Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 05:45 PM EDT

PDB ID	:	3VND
Title	:	Crystal structure of tryptophan synthase alpha-subunit from the psychrophile Shewanella frigidimarina K14-2
Authors	:	Mitsuya, D.; Tanaka, S.; Matsumura, H.; Takano, K.; Urano, N.; Ishida, M.
Deposited on	:	2012-01-12
Resolution	:	2.60 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:

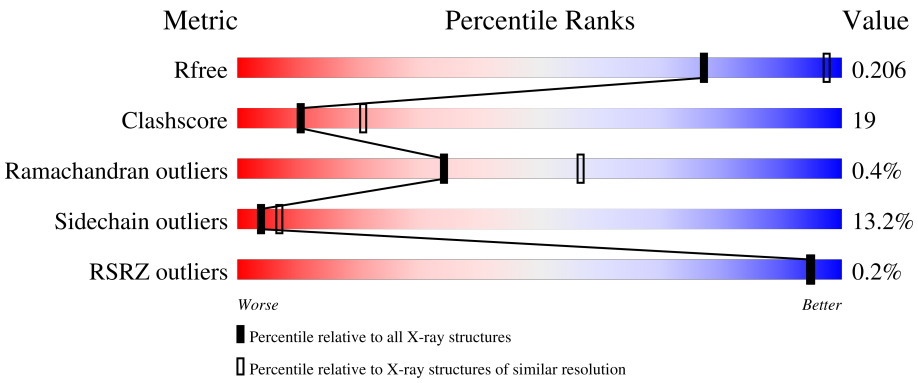
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	267	69% 22% 6% •
1	B	267	63% 28% 5% • •
1	C	267	67% 24% 5% •
1	D	267	64% 26% 6% •
1	E	267	66% 25% 5% • •

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Mol	Chain	Length	Quality of chain
1	F	267	% 63% 27% 6%
1	G	267	69% 24%
1	H	267	62% 31%

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
2	SO4	H	302	-	-	X	-

2 Entry composition (i)

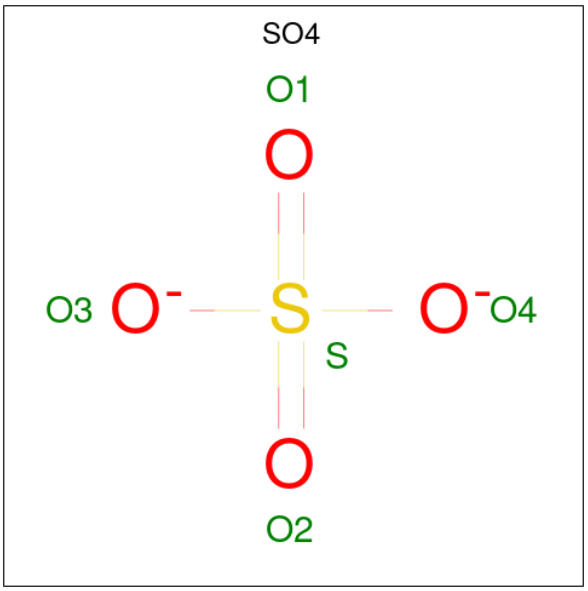
There are 4 unique types of molecules in this entry. The entry contains 16633 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	259	1907	1220	313	369	5	0	0	0
1	B	259	1907	1220	313	369	5	0	0	0
1	C	259	1907	1220	313	369	5	0	0	0
1	D	259	1907	1220	313	369	5	0	0	0
1	E	259	1907	1220	313	369	5	0	0	0
1	F	259	1907	1220	313	369	5	0	0	0
1	G	259	1907	1220	313	369	5	0	0	0
1	H	259	1907	1220	313	369	5	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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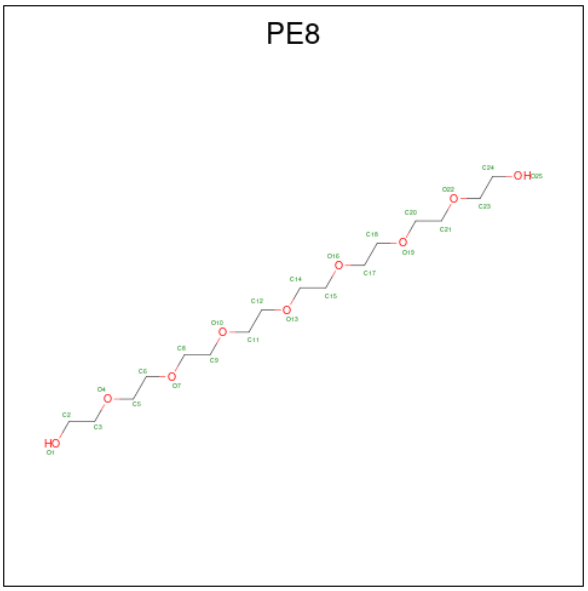
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0

- Molecule 3 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula: $C_{16}H_{34}O_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 25 16 9	0	0
3	D	1	Total C O 25 16 9	0	0
3	E	1	Total C O 25 16 9	0	0
3	G	1	Total C O 25 16 9	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	145	Total O 145 145	0	0

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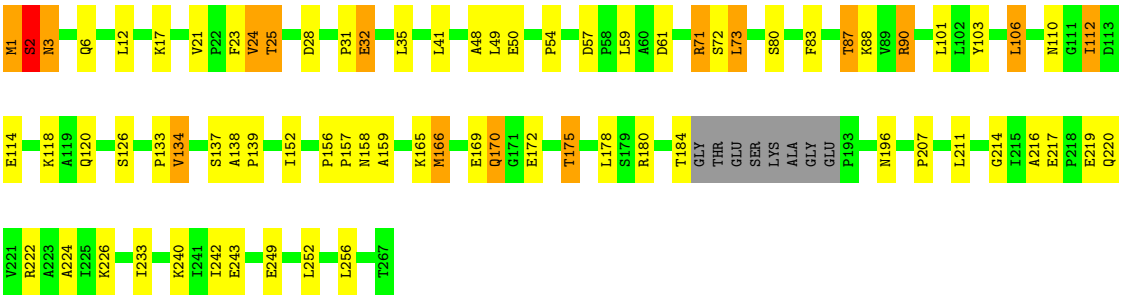
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	153	153	153	0	0
			Total	O		
4	C	156	156	156	0	0
			Total	O		
4	D	144	144	144	0	0
			Total	O		
4	E	147	147	147	0	0
			Total	O		
4	F	150	150	150	0	0
			Total	O		
4	G	149	149	149	0	0
			Total	O		
4	H	143	143	143	0	0

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.

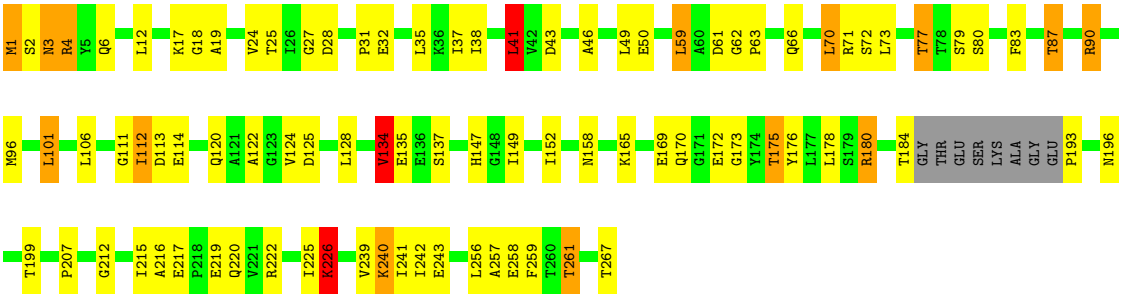
- Molecule 1: Tryptophan synthase alpha chain

Chain A:



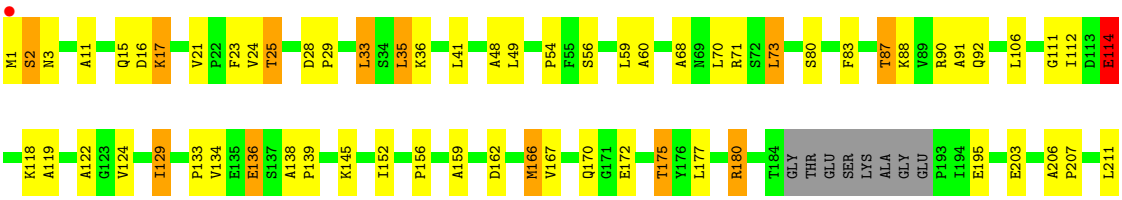
- Molecule 1: Tryptophan synthase alpha chain

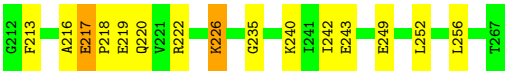
Chain B:



- Molecule 1: Tryptophan synthase alpha chain

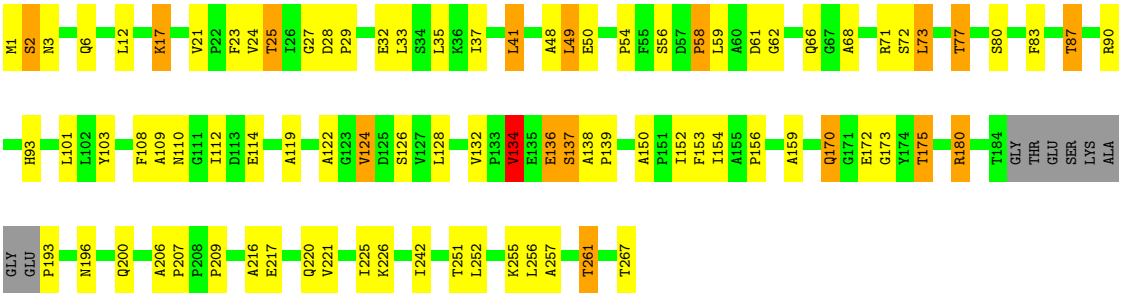
Chain C:





• Molecule 1: Tryptophan synthase alpha chain

Chain D:

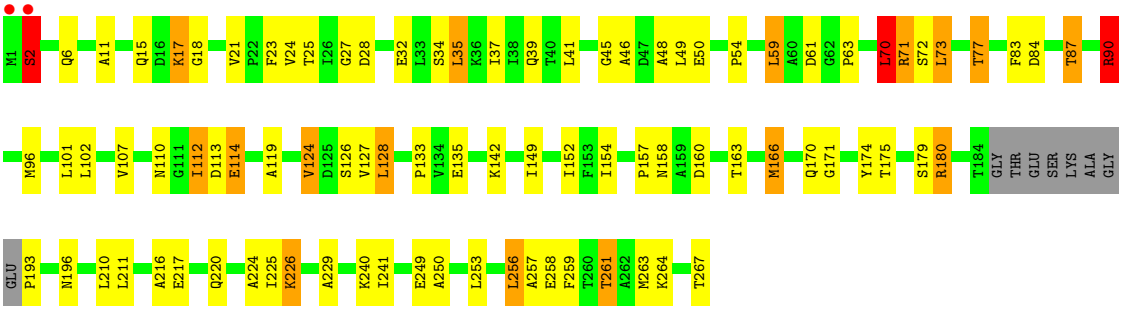


• Molecule 1: Tryptophan synthase alpha chain

Chain E:

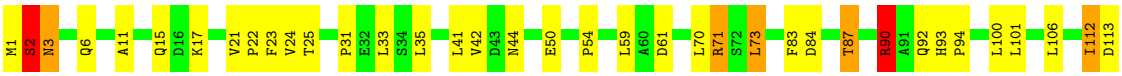
• Molecule 1: Tryptophan synthase alpha chain

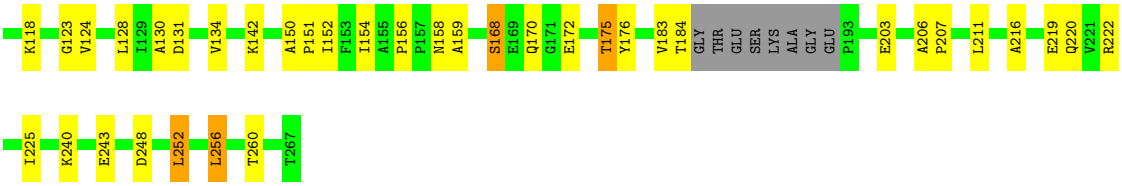
Chain F:



• Molecule 1: Tryptophan synthase alpha chain

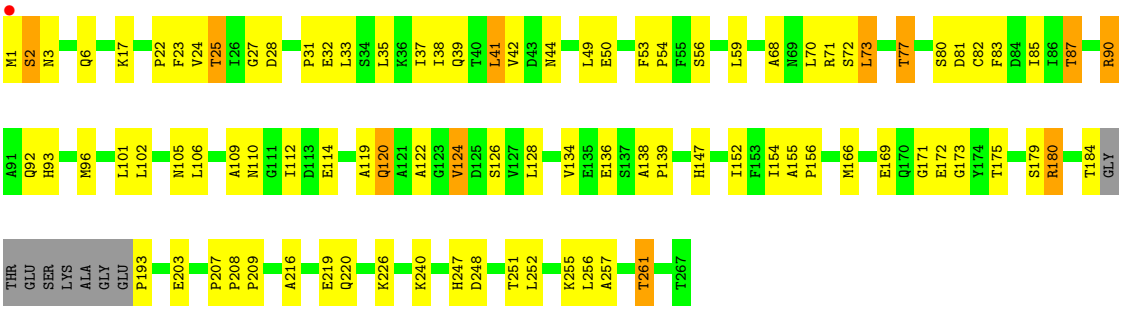
Chain G:





• Molecule 1: Tryptophan synthase alpha chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	181.14Å 182.78Å 181.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 2.60 48.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.79-2.60) 96.8 (48.74-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.173 , 0.211 0.174 , 0.206	Depositor DCC
R_{free} test set	4603 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 16.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.208 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16633	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1573e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: PE8, 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	0.95	0/1945	1.03	6/2647 (0.2%)
1	B	0.91	0/1945	1.07	13/2647 (0.5%)
1	C	0.98	1/1945 (0.1%)	1.03	4/2647 (0.2%)
1	D	1.00	1/1945 (0.1%)	1.13	5/2647 (0.2%)
1	E	0.94	0/1945	1.05	7/2647 (0.3%)
1	F	0.93	1/1945 (0.1%)	1.04	8/2647 (0.3%)
1	G	0.94	0/1945	1.05	7/2647 (0.3%)
1	H	0.94	1/1945 (0.1%)	1.01	5/2647 (0.2%)
All	All	0.95	4/15560 (0.0%)	1.05	55/21176 (0.3%)

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	2
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	2
1	F	0	1
1	G	0	2
All	All	0	11

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	114	GLU	CD-OE1	7.68	1.34	1.25
1	H	56	SER	CB-OG	6.32	1.50	1.42
1	D	32	GLU	CG-CD	5.78	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	32	GLU	CD-OE1	5.63	1.31	1.25

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	180	ARG	NE-CZ-NH2	-11.72	114.44	120.30
1	D	90	ARG	NE-CZ-NH2	-11.31	114.64	120.30
1	D	90	ARG	NE-CZ-NH1	10.90	125.75	120.30
1	E	90	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	E	180	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	F	71	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	B	90	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	H	180	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	E	180	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	C	180	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	F	180	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	D	180	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	A	71	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	E	90	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	F	90	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	B	180	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	G	248	ASP	CB-CG-OD1	-6.55	112.40	118.30
1	F	180	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	F	71	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	G	248	ASP	CB-CG-OD2	6.32	123.99	118.30
1	G	71	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	90	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	H	180	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	71	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	90	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	B	70	LEU	CA-CB-CG	6.02	129.14	115.30
1	G	90	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	F	70	LEU	CA-CB-CG	5.90	128.86	115.30
1	B	134	VAL	CB-CA-C	-5.89	100.21	111.40
1	A	57	ASP	CB-CG-OD2	5.85	123.56	118.30
1	C	35	LEU	CA-CB-CG	5.75	128.52	115.30
1	G	71	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	180	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	E	106	LEU	CA-CB-CG	5.67	128.34	115.30
1	A	57	ASP	CB-CG-OD1	-5.62	113.25	118.30
1	B	226	LYS	CD-CE-NZ	5.58	124.54	111.70
1	B	28	ASP	CB-CG-OD2	-5.57	113.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	178	LEU	CB-CG-CD1	5.51	120.37	111.00
1	F	171	GLY	N-CA-C	-5.43	99.53	113.10
1	C	129	ILE	CG1-CB-CG2	-5.42	99.47	111.40
1	A	90	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	H	166	MET	CA-CB-CG	5.38	122.45	113.30
1	C	106	LEU	CA-CB-CG	5.37	127.65	115.30
1	D	170	GLN	CA-C-N	5.37	126.94	116.20
1	G	118	LYS	CD-CE-NZ	5.29	123.86	111.70
1	B	41	LEU	CA-CB-CG	5.27	127.43	115.30
1	E	152	ILE	CB-CA-C	-5.24	101.11	111.60
1	H	171	GLY	N-CA-C	-5.24	100.01	113.10
1	G	131	ASP	CB-CG-OD2	5.22	123.00	118.30
1	F	166	MET	CA-CB-CG	5.12	122.00	113.30
1	E	170	GLN	N-CA-C	5.05	124.65	111.00
1	B	43	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	H	90	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	B	4	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	170	GLN	N-CA-C	5.01	124.54	111.00

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	GLN	Peptide
1	A	2	SER	Peptide
1	B	1	MET	Peptide
1	C	2	SER	Peptide
1	D	170	GLN	Peptide
1	D	49	LEU	Peptide
1	E	170	GLN	Peptide
1	E	2	SER	Peptide
1	F	170	GLN	Peptide
1	G	170	GLN	Peptide
1	G	2	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1907	0	1918	63	0
1	B	1907	0	1918	79	0
1	C	1907	0	1918	77	0
1	D	1907	0	1918	70	0
1	E	1907	0	1918	83	0
1	F	1907	0	1918	80	0
1	G	1907	0	1918	52	0
1	H	1907	0	1918	72	0
2	A	15	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
2	D	15	0	0	1	0
2	E	10	0	0	1	0
2	F	10	0	0	0	0
2	G	10	0	0	0	0
2	H	10	0	0	2	0
3	B	25	0	34	3	0
3	D	25	0	34	5	0
3	E	25	0	34	2	0
3	G	25	0	34	3	0
4	A	145	0	0	26	0
4	B	153	0	0	26	0
4	C	156	0	0	33	0
4	D	144	0	0	21	0
4	E	147	0	0	42	0
4	F	150	0	0	31	0
4	G	149	0	0	19	0
4	H	143	0	0	23	0
All	All	16633	0	15480	576	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 19.

All (576) 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:3:ASN:HB2	4:B:532:HOH:O	1.27	1.32
1:B:111:GLY:HA3	4:B:490:HOH:O	1.27	1.30
1:C:217:GLU:HB2	4:C:546:HOH:O	1.14	1.25
1:H:120:GLN:HG3	4:H:483:HOH:O	1.34	1.24
1:H:193:PRO:HB2	4:H:484:HOH:O	1.38	1.23
1:H:96:MET:SD	4:H:492:HOH:O	1.97	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:THR:HB	4:F:519:HOH:O	1.40	1.19
1:F:158:ASN:HA	4:F:501:HOH:O	1.45	1.15
1:H:2:SER:HA	1:H:6:GLN:HG3	1.12	1.10
1:C:3:ASN:HB3	4:C:554:HOH:O	1.54	1.08
1:G:3:ASN:HB3	4:G:545:HOH:O	1.56	1.05
1:H:2:SER:HA	1:H:6:GLN:CG	1.89	1.03
1:D:193:PRO:N	4:D:524:HOH:O	1.92	1.03
1:D:3:ASN:CB	4:D:513:HOH:O	2.05	1.02
1:C:56:SER:HA	4:C:496:HOH:O	1.60	0.99
1:D:3:ASN:HB2	4:D:513:HOH:O	1.60	0.99
1:F:72:SER:O	1:F:77:THR:HG23	1.63	0.98
1:D:3:ASN:HB3	4:D:480:HOH:O	1.64	0.97
1:E:50:GLU:CG	4:E:510:HOH:O	2.12	0.97
1:A:3:ASN:HA	4:A:480:HOH:O	1.64	0.96
1:B:2:SER:HA	1:B:6:GLN:HG3	1.48	0.95
1:C:172:GLU:HG2	4:C:549:HOH:O	1.66	0.95
1:A:50:GLU:HG2	4:A:536:HOH:O	1.66	0.95
1:F:216:ALA:H	1:F:220:GLN:NE2	1.66	0.93
1:B:72:SER:O	1:B:77:THR:HG23	1.69	0.92
1:F:225:ILE:HG13	4:F:541:HOH:O	1.70	0.92
1:B:175:THR:HG22	1:B:207:PRO:O	1.70	0.92
1:C:222:ARG:HD3	4:C:491:HOH:O	1.69	0.92
1:D:72:SER:O	1:D:77:THR:HG23	1.69	0.92
1:E:243:GLU:HG2	4:E:542:HOH:O	1.69	0.91
1:A:137:SER:HB3	4:A:496:HOH:O	1.71	0.89
1:F:225:ILE:CG1	4:F:541:HOH:O	2.20	0.89
1:D:114:GLU:HB2	4:D:424:HOH:O	1.72	0.89
1:H:255:LYS:HE3	4:H:539:HOH:O	1.73	0.89
1:E:100:LEU:HD23	4:E:517:HOH:O	1.72	0.89
1:A:243:GLU:HG2	4:A:490:HOH:O	1.72	0.88
1:H:105:ASN:HB3	4:H:497:HOH:O	1.73	0.88
1:E:165:LYS:O	1:E:169:GLU:HG3	1.75	0.86
1:B:226:LYS:HG2	4:B:547:HOH:O	1.73	0.86
1:H:42:VAL:HG13	1:H:96:MET:HE1	1.57	0.85
1:C:3:ASN:CB	4:C:543:HOH:O	2.24	0.85
1:A:175:THR:HG22	1:A:207:PRO:HG2	1.58	0.85
1:H:110:ASN:HB3	4:H:507:HOH:O	1.76	0.85
1:D:216:ALA:H	1:D:220:GLN:NE2	1.75	0.84
2:C:301:SO4:O1	4:C:537:HOH:O	1.94	0.84
1:H:42:VAL:HG13	1:H:96:MET:CE	2.08	0.84
1:A:240:LYS:HD2	4:B:527:HOH:O	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:ASN:HA	4:E:482:HOH:O	1.78	0.83
1:H:72:SER:O	1:H:77:THR:HG23	1.78	0.83
1:E:110:ASN:CA	4:E:482:HOH:O	2.25	0.83
1:A:175:THR:HG23	1:A:207:PRO:O	1.79	0.82
2:E:302:SO4:O3	4:E:461:HOH:O	1.97	0.82
1:E:193:PRO:HA	4:E:536:HOH:O	1.79	0.82
1:F:70:LEU:HB3	4:F:514:HOH:O	1.79	0.82
1:H:2:SER:CA	1:H:6:GLN:HG3	2.06	0.82
1:C:54:PRO:HB2	1:C:73:LEU:HD13	1.62	0.82
1:A:3:ASN:N	4:A:514:HOH:O	2.13	0.81
1:E:165:LYS:HE3	4:E:505:HOH:O	1.80	0.81
1:G:240:LYS:HB2	4:G:524:HOH:O	1.81	0.81
1:B:1:MET:HA	1:B:173:GLY:H	1.46	0.81
1:A:50:GLU:CG	4:A:536:HOH:O	2.27	0.80
1:G:216:ALA:H	1:G:220:GLN:NE2	1.80	0.80
1:H:120:GLN:CG	4:H:483:HOH:O	2.06	0.80
1:B:3:ASN:HA	4:B:486:HOH:O	1.82	0.80
1:G:184:THR:HG23	4:G:526:HOH:O	1.82	0.80
1:A:180:ARG:NH2	1:B:61:ASP:O	2.15	0.80
1:F:257:ALA:O	1:F:261:THR:HG22	1.83	0.79
1:E:79:SER:HB2	4:E:535:HOH:O	1.83	0.78
1:H:54:PRO:HB2	1:H:73:LEU:HD13	1.62	0.78
1:A:110:ASN:HB3	4:A:484:HOH:O	1.83	0.77
1:A:242:ILE:HA	1:A:252:LEU:HD11	1.66	0.77
1:G:2:SER:O	1:G:6:GLN:HG3	1.86	0.76
1:C:3:ASN:HB2	4:C:543:HOH:O	1.85	0.76
1:D:217:GLU:H	1:D:220:GLN:HE21	1.34	0.75
1:F:70:LEU:HD23	4:F:514:HOH:O	1.87	0.75
1:B:137:SER:HB3	4:B:544:HOH:O	1.86	0.75
1:H:44:ASN:HB3	1:H:261:THR:HG22	1.68	0.74
1:D:2:SER:HA	1:D:6:GLN:HG2	1.69	0.74
1:G:2:SER:C	4:G:516:HOH:O	2.24	0.74
1:E:222:ARG:HG3	4:E:485:HOH:O	1.87	0.74
1:B:27:GLY:HA3	1:B:77:THR:HG21	1.69	0.74
1:E:50:GLU:HG2	4:E:510:HOH:O	1.81	0.74
1:C:134:VAL:HG23	4:C:526:HOH:O	1.88	0.74
1:D:110:ASN:HB3	4:D:497:HOH:O	1.88	0.74
1:F:54:PRO:HB2	1:F:73:LEU:HD13	1.69	0.74
1:H:175:THR:HG23	1:H:207:PRO:O	1.86	0.74
1:G:216:ALA:H	1:G:220:GLN:HE22	1.34	0.73
1:C:226:LYS:HE3	4:C:505:HOH:O	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ALA:O	1:D:261:THR:CG2	2.37	0.73
1:E:32:GLU:HG2	4:E:480:HOH:O	1.87	0.73
1:C:243:GLU:CG	4:C:544:HOH:O	2.35	0.73
1:C:3:ASN:OD1	4:C:487:HOH:O	2.06	0.73
1:B:120:GLN:HG3	1:B:147:HIS:O	1.88	0.73
1:A:114:GLU:O	1:A:118:LYS:HE2	1.89	0.73
1:B:193:PRO:HA	4:B:524:HOH:O	1.88	0.73
1:A:184:THR:HA	4:A:486:HOH:O	1.87	0.72
1:B:243:GLU:HG2	4:B:526:HOH:O	1.89	0.72
1:H:1:MET:HA	1:H:173:GLY:H	1.55	0.72
1:C:243:GLU:HG2	4:C:544:HOH:O	1.89	0.71
1:D:17:LYS:HE2	4:D:505:HOH:O	1.90	0.71
1:A:21:VAL:HG22	1:A:48:ALA:HB3	1.73	0.71
1:B:222:ARG:HG2	1:B:226:LYS:HE3	1.71	0.71
3:G:303:PE8:H32	4:H:474:HOH:O	1.91	0.71
1:D:255:LYS:HE3	4:D:538:HOH:O	1.91	0.71
1:C:29:PRO:HG2	1:C:33:LEU:HD13	1.73	0.70
1:G:175:THR:HG21	1:G:206:ALA:HB1	1.71	0.70
1:B:193:PRO:N	4:B:537:HOH:O	2.24	0.70
1:A:2:SER:C	4:A:514:HOH:O	2.29	0.70
1:A:152:ILE:HD13	1:A:172:GLU:O	1.92	0.70
1:D:72:SER:O	1:D:77:THR:CG2	2.40	0.69
1:A:54:PRO:HB2	1:A:73:LEU:HD13	1.72	0.69
1:G:2:SER:O	4:G:516:HOH:O	2.09	0.69
1:B:2:SER:HA	1:B:6:GLN:CG	2.22	0.69
1:E:2:SER:O	1:E:6:GLN:HG3	1.92	0.69
1:E:174:TYR:OH	4:E:513:HOH:O	2.10	0.69
1:F:110:ASN:OD1	4:F:522:HOH:O	2.09	0.69
1:H:110:ASN:HA	4:H:534:HOH:O	1.92	0.69
1:A:2:SER:O	1:A:6:GLN:HG3	1.93	0.69
1:B:32:GLU:HB2	4:B:546:HOH:O	1.93	0.68
1:G:184:THR:HB	4:G:549:HOH:O	1.92	0.68
1:E:120:GLN:HG2	4:E:543:HOH:O	1.92	0.68
1:F:71:ARG:NH2	4:F:443:HOH:O	2.10	0.68
1:C:114:GLU:HB3	4:C:548:HOH:O	1.92	0.68
1:G:3:ASN:HB2	4:G:509:HOH:O	1.92	0.68
1:G:2:SER:C	1:G:6:GLN:HG3	2.13	0.68
1:D:2:SER:HB3	1:D:6:GLN:OE1	1.94	0.68
1:D:23:PHE:HA	1:D:50:GLU:O	1.93	0.68
1:C:114:GLU:OE2	4:C:548:HOH:O	2.11	0.67
1:E:3:ASN:OD1	4:E:483:HOH:O	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:THR:O	1:D:255:LYS:HG3	1.95	0.66
1:B:175:THR:CG2	1:B:207:PRO:O	2.42	0.66
1:B:243:GLU:CG	4:B:526:HOH:O	2.43	0.66
4:E:521:HOH:O	1:F:59:LEU:HD12	1.96	0.66
1:F:83:PHE:O	1:F:87:THR:HG22	1.96	0.66
1:D:61:ASP:OD2	1:D:103:TYR:OH	2.11	0.66
1:D:255:LYS:CE	4:D:538:HOH:O	2.42	0.66
1:E:216:ALA:H	1:E:220:GLN:NE2	1.93	0.66
1:A:240:LYS:CD	4:B:527:HOH:O	2.37	0.66
1:F:258:GLU:HB2	4:F:542:HOH:O	1.96	0.65
3:B:303:PE8:H121	4:B:518:HOH:O	1.95	0.65
1:H:83:PHE:O	1:H:87:THR:HG23	1.95	0.65
1:C:235:GLY:HA3	4:C:537:HOH:O	1.96	0.65
1:F:23:PHE:HA	1:F:50:GLU:O	1.96	0.65
1:D:175:THR:HG23	1:D:207:PRO:O	1.96	0.65
1:E:243:GLU:CG	4:E:542:HOH:O	2.37	0.65
1:E:205:ASN:ND2	4:E:518:HOH:O	2.29	0.65
1:H:257:ALA:O	1:H:261:THR:HG23	1.97	0.65
1:F:110:ASN:HB3	4:F:508:HOH:O	1.96	0.65
1:D:110:ASN:CB	4:D:497:HOH:O	2.41	0.64
1:A:50:GLU:CD	4:A:536:HOH:O	2.35	0.64
1:E:2:SER:OG	1:E:3:ASN:N	2.25	0.64
1:C:180:ARG:NH1	4:C:480:HOH:O	2.29	0.64
1:D:28:ASP:OD2	1:D:71:ARG:NH1	2.31	0.64
1:H:3:ASN:ND2	4:H:488:HOH:O	2.30	0.64
1:E:101:LEU:HD23	1:E:101:LEU:C	2.18	0.64
1:A:242:ILE:HA	1:A:252:LEU:CD1	2.27	0.64
1:C:3:ASN:N	4:C:554:HOH:O	2.31	0.64
1:E:174:TYR:HB2	1:E:208:PRO:O	1.98	0.63
1:E:61:ASP:O	1:F:180:ARG:NH2	2.31	0.63
1:E:175:THR:CG2	1:E:207:PRO:O	2.46	0.63
3:E:303:PE8:H151	4:E:507:HOH:O	1.98	0.63
1:C:83:PHE:O	1:C:87:THR:HG23	1.98	0.63
1:F:257:ALA:O	1:F:261:THR:CG2	2.47	0.63
1:B:216:ALA:H	1:B:220:GLN:NE2	1.96	0.63
1:F:216:ALA:H	1:F:220:GLN:HE22	1.45	0.63
1:C:175:THR:HG21	1:C:206:ALA:HB1	1.80	0.63
1:D:257:ALA:O	1:D:261:THR:HG22	1.98	0.62
1:G:54:PRO:HB2	1:G:73:LEU:HD13	1.80	0.62
1:A:156:PRO:HD2	1:A:159:ALA:HB2	1.80	0.62
1:C:138:ALA:N	1:C:139:PRO:HD2	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ALA:O	1:B:261:THR:HG23	1.98	0.62
1:E:78:THR:HG23	1:E:81:ASP:OD2	1.98	0.62
1:H:37:ILE:HD11	1:H:252:LEU:HD21	1.81	0.62
3:D:304:PE8:H62	4:D:472:HOH:O	2.00	0.62
1:E:25:THR:HB	4:E:427:HOH:O	1.99	0.62
1:H:28:ASP:OD2	1:H:71:ARG:NH1	2.32	0.62
1:B:257:ALA:O	1:B:261:THR:CG2	2.48	0.62
1:E:119:ALA:O	1:E:124:VAL:HG13	2.00	0.62
1:C:216:ALA:H	1:C:220:GLN:NE2	1.96	0.62
1:E:110:ASN:OD1	1:E:110:ASN:N	2.31	0.62
1:C:70:LEU:HD12	4:C:496:HOH:O	1.99	0.61
3:E:303:PE8:H212	4:E:507:HOH:O	1.99	0.61
1:D:257:ALA:O	1:D:261:THR:HG23	1.98	0.61
1:E:25:THR:HG23	1:E:68:ALA:HB1	1.82	0.61
1:H:216:ALA:H	1:H:220:GLN:NE2	1.98	0.61
1:H:32:GLU:HB3	4:H:519:HOH:O	2.00	0.61
1:C:15:GLN:HG2	1:G:92:GLN:HG2	1.83	0.60
1:B:37:ILE:HD13	1:B:242:ILE:HD13	1.83	0.60
1:F:196:ASN:HB3	4:F:487:HOH:O	2.01	0.60
1:G:151:PRO:HD2	1:G:172:GLU:HB2	1.84	0.60
1:B:18:GLY:HA3	1:B:225:ILE:HD13	1.82	0.60
1:D:25:THR:HG23	1:D:68:ALA:HB1	1.83	0.60
1:A:1:MET:HE1	1:A:207:PRO:HD3	1.83	0.60
1:B:2:SER:CA	1:B:6:GLN:HG3	2.30	0.60
1:D:62:GLY:O	1:D:66:GLN:HG3	2.02	0.60
1:G:225:ILE:O	4:G:503:HOH:O	2.17	0.60
1:C:21:VAL:HG22	1:C:48:ALA:HB3	1.83	0.59
1:G:175:THR:CG2	1:G:207:PRO:O	2.50	0.59
1:C:87:THR:HG22	1:C:122:ALA:CB	2.32	0.59
1:C:166:MET:O	1:C:170:GLN:HB2	2.02	0.59
1:D:3:ASN:CB	4:D:480:HOH:O	2.33	0.59
1:B:90:ARG:NH2	1:B:96:MET:O	2.25	0.59
1:F:225:ILE:HG12	4:F:541:HOH:O	1.96	0.59
1:C:114:GLU:HB2	4:C:485:HOH:O	2.03	0.58
1:C:23:PHE:HB3	1:C:235:GLY:HA2	1.84	0.58
1:C:60:ALA:HB1	3:D:304:PE8:H211	1.85	0.58
1:C:180:ARG:NH2	1:D:61:ASP:O	2.37	0.58
1:E:17:LYS:HE2	4:E:487:HOH:O	2.03	0.58
1:F:126:SER:HB2	1:F:152:ILE:HG12	1.84	0.58
1:A:118:LYS:HE3	4:A:484:HOH:O	2.03	0.58
1:H:110:ASN:CA	4:H:534:HOH:O	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:GLU:CD	1:F:135:GLU:H	2.07	0.58
1:F:216:ALA:H	1:F:220:GLN:HE21	1.50	0.58
1:H:42:VAL:CG1	1:H:96:MET:CE	2.80	0.58
1:C:177:LEU:N	1:C:177:LEU:HD12	2.19	0.58
1:D:3:ASN:C	4:D:480:HOH:O	2.42	0.58
2:H:302:SO4:O4	4:H:472:HOH:O	2.11	0.57
1:A:28:ASP:OD2	1:A:71:ARG:HD2	2.04	0.57
1:B:241:ILE:HG21	1:B:256:LEU:CD1	2.34	0.57
3:G:303:PE8:H81	4:G:502:HOH:O	2.05	0.57
1:D:101:LEU:C	1:D:101:LEU:HD23	2.25	0.57
1:F:158:ASN:N	4:F:535:HOH:O	2.38	0.57
1:E:180:ARG:HD2	4:F:425:HOH:O	2.04	0.57
1:C:15:GLN:CG	1:G:92:GLN:HG2	2.35	0.57
1:F:264:LYS:HE3	1:F:267:THR:OG1	2.05	0.56
1:F:28:ASP:OD2	1:F:71:ARG:HD2	2.05	0.56
1:D:56:SER:C	1:D:58:PRO:HD3	2.26	0.56
1:G:100:LEU:HD11	1:G:124:VAL:HG11	1.86	0.56
1:C:3:ASN:CB	4:C:554:HOH:O	2.31	0.56
1:C:28:ASP:OD2	1:C:71:ARG:HD2	2.05	0.56
1:E:174:TYR:HA	1:E:207:PRO:HB2	1.88	0.56
1:G:150:ALA:HB1	1:G:172:GLU:HB3	1.87	0.56
1:G:3:ASN:N	4:G:516:HOH:O	2.38	0.56
1:B:3:ASN:CG	4:B:486:HOH:O	2.44	0.56
1:H:257:ALA:O	1:H:261:THR:CG2	2.55	0.55
1:D:83:PHE:O	1:D:87:THR:HG23	2.06	0.55
1:C:217:GLU:HG3	1:C:218:PRO:HD2	1.89	0.55
1:D:37:ILE:O	1:D:41:LEU:HD22	2.07	0.55
1:C:114:GLU:CG	4:C:548:HOH:O	2.55	0.55
1:F:21:VAL:HG22	1:F:48:ALA:HB3	1.87	0.55
1:D:3:ASN:HA	1:D:6:GLN:HG2	1.89	0.55
1:F:135:GLU:OE1	1:F:135:GLU:N	2.39	0.55
1:D:37:ILE:HD13	1:D:242:ILE:HD13	1.89	0.55
1:G:113:ASP:HB3	4:G:522:HOH:O	2.06	0.55
1:F:249:GLU:HG2	4:F:529:HOH:O	2.06	0.55
1:H:128:LEU:HB2	1:H:152:ILE:HB	1.89	0.55
1:A:32:GLU:HG3	4:A:487:HOH:O	2.08	0.54
1:A:158:ASN:C	4:A:504:HOH:O	2.46	0.54
1:H:120:GLN:HG2	1:H:147:HIS:O	2.08	0.54
1:H:203:GLU:CB	4:H:498:HOH:O	2.55	0.54
4:E:521:HOH:O	1:F:59:LEU:CD1	2.53	0.54
1:E:216:ALA:H	1:E:220:GLN:HE22	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLU:OE1	4:A:520:HOH:O	2.18	0.54
1:F:217:GLU:H	1:F:220:GLN:HE21	1.55	0.54
1:G:83:PHE:O	1:G:87:THR:HG23	2.07	0.54
1:B:71:ARG:NH2	4:B:520:HOH:O	2.40	0.54
1:B:222:ARG:CG	1:B:226:LYS:HE3	2.37	0.54
1:E:171:GLY:O	1:E:172:GLU:HG3	2.08	0.54
1:E:180:ARG:NH2	1:F:61:ASP:O	2.39	0.54
1:F:216:ALA:N	1:F:220:GLN:NE2	2.47	0.54
1:G:6:GLN:HG2	4:G:505:HOH:O	2.08	0.54
1:H:110:ASN:N	4:H:534:HOH:O	2.40	0.54
1:D:128:LEU:HB2	1:D:152:ILE:HB	1.89	0.53
1:E:83:PHE:O	1:E:87:THR:HG22	2.08	0.53
1:C:226:LYS:CE	4:C:505:HOH:O	2.53	0.53
1:D:216:ALA:H	1:D:220:GLN:HE22	1.56	0.53
1:C:175:THR:CG2	1:C:207:PRO:O	2.57	0.53
1:D:175:THR:HG21	1:D:206:ALA:HB1	1.90	0.53
1:A:211:LEU:HD22	1:A:224:ALA:HB1	1.90	0.53
1:E:106:LEU:HD21	4:E:527:HOH:O	2.08	0.53
1:E:129:ILE:HD13	1:E:140:PHE:CG	2.44	0.53
1:F:35:LEU:O	1:F:39:GLN:HG3	2.09	0.53
1:B:225:ILE:HD12	1:B:267:THR:HA	1.90	0.52
1:F:216:ALA:N	1:F:220:GLN:HE22	2.06	0.52
1:H:27:GLY:HA3	1:H:77:THR:HG21	1.90	0.52
1:C:91:ALA:HA	4:C:493:HOH:O	2.09	0.52
1:H:138:ALA:O	1:H:139:PRO:C	2.44	0.52
1:G:11:ALA:O	1:G:15:GLN:HG3	2.09	0.52
1:H:23:PHE:HA	1:H:50:GLU:O	2.09	0.52
1:B:6:GLN:NE2	4:B:486:HOH:O	2.43	0.52
1:D:50:GLU:HG3	4:D:479:HOH:O	2.09	0.52
1:E:83:PHE:O	1:E:87:THR:CG2	2.57	0.52
1:F:34:SER:HA	1:F:37:ILE:HD12	1.90	0.52
1:F:107:VAL:HG12	1:F:112:ILE:HD12	1.92	0.52
1:A:120:GLN:HG3	4:A:538:HOH:O	2.10	0.52
1:D:1:MET:HA	1:D:173:GLY:H	1.75	0.52
1:A:180:ARG:HG2	4:A:463:HOH:O	2.10	0.52
1:C:240:LYS:HD3	4:D:525:HOH:O	2.08	0.52
1:A:216:ALA:H	1:A:220:GLN:NE2	2.08	0.52
1:B:83:PHE:O	1:B:87:THR:CG2	2.58	0.52
1:B:31:PRO:HD3	1:B:77:THR:HG22	1.92	0.51
1:C:111:GLY:HA3	1:C:114:GLU:HG2	1.92	0.51
1:E:120:GLN:HG2	4:E:478:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:203:GLU:HG3	4:G:525:HOH:O	2.09	0.51
1:H:106:LEU:O	1:H:106:LEU:HD23	2.10	0.51
1:A:166:MET:O	1:A:170:GLN:HG2	2.11	0.51
1:D:27:GLY:HA3	1:D:77:THR:HG21	1.92	0.51
1:C:114:GLU:H	1:C:114:GLU:CD	2.14	0.51
1:E:22:PRO:HG3	1:E:41:LEU:HG	1.92	0.51
1:H:101:LEU:O	1:H:102:LEU:HD23	2.11	0.51
1:D:226:LYS:HE2	4:D:543:HOH:O	2.10	0.51
1:G:44:ASN:O	1:G:260:THR:HG22	2.11	0.51
1:D:138:ALA:HB3	1:D:139:PRO:HD3	1.93	0.51
1:E:205:ASN:ND2	4:E:525:HOH:O	2.44	0.51
1:G:23:PHE:HB2	1:G:50:GLU:HB3	1.92	0.51
1:B:50:GLU:OE2	1:B:101:LEU:HD12	2.10	0.50
1:F:27:GLY:HA3	1:F:77:THR:HG21	1.93	0.50
1:F:193:PRO:HD2	4:F:544:HOH:O	2.12	0.50
1:F:225:ILE:CD1	1:F:267:THR:HA	2.41	0.50
1:D:193:PRO:HA	4:D:535:HOH:O	2.10	0.50
1:F:112:ILE:HG23	1:F:113:ASP:N	2.25	0.50
1:C:152:ILE:HD13	1:C:172:GLU:O	2.11	0.50
1:D:175:THR:CG2	1:D:207:PRO:O	2.60	0.50
1:C:175:THR:HG22	1:C:207:PRO:O	2.12	0.50
1:E:2:SER:C	1:E:6:GLN:HG3	2.31	0.50
1:B:87:THR:HG21	4:B:540:HOH:O	2.12	0.50
1:D:93:HIS:HB3	2:D:302:SO4:O3	2.12	0.50
1:G:175:THR:HG22	1:G:207:PRO:O	2.11	0.50
1:B:114:GLU:HG3	4:B:490:HOH:O	2.12	0.50
1:C:17:LYS:HE2	4:C:535:HOH:O	2.11	0.50
1:F:23:PHE:CD1	1:F:23:PHE:C	2.84	0.50
1:F:263:MET:HG2	4:F:482:HOH:O	2.11	0.50
1:H:31:PRO:HG3	1:H:77:THR:HB	1.94	0.50
1:F:2:SER:C	4:F:494:HOH:O	2.49	0.49
1:H:23:PHE:CD1	1:H:23:PHE:C	2.84	0.49
1:B:27:GLY:CA	1:B:77:THR:HG21	2.41	0.49
1:E:120:GLN:CG	4:E:543:HOH:O	2.55	0.49
1:F:174:TYR:CD2	1:F:210:LEU:HD12	2.46	0.49
1:E:50:GLU:HG3	4:E:510:HOH:O	1.99	0.49
1:G:90:ARG:HD2	1:G:123:GLY:HA3	1.94	0.49
1:D:3:ASN:HB3	4:D:513:HOH:O	1.87	0.49
1:H:248:ASP:OD1	1:H:251:THR:HB	2.12	0.49
1:A:165:LYS:O	1:A:169:GLU:HG3	2.12	0.49
1:A:54:PRO:HB3	1:A:72:SER:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:175:THR:HB	4:G:406:HOH:O	2.12	0.49
1:C:16:ASP:O	1:C:17:LYS:HD2	2.12	0.49
1:F:133:PRO:HA	4:F:490:HOH:O	2.12	0.49
1:F:180:ARG:HG2	4:F:480:HOH:O	2.13	0.49
1:G:154:ILE:HD13	1:G:176:TYR:CD1	2.48	0.49
1:B:128:LEU:HB2	1:B:152:ILE:HB	1.94	0.49
1:H:152:ILE:HD13	1:H:172:GLU:O	2.13	0.49
1:C:243:GLU:HG3	4:C:544:HOH:O	2.04	0.49
1:E:175:THR:HG21	1:E:206:ALA:HB1	1.95	0.49
1:A:126:SER:HB2	1:A:152:ILE:HG12	1.94	0.49
1:A:243:GLU:CG	4:A:490:HOH:O	2.46	0.49
1:B:38:ILE:HA	1:B:41:LEU:HD23	1.95	0.49
1:D:152:ILE:HD13	1:D:172:GLU:O	2.13	0.49
1:H:248:ASP:OD1	1:H:251:THR:CB	2.60	0.49
1:C:3:ASN:HB3	4:C:543:HOH:O	1.98	0.48
1:E:2:SER:O	1:E:6:GLN:CG	2.60	0.48
1:G:101:LEU:HD21	1:G:130:ALA:HB2	1.94	0.48
1:A:222:ARG:NH1	4:A:421:HOH:O	2.46	0.48
1:B:212:GLY:C	4:B:501:HOH:O	2.52	0.48
1:H:22:PRO:CG	1:H:41:LEU:HG	2.43	0.48
1:F:70:LEU:CD2	4:F:514:HOH:O	2.53	0.48
1:D:50:GLU:CG	4:D:479:HOH:O	2.62	0.48
1:F:101:LEU:O	1:F:102:LEU:HD23	2.13	0.48
1:C:3:ASN:N	4:C:501:HOH:O	2.47	0.48
1:C:60:ALA:HB1	3:D:304:PE8:H231	1.94	0.48
1:C:87:THR:HG22	1:C:122:ALA:HB1	1.95	0.48
1:C:129:ILE:N	1:C:129:ILE:HD12	2.28	0.48
1:D:180:ARG:HD2	4:D:429:HOH:O	2.13	0.48
1:A:32:GLU:OE2	1:C:219:GLU:OE1	2.32	0.48
1:A:61:ASP:O	1:B:180:ARG:NH2	2.41	0.48
1:B:83:PHE:O	1:B:87:THR:HG23	2.12	0.48
1:D:54:PRO:HB2	1:D:73:LEU:HD13	1.96	0.48
1:E:113:ASP:HB3	4:E:514:HOH:O	2.12	0.48
1:B:1:MET:HA	1:B:173:GLY:N	2.22	0.48
1:D:119:ALA:HB1	1:D:124:VAL:CG1	2.43	0.48
1:E:211:LEU:HD22	1:E:229:ALA:HB2	1.95	0.48
1:B:87:THR:HG22	1:B:122:ALA:HB1	1.94	0.48
1:B:259:PHE:HA	4:B:494:HOH:O	2.13	0.48
3:G:303:PE8:H231	4:G:490:HOH:O	2.14	0.48
1:H:25:THR:HG23	1:H:68:ALA:HB1	1.96	0.48
1:A:25:THR:HB	4:A:431:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:PRO:O	1:B:196:ASN:HB3	2.15	0.47
1:E:175:THR:HG23	1:E:207:PRO:O	2.15	0.47
1:E:180:ARG:HB3	4:E:521:HOH:O	2.13	0.47
1:G:71:ARG:NH2	1:G:243:GLU:HB2	2.29	0.47
1:B:18:GLY:HA3	1:B:225:ILE:CD1	2.44	0.47
1:B:80:SER:HB3	4:B:503:HOH:O	2.14	0.47
1:C:217:GLU:H	1:C:220:GLN:HE21	1.61	0.47
1:B:226:LYS:CG	4:B:547:HOH:O	2.47	0.47
1:B:176:TYR:CD1	1:B:176:TYR:C	2.87	0.47
4:C:417:HOH:O	1:G:94:PRO:HG3	2.15	0.47
1:E:30:SER:OG	1:E:33:LEU:HB2	2.15	0.47
1:E:175:THR:HB	4:E:477:HOH:O	2.15	0.47
1:H:87:THR:HG22	1:H:122:ALA:CB	2.44	0.47
1:B:241:ILE:O	1:B:241:ILE:CG2	2.62	0.47
1:C:249:GLU:HG2	4:C:442:HOH:O	2.15	0.47
1:B:241:ILE:O	1:B:241:ILE:HG22	2.13	0.47
1:B:241:ILE:CG2	1:B:256:LEU:CD1	2.93	0.47
1:A:21:VAL:O	1:A:233:ILE:HA	2.15	0.47
1:C:36:LYS:HE2	1:C:249:GLU:OE1	2.14	0.47
1:D:221:VAL:O	1:D:225:ILE:HD12	2.14	0.47
1:E:174:TYR:CD2	1:E:174:TYR:C	2.88	0.47
1:A:101:LEU:HD12	4:A:536:HOH:O	2.14	0.46
1:H:81:ASP:O	1:H:85:ILE:HG13	2.16	0.46
1:C:242:ILE:HA	1:C:252:LEU:CD1	2.44	0.46
1:E:110:ASN:N	4:E:482:HOH:O	2.44	0.46
1:F:241:ILE:HG21	1:F:256:LEU:HD13	1.97	0.46
1:C:11:ALA:O	1:C:15:GLN:HG3	2.16	0.46
1:G:252:LEU:HD12	1:G:256:LEU:HD22	1.96	0.46
1:A:152:ILE:CD1	1:A:172:GLU:O	2.63	0.46
1:E:129:ILE:HD13	1:E:140:PHE:CD1	2.50	0.46
1:F:152:ILE:HG13	1:F:174:TYR:CE1	2.51	0.46
1:H:22:PRO:HG3	1:H:41:LEU:HG	1.98	0.46
1:H:193:PRO:N	4:H:532:HOH:O	2.48	0.46
1:E:217:GLU:H	1:E:220:GLN:HE21	1.63	0.46
1:D:138:ALA:HB3	1:D:139:PRO:CD	2.46	0.46
1:E:182:GLY:HA2	1:F:59:LEU:HD11	1.96	0.46
1:H:248:ASP:OD1	1:H:251:THR:OG1	2.29	0.46
1:C:28:ASP:CG	1:C:71:ARG:HH11	2.19	0.46
1:D:156:PRO:HD2	1:D:159:ALA:HB2	1.98	0.46
1:H:126:SER:HB2	1:H:152:ILE:HD11	1.98	0.46
1:E:22:PRO:CG	1:E:41:LEU:HG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:THR:HG22	1:D:122:ALA:CB	2.46	0.45
1:E:50:GLU:CD	4:E:510:HOH:O	2.45	0.45
1:B:241:ILE:HG21	1:B:256:LEU:HD13	1.98	0.45
1:A:83:PHE:O	1:A:87:THR:HG22	2.17	0.45
1:H:105:ASN:O	1:H:109:ALA:HB2	2.17	0.45
1:A:73:LEU:HD12	1:A:73:LEU:HA	1.82	0.45
1:F:112:ILE:CG2	1:F:113:ASP:N	2.80	0.45
1:F:119:ALA:HB1	1:F:124:VAL:CG2	2.47	0.45
1:H:87:THR:HG22	1:H:122:ALA:HB1	1.99	0.45
1:A:252:LEU:O	1:A:256:LEU:HB2	2.17	0.45
1:B:87:THR:HG22	1:B:122:ALA:CB	2.46	0.45
1:D:21:VAL:HG22	1:D:48:ALA:HB3	1.98	0.45
1:G:168:SER:OG	1:G:206:ALA:HB2	2.17	0.45
1:D:83:PHE:O	1:D:87:THR:CG2	2.65	0.45
1:D:225:ILE:HD13	1:D:267:THR:HA	1.97	0.45
1:E:110:ASN:CB	4:E:482:HOH:O	2.63	0.45
1:F:113:ASP:HB2	4:F:527:HOH:O	2.17	0.45
1:D:209:PRO:HG3	4:D:473:HOH:O	2.15	0.45
1:C:92:GLN:HB3	1:G:15:GLN:HG2	1.99	0.45
1:D:29:PRO:HG2	1:D:33:LEU:HD23	1.98	0.45
1:E:205:ASN:CG	4:E:518:HOH:O	2.56	0.45
1:B:62:GLY:O	1:B:66:GLN:HG3	2.16	0.44
1:E:90:ARG:NH2	1:E:96:MET:O	2.40	0.44
1:C:134:VAL:HG21	1:C:167:VAL:HG22	1.98	0.44
1:G:83:PHE:O	1:G:87:THR:CG2	2.64	0.44
1:H:25:THR:HB	4:H:530:HOH:O	2.16	0.44
1:H:180:ARG:HG2	4:H:487:HOH:O	2.16	0.44
1:A:1:MET:SD	1:A:207:PRO:HA	2.57	0.44
1:E:129:ILE:CD1	1:E:140:PHE:HB3	2.48	0.44
4:E:521:HOH:O	1:F:59:LEU:HG	2.17	0.44
1:F:224:ALA:O	1:F:229:ALA:HB3	2.18	0.44
1:G:183:VAL:HG21	1:G:220:GLN:HG2	1.99	0.44
1:B:106:LEU:HD23	1:B:106:LEU:HA	1.70	0.44
1:C:88:LYS:HE2	1:C:88:LYS:HB2	1.47	0.44
1:G:3:ASN:HA	4:G:483:HOH:O	2.18	0.44
1:H:247:HIS:HB2	4:H:407:HOH:O	2.17	0.44
1:B:112:ILE:O	1:B:113:ASP:C	2.54	0.44
1:B:180:ARG:HG2	4:B:480:HOH:O	2.17	0.44
1:H:128:LEU:HD11	1:H:154:ILE:CD1	2.48	0.44
4:A:488:HOH:O	3:B:303:PE8:C5	2.65	0.44
1:D:126:SER:HA	1:D:150:ALA:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:ALA:H	1:D:220:GLN:HE21	1.59	0.44
1:B:46:ALA:O	1:B:96:MET:HE1	2.17	0.44
1:H:39:GLN:HE21	1:H:92:GLN:HE22	1.66	0.44
1:D:132:VAL:HG13	1:D:136:GLU:HB3	2.00	0.44
1:B:241:ILE:CG2	1:B:256:LEU:HD13	2.48	0.43
1:F:128:LEU:HD11	1:F:154:ILE:HG13	1.99	0.43
1:G:21:VAL:HA	1:G:22:PRO:HD2	1.87	0.43
1:A:133:PRO:O	1:A:134:VAL:C	2.56	0.43
1:C:83:PHE:O	1:C:87:THR:CG2	2.64	0.43
1:D:12:LEU:HD23	1:D:12:LEU:HA	1.75	0.43
1:D:119:ALA:HB1	1:D:124:VAL:HG11	2.00	0.43
1:F:250:ALA:HA	4:F:530:HOH:O	2.17	0.43
1:D:137:SER:O	1:D:138:ALA:C	2.57	0.43
1:F:23:PHE:CG	1:F:24:VAL:N	2.86	0.43
1:F:226:LYS:HE2	4:F:469:HOH:O	2.17	0.43
1:H:255:LYS:CE	4:H:539:HOH:O	2.48	0.43
1:B:222:ARG:HG2	1:B:226:LYS:CE	2.46	0.43
1:F:112:ILE:HG22	4:F:432:HOH:O	2.18	0.43
1:H:50:GLU:CB	4:H:493:HOH:O	2.66	0.43
1:H:83:PHE:O	1:H:87:THR:CG2	2.63	0.43
1:A:3:ASN:HB2	4:A:535:HOH:O	2.18	0.43
1:B:241:ILE:HG21	1:B:256:LEU:HD12	2.00	0.43
1:G:84:ASP:HB3	4:G:504:HOH:O	2.18	0.43
1:B:3:ASN:N	4:B:532:HOH:O	2.51	0.43
1:C:217:GLU:HG3	1:C:218:PRO:CD	2.48	0.43
1:E:158:ASN:OD1	1:E:158:ASN:N	2.45	0.43
1:F:45:GLY:O	1:F:46:ALA:C	2.57	0.43
1:G:128:LEU:HB2	1:G:152:ILE:HB	2.01	0.43
1:A:137:SER:CB	4:A:496:HOH:O	2.46	0.43
1:B:120:GLN:HB2	1:B:149:ILE:HD11	1.99	0.43
1:C:118:LYS:HE2	4:C:485:HOH:O	2.18	0.43
1:F:259:PHE:HB2	4:F:440:HOH:O	2.18	0.43
1:A:112:ILE:H	1:A:112:ILE:HG13	1.66	0.43
1:B:165:LYS:HG3	4:B:497:HOH:O	2.17	0.43
1:B:217:GLU:H	1:B:220:GLN:HE21	1.65	0.43
1:F:83:PHE:O	1:F:87:THR:CG2	2.65	0.43
1:G:59:LEU:HA	1:G:59:LEU:HD12	1.72	0.43
1:A:157:PRO:HD3	1:A:178:LEU:HB3	2.01	0.42
1:C:25:THR:HG23	1:C:68:ALA:HB1	2.01	0.42
1:F:193:PRO:N	4:F:536:HOH:O	2.51	0.42
1:B:12:LEU:CD1	1:B:19:ALA:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:LEU:C	1:E:101:LEU:CD2	2.87	0.42
1:B:219:GLU:CD	1:B:219:GLU:H	2.22	0.42
1:E:19:ALA:HA	1:E:47:ASP:OD1	2.19	0.42
1:F:15:GLN:HB2	1:F:17:LYS:HB2	2.01	0.42
1:F:160:ASP:OD1	1:F:160:ASP:N	2.47	0.42
1:E:129:ILE:HD13	1:E:140:PHE:CB	2.50	0.42
1:E:1:MET:HE1	4:E:525:HOH:O	2.18	0.42
1:E:109:ALA:C	4:E:482:HOH:O	2.57	0.42
1:F:113:ASP:O	1:F:114:GLU:C	2.53	0.42
1:G:222:ARG:HG3	4:G:507:HOH:O	2.19	0.42
1:E:22:PRO:HD2	1:E:46:ALA:HB1	2.01	0.42
1:G:158:ASN:N	1:G:158:ASN:OD1	2.53	0.42
1:D:134:VAL:HG13	1:D:153:PHE:CD1	2.54	0.42
1:E:242:ILE:HA	1:E:252:LEU:CD1	2.50	0.42
1:F:18:GLY:HA2	4:F:431:HOH:O	2.19	0.42
1:A:214:GLY:HA2	1:B:63:PRO:HD3	2.02	0.42
1:B:152:ILE:HD13	1:B:172:GLU:O	2.20	0.42
1:C:213:PHE:CE1	3:D:304:PE8:H141	2.55	0.42
1:F:2:SER:HA	1:F:6:GLN:HG3	2.02	0.42
1:C:156:PRO:HG2	1:C:159:ALA:HB2	2.02	0.42
1:C:177:LEU:N	1:C:177:LEU:CD1	2.82	0.42
1:A:23:PHE:CD1	1:A:23:PHE:C	2.93	0.41
1:B:184:THR:HG22	4:B:553:HOH:O	2.19	0.41
1:E:25:THR:CG2	1:E:68:ALA:HB1	2.49	0.41
1:A:138:ALA:N	1:A:139:PRO:HD2	2.35	0.41
4:A:488:HOH:O	3:B:303:PE8:H52	2.19	0.41
1:B:180:ARG:HG3	1:B:215:ILE:HD13	2.02	0.41
1:C:133:PRO:HD2	1:C:136:GLU:HB2	2.02	0.41
4:E:448:HOH:O	1:F:180:ARG:HD2	2.20	0.41
1:A:32:GLU:HG3	1:A:32:GLU:H	1.66	0.41
1:C:56:SER:OG	4:C:492:HOH:O	2.04	0.41
1:F:142:LYS:HD2	4:F:532:HOH:O	2.20	0.41
1:F:261:THR:HB	4:F:491:HOH:O	2.21	0.41
1:G:23:PHE:HA	1:G:50:GLU:O	2.19	0.41
1:G:61:ASP:O	1:H:180:ARG:NH2	2.53	0.41
1:H:53:PHE:CE1	1:H:82:CYS:HB2	2.56	0.41
1:B:239:VAL:O	1:B:240:LYS:C	2.59	0.41
1:E:23:PHE:HA	1:E:50:GLU:HB3	2.02	0.41
1:E:101:LEU:HD12	4:E:510:HOH:O	2.19	0.41
1:C:162:ASP:HB3	4:C:508:HOH:O	2.20	0.41
1:H:93:HIS:HA	2:H:302:SO4:O2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:203:GLU:HB3	4:H:498:HOH:O	2.21	0.41
4:A:417:HOH:O	1:B:180:ARG:CD	2.68	0.41
1:B:4:ARG:HD2	1:B:125:ASP:OD2	2.21	0.41
1:B:59:LEU:HD12	1:B:59:LEU:HA	1.80	0.41
1:F:11:ALA:O	1:F:15:GLN:HG3	2.21	0.41
1:H:208:PRO:HA	1:H:209:PRO:HD2	1.85	0.41
1:C:138:ALA:N	1:C:139:PRO:CD	2.80	0.41
1:E:90:ARG:HD2	1:E:123:GLY:HA3	2.01	0.41
1:G:156:PRO:HD2	1:G:159:ALA:HB2	2.02	0.41
4:G:508:HOH:O	1:H:180:ARG:HD2	2.20	0.41
1:A:24:VAL:HG22	4:A:530:HOH:O	2.20	0.41
1:D:28:ASP:HA	1:D:29:PRO:HA	1.90	0.41
1:E:1:MET:HB3	4:E:449:HOH:O	2.20	0.41
1:E:178:LEU:HD12	1:E:178:LEU:HA	2.00	0.41
1:G:42:VAL:HG11	1:G:93:HIS:CE1	2.55	0.41
1:H:119:ALA:HB1	1:H:124:VAL:CG1	2.51	0.41
1:E:242:ILE:HA	1:E:252:LEU:HD11	2.03	0.41
1:E:129:ILE:HD13	1:E:140:PHE:HB3	2.02	0.40
1:E:183:VAL:HG12	4:E:538:HOH:O	2.20	0.40
1:F:127:VAL:HG23	1:F:149:ILE:HG21	2.03	0.40
1:H:42:VAL:CG1	1:H:96:MET:HE1	2.40	0.40
1:D:154:ILE:HD13	3:D:304:PE8:H51	2.04	0.40
1:F:90:ARG:NH2	1:F:96:MET:O	2.39	0.40
1:G:112:ILE:H	1:G:112:ILE:HG13	1.62	0.40
1:H:38:ILE:O	1:H:41:LEU:HB2	2.20	0.40
1:A:83:PHE:O	1:A:87:THR:CG2	2.69	0.40
1:A:137:SER:O	1:A:138:ALA:C	2.59	0.40
1:C:29:PRO:HG2	1:C:33:LEU:CD1	2.48	0.40
1:E:248:ASP:O	1:E:249:GLU:C	2.59	0.40
1:H:73:LEU:HD12	1:H:73:LEU:HA	1.78	0.40
1:H:203:GLU:HB2	4:H:498:HOH:O	2.18	0.40
1:A:12:LEU:HD23	1:A:12:LEU:HA	1.68	0.40
1:A:103:TYR:O	1:A:106:LEU:HB3	2.22	0.40
1:C:119:ALA:O	1:C:124:VAL:HG13	2.22	0.40
1:E:128:LEU:HD12	1:E:129:ILE:N	2.37	0.40
1:F:253:LEU:CD2	4:F:545:HOH:O	2.70	0.40
1:H:155:ALA:HA	1:H:156:PRO:HD3	1.92	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	255/267 (96%)	239 (94%)	16 (6%)	0	100	100
1	B	255/267 (96%)	236 (92%)	17 (7%)	2 (1%)	19	39
1	C	255/267 (96%)	248 (97%)	7 (3%)	0	100	100
1	D	255/267 (96%)	239 (94%)	13 (5%)	3 (1%)	13	27
1	E	255/267 (96%)	240 (94%)	14 (6%)	1 (0%)	34	57
1	F	255/267 (96%)	237 (93%)	16 (6%)	2 (1%)	19	39
1	G	255/267 (96%)	243 (95%)	12 (5%)	0	100	100
1	H	255/267 (96%)	239 (94%)	15 (6%)	1 (0%)	34	57
All	All	2040/2136 (96%)	1921 (94%)	110 (5%)	9 (0%)	34	57

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	VAL
1	H	134	VAL
1	F	2	SER
1	D	109	ALA
1	E	3	ASN
1	B	240	LYS
1	D	134	VAL
1	F	157	PRO
1	D	58	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	196/201 (98%)	170 (87%)	26 (13%)	4 7
1	B	196/201 (98%)	171 (87%)	25 (13%)	4 8
1	C	196/201 (98%)	170 (87%)	26 (13%)	4 7
1	D	196/201 (98%)	172 (88%)	24 (12%)	5 9
1	E	196/201 (98%)	168 (86%)	28 (14%)	3 5
1	F	196/201 (98%)	170 (87%)	26 (13%)	4 7
1	G	196/201 (98%)	172 (88%)	24 (12%)	5 9
1	H	196/201 (98%)	168 (86%)	28 (14%)	3 5
All	All	1568/1608 (98%)	1361 (87%)	207 (13%)	4 7

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	SER
1	A	3	ASN
1	A	17	LYS
1	A	24	VAL
1	A	25	THR
1	A	31	PRO
1	A	32	GLU
1	A	35	LEU
1	A	41	LEU
1	A	49	LEU
1	A	59	LEU
1	A	73	LEU
1	A	80	SER
1	A	87	THR
1	A	88	LYS
1	A	90	ARG
1	A	106	LEU
1	A	112	ILE
1	A	134	VAL
1	A	166	MET
1	A	175	THR
1	A	196	ASN
1	A	217	GLU
1	A	219	GLU

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Mol	Chain	Res	Type
1	A	226	LYS
1	B	3	ASN
1	B	17	LYS
1	B	24	VAL
1	B	25	THR
1	B	35	LEU
1	B	41	LEU
1	B	49	LEU
1	B	59	LEU
1	B	70	LEU
1	B	73	LEU
1	B	77	THR
1	B	79	SER
1	B	87	THR
1	B	101	LEU
1	B	112	ILE
1	B	124	VAL
1	B	134	VAL
1	B	135	GLU
1	B	158	ASN
1	B	169	GLU
1	B	175	THR
1	B	199	THR
1	B	226	LYS
1	B	258	GLU
1	B	261	THR
1	C	1	MET
1	C	2	SER
1	C	17	LYS
1	C	24	VAL
1	C	25	THR
1	C	33	LEU
1	C	35	LEU
1	C	41	LEU
1	C	49	LEU
1	C	59	LEU
1	C	73	LEU
1	C	80	SER
1	C	87	THR
1	C	90	ARG
1	C	112	ILE
1	C	114	GLU

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Mol	Chain	Res	Type
1	C	136	GLU
1	C	145	LYS
1	C	166	MET
1	C	175	THR
1	C	195	GLU
1	C	203	GLU
1	C	211	LEU
1	C	217	GLU
1	C	226	LYS
1	C	256	LEU
1	D	2	SER
1	D	17	LYS
1	D	24	VAL
1	D	25	THR
1	D	35	LEU
1	D	41	LEU
1	D	49	LEU
1	D	59	LEU
1	D	73	LEU
1	D	77	THR
1	D	80	SER
1	D	87	THR
1	D	108	PHE
1	D	112	ILE
1	D	124	VAL
1	D	134	VAL
1	D	136	GLU
1	D	137	SER
1	D	175	THR
1	D	196	ASN
1	D	200	GLN
1	D	252	LEU
1	D	256	LEU
1	D	261	THR
1	E	2	SER
1	E	3	ASN
1	E	17	LYS
1	E	24	VAL
1	E	25	THR
1	E	31	PRO
1	E	32	GLU
1	E	33	LEU

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Mol	Chain	Res	Type
1	E	35	LEU
1	E	41	LEU
1	E	49	LEU
1	E	59	LEU
1	E	70	LEU
1	E	73	LEU
1	E	87	THR
1	E	105	ASN
1	E	108	PHE
1	E	110	ASN
1	E	112	ILE
1	E	134	VAL
1	E	175	THR
1	E	176	TYR
1	E	184	THR
1	E	197	ILE
1	E	205	ASN
1	E	211	LEU
1	E	226	LYS
1	E	256	LEU
1	F	2	SER
1	F	17	LYS
1	F	25	THR
1	F	35	LEU
1	F	41	LEU
1	F	49	LEU
1	F	59	LEU
1	F	63	PRO
1	F	70	LEU
1	F	73	LEU
1	F	77	THR
1	F	84	ASP
1	F	87	THR
1	F	90	ARG
1	F	112	ILE
1	F	114	GLU
1	F	124	VAL
1	F	128	LEU
1	F	163	THR
1	F	166	MET
1	F	179	SER
1	F	211	LEU

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Mol	Chain	Res	Type
1	F	226	LYS
1	F	240	LYS
1	F	256	LEU
1	F	261	THR
1	G	1	MET
1	G	2	SER
1	G	3	ASN
1	G	17	LYS
1	G	24	VAL
1	G	25	THR
1	G	31	PRO
1	G	33	LEU
1	G	35	LEU
1	G	41	LEU
1	G	70	LEU
1	G	73	LEU
1	G	87	THR
1	G	90	ARG
1	G	106	LEU
1	G	112	ILE
1	G	134	VAL
1	G	142	LYS
1	G	168	SER
1	G	175	THR
1	G	211	LEU
1	G	219	GLU
1	G	252	LEU
1	G	256	LEU
1	H	2	SER
1	H	17	LYS
1	H	24	VAL
1	H	25	THR
1	H	33	LEU
1	H	35	LEU
1	H	41	LEU
1	H	49	LEU
1	H	59	LEU
1	H	70	LEU
1	H	73	LEU
1	H	77	THR
1	H	80	SER
1	H	87	THR

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Mol	Chain	Res	Type
1	H	90	ARG
1	H	112	ILE
1	H	114	GLU
1	H	120	GLN
1	H	124	VAL
1	H	136	GLU
1	H	169	GLU
1	H	179	SER
1	H	184	THR
1	H	219	GLU
1	H	226	LYS
1	H	240	LYS
1	H	256	LEU
1	H	261	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	220	GLN
1	A	247	HIS
1	B	110	ASN
1	B	220	GLN
1	C	105	ASN
1	C	220	GLN
1	C	246	GLN
1	D	39	GLN
1	D	92	GLN
1	D	105	ASN
1	D	147	HIS
1	D	196	ASN
1	D	220	GLN
1	D	247	HIS
1	E	3	ASN
1	E	170	GLN
1	E	200	GLN
1	E	205	ASN
1	E	220	GLN
1	F	220	GLN
1	G	105	ASN
1	G	110	ASN
1	G	170	GLN

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Mol	Chain	Res	Type
1	G	220	GLN
1	H	39	GLN
1	H	92	GLN
1	H	105	ASN
1	H	120	GLN
1	H	220	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

22 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	PE8	G	303	-	24,24,24	0.61	0	23,23,23	1.46	2 (8%)
3	PE8	E	303	-	24,24,24	0.59	0	23,23,23	1.85	9 (39%)
2	SO4	E	302	-	4,4,4	0.34	0	6,6,6	1.02	0
3	PE8	B	303	-	24,24,24	0.57	0	23,23,23	1.85	6 (26%)
2	SO4	H	301	-	4,4,4	0.47	0	6,6,6	0.90	0
2	SO4	B	301	-	4,4,4	0.55	0	6,6,6	0.51	0
2	SO4	D	301	-	4,4,4	0.50	0	6,6,6	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	G	301	-	4,4,4	0.30	0	6,6,6	0.41	0
2	SO4	B	302	-	4,4,4	0.13	0	6,6,6	0.68	0
2	SO4	H	302	-	4,4,4	0.47	0	6,6,6	1.15	1 (16%)
2	SO4	D	303	-	4,4,4	0.32	0	6,6,6	0.53	0
2	SO4	D	302	-	4,4,4	0.47	0	6,6,6	1.16	1 (16%)
2	SO4	E	301	-	4,4,4	0.44	0	6,6,6	0.50	0
2	SO4	A	302	-	4,4,4	0.61	0	6,6,6	0.40	0
2	SO4	G	302	-	4,4,4	0.44	0	6,6,6	0.26	0
2	SO4	F	301	-	4,4,4	0.54	0	6,6,6	0.62	0
2	SO4	C	301	-	4,4,4	0.43	0	6,6,6	0.43	0
2	SO4	F	302	-	4,4,4	0.71	0	6,6,6	1.10	1 (16%)
2	SO4	A	303	-	4,4,4	0.48	0	6,6,6	1.04	0
2	SO4	C	302	-	4,4,4	0.46	0	6,6,6	0.79	0
2	SO4	A	301	-	4,4,4	0.37	0	6,6,6	0.79	0
3	PE8	D	304	-	24,24,24	0.68	0	23,23,23	1.60	4 (17%)

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	PE8	B	303	-	-	14/22/22/22	-
3	PE8	G	303	-	-	14/22/22/22	-
3	PE8	E	303	-	-	13/22/22/22	-
3	PE8	D	304	-	-	15/22/22/22	-

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	303	PE8	O22-C21-C20	3.30	125.41	110.35
3	B	303	PE8	O10-C9-C8	3.25	125.17	110.35
3	B	303	PE8	O13-C12-C11	3.14	124.66	110.35
3	B	303	PE8	O4-C5-C6	2.95	123.78	110.35
3	D	304	PE8	O22-C23-C24	2.71	122.04	110.11
3	B	303	PE8	C8-O7-C6	2.62	124.71	113.26
3	G	303	PE8	O7-C6-C5	2.61	122.23	110.35
3	E	303	PE8	C20-O19-C18	2.58	124.53	113.26
3	E	303	PE8	C8-O7-C6	2.48	124.11	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	303	PE8	O19-C20-C21	2.40	121.29	110.35
3	D	304	PE8	O22-C21-C20	2.39	121.24	110.35
3	G	303	PE8	O4-C3-C2	2.33	120.36	110.11
3	E	303	PE8	O16-C15-C14	2.29	120.77	110.35
2	D	302	SO4	O3-S-O2	-2.28	97.64	109.56
3	D	304	PE8	C23-O22-C21	2.26	123.14	113.26
2	H	302	SO4	O4-S-O1	-2.22	97.96	109.56
3	E	303	PE8	O22-C23-C24	2.16	119.61	110.11
3	D	304	PE8	C17-O16-C15	2.15	122.67	113.26
3	E	303	PE8	C5-O4-C3	2.11	122.49	113.26
3	B	303	PE8	O19-C18-C17	2.09	119.90	110.35
3	E	303	PE8	O4-C5-C6	2.07	119.80	110.35
3	B	303	PE8	C5-O4-C3	2.03	122.14	113.26
2	F	302	SO4	O3-S-O2	2.03	120.16	109.56
3	E	303	PE8	O16-C17-C18	2.02	119.54	110.35

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	303	PE8	O10-C11-C12-O13
3	G	303	PE8	O19-C20-C21-O22
3	B	303	PE8	O16-C17-C18-O19
3	G	303	PE8	O10-C11-C12-O13
3	G	303	PE8	O16-C17-C18-O19
3	D	304	PE8	O4-C5-C6-O7
3	B	303	PE8	O13-C14-C15-O16
3	D	304	PE8	O7-C8-C9-O10
3	E	303	PE8	O10-C11-C12-O13
3	D	304	PE8	O1-C2-C3-O4
3	E	303	PE8	O22-C23-C24-O25
3	B	303	PE8	O19-C20-C21-O22
3	B	303	PE8	O1-C2-C3-O4
3	G	303	PE8	O4-C5-C6-O7
3	D	304	PE8	C6-C5-O4-C3
3	B	303	PE8	O4-C5-C6-O7
3	D	304	PE8	O10-C11-C12-O13
3	E	303	PE8	O1-C2-C3-O4
3	G	303	PE8	C12-C11-O10-C9
3	E	303	PE8	O19-C20-C21-O22
3	G	303	PE8	O7-C8-C9-O10
3	E	303	PE8	O16-C17-C18-O19

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Mol	Chain	Res	Type	Atoms
3	B	303	PE8	O7-C8-C9-O10
3	G	303	PE8	O22-C23-C24-O25
3	D	304	PE8	C11-C12-O13-C14
3	D	304	PE8	O13-C14-C15-O16
3	E	303	PE8	C15-C14-O13-C12
3	D	304	PE8	C8-C9-O10-C11
3	D	304	PE8	C20-C21-O22-C23
3	E	303	PE8	C8-C9-O10-C11
3	G	303	PE8	C8-C9-O10-C11
3	D	304	PE8	C24-C23-O22-C21
3	D	304	PE8	C18-C17-O16-C15
3	G	303	PE8	O1-C2-C3-O4
3	D	304	PE8	C5-C6-O7-C8
3	B	303	PE8	C20-C21-O22-C23
3	B	303	PE8	O22-C23-C24-O25
3	B	303	PE8	C2-C3-O4-C5
3	G	303	PE8	C20-C21-O22-C23
3	B	303	PE8	C17-C18-O19-C20
3	E	303	PE8	O13-C14-C15-O16
3	E	303	PE8	C11-C12-O13-C14
3	D	304	PE8	C14-C15-O16-C17
3	E	303	PE8	C17-C18-O19-C20
3	B	303	PE8	C18-C17-O16-C15
3	E	303	PE8	C20-C21-O22-C23
3	E	303	PE8	C18-C17-O16-C15
3	E	303	PE8	C21-C20-O19-C18
3	G	303	PE8	C5-C6-O7-C8
3	D	304	PE8	C21-C20-O19-C18
3	B	303	PE8	C14-C15-O16-C17
3	G	303	PE8	O13-C14-C15-O16
3	G	303	PE8	C9-C8-O7-C6
3	G	303	PE8	C21-C20-O19-C18
3	B	303	PE8	C9-C8-O7-C6
3	D	304	PE8	O19-C20-C21-O22

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	303	PE8	3	0
3	E	303	PE8	2	0
2	E	302	SO4	1	0

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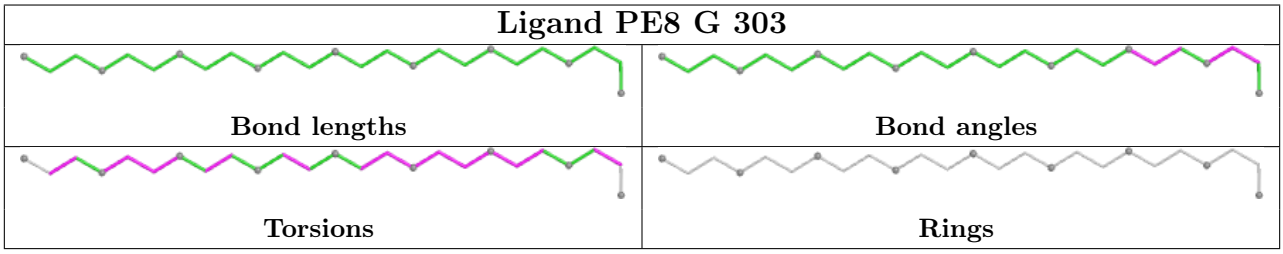
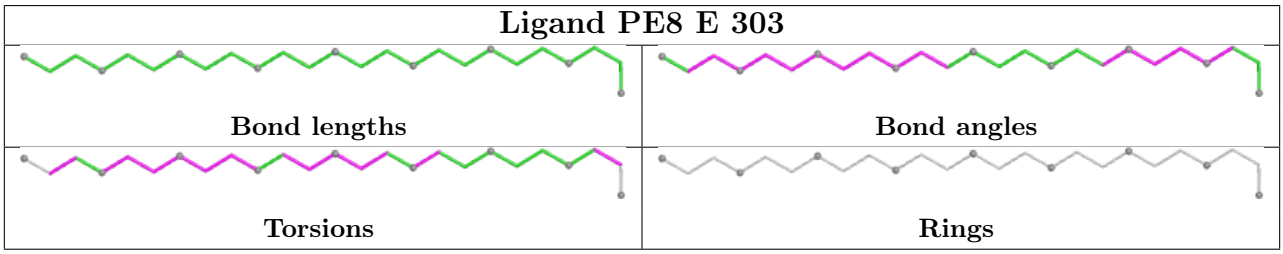
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	303	PE8	3	0
2	H	302	SO4	2	0
2	D	302	SO4	1	0
2	C	301	SO4	1	0
3	D	304	PE8	5	0

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.

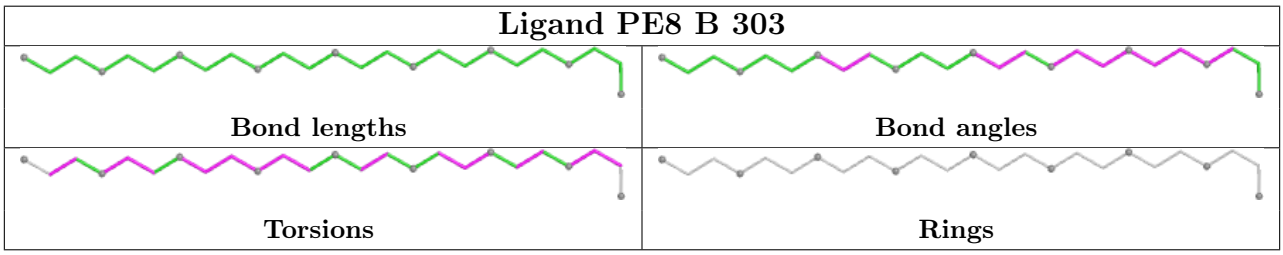
Ligand PE8 G 303

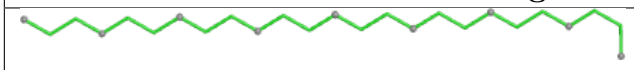
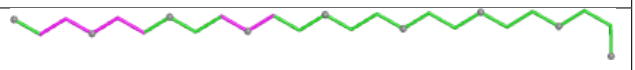
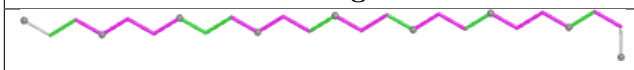
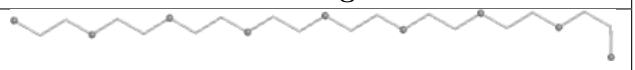


Ligand PE8 E 303



Ligand PE8 B 303



Ligand PE8 D 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	259/267 (97%)	-0.56	0	100	100	17, 28, 54, 63	0
1	B	259/267 (97%)	-0.51	0	100	100	18, 29, 53, 67	0
1	C	259/267 (97%)	-0.53	1 (0%)	92	91	19, 28, 51, 74	0
1	D	259/267 (97%)	-0.50	0	100	100	17, 27, 53, 66	0
1	E	259/267 (97%)	-0.51	0	100	100	16, 28, 53, 67	0
1	F	259/267 (97%)	-0.49	2 (0%)	86	84	18, 28, 59, 80	0
1	G	259/267 (97%)	-0.52	0	100	100	18, 28, 49, 70	0
1	H	259/267 (97%)	-0.51	1 (0%)	92	91	19, 29, 56, 71	0
All	All	2072/2136 (97%)	-0.52	4 (0%)	95	95	16, 28, 54, 80	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1	MET	3.9
1	H	1	MET	3.4
1	F	2	SER	3.0
1	C	1	MET	2.2

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 monosaccharides in this entry.

6.4 Ligands (i)

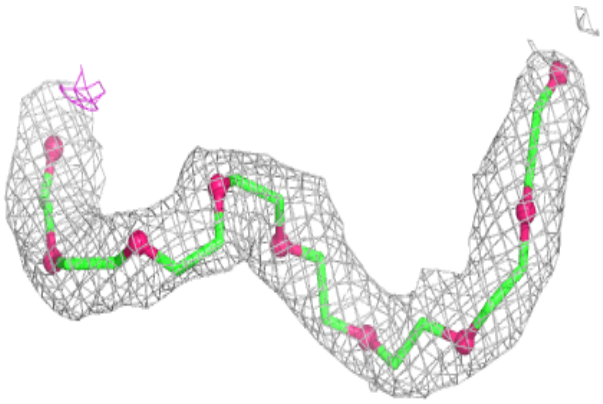
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

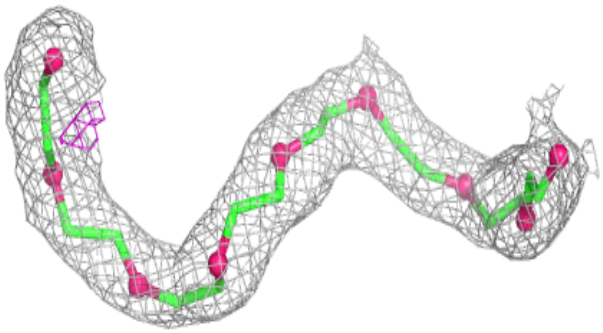
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	302	5/5	0.90	0.31	104,106,110,118	0
2	SO4	D	301	5/5	0.92	0.35	85,90,104,114	0
3	PE8	G	303	25/25	0.93	0.20	41,49,60,62	0
3	PE8	B	303	25/25	0.94	0.16	39,51,54,56	0
3	PE8	E	303	25/25	0.95	0.18	39,45,55,56	0
3	PE8	D	304	25/25	0.96	0.17	40,50,54,57	0
2	SO4	F	302	5/5	0.98	0.15	34,36,42,46	0
2	SO4	D	302	5/5	0.99	0.13	32,41,48,49	0
2	SO4	D	303	5/5	0.99	0.13	21,24,26,28	0
2	SO4	E	301	5/5	0.99	0.14	26,29,31,35	0
2	SO4	E	302	5/5	0.99	0.16	36,39,42,43	0
2	SO4	F	301	5/5	0.99	0.12	23,23,24,28	0
2	SO4	A	303	5/5	0.99	0.15	26,28,29,32	0
2	SO4	G	301	5/5	0.99	0.14	40,41,43,44	0
2	SO4	G	302	5/5	0.99	0.11	29,29,34,40	0
2	SO4	H	302	5/5	0.99	0.13	31,38,41,41	0
2	SO4	B	301	5/5	0.99	0.14	42,46,47,55	0
2	SO4	C	301	5/5	0.99	0.15	26,26,29,31	0
2	SO4	C	302	5/5	0.99	0.14	33,42,44,44	0
2	SO4	A	301	5/5	0.99	0.15	23,23,25,28	0
2	SO4	H	301	5/5	1.00	0.12	21,25,26,28	0
2	SO4	B	302	5/5	1.00	0.13	23,23,25,26	0

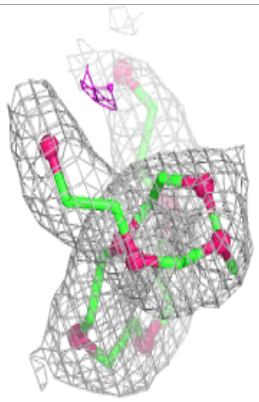
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PE8 G 303:

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

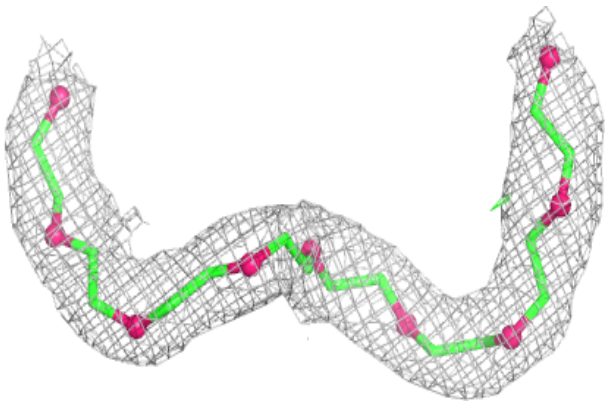


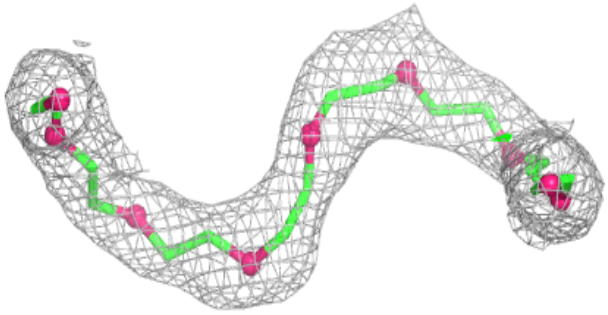


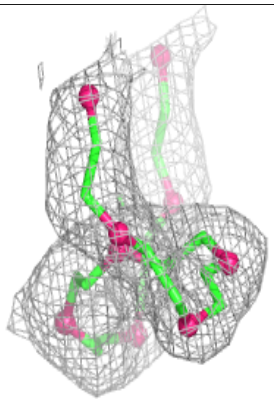


Electron density around PE8 B 303:

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

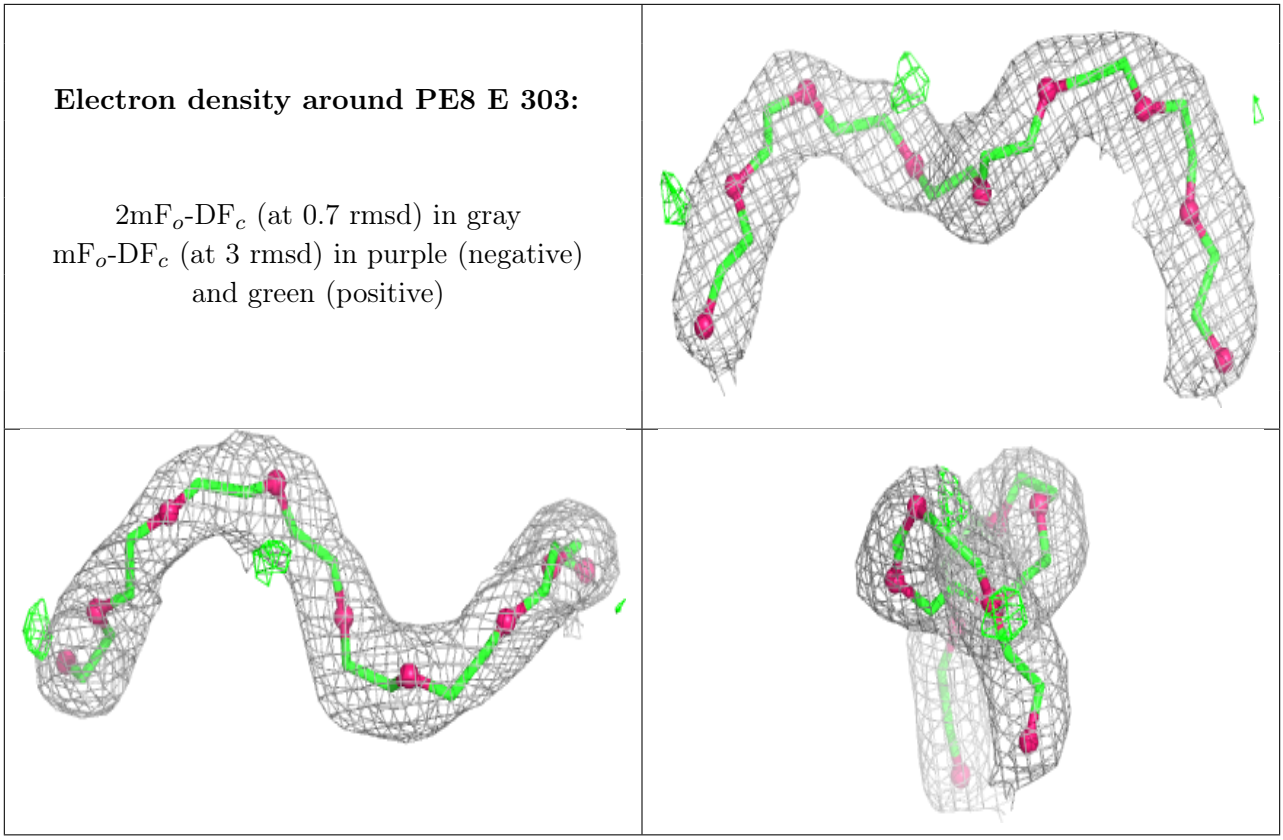






Electron density around PE8 E 303:

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



Electron density around PE8 D 304:

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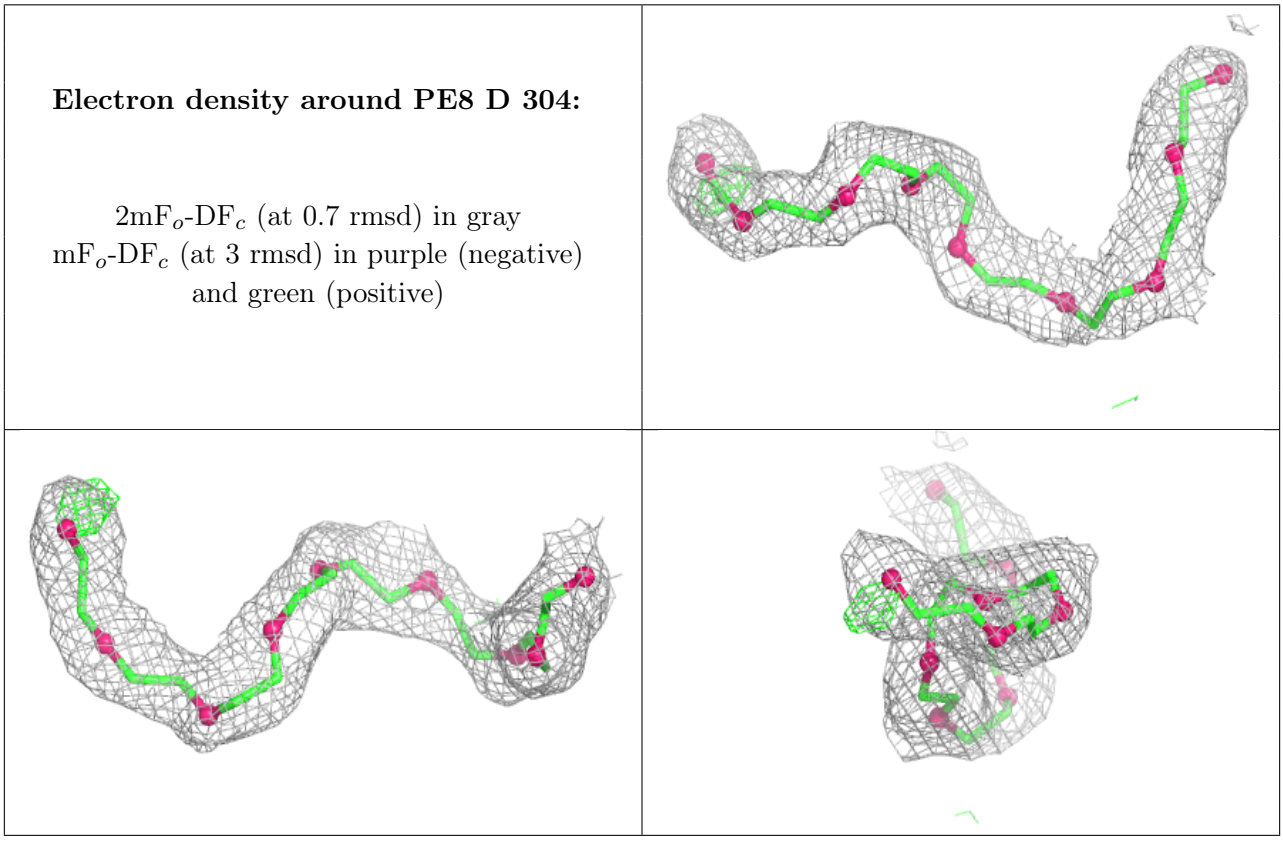
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.