Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 06:39 PM EDT

PDB ID	:	3HLB
Title	:	Simvastatin Synthase (LovD) from Aspergillus terreus, unliganded, selenomethionyl derivative
Authors	:	Sawaya, M.R.; Yeates, T.O.; Laidman, J.; Pashkov, I.; Gao, X.; Tang, Y.
Deposited on	:	2009-05-27
Resolution	:	2.50 Å(reported)

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

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

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

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

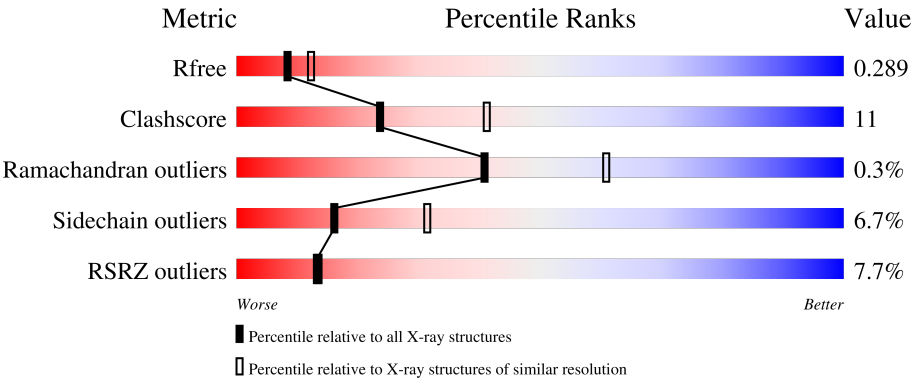
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	432	5% 70% 22% • 6%
1	B	432	9% 73% 19% • 6%
1	C	432	8% 70% 20% • 8%
1	D	432	7% 67% 22% • 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12633 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 Transesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3173	1991	574	587	21			
1	B	404	Total	C	N	O	S	0	0	0
			3173	1991	574	587	21			
1	C	398	Total	C	N	O	S	0	0	0
			3118	1955	565	577	21			
1	D	393	Total	C	N	O	S	0	0	0
			3083	1936	560	566	21			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP Q9Y7D1
A	-17	SER	-	expression tag	UNP Q9Y7D1
A	-16	SER	-	expression tag	UNP Q9Y7D1
A	-15	HIS	-	expression tag	UNP Q9Y7D1
A	-14	HIS	-	expression tag	UNP Q9Y7D1
A	-13	HIS	-	expression tag	UNP Q9Y7D1
A	-12	HIS	-	expression tag	UNP Q9Y7D1
A	-11	HIS	-	expression tag	UNP Q9Y7D1
A	-10	HIS	-	expression tag	UNP Q9Y7D1
A	-9	SER	-	expression tag	UNP Q9Y7D1
A	-8	SER	-	expression tag	UNP Q9Y7D1
A	-7	GLY	-	expression tag	UNP Q9Y7D1
A	-6	LEU	-	expression tag	UNP Q9Y7D1
A	-5	VAL	-	expression tag	UNP Q9Y7D1
A	-4	PRO	-	expression tag	UNP Q9Y7D1
A	-3	ARG	-	expression tag	UNP Q9Y7D1
A	-2	GLY	-	expression tag	UNP Q9Y7D1
A	-1	SER	-	expression tag	UNP Q9Y7D1
A	0	HIS	-	expression tag	UNP Q9Y7D1
A	40	ALA	CYS	engineered mutation	UNP Q9Y7D1
A	60	ASN	CYS	engineered mutation	UNP Q9Y7D1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q9Y7D1
B	-17	SER	-	expression tag	UNP Q9Y7D1
B	-16	SER	-	expression tag	UNP Q9Y7D1
B	-15	HIS	-	expression tag	UNP Q9Y7D1
B	-14	HIS	-	expression tag	UNP Q9Y7D1
B	-13	HIS	-	expression tag	UNP Q9Y7D1
B	-12	HIS	-	expression tag	UNP Q9Y7D1
B	-11	HIS	-	expression tag	UNP Q9Y7D1
B	-10	HIS	-	expression tag	UNP Q9Y7D1
B	-9	SER	-	expression tag	UNP Q9Y7D1
B	-8	SER	-	expression tag	UNP Q9Y7D1
B	-7	GLY	-	expression tag	UNP Q9Y7D1
B	-6	LEU	-	expression tag	UNP Q9Y7D1
B	-5	VAL	-	expression tag	UNP Q9Y7D1
B	-4	PRO	-	expression tag	UNP Q9Y7D1
B	-3	ARG	-	expression tag	UNP Q9Y7D1
B	-2	GLY	-	expression tag	UNP Q9Y7D1
B	-1	SER	-	expression tag	UNP Q9Y7D1
B	0	HIS	-	expression tag	UNP Q9Y7D1
B	40	ALA	CYS	engineered mutation	UNP Q9Y7D1
B	60	ASN	CYS	engineered mutation	UNP Q9Y7D1
C	-18	GLY	-	expression tag	UNP Q9Y7D1
C	-17	SER	-	expression tag	UNP Q9Y7D1
C	-16	SER	-	expression tag	UNP Q9Y7D1
C	-15	HIS	-	expression tag	UNP Q9Y7D1
C	-14	HIS	-	expression tag	UNP Q9Y7D1
C	-13	HIS	-	expression tag	UNP Q9Y7D1
C	-12	HIS	-	expression tag	UNP Q9Y7D1
C	-11	HIS	-	expression tag	UNP Q9Y7D1
C	-10	HIS	-	expression tag	UNP Q9Y7D1
C	-9	SER	-	expression tag	UNP Q9Y7D1
C	-8	SER	-	expression tag	UNP Q9Y7D1
C	-7	GLY	-	expression tag	UNP Q9Y7D1
C	-6	LEU	-	expression tag	UNP Q9Y7D1
C	-5	VAL	-	expression tag	UNP Q9Y7D1
C	-4	PRO	-	expression tag	UNP Q9Y7D1
C	-3	ARG	-	expression tag	UNP Q9Y7D1
C	-2	GLY	-	expression tag	UNP Q9Y7D1
C	-1	SER	-	expression tag	UNP Q9Y7D1
C	0	HIS	-	expression tag	UNP Q9Y7D1
C	40	ALA	CYS	engineered mutation	UNP Q9Y7D1
C	60	ASN	CYS	engineered mutation	UNP Q9Y7D1

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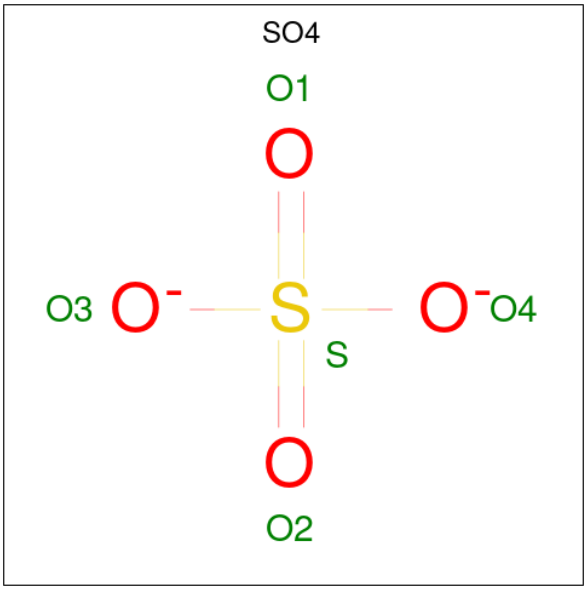
Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	GLY	-	expression tag	UNP Q9Y7D1
D	-17	SER	-	expression tag	UNP Q9Y7D1
D	-16	SER	-	expression tag	UNP Q9Y7D1
D	-15	HIS	-	expression tag	UNP Q9Y7D1
D	-14	HIS	-	expression tag	UNP Q9Y7D1
D	-13	HIS	-	expression tag	UNP Q9Y7D1
D	-12	HIS	-	expression tag	UNP Q9Y7D1
D	-11	HIS	-	expression tag	UNP Q9Y7D1
D	-10	HIS	-	expression tag	UNP Q9Y7D1
D	-9	SER	-	expression tag	UNP Q9Y7D1
D	-8	SER	-	expression tag	UNP Q9Y7D1
D	-7	GLY	-	expression tag	UNP Q9Y7D1
D	-6	LEU	-	expression tag	UNP Q9Y7D1
D	-5	VAL	-	expression tag	UNP Q9Y7D1
D	-4	PRO	-	expression tag	UNP Q9Y7D1
D	-3	ARG	-	expression tag	UNP Q9Y7D1
D	-2	GLY	-	expression tag	UNP Q9Y7D1
D	-1	SER	-	expression tag	UNP Q9Y7D1
D	0	HIS	-	expression tag	UNP Q9Y7D1
D	40	ALA	CYS	engineered mutation	UNP Q9Y7D1
D	60	ASN	CYS	engineered mutation	UNP Q9Y7D1

- 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

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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	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	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

- Molecule 3 is water.

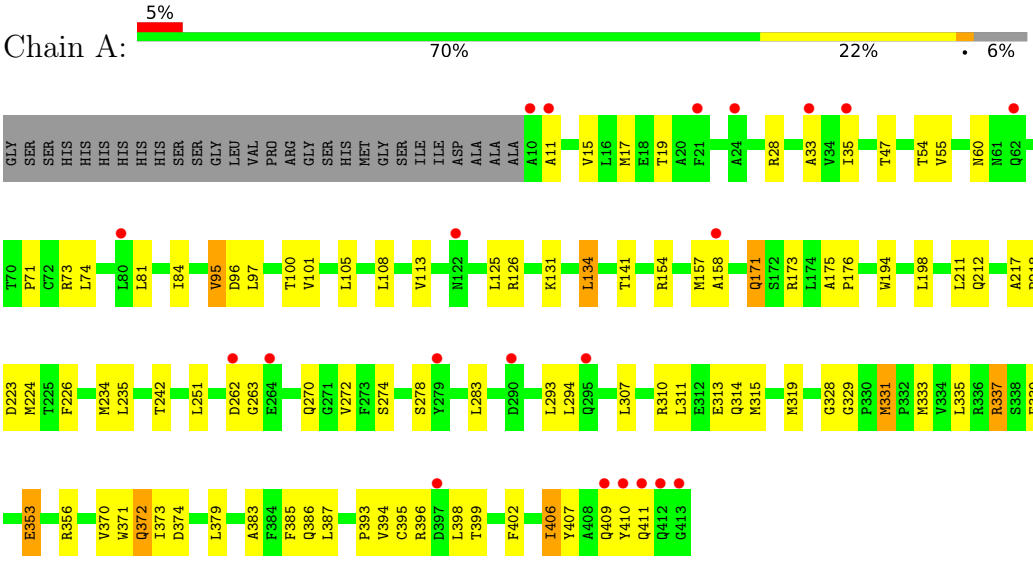
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	11	Total O 11 11	0	0
3	B	3	Total O 3 3	0	0
3	C	4	Total O 4 4	0	0
3	D	3	Total O 3 3	0	0

3 Residue-property plots (i)

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

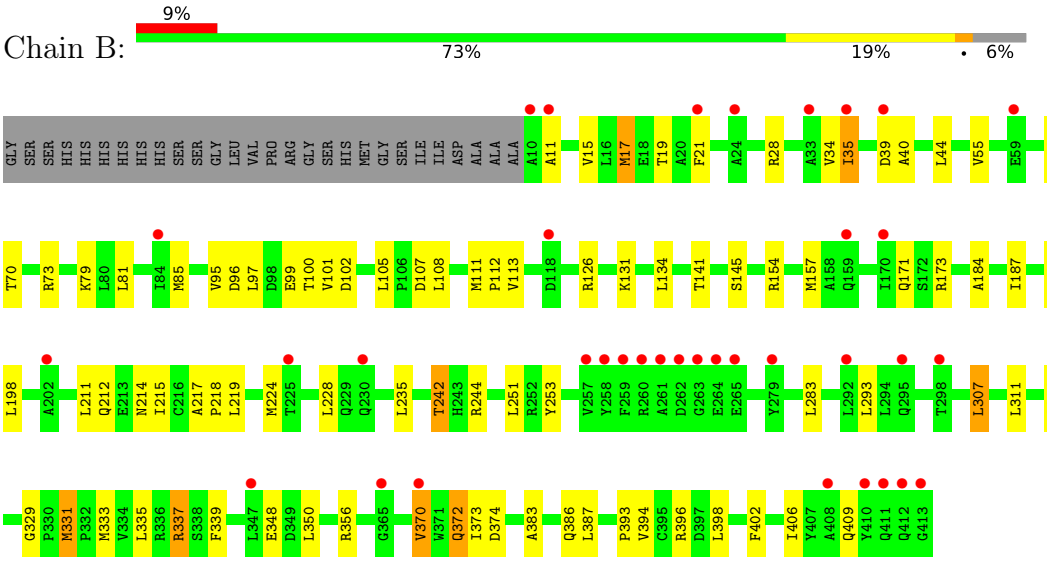
• Molecule 1: Transesterase

Chain A:



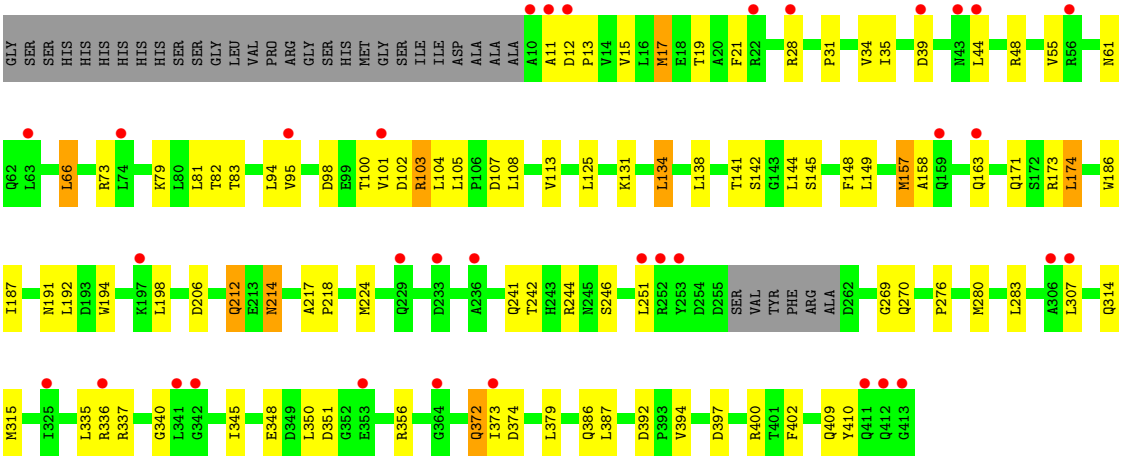
• Molecule 1: Transesterase

Chain B:

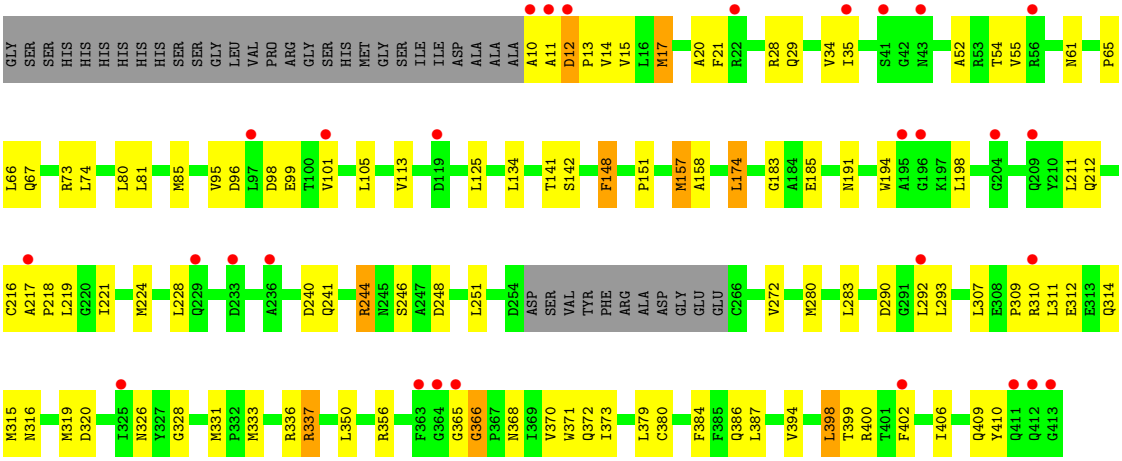


• Molecule 1: Transesterase

Chain C:



- Molecule 1: Transesterase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	209.47Å 85.22Å 104.05Å 90.00° 117.48° 90.00°	Depositor
Resolution (Å)	54.39 – 2.50 54.41 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.4 (54.39-2.50) 89.5 (54.41-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.248 , 0.290 0.250 , 0.289	Depositor DCC
R_{free} test set	2518 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	49.4	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.017 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12633	wwPDB-VP
Average B, all atoms (Å^2)	51.0	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 23.97 % 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 4.1978e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.34	0/3241	0.55	0/4388
1	B	0.34	0/3241	0.55	0/4388
1	C	0.34	0/3183	0.54	0/4308
1	D	0.34	0/3148	0.55	0/4261
All	All	0.34	0/12813	0.55	0/17345

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3173	0	3134	79	0
1	B	3173	0	3134	75	0
1	C	3118	0	3081	65	0
1	D	3083	0	3060	80	0
2	A	20	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
3	A	11	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	1	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
All	All	12633	0	12409	280	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 11.

All (280) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:HD22	1:A:373:ILE:HD11	1.45	0.98
1:A:60:ASN:HD22	1:D:151:PRO:HG2	1.32	0.94
1:D:95:VAL:HG11	1:D:198:LEU:HD11	1.52	0.89
1:D:55:VAL:HG11	1:D:251:LEU:HD13	1.55	0.89
1:B:101:VAL:CG2	1:B:105:LEU:HD12	2.05	0.87
1:B:283:LEU:HD22	1:B:373:ILE:HD11	1.60	0.83
1:A:407:TYR:O	1:A:411:GLN:HG2	1.79	0.82
1:A:370:VAL:HG13	1:A:383:ALA:HB3	1.63	0.81
1:B:35:ILE:HG23	1:B:402:PHE:CE1	2.17	0.80
1:A:81:LEU:HD13	1:A:224:MET:CE	2.11	0.80
1:D:370:VAL:HG11	1:D:399:THR:HG21	1.62	0.79
1:C:148:PHE:CG	1:D:246:SER:HB2	2.17	0.79
1:B:101:VAL:HG21	1:B:105:LEU:HD12	1.66	0.78
1:A:101:VAL:HG21	1:A:105:LEU:HD12	1.63	0.78
1:D:81:LEU:HD13	1:D:224:MET:HE3	1.66	0.77
1:B:307:LEU:HD12	1:B:311:LEU:HB3	1.69	0.74
1:A:55:VAL:HG13	1:A:242:THR:HG21	1.70	0.74
1:C:246:SER:HB2	1:D:148:PHE:CG	2.23	0.74
1:A:35:ILE:HG23	1:A:402:PHE:CE1	2.23	0.73
1:C:55:VAL:HG11	1:C:251:LEU:HD13	1.69	0.73
1:D:101:VAL:HG21	1:D:105:LEU:HD12	1.71	0.72
1:B:95:VAL:HG11	1:B:198:LEU:HD11	1.71	0.71
1:D:219:LEU:HD23	1:D:292:LEU:HD11	1.71	0.71
1:D:74:LEU:HD12	1:D:272:VAL:HG12	1.72	0.71
1:A:307:LEU:HD12	1:A:311:LEU:HB3	1.71	0.71
1:A:55:VAL:HG11	1:A:251:LEU:HD13	1.71	0.70
1:A:370:VAL:HG11	1:A:399:THR:HG21	1.73	0.70
1:B:81:LEU:HD13	1:B:224:MET:HE2	1.74	0.69
1:D:35:ILE:HG23	1:D:402:PHE:CE1	2.27	0.69
1:A:81:LEU:HD13	1:A:224:MET:HE2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:GLU:O	1:A:411:GLN:NE2	2.27	0.67
1:D:142:SER:OG	1:D:191:ASN:ND2	2.26	0.67
1:A:84:ILE:HD12	1:A:294:LEU:HD22	1.77	0.67
1:B:81:LEU:HD13	1:B:224:MET:CE	2.25	0.67
1:A:283:LEU:CD2	1:A:373:ILE:HD11	2.24	0.66
1:D:219:LEU:CD2	1:D:292:LEU:HD11	2.24	0.66
1:A:100:THR:HG23	1:A:131:LYS:HB3	1.77	0.66
1:D:373:ILE:HD13	1:D:380:CYS:HB2	1.75	0.66
1:D:141:THR:O	1:D:141:THR:HG22	1.96	0.66
1:A:81:LEU:CD1	1:A:224:MET:HE3	2.27	0.65
1:C:157:MET:HE1	1:D:244:ARG:HH21	1.62	0.65
1:A:158:ALA:HA	1:B:394:VAL:HG12	1.79	0.64
1:C:35:ILE:HG23	1:C:402:PHE:CE1	2.33	0.64
1:B:244:ARG:NH1	1:B:387:LEU:HD21	2.13	0.63
1:C:148:PHE:CD2	1:D:246:SER:HB2	2.34	0.63
1:B:34:VAL:HG23	1:B:66:LEU:HD13	1.81	0.63
1:D:81:LEU:HD13	1:D:224:MET:CE	2.29	0.63
1:A:15:VAL:O	1:A:19:THR:HG23	1.99	0.63
1:A:60:ASN:HD22	1:D:151:PRO:CG	2.10	0.62
1:C:241:GLN:HE22	1:C:386:GLN:NE2	1.96	0.62
1:C:246:SER:HB2	1:D:148:PHE:CD2	2.35	0.62
1:A:73:ARG:H	1:A:386:GLN:HE22	1.47	0.61
1:A:97:LEU:HD23	1:A:134:LEU:CD1	2.32	0.60
1:A:101:VAL:CG2	1:A:105:LEU:HD12	2.31	0.60
1:A:217:ALA:HB3	1:A:218:PRO:HD3	1.84	0.60
1:B:253:TYR:CZ	1:D:309:PRO:HG2	2.37	0.60
1:D:55:VAL:HG11	1:D:251:LEU:CD1	2.30	0.60
1:C:244:ARG:HH12	1:C:387:LEU:HD21	1.66	0.60
1:C:379:LEU:HD21	1:C:410:TYR:CD2	2.37	0.60
1:A:35:ILE:HD12	1:A:402:PHE:CG	2.37	0.59
1:A:393:PRO:HG3	1:B:154:ARG:HD2	1.85	0.59
1:C:392:ASP:OD1	1:C:394:VAL:HG22	2.01	0.59
1:B:101:VAL:HG22	1:B:105:LEU:HD12	1.83	0.58
1:B:217:ALA:HB3	1:B:218:PRO:HD3	1.85	0.58
1:D:34:VAL:HG23	1:D:66:LEU:HD13	1.84	0.58
1:C:103:ARG:CZ	1:C:104:LEU:HD21	2.34	0.58
1:D:241:GLN:HE22	1:D:386:GLN:NE2	2.02	0.58
1:C:100:THR:HG23	1:C:131:LYS:HB3	1.86	0.57
1:C:217:ALA:HB3	1:C:218:PRO:HD3	1.86	0.57
1:C:101:VAL:HG21	1:C:105:LEU:HD12	1.86	0.57
1:A:307:LEU:HD21	1:A:339:PHE:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ILE:HD12	1:B:402:PHE:CD2	2.39	0.57
1:D:11:ALA:HB2	1:D:409:GLN:NE2	2.19	0.57
1:A:226:PHE:CE2	1:A:272:VAL:HG23	2.39	0.57
1:B:319:MET:CE	1:B:337:ARG:HD3	2.34	0.57
1:C:144:LEU:HD12	1:C:144:LEU:O	2.05	0.57
1:D:11:ALA:HB2	1:D:409:GLN:HG3	1.88	0.56
1:B:11:ALA:HB2	1:B:409:GLN:HE21	1.69	0.56
1:B:319:MET:HE3	1:B:337:ARG:HD3	1.88	0.56
1:A:33:ALA:HB2	1:A:385:PHE:CE1	2.42	0.55
1:A:11:ALA:HB2	1:A:409:GLN:HG3	1.88	0.55
1:D:11:ALA:O	1:D:15:VAL:HG22	2.07	0.55
1:C:394:VAL:HG12	1:D:158:ALA:HA	1.88	0.55
1:A:370:VAL:CG1	1:A:383:ALA:HB3	2.35	0.55
1:D:217:ALA:HB3	1:D:218:PRO:HD3	1.87	0.55
1:B:242:THR:OG1	1:B:387:LEU:HD12	2.06	0.55
1:A:211:LEU:HD11	1:A:224:MET:CE	2.37	0.54
1:B:331:MET:HE3	3:B:417:HOH:O	2.07	0.54
1:D:81:LEU:HD22	1:D:224:MET:HE1	1.88	0.54
1:A:331:MET:HE2	3:A:421:HOH:O	2.06	0.54
1:D:319:MET:HE3	1:D:337:ARG:HD3	1.89	0.54
1:C:244:ARG:NH1	1:C:387:LEU:HD21	2.23	0.54
1:C:15:VAL:O	1:C:19:THR:HG23	2.08	0.54
1:D:310:ARG:HD3	1:D:311:LEU:HD23	1.89	0.54
1:D:11:ALA:HB2	1:D:409:GLN:CG	2.38	0.54
1:A:372:GLN:HE22	1:A:374:ASP:HB2	1.73	0.53
1:D:283:LEU:HB3	1:D:373:ILE:HD11	1.91	0.53
1:C:350:LEU:HD13	1:C:356:ARG:HB2	1.89	0.53
1:A:350:LEU:HD22	1:A:356:ARG:HB2	1.90	0.53
1:B:81:LEU:CD1	1:B:224:MET:CE	2.87	0.53
1:C:144:LEU:HD12	1:C:144:LEU:C	2.29	0.53
1:C:171:GLN:HB2	1:C:174:LEU:HD23	1.91	0.53
1:B:73:ARG:H	1:B:386:GLN:HE22	1.56	0.52
1:C:17:MET:HE2	1:C:21:PHE:CD2	2.43	0.52
1:B:315:MET:HG2	1:B:319:MET:HE2	1.92	0.52
1:A:211:LEU:HD11	1:A:224:MET:HE2	1.92	0.52
1:B:100:THR:HG23	1:B:131:LYS:HB3	1.92	0.52
1:B:107:ASP:OD1	1:B:107:ASP:N	2.43	0.51
1:D:244:ARG:HH12	1:D:387:LEU:HD21	1.75	0.51
1:D:219:LEU:HD11	1:D:293:LEU:HD11	1.93	0.51
1:A:60:ASN:ND2	1:D:151:PRO:HG2	2.13	0.51
1:C:244:ARG:HH21	1:D:157:MET:HE3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:MET:HE3	1:A:337:ARG:HG2	1.93	0.51
1:A:154:ARG:HD2	1:B:393:PRO:HG3	1.92	0.51
1:B:370:VAL:HG13	1:B:383:ALA:HB3	1.92	0.51
1:C:73:ARG:H	1:C:386:GLN:HE22	1.59	0.51
1:C:82:THR:HB	1:C:192:LEU:HD12	1.93	0.51
1:C:55:VAL:HG13	1:C:242:THR:HG21	1.93	0.50
1:A:319:MET:HE3	1:A:337:ARG:HD3	1.94	0.50
1:C:11:ALA:HB2	1:C:409:GLN:NE2	2.26	0.50
1:D:10:ALA:HB3	1:D:15:VAL:CG1	2.42	0.50
1:B:11:ALA:HB2	1:B:409:GLN:HG3	1.94	0.50
1:C:11:ALA:HB2	1:C:409:GLN:CG	2.42	0.50
1:D:85:MET:HE1	1:D:211:LEU:HB2	1.93	0.50
1:D:394:VAL:O	1:D:398:LEU:HD13	2.12	0.50
1:B:335:LEU:HD22	1:B:348:GLU:OE1	2.11	0.50
1:B:350:LEU:HD13	1:B:356:ARG:HB2	1.93	0.50
1:A:81:LEU:CD2	1:A:224:MET:HE3	2.42	0.50
1:B:85:MET:CE	1:B:211:LEU:HA	2.42	0.50
1:D:17:MET:HE2	1:D:21:PHE:CD2	2.47	0.50
1:A:108:LEU:HD13	1:A:194:TRP:CE2	2.46	0.50
1:C:283:LEU:HB3	1:C:373:ILE:HD11	1.94	0.49
1:B:15:VAL:O	1:B:19:THR:HG23	2.12	0.49
1:D:312:GLU:O	1:D:316:ASN:ND2	2.45	0.49
1:B:108:LEU:HD13	1:B:194:TRP:CE2	2.47	0.49
1:D:74:LEU:HD12	1:D:272:VAL:CG1	2.41	0.49
1:B:85:MET:HE3	1:B:211:LEU:HA	1.94	0.49
1:C:214:ASN:HD22	1:C:214:ASN:N	2.10	0.49
1:A:71:PRO:HG2	1:A:234:MET:O	2.12	0.49
1:C:335:LEU:HD13	1:C:336:ARG:N	2.28	0.49
1:B:219:LEU:HD11	1:B:293:LEU:HD11	1.95	0.49
1:C:142:SER:OG	1:C:191:ASN:ND2	2.43	0.49
1:C:55:VAL:HG11	1:C:251:LEU:CD1	2.41	0.48
1:C:158:ALA:HA	1:D:394:VAL:HG12	1.95	0.48
1:C:379:LEU:HD21	1:C:410:TYR:CG	2.47	0.48
1:C:108:LEU:HD13	1:C:194:TRP:CE2	2.48	0.48
1:C:163:GLN:HE21	1:D:29:GLN:HG3	1.79	0.48
1:A:113:VAL:HG11	1:A:126:ARG:HH21	1.79	0.48
1:C:11:ALA:HB2	1:C:409:GLN:HG3	1.94	0.48
1:B:141:THR:O	1:B:141:THR:HG22	2.14	0.48
1:A:315:MET:HG2	1:A:319:MET:HE2	1.96	0.48
1:D:328:GLY:O	1:D:331:MET:HG2	2.13	0.48
1:A:55:VAL:CG1	1:A:251:LEU:HD13	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:ASP:HB3	1:D:99:GLU:HB2	1.97	0.47
1:D:141:THR:HG22	1:D:183:GLY:H	1.80	0.47
1:D:244:ARG:NH1	1:D:387:LEU:HD21	2.30	0.47
1:A:35:ILE:HD12	1:A:402:PHE:CD2	2.49	0.47
1:A:141:THR:HG22	1:A:141:THR:O	2.14	0.47
1:C:145:SER:HB2	1:C:187:ILE:HG21	1.96	0.47
1:C:212:GLN:HE21	1:C:212:GLN:HA	1.80	0.47
1:B:35:ILE:HD12	1:B:402:PHE:CG	2.50	0.47
1:C:186:TRP:CE2	1:C:315:MET:HE3	2.50	0.47
1:B:244:ARG:HH12	1:B:387:LEU:HD21	1.78	0.47
1:B:11:ALA:CB	1:B:409:GLN:HE21	2.27	0.47
1:B:214:ASN:N	1:B:214:ASN:HD22	2.13	0.47
1:A:134:LEU:O	1:A:134:LEU:HD22	2.14	0.47
1:A:73:ARG:N	1:A:386:GLN:HE22	2.11	0.46
1:D:315:MET:HG2	1:D:319:MET:HE2	1.97	0.46
1:C:83:THR:HG23	1:C:138:LEU:HD22	1.98	0.46
1:A:333:MET:HE3	1:A:396:ARG:NE	2.29	0.46
1:B:307:LEU:CD1	1:B:311:LEU:HB3	2.43	0.46
1:D:85:MET:HE3	1:D:211:LEU:HA	1.97	0.46
1:B:211:LEU:HD12	1:B:215:ILE:HD12	1.97	0.46
1:A:319:MET:CE	1:A:337:ARG:HD3	2.46	0.46
1:D:10:ALA:HB3	1:D:15:VAL:HG13	1.98	0.46
1:A:379:LEU:HD11	1:A:410:TYR:CD2	2.51	0.46
1:C:100:THR:HG22	1:C:102:ASP:H	1.81	0.46
1:B:198:LEU:C	1:B:198:LEU:HD13	2.37	0.45
1:A:97:LEU:HD23	1:A:134:LEU:HD12	1.97	0.45
1:C:198:LEU:HD13	1:C:198:LEU:C	2.37	0.45
1:D:141:THR:HG23	1:D:185:GLU:O	2.16	0.45
1:B:55:VAL:HG11	1:B:251:LEU:HD13	1.97	0.45
1:B:79:LYS:HD3	1:B:192:LEU:HD23	1.98	0.45
1:A:113:VAL:HG11	1:A:126:ARG:NH2	2.32	0.45
1:A:387:LEU:HD23	1:A:395:CYS:SG	2.56	0.45
1:D:11:ALA:HB3	1:D:14:VAL:HG23	1.99	0.45
1:B:66:LEU:HD23	1:B:70:THR:HG21	1.97	0.45
1:A:235:LEU:HD23	1:A:235:LEU:O	2.16	0.45
1:A:81:LEU:HD13	1:A:224:MET:HE3	1.83	0.45
1:B:101:VAL:HG22	1:B:105:LEU:HB2	1.99	0.45
1:C:11:ALA:HB2	1:C:409:GLN:CD	2.37	0.45
1:D:17:MET:O	1:D:20:ALA:HB3	2.16	0.45
1:D:368:ASN:ND2	1:D:387:LEU:O	2.44	0.45
1:D:12:ASP:HB2	1:D:13:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LEU:HD12	1:A:337:ARG:HG3	1.99	0.44
1:D:216:CYS:HA	1:D:221:ILE:HB	1.99	0.44
1:A:328:GLY:O	3:A:418:HOH:O	2.21	0.44
1:B:113:VAL:HG11	1:B:126:ARG:NH2	2.32	0.44
1:B:228:LEU:CD1	1:B:235:LEU:HD12	2.48	0.44
1:C:39:ASP:HB2	1:C:44:LEU:HB3	1.98	0.44
1:A:219:LEU:HG	1:A:293:LEU:HD21	1.98	0.44
1:A:235:LEU:HD22	1:D:320:ASP:HB3	1.98	0.44
1:B:81:LEU:CD2	1:B:224:MET:HE3	2.47	0.44
1:B:96:ASP:HB3	1:B:99:GLU:HB2	1.99	0.44
1:A:198:LEU:HD13	1:A:198:LEU:C	2.38	0.44
1:B:113:VAL:HG13	1:B:126:ARG:HB3	2.00	0.44
1:B:145:SER:HB2	1:B:187:ILE:HG21	1.99	0.44
1:C:12:ASP:HB2	1:C:13:PRO:HD3	2.00	0.44
1:C:34:VAL:HG23	1:C:66:LEU:HD13	2.00	0.44
1:C:335:LEU:HD22	1:C:348:GLU:OE1	2.18	0.44
1:D:35:ILE:HD12	1:D:402:PHE:CG	2.53	0.44
1:A:74:LEU:HD12	1:A:272:VAL:HG12	2.00	0.44
1:A:97:LEU:HD23	1:A:134:LEU:HD13	1.97	0.44
1:B:111:MET:HE3	1:B:112:PRO:HD2	2.00	0.44
1:A:171:GLN:HA	1:A:171:GLN:HE21	1.83	0.43
1:B:85:MET:HE1	1:B:211:LEU:HB2	2.00	0.43
1:C:95:VAL:HG11	1:C:198:LEU:HD11	1.99	0.43
1:B:372:GLN:HE22	1:B:374:ASP:HB2	1.84	0.43
1:D:11:ALA:HB3	1:D:14:VAL:CG2	2.49	0.43
1:D:52:ALA:HA	1:D:65:PRO:HA	2.00	0.43
1:D:73:ARG:H	1:D:386:GLN:HE22	1.66	0.43
1:A:175:ALA:N	1:A:176:PRO:HD2	2.33	0.43
1:B:307:LEU:HD21	1:B:339:PHE:HB3	2.01	0.43
1:C:79:LYS:NZ	1:C:269:GLY:O	2.52	0.43
1:C:171:GLN:HB2	1:C:174:LEU:CD2	2.49	0.43
1:B:406:ILE:C	1:B:406:ILE:HD12	2.39	0.43
1:C:141:THR:HG22	1:C:141:THR:O	2.19	0.43
1:D:54:THR:HG22	1:D:240:ASP:HB2	2.00	0.43
1:A:95:VAL:HG11	1:A:198:LEU:HD11	2.01	0.43
1:C:17:MET:HG3	1:C:402:PHE:HA	2.01	0.43
1:C:134:LEU:O	1:C:134:LEU:HD22	2.19	0.43
1:B:235:LEU:O	1:B:235:LEU:HD23	2.19	0.42
1:D:406:ILE:C	1:D:406:ILE:HD12	2.40	0.42
1:C:107:ASP:N	1:C:107:ASP:OD1	2.53	0.42
1:A:81:LEU:HD22	1:A:224:MET:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASP:OD2	1:A:97:LEU:N	2.52	0.42
1:B:85:MET:CE	1:B:211:LEU:CA	2.97	0.42
1:C:94:LEU:O	1:C:95:VAL:HG13	2.19	0.42
1:C:148:PHE:CZ	1:C:149:LEU:HD21	2.53	0.42
1:D:183:GLY:O	1:D:311:LEU:HD11	2.20	0.42
1:D:379:LEU:HD21	1:D:410:TYR:CG	2.55	0.42
1:A:221:ILE:HD13	1:A:278:SER:HB3	2.01	0.42
1:B:81:LEU:CD1	1:B:224:MET:HE3	2.50	0.42
1:B:333:MET:HE2	1:B:396:ARG:NH2	2.35	0.42
1:D:80:LEU:HD13	1:D:371:TRP:CZ2	2.55	0.42
1:A:283:LEU:HD22	1:A:373:ILE:CD1	2.33	0.42
1:B:39:ASP:HB2	1:B:44:LEU:HB3	2.02	0.42
1:B:350:LEU:HD22	1:B:356:ARG:HG3	2.02	0.42
1:D:251:LEU:HD12	1:D:251:LEU:O	2.20	0.42
1:A:406:ILE:HD12	1:A:406:ILE:C	2.41	0.41
1:C:372:GLN:HE22	1:C:374:ASP:HB2	1.84	0.41
1:D:11:ALA:HB2	1:D:409:GLN:HE21	1.84	0.41
1:B:97:LEU:HD23	1:B:134:LEU:CD1	2.49	0.41
1:D:365:GLY:O	1:D:366:GLY:C	2.59	0.41
1:D:174:LEU:HD12	1:D:194:TRP:CE2	2.55	0.41
1:A:223:ASP:O	1:A:274:SER:HA	2.20	0.41
1:A:283:LEU:HD11	1:A:371:TRP:HB2	2.01	0.41
1:D:17:MET:HE2	1:D:17:MET:O	2.21	0.41
1:D:228:LEU:HD13	1:D:228:LEU:O	2.21	0.41
1:B:97:LEU:HD23	1:B:134:LEU:HD12	2.03	0.41
1:B:100:THR:HG22	1:B:102:ASP:H	1.86	0.41
1:C:35:ILE:HD12	1:C:402:PHE:CD2	2.56	0.41
1:C:81:LEU:CD2	1:C:224:MET:HE1	2.50	0.41
1:D:350:LEU:HD13	1:D:356:ARG:HB2	2.01	0.41
1:A:81:LEU:CD1	1:A:224:MET:CE	2.85	0.41
1:A:307:LEU:CD2	1:A:339:PHE:HB3	2.51	0.41
1:A:335:LEU:HD22	1:A:348:GLU:OE1	2.21	0.41
1:C:108:LEU:HD22	1:C:194:TRP:CD2	2.56	0.41
1:C:173:ARG:HA	1:D:248:ASP:HB3	2.02	0.41
1:D:74:LEU:CD1	1:D:272:VAL:HG12	2.48	0.41
1:D:326:ASN:HD21	1:D:333:MET:HE3	1.86	0.41
1:B:39:ASP:OD1	1:B:40:ALA:N	2.54	0.41
1:B:319:MET:HE1	1:B:337:ARG:HD3	2.03	0.41
1:B:113:VAL:HG11	1:B:126:ARG:HH21	1.85	0.40
1:C:340:GLY:HA3	1:C:345:ILE:HD11	2.02	0.40
1:A:60:ASN:HA	1:D:151:PRO:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:MET:HE2	1:B:21:PHE:CD2	2.57	0.40
1:B:335:LEU:HD12	1:B:337:ARG:HG3	2.02	0.40
1:B:184:ALA:C	1:B:311:LEU:HD21	2.41	0.40
1:B:350:LEU:HD22	1:B:356:ARG:HB2	2.03	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	402/432 (93%)	381 (95%)	19 (5%)	2 (0%)	29	48
1	B	402/432 (93%)	384 (96%)	17 (4%)	1 (0%)	47	68
1	C	394/432 (91%)	374 (95%)	19 (5%)	1 (0%)	41	61
1	D	389/432 (90%)	372 (96%)	16 (4%)	1 (0%)	41	61
All	All	1587/1728 (92%)	1511 (95%)	71 (4%)	5 (0%)	41	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	GLY
1	B	329	GLY
1	D	366	GLY
1	A	263	GLY
1	C	31	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	335/356 (94%)	311 (93%)	24 (7%)	14	28
1	B	335/356 (94%)	319 (95%)	16 (5%)	25	48
1	C	329/356 (92%)	304 (92%)	25 (8%)	13	25
1	D	326/356 (92%)	302 (93%)	24 (7%)	13	27
All	All	1325/1424 (93%)	1236 (93%)	89 (7%)	16	31

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	MET
1	A	28	ARG
1	A	47	THR
1	A	54	THR
1	A	69	ASP
1	A	95	VAL
1	A	125	LEU
1	A	134	LEU
1	A	157	MET
1	A	171	GLN
1	A	173	ARG
1	A	212	GLN
1	A	262	ASP
1	A	270	GLN
1	A	310	ARG
1	A	313	GLU
1	A	314	GLN
1	A	331	MET
1	A	337	ARG
1	A	353	GLU
1	A	372	GLN
1	A	394	VAL
1	A	398	LEU
1	A	406	ILE
1	B	17	MET
1	B	28	ARG
1	B	35	ILE
1	B	67	GLN
1	B	157	MET
1	B	171	GLN

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Mol	Chain	Res	Type
1	B	173	ARG
1	B	212	GLN
1	B	242	THR
1	B	307	LEU
1	B	314	GLN
1	B	331	MET
1	B	337	ARG
1	B	370	VAL
1	B	372	GLN
1	B	398	LEU
1	C	17	MET
1	C	28	ARG
1	C	48	ARG
1	C	61	ASN
1	C	66	LEU
1	C	98	ASP
1	C	103	ARG
1	C	113	VAL
1	C	125	LEU
1	C	134	LEU
1	C	157	MET
1	C	174	LEU
1	C	206	ASP
1	C	212	GLN
1	C	214	ASN
1	C	270	GLN
1	C	276	PRO
1	C	280	MET
1	C	307	LEU
1	C	314	GLN
1	C	337	ARG
1	C	351	ASP
1	C	372	GLN
1	C	397	ASP
1	C	400	ARG
1	D	12	ASP
1	D	17	MET
1	D	28	ARG
1	D	61	ASN
1	D	67	GLN
1	D	98	ASP
1	D	113	VAL

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Mol	Chain	Res	Type
1	D	125	LEU
1	D	134	LEU
1	D	148	PHE
1	D	157	MET
1	D	174	LEU
1	D	212	GLN
1	D	244	ARG
1	D	280	MET
1	D	290	ASP
1	D	307	LEU
1	D	314	GLN
1	D	336	ARG
1	D	337	ARG
1	D	372	GLN
1	D	384	PHE
1	D	398	LEU
1	D	400	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	61	ASN
1	A	122	ASN
1	A	150	HIS
1	A	163	GLN
1	A	171	GLN
1	A	191	ASN
1	A	212	GLN
1	A	245	ASN
1	A	295	GLN
1	A	317	GLN
1	A	372	GLN
1	A	386	GLN
1	A	409	GLN
1	B	171	GLN
1	B	191	ASN
1	B	212	GLN
1	B	214	ASN
1	B	245	ASN
1	B	372	GLN
1	B	386	GLN

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Mol	Chain	Res	Type
1	B	409	GLN
1	C	29	GLN
1	C	61	ASN
1	C	150	HIS
1	C	163	GLN
1	C	171	GLN
1	C	191	ASN
1	C	212	GLN
1	C	229	GLN
1	C	317	GLN
1	C	372	GLN
1	C	386	GLN
1	C	409	GLN
1	D	61	ASN
1	D	171	GLN
1	D	191	ASN
1	D	212	GLN
1	D	295	GLN
1	D	372	GLN
1	D	386	GLN
1	D	409	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)

13 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	$\#\|Z\| > 2$
2	SO4	A	416	-	4,4,4	0.12	0	6,6,6	0.16	0
2	SO4	B	415	-	4,4,4	0.16	0	6,6,6	0.14	0
2	SO4	C	415	-	4,4,4	0.14	0	6,6,6	0.22	0
2	SO4	C	416	-	4,4,4	0.11	0	6,6,6	0.10	0
2	SO4	D	415	-	4,4,4	0.13	0	6,6,6	0.21	0
2	SO4	B	416	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	C	414	-	4,4,4	0.15	0	6,6,6	0.16	0
2	SO4	D	416	-	4,4,4	0.12	0	6,6,6	0.14	0
2	SO4	D	414	-	4,4,4	0.18	0	6,6,6	0.23	0
2	SO4	A	415	-	4,4,4	0.12	0	6,6,6	0.15	0
2	SO4	A	417	-	4,4,4	0.16	0	6,6,6	0.17	0
2	SO4	A	414	-	4,4,4	0.16	0	6,6,6	0.10	0
2	SO4	B	414	-	4,4,4	0.17	0	6,6,6	0.16	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	404/432 (93%)	0.62	23 (5%) 23 25	41, 51, 60, 83	0
1	B	404/432 (93%)	0.73	37 (9%) 9 9	40, 51, 61, 98	0
1	C	398/432 (92%)	0.79	34 (8%) 10 10	41, 51, 60, 87	0
1	D	393/432 (90%)	0.72	29 (7%) 14 15	41, 51, 58, 79	0
All	All	1599/1728 (92%)	0.71	123 (7%) 13 13	40, 51, 60, 98	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	10	ALA	19.7
1	D	11	ALA	8.7
1	D	10	ALA	8.5
1	A	413	GLY	7.9
1	C	411	GLN	7.2
1	B	413	GLY	6.8
1	B	411	GLN	6.5
1	B	263	GLY	6.3
1	B	10	ALA	6.0
1	C	413	GLY	5.8
1	B	412	GLN	5.7
1	B	258	TYR	5.7
1	C	22	ARG	5.6
1	D	22	ARG	5.3
1	C	11	ALA	5.2
1	C	412	GLN	5.1
1	A	412	GLN	4.9
1	B	261	ALA	4.9
1	D	413	GLY	4.7
1	C	229	GLN	4.5
1	B	264	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	101	VAL	4.5
1	A	10	ALA	4.4
1	A	62	GLN	4.4
1	C	233	ASP	4.3
1	A	11	ALA	3.9
1	B	265	GLU	3.9
1	D	101	VAL	3.9
1	B	262	ASP	3.8
1	D	292	LEU	3.7
1	A	397	ASP	3.7
1	B	11	ALA	3.7
1	A	264	GLU	3.6
1	A	35	ILE	3.6
1	B	279	TYR	3.6
1	D	12	ASP	3.5
1	D	412	GLN	3.4
1	B	21	PHE	3.3
1	C	336	ARG	3.3
1	D	411	GLN	3.3
1	D	402	PHE	3.3
1	B	202	ALA	3.2
1	B	170	ILE	3.2
1	A	262	ASP	3.2
1	A	411	GLN	3.2
1	B	259	PHE	3.2
1	C	12	ASP	3.1
1	B	257	VAL	3.1
1	B	410	TYR	3.1
1	B	260	ARG	3.1
1	C	56	ARG	3.0
1	B	159	GLN	3.0
1	C	306	ALA	2.9
1	C	43	ASN	2.9
1	C	325	ILE	2.9
1	D	195	ALA	2.8
1	B	370	VAL	2.8
1	C	342	GLY	2.8
1	D	97	LEU	2.8
1	C	197	LYS	2.7
1	D	41	SER	2.7
1	C	95	VAL	2.7
1	B	35	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	295	GLN	2.6
1	A	33	ALA	2.6
1	C	63	LEU	2.6
1	B	59	GLU	2.6
1	D	196	GLY	2.6
1	B	24	ALA	2.6
1	D	363	PHE	2.6
1	B	84	ILE	2.5
1	C	373	ILE	2.5
1	B	39	ASP	2.5
1	D	43	ASN	2.5
1	B	298	THR	2.5
1	B	292	LEU	2.5
1	C	236	ALA	2.4
1	D	119	ASP	2.4
1	A	279	TYR	2.4
1	C	353	GLU	2.4
1	B	408	ALA	2.4
1	C	39	ASP	2.4
1	C	341	LEU	2.3
1	A	68	VAL	2.3
1	D	233	ASP	2.3
1	A	24	ALA	2.3
1	D	236	ALA	2.3
1	D	229	GLN	2.3
1	D	325	ILE	2.3
1	D	364	GLY	2.3
1	C	163	GLN	2.3
1	A	410	TYR	2.3
1	C	44	LEU	2.3
1	C	74	LEU	2.2
1	C	307	LEU	2.2
1	D	56	ARG	2.2
1	A	122	ASN	2.2
1	D	209	GLN	2.2
1	A	66	LEU	2.2
1	A	409	GLN	2.2
1	B	230	GLN	2.1
1	A	21	PHE	2.1
1	A	158	ALA	2.1
1	B	118	ASP	2.1
1	C	253	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	80	LEU	2.1
1	D	204	GLY	2.1
1	B	68	VAL	2.1
1	D	217	ALA	2.1
1	B	225	THR	2.1
1	B	347	LEU	2.1
1	B	33	ALA	2.1
1	A	290	ASP	2.1
1	D	35	ILE	2.1
1	C	251	LEU	2.1
1	C	364	GLY	2.1
1	C	252	ARG	2.1
1	A	295	GLN	2.0
1	B	365	GLY	2.0
1	C	28	ARG	2.0
1	C	159	GLN	2.0
1	D	365	GLY	2.0
1	D	310	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	D	416	5/5	0.84	0.28	71,72,73,73	0
2	SO4	B	416	5/5	0.85	0.23	85,85,86,86	0
2	SO4	A	416	5/5	0.88	0.25	86,87,87,88	0
2	SO4	A	417	5/5	0.89	0.26	71,72,73,73	0
2	SO4	C	414	5/5	0.93	0.17	73,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	C	416	5/5	0.94	0.29	72,72,73,73	0
2	SO4	D	414	5/5	0.95	0.14	50,50,51,51	0
2	SO4	B	414	5/5	0.95	0.21	58,58,59,59	0
2	SO4	C	415	5/5	0.96	0.09	47,48,48,48	0
2	SO4	B	415	5/5	0.96	0.12	59,61,61,61	0
2	SO4	A	415	5/5	0.96	0.32	66,66,67,67	0
2	SO4	A	414	5/5	0.96	0.24	63,63,64,64	0
2	SO4	D	415	5/5	0.97	0.19	67,67,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.