HA	1.90	0.53
2:H:79:LEU:HB3	2:H:87:ILE:HD11	1.90	0.53
1:A:56:ARG:HG3	1:A:56:ARG:HH11	1.74	0.53
1:A:214:MET:HE1	2:C:88:LEU:HG	1.91	0.53
1:A:589:GLU:OE2	1:A:652:GLY:N	2.34	0.53
1:F:701:ARG:HD2	1:F:708:PRO:HB3	1.90	0.53
2:H:103:GLU:O	2:H:107:ILE:HD12	2.09	0.53
1:B:9:VAL:O	1:B:13:ARG:HG2	2.09	0.52
1:B:464:MET:HA	1:B:467:ARG:HD3	1.90	0.52
1:B:573:LEU:HD11	1:B:619:ILE:HD12	1.91	0.52
1:E:171:GLU:HA	1:E:201:GLN:HG3	1.90	0.52
1:B:30:ILE:O	1:B:277:MET:HG3	2.09	0.52
1:E:118:MET:HG3	1:E:323:ILE:HD11	1.92	0.52
1:E:520:ASN:OD1	1:E:520:ASN:N	2.39	0.52
1:F:141:ASN:ND2	1:F:399:GLY:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:34:LEU:O	2:G:34:LEU:HD23	2.09	0.52
1:A:160:ALA:O	1:A:164:ILE:HG23	2.09	0.52
1:E:464:MET:HG3	1:E:469:ILE:HD12	1.91	0.52
1:E:577:GLU:OE2	1:E:600:LYS:HE3	2.10	0.52
1:F:145:VAL:CG2	1:F:170:GLN:HG2	2.40	0.52
1:E:319:ALA:O	1:E:323:ILE:HG13	2.09	0.52
1:B:740:GLN:OE1	1:B:741:ASP:OD2	2.27	0.52
1:A:484:GLU:H	1:A:484:GLU:CD	2.17	0.52
1:E:222:GLU:O	1:E:224:VAL:N	2.38	0.52
3:E:2602:B12:H261	3:E:2602:B12:H601	1.92	0.52
1:A:317:VAL:O	1:A:320:GLU:HG2	2.10	0.52
1:E:265:SER:O	1:E:269:MET:HG3	2.09	0.52
1:E:575:THR:HB	1:E:747:LEU:HD22	1.92	0.52
1:A:691:THR:O	1:A:695:ILE:HG13	2.09	0.52
1:B:354:MET:HA	1:B:361:ILE:HD13	1.92	0.52
2:G:101:GLN:O	2:G:105:LEU:HD12	2.09	0.52
1:B:62:MET:HG2	2:D:134:ARG:HG3	1.91	0.52
1:B:86:VAL:O	1:B:90:ARG:HG3	2.10	0.52
1:A:148:LEU:HD11	1:B:713:VAL:O	2.09	0.52
2:C:110:GLU:O	2:C:114:THR:OG1	2.26	0.52
1:F:126:MET:HE1	1:F:315:ARG:HG3	1.92	0.51
1:B:619:ILE:HG23	1:B:629:ALA:HB3	1.93	0.51
1:F:318:LEU:HD12	1:F:318:LEU:O	2.10	0.51
1:F:391:LEU:O	1:F:395:LEU:HD12	2.10	0.51
2:G:39:SER:HB2	2:G:41:GLU:OE1	2.11	0.51
1:A:67:ILE:HD13	1:A:286:PHE:CB	2.40	0.51
1:B:225:SER:O	1:B:243:LYS:HE2	2.11	0.51
1:B:589:GLU:HA	1:B:628:HIS:O	2.10	0.51
1:B:624:GLU:O	1:B:624:GLU:CG	2.58	0.51
2:D:18:PRO:N	2:D:19:GLU:OE1	2.43	0.51
1:B:273:GLU:O	1:B:275:LYS:NZ	2.38	0.51
3:E:2601:B12:O4	1:F:664:THR:OG1	2.27	0.51
1:B:511:ARG:HH11	1:B:511:ARG:HB2	1.73	0.51
1:F:210:LEU:HD22	1:F:246:LEU:HD11	1.93	0.51
1:B:655:ILE:HG13	1:B:703:ALA:HA	1.93	0.51
1:E:680:LEU:CD2	3:E:2602:B12:H301	2.41	0.51
1:A:619:ILE:O	1:A:623:GLU:HG3	2.11	0.51
2:G:6:MET:HG3	2:G:56:TYR:CG	2.46	0.51
1:E:199:LEU:HB3	1:E:220:TYR:CD1	2.46	0.51
1:E:222:GLU:O	1:E:260:THR:OG1	2.29	0.51
1:A:472:LEU:HA	1:A:475:VAL:CG2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:MET:HE1	1:B:105:ILE:CD1	2.42	0.50
1:B:232:VAL:HG21	1:B:266:GLU:HA	1.92	0.50
1:E:483:PHE:HD1	1:E:486:ILE:HD13	1.75	0.50
1:E:713:VAL:HG11	1:F:374:MET:HE1	1.93	0.50
3:E:2601:B12:H332	1:F:677:ASN:ND2	2.09	0.50
1:A:133:MET:HE3	1:A:133:MET:HA	1.93	0.50
1:A:713:VAL:HG11	1:B:374:MET:HE1	1.92	0.50
1:B:681:PHE:HE1	1:B:711:VAL:HB	1.75	0.50
1:F:86:VAL:O	1:F:90:ARG:HG3	2.11	0.50
1:F:478:LEU:HD22	1:F:486:ILE:CG1	2.41	0.50
1:F:576:ARG:HH11	1:F:576:ARG:HG3	1.76	0.50
1:A:493:MET:CE	1:A:509:LEU:HD11	2.42	0.50
1:E:121:MET:HE2	1:E:126:MET:HG2	1.93	0.50
1:E:227:TYR:HB3	1:E:232:VAL:HG12	1.93	0.50
3:E:2601:B12:H351	3:E:2601:B12:H363	1.93	0.50
1:F:6:ARG:HG2	1:F:6:ARG:HH11	1.77	0.50
1:A:474:ILE:HG22	1:A:478:LEU:HD11	1.93	0.50
1:B:118:MET:HE1	1:B:121:MET:HE1	1.93	0.50
1:B:141:ASN:HB3	1:B:167:PHE:CD1	2.47	0.50
1:F:577:GLU:HB3	1:F:745:VAL:HG11	1.93	0.50
1:A:147:ASN:HD21	1:A:151:ASN:H	1.59	0.50
1:A:715:ASN:HD21	1:B:376:ALA:HA	1.76	0.50
1:B:224:VAL:HG21	1:B:257:MET:HE2	1.94	0.50
1:B:584:ASP:OD1	1:B:670:ARG:NH2	2.45	0.50
1:B:395:LEU:HB2	1:B:397:VAL:HG12	1.94	0.50
1:F:258:ARG:NH2	1:F:330:GLU:OE2	2.41	0.50
1:B:216:GLY:HA2	1:B:497:ARG:NH2	2.26	0.50
1:E:636:ARG:HD3	1:E:646:ASP:OD2	2.12	0.50
1:E:692:TYR:HA	1:E:695:ILE:HD12	1.92	0.50
1:A:7:PHE:HA	1:A:10:LEU:HB2	1.93	0.50
1:E:173:THR:OG1	3:E:2601:B12:C26	2.59	0.50
2:H:112:GLU:OE2	2:H:113:HIS:CE1	2.61	0.50
1:B:677:ASN:OD1	3:B:2601:B12:N33	2.45	0.49
1:E:269:MET:HE3	3:E:2601:B12:N52	2.20	0.49
1:E:493:MET:HE3	1:E:493:MET:HA	1.94	0.49
1:E:551:PRO:HG2	1:F:24:TRP:HB2	1.93	0.49
1:F:117:VAL:HG12	1:F:118:MET:HE2	1.93	0.49
1:A:577:GLU:HG3	1:A:745:VAL:HG11	1.94	0.49
1:E:237:ASP:O	2:G:95:ARG:HD3	2.12	0.49
2:G:63:GLN:N	2:G:63:GLN:OE1	2.45	0.49
1:A:171:GLU:OE2	1:A:203:SER:OG	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:49:ILE:HD13	2:C:54:LEU:HG	1.93	0.49
3:E:2601:B12:C10	3:E:2601:B12:N45	2.67	0.49
1:F:478:LEU:HD22	1:F:486:ILE:CD1	2.43	0.49
2:G:51:ARG:HG2	2:G:77:ALA:HB1	1.94	0.49
2:D:5:THR:HA	2:D:59:GLN:NE2	2.27	0.49
1:E:257:MET:HE1	1:E:259:TYR:CE1	2.47	0.49
2:C:101:GLN:HB2	2:C:137:LEU:HD21	1.94	0.49
1:E:644:ALA:HB1	1:E:668:HIS:HB2	1.95	0.49
2:G:139:LYS:HD2	2:G:140:GLY:H	1.77	0.49
1:A:395:LEU:HB3	1:B:123:VAL:HG11	1.93	0.49
1:A:636:ARG:NH1	1:A:646:ASP:OD1	2.46	0.49
1:B:308:GLY:O	1:B:345:ARG:NH2	2.44	0.49
1:E:147:ASN:HD21	1:E:151:ASN:N	2.10	0.49
1:E:333:SER:HB2	1:E:353:GLN:HG2	1.94	0.49
1:F:145:VAL:HG21	1:F:170:GLN:HG2	1.93	0.49
2:G:59:GLN:O	2:G:63:GLN:OE1	2.30	0.49
1:A:99:ARG:O	1:A:103:ILE:HG12	2.12	0.49
2:D:12:PRO:HD2	2:D:16:ARG:HG3	1.93	0.49
1:F:732:ILE:O	1:F:736:LYS:CE	2.61	0.49
2:H:45:GLN:HG3	2:H:45:GLN:O	2.12	0.49
2:D:10:ASP:HB3	2:D:17:CYS:SG	2.52	0.49
2:H:85:GLU:H	2:H:85:GLU:CD	2.21	0.49
1:A:690:GLU:O	1:A:694:GLN:HG2	2.12	0.49
1:B:292:GLY:HA3	2:D:72:ASN:HB2	1.94	0.49
1:E:213:GLY:HA3	1:E:255:LEU:HD11	1.95	0.49
1:E:301:VAL:HG22	1:E:334:ALA:HB2	1.95	0.49
1:E:302:SER:HB3	3:E:2601:B12:C53	2.14	0.49
1:F:576:ARG:HG3	1:F:576:ARG:NH1	2.27	0.49
1:F:686:LEU:HD21	1:F:719:VAL:HG22	1.92	0.49
1:F:118:MET:HG3	1:F:323:ILE:HD11	1.94	0.49
1:F:402:ARG:HG2	1:F:402:ARG:HH11	1.78	0.49
1:F:457:ASP:O	1:F:461:VAL:HG23	2.12	0.49
1:A:5:LYS:O	1:A:8:ALA:HB3	2.13	0.48
2:D:28:PRO:HG2	2:D:31:ASP:OD1	2.13	0.48
1:E:602:GLN:HE22	1:E:733:LYS:HB2	1.77	0.48
2:G:103:GLU:OE1	2:G:138:ARG:NH2	2.45	0.48
1:A:333:SER:HB2	1:A:353:GLN:HG2	1.95	0.48
1:A:376:ALA:HB2	3:B:2601:B12:H541	1.95	0.48
1:A:472:LEU:HD11	2:C:47:VAL:HG21	1.95	0.48
1:E:716:ASP:HB3	1:E:719:VAL:HG23	1.95	0.48
1:E:717:GLN:HB3	1:F:370:ASN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:232:VAL:HG23	1:F:271:TYR:HB2	1.96	0.48
2:H:11:TYR:HB3	2:H:12:PRO:HD3	1.95	0.48
2:G:23:THR:HG23	2:G:27:LYS:O	2.13	0.48
1:B:188:LEU:HD12	1:B:188:LEU:C	2.33	0.48
1:B:246:LEU:HD13	2:D:91:TYR:CD1	2.49	0.48
2:D:11:TYR:HA	2:D:60:ILE:HD13	1.95	0.48
2:D:17:CYS:C	2:D:19:GLU:OE1	2.56	0.48
3:E:2601:B12:H473	3:E:2601:B12:C50	2.43	0.48
1:F:316:ALA:O	1:F:320:GLU:OE1	2.31	0.48
1:F:573:LEU:HD21	1:F:619:ILE:HD12	1.95	0.48
3:B:2601:B12:H562	3:B:2601:B12:H4R	1.96	0.48
2:H:49:ILE:CD1	2:H:54:LEU:HG	2.44	0.48
1:B:588:ASP:OD1	1:B:588:ASP:N	2.30	0.48
1:E:43:LYS:HB3	1:E:51:GLU:HB3	1.94	0.48
1:A:56:ARG:HG3	1:A:56:ARG:NH1	2.28	0.48
1:A:366:SER:OG	1:A:368:VAL:O	2.28	0.48
1:B:43:LYS:HG3	1:B:51:GLU:HB3	1.95	0.48
1:E:395:LEU:HB2	1:E:397:VAL:HG12	1.96	0.48
1:A:56:ARG:NH1	1:A:59:GLN:OE1	2.47	0.48
1:A:73:ASN:O	1:A:77:THR:OG1	2.32	0.48
1:A:201:GLN:NE2	1:A:222:GLU:HB3	2.29	0.48
1:B:106:THR:CG2	1:B:326:MET:HE3	2.44	0.48
1:F:478:LEU:CD2	1:F:486:ILE:HD11	2.43	0.48
2:G:129:GLU:O	2:G:133:GLN:HG3	2.13	0.48
1:E:205:GLU:HA	3:E:2601:B12:H362	1.95	0.48
1:F:247:ALA:CB	1:F:257:MET:HE3	2.43	0.48
1:F:389:ASN:HA	1:F:392:GLN:HE21	1.78	0.48
2:G:135:HIS:C	2:G:136:LYS:HD3	2.39	0.48
2:H:24:PRO:HG2	2:H:48:ARG:HB2	1.96	0.48
1:A:355:LEU:HD22	1:B:123:VAL:HG21	1.96	0.47
1:A:586:ARG:HG3	1:A:589:GLU:HB3	1.96	0.47
1:B:573:LEU:HD23	1:B:751:LEU:HD23	1.94	0.47
1:B:585:GLU:HG3	1:B:630:ARG:CZ	2.43	0.47
2:D:6:MET:H	2:D:59:GLN:NE2	2.12	0.47
1:E:299:GLY:C	1:E:301:VAL:H	2.21	0.47
1:A:365:TYR:CE1	1:A:385:PHE:CE1	3.02	0.47
1:B:609:MET:HE1	1:B:688:THR:HA	1.96	0.47
1:E:224:VAL:HG11	1:E:257:MET:HE2	1.95	0.47
1:E:624:GLU:HB3	1:E:697:LYS:HZ1	1.76	0.47
1:F:392:GLN:HG2	1:F:399:GLY:H	1.79	0.47
1:F:732:ILE:O	1:F:736:LYS:HE3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:108:ALA:HA	2:D:111:LEU:HD12	1.96	0.47
1:E:123:VAL:O	1:E:127:MET:HG3	2.15	0.47
3:B:2601:B12:C2B	3:B:2601:B12:N23	2.78	0.47
1:E:174:VAL:HG21	1:E:177:ALA:HA	1.97	0.47
1:E:586:ARG:HH21	1:E:588:ASP:CG	2.22	0.47
1:F:261:SER:OG	1:F:262:GLY:N	2.45	0.47
1:A:352:MET:HE1	1:B:355:LEU:HD11	1.97	0.47
3:B:2601:B12:H2B	3:B:2601:B12:N23	2.30	0.47
2:C:35:GLU:CD	2:C:35:GLU:H	2.23	0.47
1:E:136:ARG:NH1	1:E:506:SER:HB3	2.29	0.47
1:F:142:GLN:NE2	1:F:169:GLU:OE1	2.47	0.47
1:A:67:ILE:HD13	1:A:286:PHE:HB3	1.97	0.47
1:B:600:LYS:HD2	1:B:601:HIS:CE1	2.50	0.47
1:E:351:LEU:HD23	1:E:354:MET:HE3	1.96	0.47
1:F:606:LEU:HD21	1:F:727:ALA:HA	1.95	0.47
1:F:641:SER:HB2	1:F:674:PRO:O	2.15	0.47
1:A:63:ILE:HB	1:A:283:ARG:HH21	1.79	0.47
1:B:136:ARG:HB2	1:B:506:SER:HB3	1.97	0.47
1:B:726:LYS:HA	1:B:729:LEU:HD12	1.97	0.47
2:D:6:MET:HG3	2:D:10:ASP:HB2	1.97	0.47
1:E:335:ASN:HD21	1:E:353:GLN:HB2	1.80	0.47
1:E:549:VAL:HG23	1:F:21:ILE:HG22	1.95	0.47
1:F:199:LEU:HD23	1:F:493:MET:HE1	1.96	0.47
1:F:323:ILE:O	1:F:327:LEU:HD23	2.14	0.47
1:A:132:LYS:HA	1:A:525:TYR:HB3	1.96	0.47
1:A:216:GLY:HA2	1:A:497:ARG:NH2	2.30	0.47
1:B:499:THR:HG22	2:D:29:LEU:HD11	1.97	0.47
2:C:55:GLU:OE2	2:C:74:ARG:NH1	2.45	0.47
2:C:70:ALA:O	2:C:74:ARG:HG3	2.14	0.47
1:F:142:GLN:HB3	1:F:363:SER:HA	1.97	0.47
1:F:194:GLY:HA2	1:F:412:ILE:HG12	1.96	0.47
1:A:143:CYS:SG	1:A:170:GLN:HG2	2.55	0.47
1:B:179:TYR:CE2	1:B:454:VAL:HG13	2.50	0.47
1:B:195:ARG:HD3	1:B:511:ARG:HG2	1.97	0.47
1:E:237:ASP:OD2	2:G:98:ARG:NH2	2.48	0.47
2:H:86:ARG:NH1	2:H:110:GLU:OE1	2.47	0.47
1:E:678:LEU:HD13	1:E:702:TYR:CD1	2.50	0.46
1:F:93:VAL:HG12	1:F:128:MET:CG	2.46	0.46
2:G:99:SER:HB3	2:G:104:LEU:HG	1.98	0.46
1:A:179:TYR:CE2	1:A:454:VAL:HG13	2.50	0.46
1:A:475:VAL:HG13	1:A:487:ALA:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:ALA:HB3	1:B:437:VAL:HG13	1.97	0.46
1:E:573:LEU:HD21	1:E:749:ILE:HG23	1.96	0.46
1:A:431:PRO:O	1:A:452:ARG:NH2	2.46	0.46
1:A:442:TYR:CE2	1:B:2:LYS:HE2	2.51	0.46
2:D:32:ILE:HD12	2:D:32:ILE:N	2.29	0.46
1:F:134:ARG:NH1	1:F:357:GLY:O	2.40	0.46
1:F:573:LEU:CD1	1:F:616:LYS:HG3	2.38	0.46
1:A:115:VAL:HG11	1:A:279:TYR:HA	1.97	0.46
1:A:224:VAL:HG11	1:A:259:TYR:CE1	2.50	0.46
1:A:582:SER:O	1:A:630:ARG:NH1	2.29	0.46
2:D:85:GLU:H	2:D:85:GLU:CD	2.24	0.46
1:E:133:MET:SD	1:E:326:MET:HB3	2.55	0.46
1:F:182:PHE:CD1	1:F:461:VAL:HG22	2.50	0.46
1:F:206:GLU:OE2	1:F:243:LYS:NZ	2.47	0.46
2:G:6:MET:HG3	2:G:56:TYR:CD1	2.49	0.46
2:H:129:GLU:O	2:H:133:GLN:HG3	2.16	0.46
1:A:619:ILE:HG23	1:A:629:ALA:HB3	1.98	0.46
1:B:94:ASP:OD1	1:B:95:ILE:N	2.49	0.46
1:B:504:GLN:HG3	2:D:11:TYR:CE1	2.46	0.46
1:E:701:ARG:HD2	1:E:708:PRO:HB3	1.96	0.46
1:F:253:ARG:NH2	2:H:82:ILE:O	2.44	0.46
2:D:19:GLU:OE2	2:H:9:GLN:HB3	2.16	0.46
1:E:718:MET:C	1:E:721:PRO:HD2	2.41	0.46
1:F:265:SER:O	1:F:269:MET:HG3	2.15	0.46
1:A:398:ASP:CG	1:A:538:ARG:HE	2.23	0.46
3:A:2601:B12:H561	3:A:2601:B12:C53	2.44	0.46
1:B:98:SER:O	1:B:102:ILE:HG13	2.15	0.46
1:B:539:TRP:O	1:B:543:LYS:HG3	2.16	0.46
1:E:63:ILE:HG12	1:E:287:ILE:HD11	1.98	0.46
1:E:600:LYS:HD3	1:E:601:HIS:NE2	2.31	0.46
1:A:145:VAL:HB	1:A:187:LEU:HD11	1.98	0.46
1:A:484:GLU:OE1	1:A:484:GLU:N	2.45	0.46
1:B:224:VAL:HG13	1:B:246:LEU:HD23	1.97	0.46
2:C:56:TYR:O	2:C:60:ILE:HG12	2.16	0.46
1:E:258:ARG:NE	1:E:330:GLU:OE1	2.41	0.46
1:F:143:CYS:SG	1:F:170:GLN:HG3	2.56	0.46
1:F:232:VAL:HG21	1:F:266:GLU:HA	1.98	0.46
2:G:99:SER:CB	2:G:104:LEU:HD21	2.46	0.46
1:A:571:PHE:HD1	1:A:571:PHE:H	1.63	0.46
1:E:222:GLU:HG3	1:E:258:ARG:HD2	1.98	0.46
3:E:2602:B12:H562	3:E:2602:B12:H541	1.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:609:MET:HE1	1:F:688:THR:HA	1.98	0.46
2:G:20:HIS:HB3	2:G:56:TYR:HE2	1.80	0.46
1:A:500:GLY:HA2	1:A:503:LEU:HD13	1.98	0.46
1:A:526:GLN:HB2	1:A:530:THR:HG21	1.98	0.46
1:B:106:THR:C	1:B:108:ALA:N	2.67	0.46
2:C:11:TYR:C	2:C:13:LEU:HD12	2.41	0.46
2:H:62:GLU:OE2	2:H:74:ARG:NH2	2.47	0.46
1:A:42:VAL:HG21	1:A:77:THR:HG21	1.98	0.45
1:B:141:ASN:ND2	1:B:399:GLY:O	2.49	0.45
1:E:252:SER:OG	1:E:253:ARG:NH1	2.38	0.45
1:F:436:GLU:OE1	1:F:452:ARG:NH1	2.49	0.45
1:A:533:ARG:HA	1:A:533:ARG:HD3	1.83	0.45
1:A:667:ILE:HB	1:A:679:GLU:HB2	1.97	0.45
2:D:59:GLN:O	2:D:63:GLN:HG2	2.15	0.45
1:E:574:LYS:HG2	1:E:575:THR:N	2.30	0.45
1:F:343:ASP:HA	1:F:346:ARG:HG2	1.99	0.45
1:F:346:ARG:HH12	1:F:384:ASP:CG	2.24	0.45
1:E:393:ARG:HH12	1:F:20:LEU:HD12	1.81	0.45
3:E:2601:B12:H351	3:E:2601:B12:C36	2.46	0.45
1:F:317:VAL:O	1:F:320:GLU:HG2	2.16	0.45
1:A:201:GLN:HE22	1:A:222:GLU:HB3	1.81	0.45
1:A:495:ARG:NH1	2:C:32:ILE:O	2.49	0.45
3:B:2601:B12:H2B	3:B:2601:B12:C15	2.47	0.45
1:E:24:TRP:HB2	1:F:551:PRO:HG2	1.97	0.45
1:E:232:VAL:HG11	1:E:266:GLU:HG3	1.98	0.45
1:B:146:THR:OG1	1:B:372:ASP:O	2.34	0.45
2:C:129:GLU:O	2:C:133:GLN:HG3	2.17	0.45
1:F:83:LEU:O	1:F:113:LYS:NZ	2.38	0.45
2:G:8:VAL:HG21	2:G:64:MET:HE3	1.98	0.45
1:A:492:ASN:HA	1:A:495:ARG:HD3	1.97	0.45
1:B:63:ILE:HG23	1:B:287:ILE:HD11	1.99	0.45
1:B:89:ALA:O	1:B:93:VAL:HG22	2.17	0.45
1:B:283:ARG:O	1:B:287:ILE:HG13	2.17	0.45
1:B:694:GLN:HE22	1:B:697:LYS:HE3	1.82	0.45
1:A:98:SER:OG	1:A:101:GLU:HG3	2.17	0.45
1:A:299:GLY:C	1:A:301:VAL:N	2.73	0.45
1:A:386:ASP:O	1:A:390:ILE:HG13	2.17	0.45
3:B:2601:B12:C10	3:B:2601:B12:H422	2.47	0.45
3:B:2601:B12:H301	3:B:2601:B12:H253	1.50	0.45
1:F:216:GLY:HA2	1:F:497:ARG:HH22	1.79	0.45
3:A:2601:B12:H203	3:A:2601:B12:H302	1.93	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2601:B12:C49	3:B:2601:B12:H473	2.47	0.45
1:E:241:TRP:CZ2	2:G:130:VAL:HG21	2.51	0.45
1:E:321:ASN:HD22	1:E:353:GLN:HE21	1.64	0.45
1:F:532:TYR:O	1:F:533:ARG:HD2	2.16	0.45
2:H:13:LEU:HB3	2:H:21:ILE:HD11	1.98	0.45
1:B:43:LYS:HG3	1:B:51:GLU:OE1	2.17	0.45
1:B:81:MET:SD	1:B:110:THR:HG23	2.57	0.45
1:F:172:THR:HB	1:F:187:LEU:HD22	1.99	0.45
1:A:259:TYR:CZ	1:A:293:VAL:HG21	2.52	0.45
1:A:334:ALA:C	1:A:336:ASP:N	2.68	0.45
1:A:644:ALA:HB1	1:A:668:HIS:HB2	1.99	0.45
1:B:299:GLY:C	1:B:301:VAL:H	2.24	0.45
1:B:522:ILE:H	1:B:522:ILE:CD1	2.27	0.45
2:D:132:GLN:HA	2:D:137:LEU:HD21	1.99	0.45
1:E:662:LYS:NZ	3:E:2602:B12:O5	2.50	0.45
1:F:115:VAL:HG11	1:F:278:LEU:HG	1.98	0.45
1:F:24:TRP:HB3	1:F:29:LEU:HB2	1.99	0.44
1:F:471:GLY:O	1:F:475:VAL:HG23	2.17	0.44
1:B:134:ARG:HD3	1:B:357:GLY:O	2.18	0.44
1:E:148:LEU:HB2	1:E:372:ASP:OD1	2.18	0.44
1:E:384:ASP:O	1:E:387:ASP:HB2	2.17	0.44
1:A:193:CYS:SG	1:A:486:ILE:HD12	2.58	0.44
1:F:668:HIS:NE2	1:F:676:SER:O	2.51	0.44
2:H:36:LYS:NZ	2:H:41:GLU:OE2	2.44	0.44
1:A:161:GLU:O	1:A:165:ARG:HG3	2.17	0.44
1:A:269:MET:CE	3:B:2601:B12:N45	2.79	0.44
1:A:609:MET:HE3	1:A:609:MET:HB2	1.69	0.44
1:E:159:ALA:HB1	1:E:170:GLN:HE22	1.83	0.44
1:E:690:GLU:H	1:E:690:GLU:CD	2.21	0.44
1:F:343:ASP:OD1	1:F:346:ARG:NH2	2.46	0.44
3:A:2601:B12:H621	3:A:2601:B12:H18	1.64	0.44
1:B:649:ASN:HA	1:B:670:ARG:HG3	1.99	0.44
1:E:6:ARG:NH1	1:F:161:GLU:OE2	2.50	0.44
1:E:30:ILE:HG21	1:E:34:SER:HB2	2.00	0.44
1:E:134:ARG:HD3	1:E:357:GLY:O	2.17	0.44
1:E:151:ASN:HA	1:E:152:PRO:HD3	1.85	0.44
1:E:281:GLU:HG2	1:E:320:GLU:HB2	1.99	0.44
1:E:426:GLU:OE2	1:E:480:ARG:HB2	2.16	0.44
1:E:444:HIS:O	1:F:6:ARG:NH2	2.50	0.44
1:E:722:LYS:HG3	1:F:341:HIS:CE1	2.52	0.44
1:F:362:PHE:HE1	1:F:388:TYR:CZ	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:464:MET:HG2	1:F:469:ILE:HG13	1.99	0.44
1:A:51:GLU:C	1:A:51:GLU:OE1	2.61	0.44
1:A:675:LEU:HD22	3:A:2601:B12:H411	2.00	0.44
2:G:99:SER:HB2	2:G:104:LEU:HD21	1.99	0.44
1:A:645:TRP:O	1:A:649:ASN:ND2	2.38	0.44
1:B:645:TRP:HB2	1:B:668:HIS:CE1	2.53	0.44
3:B:2601:B12:H261	3:B:2601:B12:H91	1.69	0.44
1:A:34:SER:HB2	1:A:276:SER:HB3	2.00	0.44
1:A:728:ALA:HB2	1:B:306:MET:SD	2.58	0.44
1:B:133:MET:HG3	1:B:326:MET:HB3	1.99	0.44
1:B:606:LEU:CD2	1:B:726:LYS:HG2	2.38	0.44
1:E:153:VAL:HG22	1:E:432:ILE:HD13	1.99	0.44
1:F:389:ASN:O	1:F:392:GLN:HB2	2.17	0.44
1:A:387:ASP:O	1:A:391:LEU:HG	2.18	0.44
1:B:259:TYR:HB2	1:B:288:THR:HG23	2.00	0.44
2:C:97:PHE:CE1	2:C:136:LYS:HA	2.51	0.44
1:E:680:LEU:HD21	3:E:2602:B12:C20	2.44	0.44
3:E:2602:B12:H541	3:E:2602:B12:H602	1.35	0.44
1:B:317:VAL:HA	1:B:320:GLU:OE1	2.18	0.43
1:B:476:GLY:HA2	2:D:38:LEU:HD21	2.00	0.43
1:B:686:LEU:HD21	1:B:719:VAL:HG21	1.98	0.43
2:C:12:PRO:HD2	2:C:16:ARG:HD2	2.00	0.43
1:E:510:ASP:OD1	1:E:510:ASP:N	2.46	0.43
1:A:311:PRO:HD3	1:B:393:ARG:NH2	2.33	0.43
1:E:273:GLU:O	1:E:275:LYS:NZ	2.51	0.43
1:E:483:PHE:CD1	1:E:486:ILE:HD13	2.53	0.43
1:E:533:ARG:HH12	1:F:122:ASN:ND2	2.16	0.43
1:A:640:VAL:HB	1:A:660:GLN:NE2	2.33	0.43
1:B:643:MET:HE1	1:B:659:ILE:O	2.18	0.43
1:E:624:GLU:CD	1:E:697:LYS:NZ	2.76	0.43
1:F:182:PHE:O	1:F:185:LEU:HB3	2.18	0.43
1:F:201:GLN:OE1	1:F:222:GLU:HG2	2.18	0.43
1:F:213:GLY:O	1:F:497:ARG:NH2	2.51	0.43
1:F:323:ILE:O	1:F:326:MET:HG2	2.18	0.43
1:F:643:MET:HE1	1:F:660:GLN:HG3	1.99	0.43
1:F:644:ALA:HB1	1:F:668:HIS:HB2	1.99	0.43
1:A:83:LEU:HD13	1:A:91:MET:HE1	2.01	0.43
1:A:154:GLN:NE2	1:A:158:ASP:OD2	2.50	0.43
1:A:169:GLU:HG2	1:A:199:LEU:HB2	2.00	0.43
1:B:313:GLY:O	1:B:317:VAL:HG23	2.19	0.43
2:C:9:GLN:O	2:C:16:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:574:LYS:HG2	1:E:575:THR:H	1.82	0.43
1:F:48:LEU:HD21	1:F:57:ARG:CZ	2.49	0.43
1:F:73:ASN:O	1:F:77:THR:HB	2.18	0.43
1:F:307:THR:O	1:F:313:GLY:HA3	2.18	0.43
1:A:268:LEU:HD21	3:B:2601:B12:H5R2	2.00	0.43
1:A:444:HIS:ND1	1:B:6:ARG:HD3	2.34	0.43
1:B:253:ARG:HH21	2:D:84:ASP:HA	1.83	0.43
1:B:586:ARG:HH21	1:B:588:ASP:CG	2.26	0.43
1:B:664:THR:HG21	3:B:2601:B12:H2R	2.00	0.43
2:C:98:ARG:O	2:C:138:ARG:NH2	2.38	0.43
1:E:173:THR:HG23	1:E:174:VAL:N	2.33	0.43
1:E:444:HIS:CE1	1:F:6:ARG:HE	2.36	0.43
1:E:602:GLN:NE2	1:E:733:LYS:CB	2.82	0.43
1:F:717:GLN:HG3	1:F:718:MET:HE2	2.00	0.43
1:E:224:VAL:HG11	1:E:257:MET:CE	2.48	0.43
1:E:321:ASN:ND2	1:E:353:GLN:HE21	2.17	0.43
1:A:67:ILE:HD13	1:A:286:PHE:HB2	2.01	0.43
1:A:458:LEU:O	1:A:461:VAL:HG12	2.19	0.43
1:B:649:ASN:O	1:B:670:ARG:NH2	2.52	0.43
1:E:106:THR:HG21	1:E:326:MET:HB2	1.99	0.43
1:F:132:LYS:HA	1:F:525:TYR:HB3	2.01	0.43
1:B:91:MET:HE1	1:B:105:ILE:HD12	1.99	0.43
3:B:2601:B12:H562	3:B:2601:B12:O2	2.18	0.43
1:F:189:VAL:HG21	1:F:423:VAL:HG21	2.01	0.43
1:B:494:LEU:HB3	2:D:47:VAL:HG11	2.00	0.43
1:E:417:ALA:HB1	1:E:437:VAL:HG22	1.99	0.43
1:F:99:ARG:O	1:F:103:ILE:HG12	2.18	0.43
1:F:263:THR:HG23	1:F:281:GLU:HG3	1.99	0.43
2:H:47:VAL:HG23	2:H:47:VAL:O	2.18	0.43
1:B:54:GLY:C	1:B:55:LYS:HD3	2.43	0.43
1:E:73:ASN:HD22	1:E:75:GLU:H	1.67	0.43
1:E:492:ASN:HD22	1:E:492:ASN:HA	1.60	0.43
2:H:49:ILE:O	2:H:80:ILE:HD13	2.19	0.43
1:A:137:ARG:HG3	1:A:523:ASN:HA	2.00	0.42
1:A:263:THR:HB	1:A:277:MET:HB3	2.01	0.42
1:A:349:ARG:CD	1:A:349:ARG:C	2.92	0.42
1:E:502:TYR:HA	1:E:507:ALA:HB1	2.01	0.42
1:F:294:GLN:OE1	1:F:330:GLU:OE1	2.36	0.42
1:F:314:ILE:HG23	1:F:349:ARG:HG2	2.00	0.42
1:A:65:ARG:NH1	2:C:130:VAL:HG22	2.34	0.42
1:A:141:ASN:HB3	1:A:167:PHE:CD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ARG:HD2	1:A:379:ASN:O	2.20	0.42
1:B:61:ASP:HB2	1:B:230:GLU:CD	2.44	0.42
1:B:398:ASP:OD2	1:B:532:TYR:OH	2.23	0.42
1:E:375:PHE:CA	3:E:2601:B12:H602	2.20	0.42
1:E:391:LEU:HD23	1:E:391:LEU:HA	1.82	0.42
1:E:682:SER:HB3	3:E:2602:B12:H201	2.01	0.42
1:A:223:THR:HA	1:A:260:THR:OG1	2.19	0.42
1:A:335:ASN:HD21	1:A:353:GLN:HB2	1.83	0.42
1:A:690:GLU:OE1	1:A:690:GLU:HA	2.18	0.42
1:A:720:ARG:CZ	1:B:337:GLN:HB3	2.49	0.42
2:D:54:LEU:HD23	2:D:54:LEU:HA	1.93	0.42
1:E:573:LEU:CD2	1:E:615:LEU:HD23	2.50	0.42
1:E:609:MET:HE3	1:E:614:ILE:HD11	2.01	0.42
1:F:130:LEU:HD11	1:F:358:THR:HG22	2.02	0.42
1:F:148:LEU:HD23	1:F:148:LEU:HA	1.87	0.42
1:B:81:MET:HE1	1:B:113:LYS:HB2	2.01	0.42
1:B:194:GLY:HA2	1:B:412:ILE:HG12	2.00	0.42
3:B:2601:B12:H4R	3:B:2601:B12:C56	2.49	0.42
1:E:369:PRO:HG3	1:E:444:HIS:CD2	2.54	0.42
1:E:637:THR:HG21	1:E:642:PHE:HB2	2.00	0.42
1:F:143:CYS:HB3	1:F:167:PHE:CE1	2.55	0.42
2:G:64:MET:HA	2:G:64:MET:HE2	2.01	0.42
1:B:88:ILE:O	1:B:92:LEU:HG	2.20	0.42
1:F:539:TRP:NE1	1:F:543:LYS:HD3	2.35	0.42
1:A:694:GLN:NE2	1:A:694:GLN:HA	2.35	0.42
1:B:158:ASP:HA	1:B:413:ARG:HH12	1.84	0.42
1:E:693:ARG:O	1:E:697:LYS:HG3	2.19	0.42
2:H:49:ILE:HG13	2:H:53:THR:HB	2.01	0.42
1:A:669:GLN:HB3	1:A:672:LEU:HD12	2.01	0.42
3:B:2601:B12:H541	3:B:2601:B12:H602	1.86	0.42
1:E:299:GLY:HA2	1:E:317:VAL:HG13	2.00	0.42
1:F:681:PHE:CZ	1:F:695:ILE:HG12	2.54	0.42
1:A:259:TYR:CE2	1:A:293:VAL:HG21	2.55	0.42
1:B:586:ARG:NH2	1:B:588:ASP:OD1	2.52	0.42
1:A:683:GLN:OE1	1:A:715:ASN:HA	2.20	0.42
1:B:246:LEU:HD13	2:D:91:TYR:CE1	2.55	0.42
2:D:78:GLU:HB2	2:D:120:ASN:ND2	2.34	0.42
1:E:56:ARG:NH1	1:E:58:ASP:OD1	2.42	0.42
3:E:2601:B12:H2B	3:E:2601:B12:H492	2.01	0.42
1:F:551:PRO:HA	1:F:554:ILE:HD12	2.01	0.42
1:A:210:LEU:O	1:A:214:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:ASP:HB3	1:B:719:VAL:HG23	2.02	0.42
1:E:366:SER:HB3	1:E:381:ASP:HA	2.00	0.42
1:E:573:LEU:HD13	1:E:616:LYS:HA	2.02	0.42
1:A:721:PRO:O	1:B:19:GLY:N	2.49	0.41
3:B:2601:B12:H363	3:B:2601:B12:H412	1.49	0.41
2:C:11:TYR:HA	2:C:13:LEU:HD12	2.01	0.41
1:E:136:ARG:NH2	1:E:359:ASP:O	2.53	0.41
1:E:146:THR:OG1	1:E:374:MET:HG2	2.20	0.41
1:F:146:THR:HB	1:F:374:MET:HG2	2.02	0.41
1:F:496:GLN:HG3	1:F:509:LEU:HD11	2.01	0.41
1:A:42:VAL:HG11	1:A:77:THR:HG22	2.02	0.41
1:A:324:ALA:O	1:A:329:LEU:HB2	2.20	0.41
1:B:215:ARG:NH2	1:B:465:MET:O	2.53	0.41
2:C:59:GLN:O	2:C:63:GLN:HG2	2.20	0.41
1:E:504:GLN:HG3	2:G:11:TYR:CE1	2.55	0.41
1:F:526:GLN:HB3	1:F:530:THR:HG21	2.02	0.41
1:F:658:GLY:O	1:F:665:THR:HA	2.19	0.41
3:A:2601:B12:C2B	3:A:2601:B12:H492	2.50	0.41
1:B:77:THR:HA	1:B:108:ALA:HB1	2.02	0.41
1:B:106:THR:O	1:B:109:ILE:HG12	2.20	0.41
1:E:348:ALA:HA	1:F:351:LEU:HD11	2.03	0.41
1:E:160:ALA:HB2	1:E:416:ALA:HB2	2.02	0.41
1:E:339:PHE:C	1:F:721:PRO:HB3	2.45	0.41
1:E:340:SER:O	1:E:346:ARG:NH2	2.52	0.41
1:F:171:GLU:HG2	1:F:375:PHE:CZ	2.56	0.41
1:A:118:MET:HE1	1:A:322:LEU:HG	2.03	0.41
1:A:376:ALA:CB	3:B:2601:B12:H541	2.50	0.41
1:B:136:ARG:HE	1:B:506:SER:HB3	1.84	0.41
1:B:526:GLN:N	1:B:530:THR:OG1	2.45	0.41
1:E:128:MET:HE1	1:E:525:TYR:OH	2.21	0.41
1:F:504:GLN:HG3	2:H:11:TYR:CE1	2.55	0.41
2:H:103:GLU:O	2:H:107:ILE:CD1	2.69	0.41
1:A:146:THR:OG1	1:A:373:ASN:HA	2.21	0.41
1:A:681:PHE:CZ	1:A:695:ILE:HG12	2.56	0.41
1:B:543:LYS:HB2	1:B:543:LYS:HE2	1.91	0.41
1:E:132:LYS:HA	1:E:525:TYR:HB3	2.02	0.41
1:E:299:GLY:CA	1:E:317:VAL:HG13	2.51	0.41
1:F:201:GLN:HG2	1:F:202:CYS:N	2.35	0.41
1:A:193:CYS:O	1:A:412:ILE:HD11	2.20	0.41
1:A:334:ALA:HA	1:A:363:SER:OG	2.20	0.41
1:E:386:ASP:OD1	1:F:10:LEU:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:2601:B12:N22	3:E:2601:B12:H422	2.25	0.41
1:F:209:GLU:OE2	1:F:221:ALA:HB1	2.21	0.41
1:F:306:MET:HE3	1:F:306:MET:HB3	1.79	0.41
1:B:32:MET:HE3	1:B:278:LEU:HD23	2.02	0.41
1:B:227:TYR:HB3	1:B:232:VAL:HG12	2.03	0.41
1:B:415:LYS:HZ1	1:B:486:ILE:HD11	1.86	0.41
1:E:140:SER:OG	1:E:168:SER:OG	2.22	0.41
1:F:573:LEU:HD22	1:F:616:LYS:N	2.34	0.41
2:G:95:ARG:HB2	2:G:98:ARG:HG3	2.01	0.41
1:A:609:MET:HG2	1:A:614:ILE:HD11	2.03	0.41
2:C:55:GLU:CD	2:C:74:ARG:NH1	2.79	0.41
2:D:9:GLN:OE1	2:D:9:GLN:N	2.49	0.41
1:E:83:LEU:O	1:E:113:LYS:NZ	2.53	0.41
1:F:321:ASN:ND2	1:F:333:SER:HB2	2.36	0.41
1:F:332:ALA:HB1	1:F:363:SER:HB2	2.03	0.41
1:F:420:ILE:HD12	1:F:420:ILE:HA	1.86	0.41
1:F:538:ARG:O	1:F:542:ILE:HG13	2.20	0.41
2:G:10:ASP:O	2:G:13:LEU:HD23	2.21	0.41
2:G:59:GLN:O	2:G:62:GLU:HB2	2.21	0.41
2:G:135:HIS:O	2:G:136:LYS:HD3	2.20	0.41
1:E:255:LEU:HD23	1:E:255:LEU:HA	1.80	0.41
1:E:257:MET:SD	1:E:257:MET:C	3.04	0.41
1:E:279:TYR:CE2	1:E:283:ARG:HD2	2.55	0.41
3:E:2601:B12:HM63	3:E:2601:B12:HM51	1.92	0.41
1:A:179:TYR:HE2	1:A:454:VAL:HG13	1.86	0.40
3:A:2601:B12:C19	3:A:2601:B12:C27	2.99	0.40
1:B:40:SER:HB2	1:B:81:MET:HE1	2.02	0.40
1:E:199:LEU:HB3	1:E:220:TYR:CE1	2.57	0.40
1:E:286:PHE:CE1	1:E:327:LEU:HD21	2.55	0.40
1:E:503:LEU:HD23	1:E:503:LEU:HA	1.88	0.40
1:F:143:CYS:HB3	1:F:167:PHE:CD1	2.55	0.40
2:G:21:ILE:C	2:G:22:LEU:HD12	2.46	0.40
1:A:224:VAL:CG1	1:A:259:TYR:CE1	3.04	0.40
1:B:121:MET:HB3	1:B:125:GLU:HB3	2.03	0.40
2:D:92:ASN:O	2:D:98:ARG:HG3	2.20	0.40
1:E:715:ASN:HB3	1:F:148:LEU:HD21	2.03	0.40
1:F:337:GLN:HE22	1:F:375:PHE:HB3	1.86	0.40
1:F:478:LEU:HD22	1:F:486:ILE:HG13	2.02	0.40
1:B:720:ARG:HB3	1:B:721:PRO:HD3	2.01	0.40
2:C:90:ILE:HG12	2:C:107:ILE:CG2	2.52	0.40
1:E:591:VAL:HA	1:E:630:ARG:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:294:GLN:CD	1:F:330:GLU:OE1	2.64	0.40
1:F:643:MET:HE1	1:F:660:GLN:CG	2.51	0.40
1:A:408:GLU:H	1:A:408:GLU:HG2	1.63	0.40
2:C:22:LEU:HD23	2:C:26:GLY:HA2	2.03	0.40
1:E:228:GLY:O	1:E:283:ARG:NH1	2.54	0.40
1:E:317:VAL:O	1:E:320:GLU:HG2	2.22	0.40
1:E:678:LEU:HD13	1:E:702:TYR:CZ	2.57	0.40
1:F:62:MET:HE2	1:F:230:GLU:HG2	2.04	0.40
1:F:98:SER:HB3	1:F:526:GLN:HE22	1.87	0.40
2:G:35:GLU:H	2:G:35:GLU:CD	2.29	0.40
1:A:127:MET:O	1:A:356:PRO:HB3	2.21	0.40
1:A:254:GLY:O	1:A:497:ARG:HA	2.21	0.40
3:A:2601:B12:H482	3:A:2601:B12:H473	1.78	0.40
1:B:117:VAL:O	1:B:121:MET:HE2	2.22	0.40
1:B:667:ILE:HG13	1:B:681:PHE:HE2	1.86	0.40
2:G:72:ASN:C	2:G:72:ASN:ND2	2.78	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	733/754 (97%)	702 (96%)	29 (4%)	2 (0%)	36	64
1	B	732/754 (97%)	698 (95%)	32 (4%)	2 (0%)	36	64
1	E	733/754 (97%)	692 (94%)	36 (5%)	5 (1%)	18	46
1	F	735/754 (98%)	701 (95%)	31 (4%)	3 (0%)	30	58
2	C	137/141 (97%)	131 (96%)	5 (4%)	1 (1%)	18	46
2	D	136/141 (96%)	128 (94%)	8 (6%)	0	100	100
2	G	135/141 (96%)	127 (94%)	7 (5%)	1 (1%)	18	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	136/141 (96%)	131 (96%)	2 (2%)	3 (2%)	5 19
All	All	3477/3580 (97%)	3310 (95%)	150 (4%)	17 (0%)	24 53

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	12	PRO
2	H	12	PRO
1	A	301	VAL
1	A	364	GLY
1	E	223	THR
1	E	544	ASN
2	G	12	PRO
2	H	11	TYR
1	E	364	GLY
1	F	364	GLY
1	B	364	GLY
1	F	301	VAL
1	B	301	VAL
1	E	301	VAL
2	H	47	VAL
1	F	569	PRO
1	E	551	PRO

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	588/619 (95%)	584 (99%)	4 (1%)	76 91
1	B	600/619 (97%)	595 (99%)	5 (1%)	73 89
1	E	594/619 (96%)	586 (99%)	8 (1%)	61 84
1	F	599/619 (97%)	595 (99%)	4 (1%)	76 91
2	C	115/120 (96%)	115 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	117/120 (98%)	115 (98%)	2 (2%)	53	80
2	G	115/120 (96%)	114 (99%)	1 (1%)	70	88
2	H	116/120 (97%)	116 (100%)	0	100	100
All	All	2844/2956 (96%)	2820 (99%)	24 (1%)	73	89

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	PHE
1	A	384	ASP
1	A	502	TYR
1	A	573	LEU
1	B	42	VAL
1	B	174	VAL
1	B	233	PHE
1	B	502	TYR
1	B	664	THR
2	D	15	THR
2	D	39	SER
1	E	73	ASN
1	E	88	ILE
1	E	153	VAL
1	E	469	ILE
1	E	502	TYR
1	E	520	ASN
1	E	570	SER
1	E	736	LYS
1	F	153	VAL
1	F	179	TYR
1	F	412	ILE
1	F	502	TYR
2	G	30	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	120	GLN
1	A	142	GLN
1	A	151	ASN

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Mol	Chain	Res	Type
1	A	297	GLN
1	A	321	ASN
1	A	353	GLN
1	A	604	HIS
1	A	677	ASN
1	A	694	GLN
1	A	715	ASN
1	B	79	GLN
1	B	131	GLN
1	B	142	GLN
1	B	468	ASN
1	B	604	HIS
1	B	668	HIS
1	B	694	GLN
2	C	59	GLN
2	C	63	GLN
2	C	92	ASN
2	D	59	GLN
2	D	63	GLN
2	D	65	GLN
1	E	73	ASN
1	E	170	GLN
1	E	321	ASN
1	E	337	GLN
1	E	492	ASN
1	F	59	GLN
1	F	73	ASN
1	F	321	ASN
1	F	335	ASN
1	F	414	GLN
1	F	748	HIS
2	G	72	ASN
2	G	113	HIS
2	G	133	GLN
2	H	120	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)

4 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	B	2601	-	93,101,101	1.31	9 (9%)	146,166,166	1.93	21 (14%)
3	B12	E	2602	-	93,101,101	1.50	13 (13%)	146,166,166	2.09	41 (28%)
3	B12	E	2601	1	93,101,101	1.38	11 (11%)	146,166,166	1.71	32 (21%)
3	B12	A	2601	-	93,101,101	1.61	13 (13%)	146,166,166	2.83	48 (32%)

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	B	2601	-	-	22/56/223/223	0/3/11/11
3	B12	E	2602	-	-	17/56/223/223	0/3/11/11
3	B12	E	2601	1	-	24/56/223/223	0/3/11/11
3	B12	A	2601	-	-	20/56/223/223	0/3/11/11

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2601	B12	C14-N23	-5.92	1.27	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2601	B12	C14-N23	5.61	1.42	1.35
3	E	2601	B12	C14-N23	5.57	1.42	1.35
3	A	2601	B12	C1-C19	-5.15	1.44	1.55
3	E	2602	B12	C14-N23	-4.71	1.29	1.35
3	B	2601	B12	C8B-C9B	4.58	1.48	1.40
3	A	2601	B12	C8B-C9B	4.57	1.48	1.40
3	E	2602	B12	C9B-N3B	-4.49	1.31	1.39
3	E	2602	B12	C8B-C9B	4.18	1.47	1.40
3	E	2601	B12	C1-C2	-4.12	1.49	1.58
3	E	2601	B12	C8B-C9B	4.11	1.47	1.40
3	A	2601	B12	C16-C15	-3.86	1.33	1.44
3	A	2601	B12	C9B-N3B	-3.77	1.32	1.39
3	E	2601	B12	C9B-N3B	-3.71	1.33	1.39
3	E	2602	B12	C9-N22	3.49	1.39	1.30
3	A	2601	B12	C9-N22	3.48	1.39	1.30
3	E	2602	B12	C2B-N1B	-3.22	1.31	1.37
3	A	2601	B12	C1-C2	-3.20	1.51	1.58
3	E	2601	B12	C8B-N1B	-3.17	1.33	1.39
3	B	2601	B12	C8B-N1B	-3.15	1.33	1.39
3	E	2601	B12	C6B-C5B	3.12	1.48	1.40
3	B	2601	B12	C6B-C5B	3.06	1.48	1.40
3	B	2601	B12	C9B-N3B	-3.04	1.34	1.39
3	E	2602	B12	C20-C1	-3.03	1.47	1.53
3	A	2601	B12	C6B-C5B	3.00	1.48	1.40
3	E	2602	B12	C8B-N1B	-2.99	1.33	1.39
3	A	2601	B12	C11-N23	-2.99	1.31	1.37
3	E	2602	B12	C16-C15	-2.97	1.36	1.44
3	E	2601	B12	C6-C5	2.96	1.44	1.36
3	E	2601	B12	C9-N22	2.95	1.38	1.30
3	A	2601	B12	C8B-N1B	-2.91	1.33	1.39
3	B	2601	B12	C9-N22	2.91	1.38	1.30
3	A	2601	B12	C10-C9	2.82	1.47	1.39
3	E	2602	B12	C6B-C5B	2.69	1.47	1.40
3	E	2602	B12	C4B-C5B	-2.68	1.35	1.39
3	E	2601	B12	C19-N24	2.68	1.53	1.48
3	E	2602	B12	C19-N24	2.67	1.53	1.48
3	B	2601	B12	C18-C19	-2.67	1.48	1.53
3	E	2601	B12	C2B-N1B	-2.52	1.33	1.37
3	A	2601	B12	C8-C9	-2.51	1.45	1.51
3	B	2601	B12	C2B-N1B	-2.41	1.33	1.37
3	A	2601	B12	C2B-N1B	-2.38	1.33	1.37
3	E	2602	B12	C10-C11	-2.28	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2602	B12	C14-C15	2.26	1.48	1.38
3	B	2601	B12	C11-N23	2.12	1.41	1.37
3	E	2601	B12	C11-N23	2.11	1.41	1.37

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2601	B12	C1-C19-N24	17.49	125.92	106.24
3	B	2601	B12	C1-C19-N24	9.73	117.19	106.24
3	B	2601	B12	C20-C1-C19	-7.56	102.07	109.36
3	B	2601	B12	C18-C19-N24	7.55	113.81	102.31
3	A	2601	B12	C35-C5-C6	6.67	133.06	122.43
3	E	2602	B12	C18-C17-C16	6.67	108.77	100.67
3	A	2601	B12	C18-C19-N24	6.64	112.41	102.31
3	E	2602	B12	C54-C17-C18	-6.56	103.29	112.98
3	A	2601	B12	C41-C8-C9	-6.35	99.99	111.19
3	E	2602	B12	C20-C1-C2	6.30	123.81	113.28
3	A	2601	B12	C2-C1-N21	6.27	110.51	101.77
3	E	2601	B12	C6-C5-C4	-6.06	110.69	121.54
3	A	2601	B12	C20-C1-C19	-6.01	103.56	109.36
3	B	2601	B12	C18-C60-C61	-5.92	99.21	113.97
3	B	2601	B12	C18-C17-C16	5.63	107.51	100.67
3	A	2601	B12	C15-C16-N24	-5.54	114.44	122.42
3	E	2602	B12	C60-C18-C19	-5.24	100.95	114.62
3	A	2601	B12	C26-C2-C3	5.13	116.49	107.41
3	E	2602	B12	C20-C1-C19	5.08	114.25	109.36
3	A	2601	B12	C53-C15-C16	5.03	129.04	120.38
3	A	2601	B12	C55-C56-C57	5.00	122.15	111.23
3	E	2601	B12	C5-C6-N22	-4.96	116.31	123.88
3	A	2601	B12	C1-C19-C18	-4.95	113.76	121.88
3	E	2602	B12	C20-C1-N21	-4.86	102.30	110.27
3	B	2601	B12	C2-C3-C4	4.83	107.12	101.63
3	E	2601	B12	C7-C6-C5	4.82	135.65	128.07
3	A	2601	B12	C37-C7-C6	4.79	122.18	107.12
3	E	2601	B12	C2-C3-C4	4.68	106.95	101.63
3	A	2601	B12	C30-C3-C2	-4.67	109.20	119.09
3	E	2602	B12	C48-C13-C14	4.65	120.08	108.49
3	A	2601	B12	C26-C2-C1	4.60	117.17	110.01
3	A	2601	B12	C1-C2-C3	-4.60	95.73	101.60
3	A	2601	B12	C2-C1-C19	4.59	125.85	118.60
3	A	2601	B12	C9-C10-C11	-4.38	119.63	125.97
3	A	2601	B12	C60-C18-C19	4.37	126.03	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2602	B12	C19-C1-N21	-4.33	97.73	102.16
3	A	2601	B12	C18-C60-C61	-4.29	103.26	113.97
3	A	2601	B12	C13-C14-C15	-4.25	117.83	124.32
3	B	2601	B12	C3-C4-N21	-4.23	106.67	111.97
3	E	2601	B12	C8B-C9B-N3B	-4.20	105.33	109.97
3	E	2602	B12	C8B-C9B-N3B	-4.20	105.34	109.97
3	E	2602	B12	C1-C2-C3	4.18	106.94	101.60
3	E	2601	B12	C30-C3-C2	-4.17	110.27	119.09
3	A	2601	B12	C12-C13-C14	-4.02	95.53	102.26
3	A	2601	B12	C35-C5-C4	-4.02	108.59	116.79
3	E	2601	B12	C9B-N3B-C2B	3.99	109.20	104.44
3	E	2602	B12	C9-C10-C11	-3.87	120.37	125.97
3	A	2601	B12	C36-C7-C6	-3.84	92.48	112.40
3	B	2601	B12	C17-C16-C15	3.79	132.23	126.26
3	E	2601	B12	C48-C13-C14	3.77	117.89	108.49
3	B	2601	B12	C20-C1-N21	3.77	116.45	110.27
3	A	2601	B12	C54-C17-C18	-3.70	107.52	112.98
3	E	2602	B12	C55-C56-C57	-3.61	103.35	111.23
3	A	2601	B12	C13-C14-N23	3.61	114.01	109.10
3	E	2602	B12	C9B-C8B-N1B	3.59	106.86	105.35
3	E	2602	B12	C4B-C9B-C8B	3.57	123.58	120.15
3	E	2601	B12	C35-C5-C4	3.51	123.96	116.79
3	A	2601	B12	C10-C9-N22	3.50	129.75	125.73
3	B	2601	B12	C54-C17-C18	-3.49	107.82	112.98
3	A	2601	B12	C12-C11-C10	3.46	127.87	123.37
3	B	2601	B12	C8B-C9B-N3B	-3.39	106.23	109.97
3	E	2602	B12	C5-C6-N22	-3.39	118.70	123.88
3	A	2601	B12	C25-C2-C1	-3.38	108.68	113.78
3	E	2602	B12	C7B-C8B-C9B	-3.38	118.51	122.52
3	A	2601	B12	C48-C13-C14	3.36	116.85	108.49
3	E	2602	B12	C17-C16-C15	3.34	131.53	126.26
3	E	2601	B12	C20-C1-C19	-3.32	106.15	109.36
3	A	2601	B12	O3-C2P-C1P	3.31	113.52	106.92
3	E	2602	B12	C25-C2-C26	-3.25	103.14	109.71
3	E	2601	B12	C18-C60-C61	-3.24	105.88	113.97
3	E	2601	B12	C2-C26-C27	-3.23	106.14	115.22
3	E	2602	B12	C9B-N3B-C2B	3.22	108.28	104.44
3	E	2601	B12	C3-C4-N21	-3.21	107.94	111.97
3	B	2601	B12	C26-C2-C3	3.21	113.09	107.41
3	E	2602	B12	C2-C1-N21	-3.20	97.30	101.77
3	A	2601	B12	C8B-C9B-N3B	-3.16	106.48	109.97
3	E	2602	B12	C7-C8-C9	-3.13	96.91	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2602	B12	C12-C11-C10	-3.09	119.34	123.37
3	E	2602	B12	C8B-N1B-C1R	3.08	130.62	125.39
3	B	2601	B12	C2P-C1P-N59	-2.99	108.53	112.93
3	E	2601	B12	C2-C1-C19	-2.99	113.89	118.60
3	A	2601	B12	C17-C16-C15	2.97	130.93	126.26
3	E	2602	B12	C17-C16-N24	-2.96	106.59	111.15
3	A	2601	B12	C56-C55-C17	2.96	121.22	115.52
3	B	2601	B12	C30-C3-C2	-2.90	112.94	119.09
3	E	2601	B12	C7-C6-N22	-2.90	102.64	107.94
3	E	2602	B12	C53-C15-C14	-2.90	112.60	118.43
3	E	2601	B12	C30-C31-C32	-2.89	102.79	112.59
3	B	2601	B12	C15-C16-N24	-2.88	118.27	122.42
3	A	2601	B12	C53-C15-C14	-2.86	112.67	118.43
3	A	2601	B12	C36-C7-C37	2.85	115.50	110.80
3	A	2601	B12	C8-C9-N22	-2.84	105.11	110.77
3	A	2601	B12	C20-C1-N21	-2.83	105.62	110.27
3	E	2601	B12	C8B-N1B-C2B	2.80	108.98	106.37
3	B	2601	B12	C9B-C8B-N1B	2.80	106.53	105.35
3	E	2602	B12	C7B-C6B-C5B	2.70	123.53	119.67
3	E	2602	B12	O3-C2P-C1P	2.68	112.26	106.92
3	E	2601	B12	O3-C2P-C1P	2.66	112.23	106.92
3	E	2602	B12	C2-C1-C19	-2.64	114.43	118.60
3	E	2601	B12	C48-C13-C12	-2.63	109.26	116.63
3	E	2602	B12	C53-C15-C16	2.60	124.85	120.38
3	E	2602	B12	C3R-C2R-C1R	2.59	105.63	99.89
3	E	2601	B12	C56-C55-C17	2.58	120.49	115.52
3	E	2601	B12	C56-C57-N59	2.56	120.74	116.42
3	E	2602	B12	C26-C2-C1	2.56	114.00	110.01
3	E	2601	B12	C18-C17-C16	2.54	103.75	100.67
3	E	2601	B12	C26-C2-C1	-2.54	106.05	110.01
3	E	2601	B12	C8-C9-N22	-2.54	105.71	110.77
3	E	2602	B12	C13-C14-N23	2.53	112.55	109.10
3	A	2601	B12	C5-C4-N21	-2.53	120.09	124.19
3	E	2601	B12	N1B-C2B-N3B	-2.51	110.47	113.91
3	A	2601	B12	C7B-C8B-C9B	-2.51	119.54	122.52
3	B	2601	B12	C5-C4-N21	2.50	128.25	124.19
3	B	2601	B12	C48-C13-C12	-2.49	109.66	116.63
3	E	2602	B12	C37-C7-C6	2.48	114.91	107.12
3	E	2602	B12	C60-C18-C17	-2.45	109.82	115.74
3	E	2602	B12	C13-C12-C11	-2.43	98.21	100.97
3	E	2601	B12	C20-C1-N21	2.41	114.22	110.27
3	E	2602	B12	C30-C31-C32	-2.41	104.43	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2601	B12	C17-C16-N24	-2.39	107.47	111.15
3	A	2601	B12	C9B-C8B-N1B	2.35	106.34	105.35
3	A	2601	B12	C20-C1-C2	-2.32	109.41	113.28
3	A	2601	B12	C16-C15-C14	-2.32	117.73	121.25
3	E	2602	B12	O5-P-O4	2.29	123.55	112.24
3	A	2601	B12	C3-C4-N21	2.28	114.82	111.97
3	E	2602	B12	C7-C37-C38	2.26	121.04	114.25
3	E	2602	B12	C56-C55-C17	-2.25	111.18	115.52
3	E	2601	B12	C26-C2-C3	2.23	111.36	107.41
3	E	2601	B12	C15-C16-N24	-2.22	119.22	122.42
3	E	2601	B12	C13-C12-C11	2.22	103.48	100.97
3	E	2601	B12	C5-C4-N21	2.19	127.74	124.19
3	A	2601	B12	C9B-N3B-C2B	2.16	107.02	104.44
3	A	2601	B12	C41-C42-C43	-2.16	105.25	112.59
3	E	2602	B12	C1R-N1B-C2B	-2.14	122.31	127.14
3	A	2601	B12	C12-C11-N23	-2.11	108.88	111.83
3	B	2601	B12	C25-C2-C1	-2.11	110.60	113.78
3	A	2601	B12	C13-C12-C11	-2.10	98.59	100.97
3	A	2601	B12	C19-C1-N21	-2.10	100.02	102.16
3	B	2601	B12	C55-C17-C18	-2.05	107.18	111.15
3	E	2602	B12	O58-C57-C56	-2.02	118.33	122.02
3	E	2601	B12	C54-C17-C18	-2.02	110.01	112.98
3	E	2601	B12	C7B-C8B-C9B	-2.01	120.14	122.52

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2601	B12	C1-C2-C26-C27
3	A	2601	B12	C25-C2-C26-C27
3	A	2601	B12	C38-C37-C7-C6
3	A	2601	B12	C38-C37-C7-C36
3	A	2601	B12	C38-C37-C7-C8
3	A	2601	B12	C14-C13-C48-C49
3	B	2601	B12	C1-C2-C26-C27
3	B	2601	B12	C25-C2-C26-C27
3	B	2601	B12	C3-C2-C26-C27
3	B	2601	B12	C38-C37-C7-C36
3	B	2601	B12	C42-C41-C8-C9
3	B	2601	B12	C56-C57-N59-C1P
3	B	2601	B12	N59-C1P-C2P-O3
3	E	2601	B12	C1-C2-C26-C27

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Mol	Chain	Res	Type	Atoms
3	E	2601	B12	C25-C2-C26-C27
3	E	2601	B12	C3-C2-C26-C27
3	E	2601	B12	C42-C41-C8-C7
3	E	2601	B12	C42-C41-C8-C9
3	E	2601	B12	C16-C17-C55-C56
3	E	2601	B12	C54-C17-C55-C56
3	E	2601	B12	C18-C17-C55-C56
3	E	2601	B12	N59-C1P-C2P-C3P
3	E	2601	B12	N59-C1P-C2P-O3
3	E	2601	B12	C1P-C2P-O3-P
3	E	2601	B12	C3P-C2P-O3-P
3	E	2602	B12	C16-C17-C55-C56
3	E	2602	B12	C54-C17-C55-C56
3	E	2602	B12	N59-C1P-C2P-C3P
3	E	2602	B12	N59-C1P-C2P-O3
3	E	2602	B12	C2P-O3-P-O5
3	B	2601	B12	O58-C57-N59-C1P
3	E	2602	B12	O6R-C4R-C5R-O8R
3	E	2602	B12	C3R-C4R-C5R-O8R
3	A	2601	B12	C2-C3-C30-C31
3	B	2601	B12	C42-C41-C8-C7
3	E	2601	B12	C3R-C4R-C5R-O8R
3	B	2601	B12	C4-C3-C30-C31
3	B	2601	B12	C2P-C1P-N59-C57
3	E	2601	B12	C13-C48-C49-C50
3	E	2601	B12	O6R-C4R-C5R-O8R
3	A	2601	B12	C7-C37-C38-N40
3	E	2601	B12	C56-C57-N59-C1P
3	E	2601	B12	O58-C57-N59-C1P
3	B	2601	B12	C17-C55-C56-C57
3	B	2601	B12	C2-C3-C30-C31
3	A	2601	B12	C16-C17-C55-C56
3	B	2601	B12	N59-C1P-C2P-C3P
3	A	2601	B12	C7-C37-C38-O39
3	B	2601	B12	C38-C37-C7-C8
3	A	2601	B12	C17-C55-C56-C57
3	A	2601	B12	O6R-C4R-C5R-O8R
3	E	2602	B12	C2-C3-C30-C31
3	E	2601	B12	C14-C13-C48-C49
3	B	2601	B12	C12-C13-C48-C49
3	E	2602	B12	C2P-O3-P-O2
3	A	2601	B12	C4-C3-C30-C31

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Mol	Chain	Res	Type	Atoms
3	B	2601	B12	C38-C37-C7-C6
3	B	2601	B12	C41-C42-C43-O44
3	B	2601	B12	C41-C42-C43-N45
3	E	2601	B12	C3R-O2-P-O4
3	E	2602	B12	C2P-O3-P-O4
3	E	2602	B12	C4-C3-C30-C31
3	E	2602	B12	C17-C55-C56-C57
3	B	2601	B12	C18-C17-C55-C56
3	A	2601	B12	C3-C2-C26-C27
3	E	2602	B12	C1-C2-C26-C27
3	E	2602	B12	C25-C2-C26-C27
3	A	2601	B12	C12-C13-C48-C49
3	A	2601	B12	C42-C41-C8-C9
3	E	2602	B12	C18-C17-C55-C56
3	E	2601	B12	C8-C41-C42-C43
3	A	2601	B12	C18-C60-C61-N62
3	E	2602	B12	C42-C41-C8-C9
3	B	2601	B12	C55-C56-C57-O58
3	A	2601	B12	C18-C17-C55-C56
3	A	2601	B12	C18-C60-C61-O63
3	E	2601	B12	C3R-O2-P-O3
3	B	2601	B12	C55-C56-C57-N59
3	A	2601	B12	C56-C57-N59-C1P
3	E	2602	B12	C8-C41-C42-C43
3	E	2601	B12	O6R-C1R-N1B-C8B
3	E	2601	B12	C17-C18-C60-C61
3	E	2601	B12	C19-C18-C60-C61

There are no ring outliers.

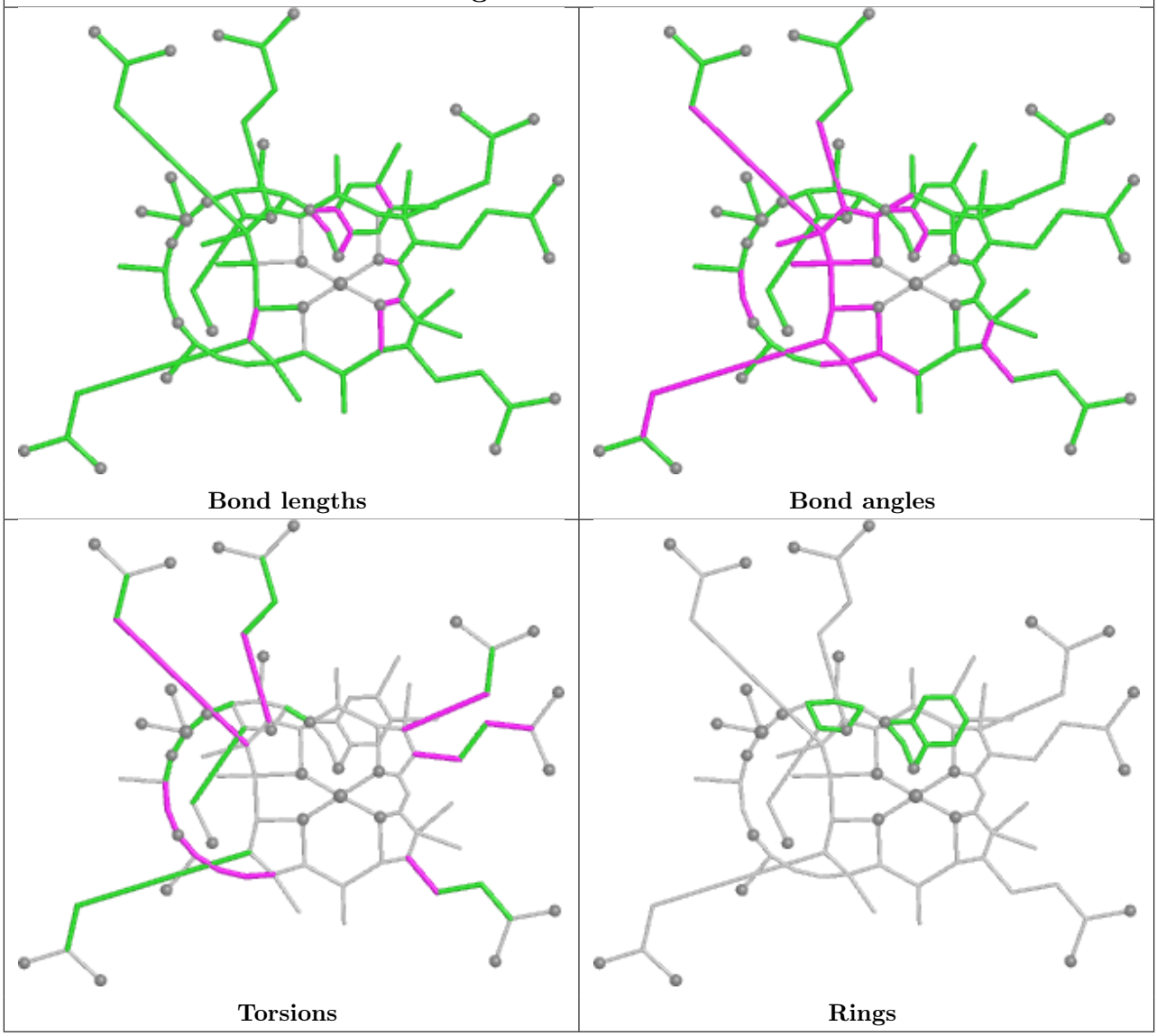
4 monomers are involved in 96 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2601	B12	31	0
3	E	2602	B12	13	0
3	E	2601	B12	36	0
3	A	2601	B12	16	0

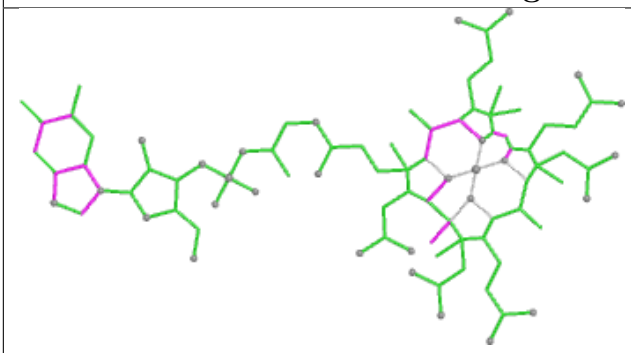
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

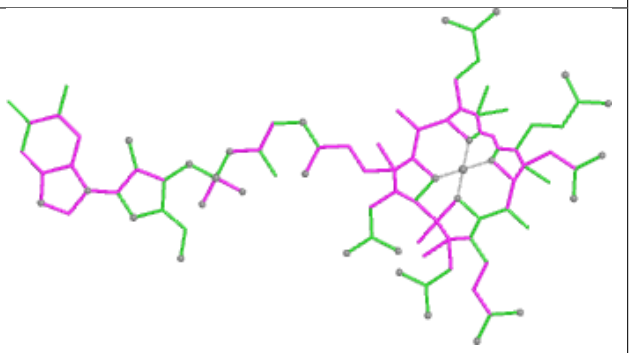
Ligand B12 B 2601



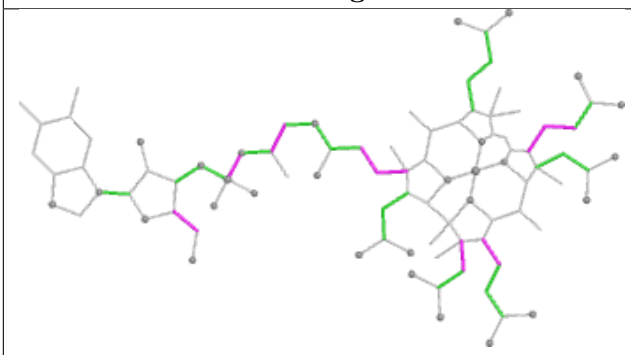
Ligand B12 E 2602



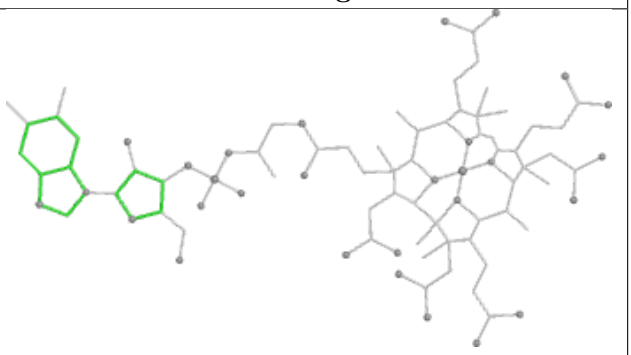
Bond lengths



Bond angles

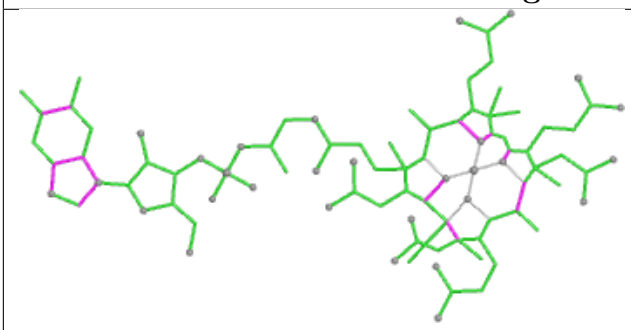


Torsions

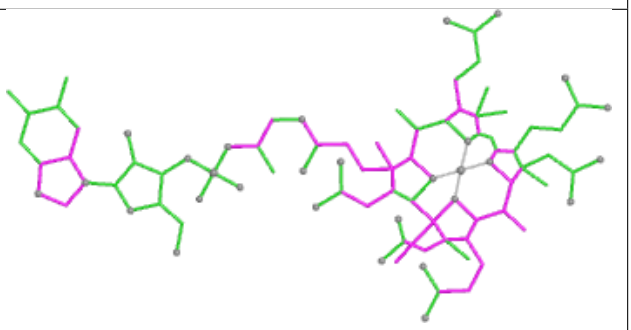


Rings

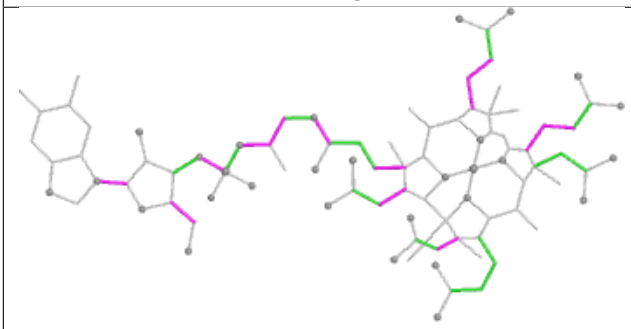
Ligand B12 E 2601



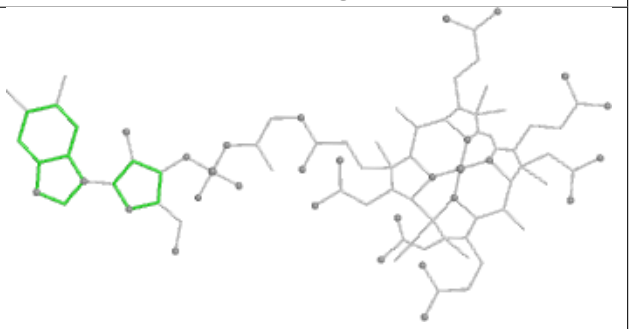
Bond lengths



Bond angles

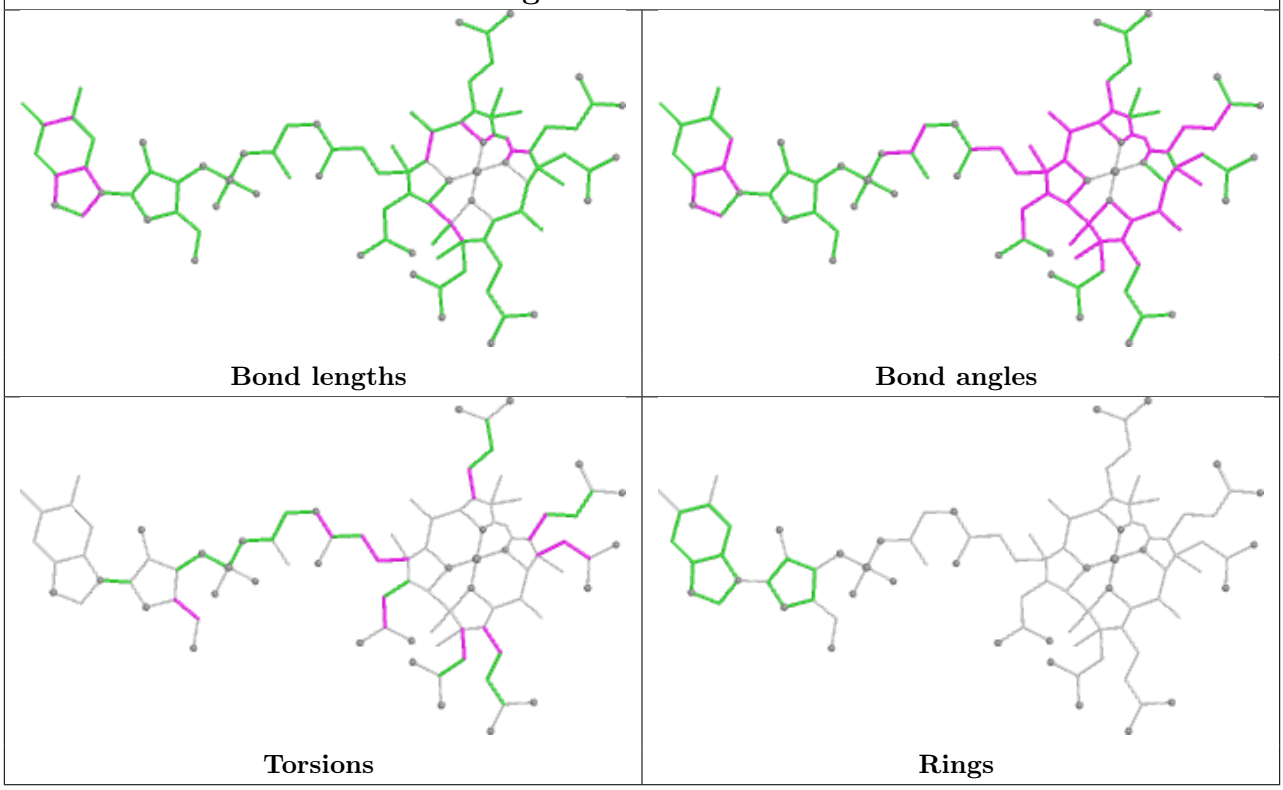


Torsions



Rings

Ligand B12 A 2601



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	737/754 (97%)	-1.41	0	100	100	25, 40, 54, 94	0
1	B	736/754 (97%)	-1.41	0	100	100	24, 37, 49, 66	0
1	E	737/754 (97%)	-1.41	0	100	100	28, 41, 56, 84	0
1	F	739/754 (98%)	-1.42	0	100	100	23, 39, 51, 80	0
2	C	139/141 (98%)	-1.39	0	100	100	34, 48, 65, 79	0
2	D	138/141 (97%)	-1.44	0	100	100	32, 42, 58, 71	0
2	G	137/141 (97%)	-1.38	0	100	100	36, 48, 65, 72	0
2	H	138/141 (97%)	-1.40	0	100	100	33, 47, 59, 73	0
All	All	3501/3580 (97%)	-1.41	0	100	100	23, 40, 56, 94	0

There are no RSRZ outliers to report.

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)

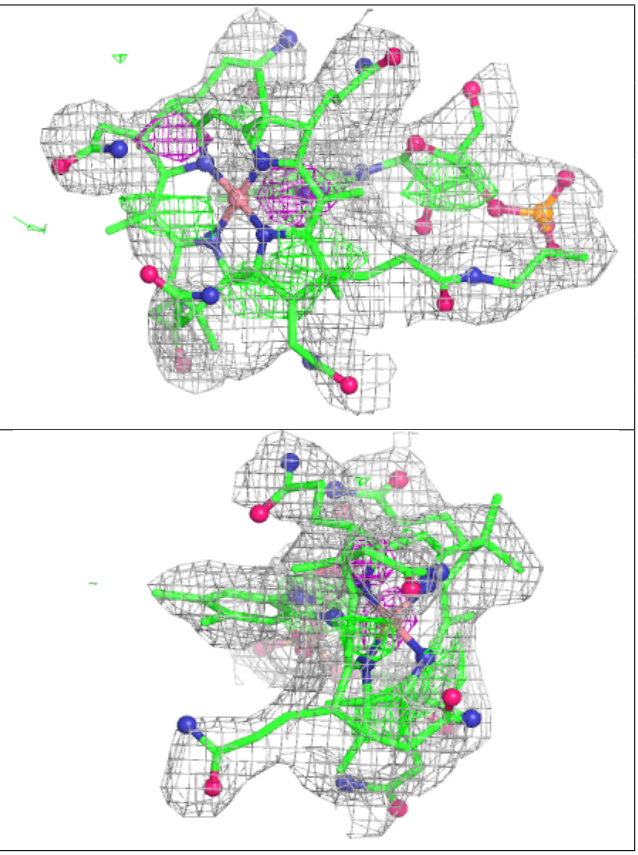
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	B12	A	2601	91/91	0.99	0.06	27,45,61,66	0
3	B12	B	2601	91/91	0.99	0.04	21,38,46,51	0
3	B12	E	2601	91/91	0.99	0.05	28,48,63,70	0
3	B12	E	2602	91/91	0.99	0.04	30,46,58,72	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.

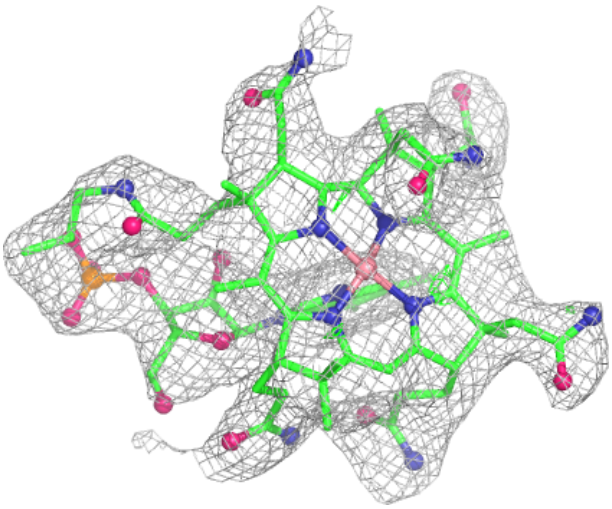
Electron density around B12 A 2601:

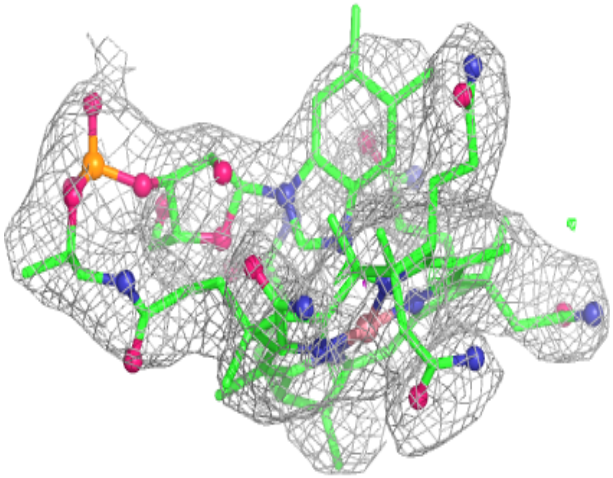
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

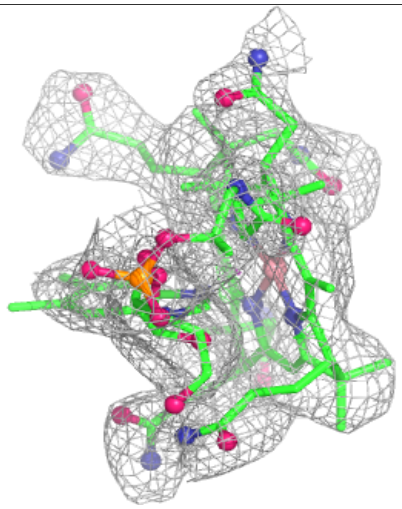


Electron density around B12 B 2601:

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

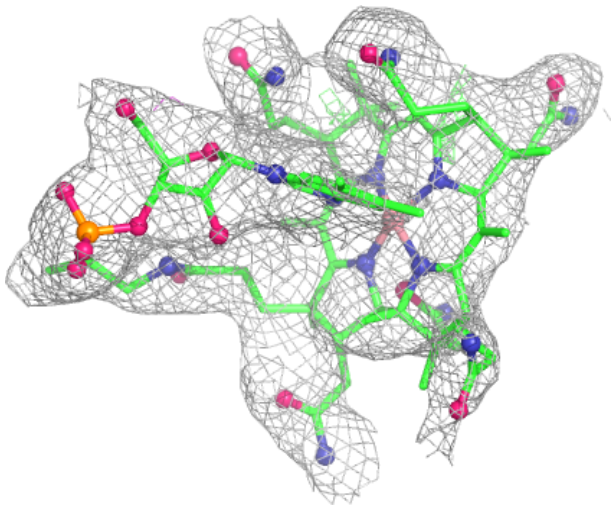


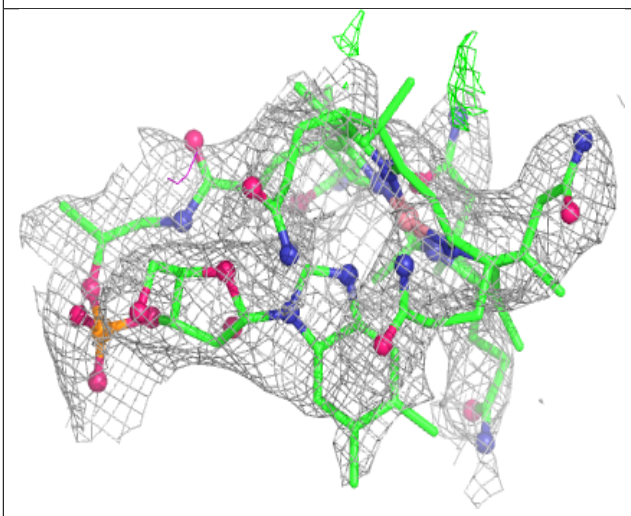


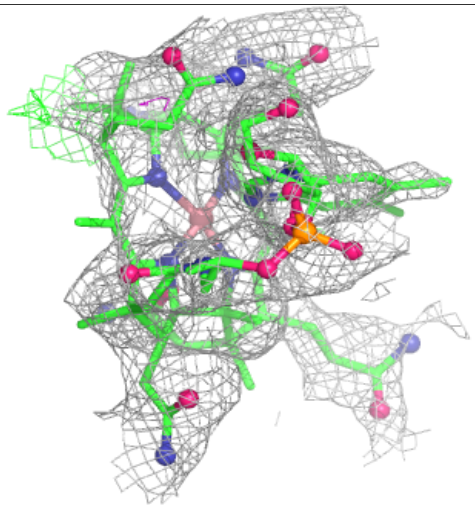


Electron density around B12 E 2601:

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

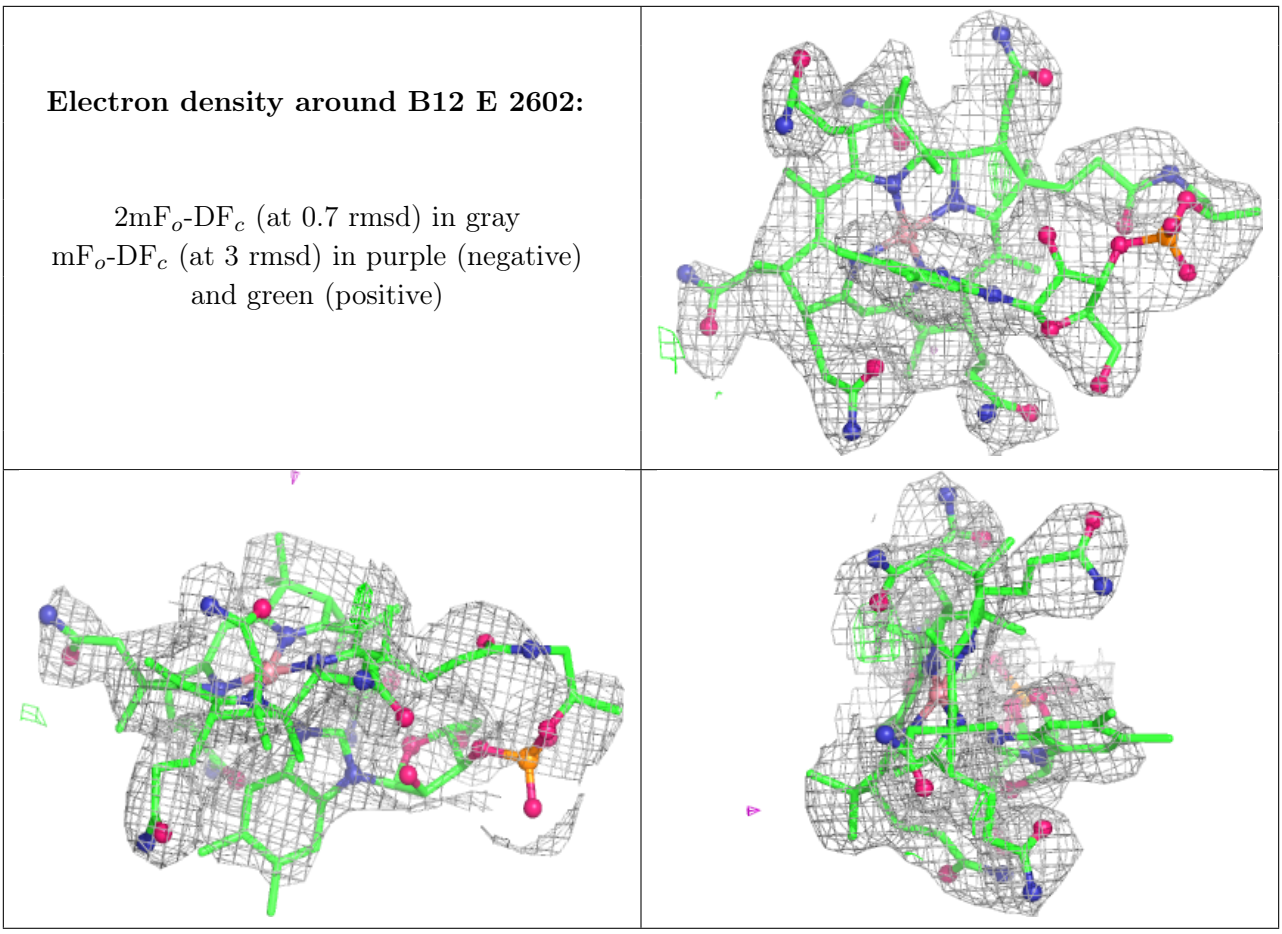






Electron density around B12 E 2602:

$2mF_o$-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.