



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:22 AM UTC

PDB ID : 5Y57 / pdb_00005y57
Title : Crystal structure of a Novel Pyrethroid Hydrolase from *Sphingobium faniae* JZ-2
Authors : Xu, D.Q.; Ran, T.T.; He, J.; Wang, W.W.
Deposited on : 2017-08-07
Resolution : 1.96 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

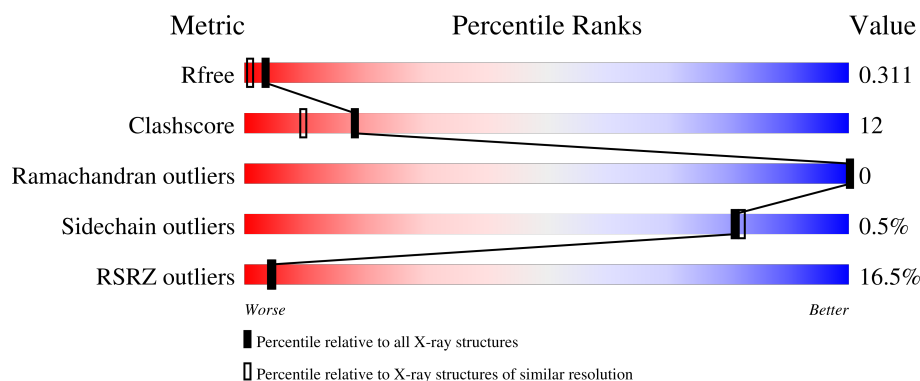
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 $\leq 5\%$. 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	288	2% 77% 10% 13%
1	B	288	2% 74% 12% 12%
1	C	288	3% 70% 18% 12%
1	D	288	2% 74% 13% 12%
1	E	288	29% 57% 30% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	288	49% 57% 30% 12%

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	PMS	F	301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11971 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 Pyrethroid hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	Se	0	1	0
			1916	1219	331	359	1	6			
1	B	252	Total	C	N	O	S	Se	0	1	0
			1920	1221	332	360	1	6			
1	C	253	Total	C	N	O	S	Se	0	1	0
			1923	1223	330	363	1	6			
1	D	252	Total	C	N	O	S	Se	0	1	0
			1920	1221	332	360	1	6			
1	E	251	Total	C	N	O	S	Se	0	1	0
			1899	1210	327	355	1	6			
1	F	253	Total	C	N	O	S	Se	0	1	0
			1873	1192	320	354	1	6			

There are 54 discrepancies between the modelled and reference sequences:

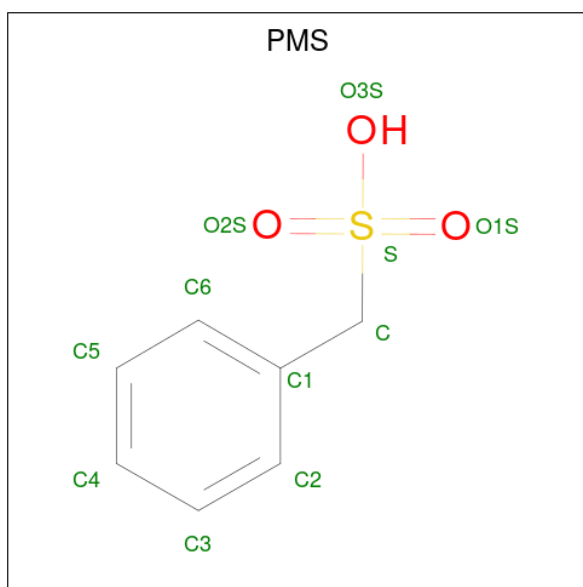
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP D0VUS3
A	281	LEU	-	expression tag	UNP D0VUS3
A	282	GLU	-	expression tag	UNP D0VUS3
A	283	HIS	-	expression tag	UNP D0VUS3
A	284	HIS	-	expression tag	UNP D0VUS3
A	285	HIS	-	expression tag	UNP D0VUS3
A	286	HIS	-	expression tag	UNP D0VUS3
A	287	HIS	-	expression tag	UNP D0VUS3
A	288	HIS	-	expression tag	UNP D0VUS3
B	1	MSE	-	initiating methionine	UNP D0VUS3
B	281	LEU	-	expression tag	UNP D0VUS3
B	282	GLU	-	expression tag	UNP D0VUS3
B	283	HIS	-	expression tag	UNP D0VUS3
B	284	HIS	-	expression tag	UNP D0VUS3
B	285	HIS	-	expression tag	UNP D0VUS3
B	286	HIS	-	expression tag	UNP D0VUS3
B	287	HIS	-	expression tag	UNP D0VUS3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	288	HIS	-	expression tag	UNP D0VUS3
C	1	MSE	-	initiating methionine	UNP D0VUS3
C	281	LEU	-	expression tag	UNP D0VUS3
C	282	GLU	-	expression tag	UNP D0VUS3
C	283	HIS	-	expression tag	UNP D0VUS3
C	284	HIS	-	expression tag	UNP D0VUS3
C	285	HIS	-	expression tag	UNP D0VUS3
C	286	HIS	-	expression tag	UNP D0VUS3
C	287	HIS	-	expression tag	UNP D0VUS3
C	288	HIS	-	expression tag	UNP D0VUS3
D	1	MSE	-	initiating methionine	UNP D0VUS3
D	281	LEU	-	expression tag	UNP D0VUS3
D	282	GLU	-	expression tag	UNP D0VUS3
D	283	HIS	-	expression tag	UNP D0VUS3
D	284	HIS	-	expression tag	UNP D0VUS3
D	285	HIS	-	expression tag	UNP D0VUS3
D	286	HIS	-	expression tag	UNP D0VUS3
D	287	HIS	-	expression tag	UNP D0VUS3
D	288	HIS	-	expression tag	UNP D0VUS3
E	1	MSE	-	initiating methionine	UNP D0VUS3
E	281	LEU	-	expression tag	UNP D0VUS3
E	282	GLU	-	expression tag	UNP D0VUS3
E	283	HIS	-	expression tag	UNP D0VUS3
E	284	HIS	-	expression tag	UNP D0VUS3
E	285	HIS	-	expression tag	UNP D0VUS3
E	286	HIS	-	expression tag	UNP D0VUS3
E	287	HIS	-	expression tag	UNP D0VUS3
E	288	HIS	-	expression tag	UNP D0VUS3
F	1	MSE	-	initiating methionine	UNP D0VUS3
F	281	LEU	-	expression tag	UNP D0VUS3
F	282	GLU	-	expression tag	UNP D0VUS3
F	283	HIS	-	expression tag	UNP D0VUS3
F	284	HIS	-	expression tag	UNP D0VUS3
F	285	HIS	-	expression tag	UNP D0VUS3
F	286	HIS	-	expression tag	UNP D0VUS3
F	287	HIS	-	expression tag	UNP D0VUS3
F	288	HIS	-	expression tag	UNP D0VUS3

- Molecule 2 is phenylmethanesulfonic acid (CCD ID: PMS) (formula: C₇H₈O₃S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			10	7	2	1		
2	B	1	Total	C	O	S	0	0
			10	7	2	1		
2	C	1	Total	C	O	S	0	0
			10	7	2	1		
2	D	1	Total	C	O	S	0	0
			10	7	2	1		
2	E	1	Total	C	O	S	0	0
			10	7	2	1		
2	F	1	Total	C	O	S	0	0
			10	7	2	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

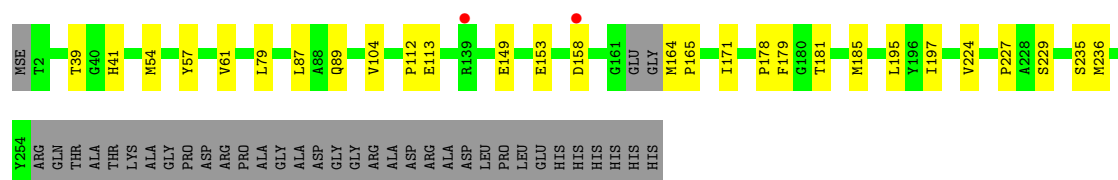
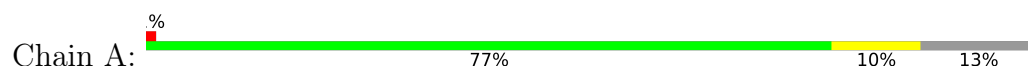
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total	O	0	0
			105	105		
4	B	96	Total	O	0	0
			96	96		
4	C	85	Total	O	0	0
			85	85		
4	D	97	Total	O	0	0
			97	97		
4	E	29	Total	O	0	0
			29	29		
4	F	18	Total	O	0	0
			18	18		

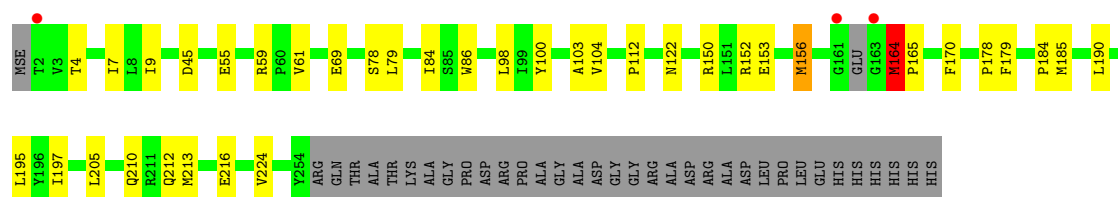
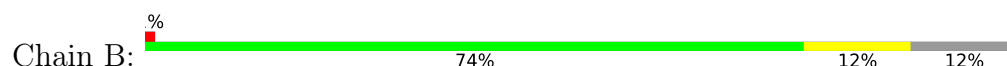
3 Residue-property plots [i](#)

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.

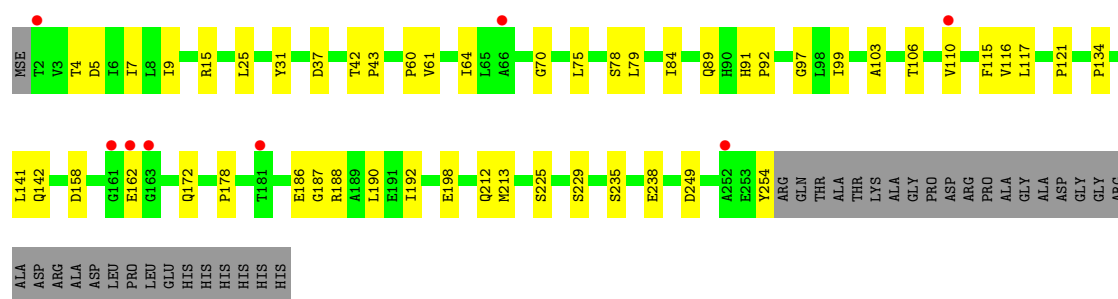
• Molecule 1: Pyrethroid hydrolase



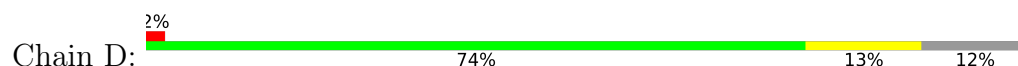
• Molecule 1: Pyrethroid hydrolase

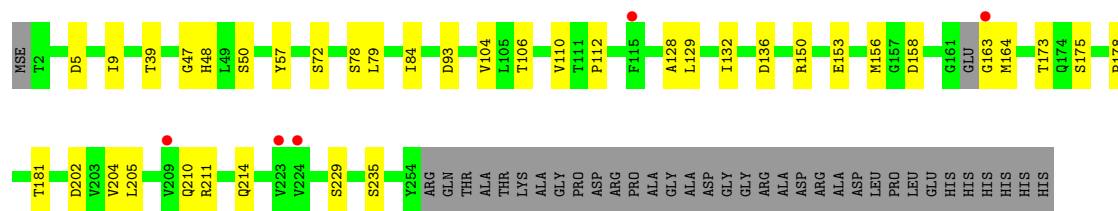


• Molecule 1: Pyrethroid hydrolase

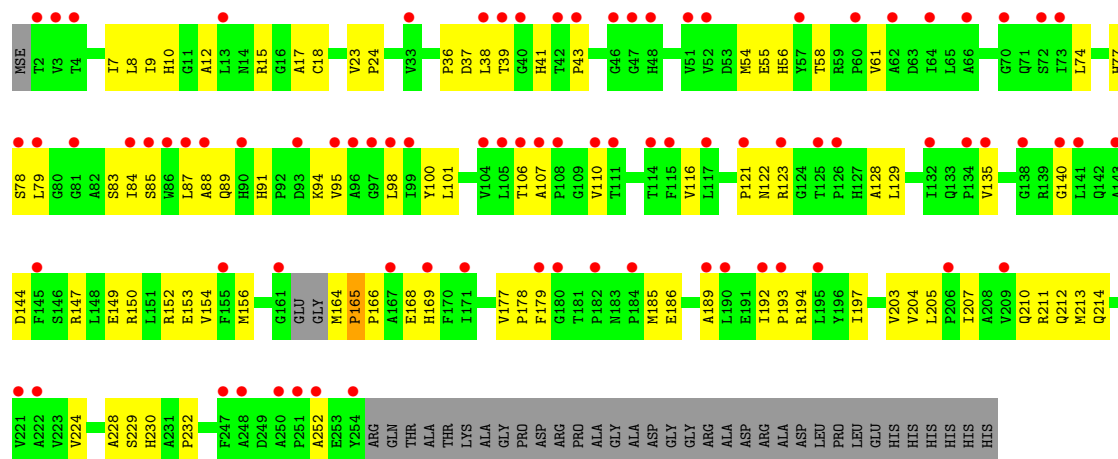


• Molecule 1: Pyrethroid hydrolase

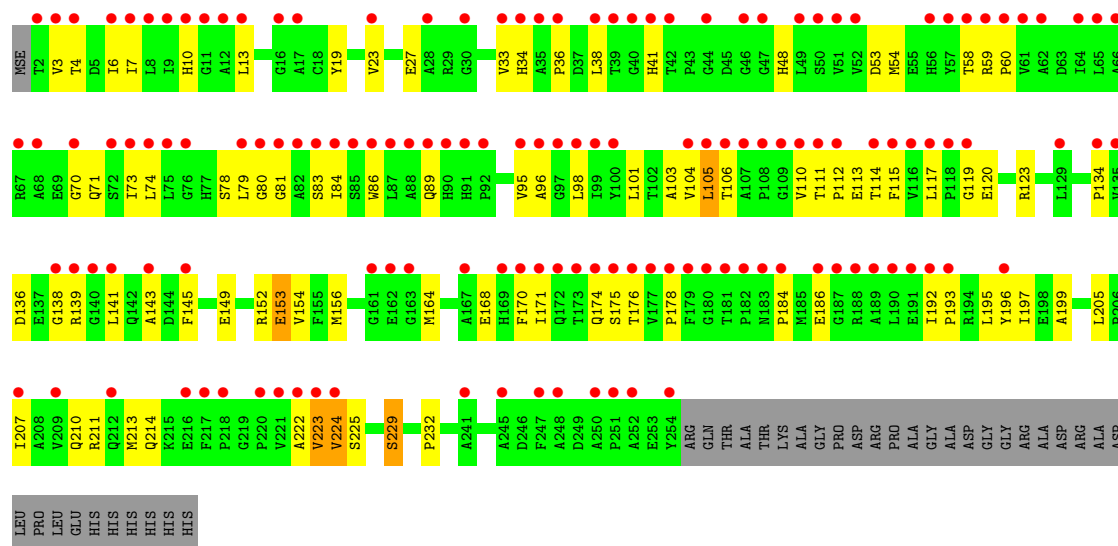




• Molecule 1: Pyrethroid hydrolase



• Molecule 1: Pyrethroid hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	168.45Å 168.45Å 123.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.85 – 1.96 19.85 – 1.96	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.85-1.96) 98.8 (19.85-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.96Å)	Xtriage
Refinement program	PHENIX (dev_2247: ???)	Depositor
R, R_{free}	0.255 , 0.309 0.260 , 0.311	Depositor DCC
R_{free} test set	6276 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11971	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: PMS, 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	0.43	0/1963	0.63	0/2678
1	B	0.53	2/1966 (0.1%)	0.71	4/2680 (0.1%)
1	C	0.41	0/1970	0.61	0/2688
1	D	0.49	0/1966	0.64	0/2680
1	E	0.46	0/1946	0.67	2/2658 (0.1%)
1	F	0.42	0/1919	0.69	3/2625 (0.1%)
All	All	0.46	2/11730 (0.0%)	0.66	9/16009 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	MSE	C-N	5.33	1.39	1.33
1	B	165	PRO	C-O	-5.15	1.18	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	MSE	N-CA-CB	-6.63	102.04	109.74
1	F	223	VAL	N-CA-C	6.59	117.60	108.12
1	B	156	MSE	N-CA-C	6.36	121.09	112.88
1	F	224	VAL	N-CA-C	-5.89	99.64	108.12
1	F	154	VAL	N-CA-C	5.83	116.01	110.53
1	E	165	PRO	CA-C-N	-5.26	114.83	120.03
1	E	165	PRO	C-N-CA	-5.26	114.83	120.03
1	B	164	MSE	CA-C-N	-5.15	115.08	120.38
1	B	164	MSE	C-N-CA	-5.15	115.08	120.38

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	1916	0	1875	15	0
1	B	1920	0	1879	29	0
1	C	1923	0	1874	34	0
1	D	1920	0	1878	26	0
1	E	1899	0	1848	99	0
1	F	1873	0	1792	76	0
2	A	10	0	7	0	0
2	B	10	0	7	0	0
2	C	10	0	7	0	0
2	D	10	0	7	0	0
2	E	10	0	7	3	0
2	F	10	0	7	5	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	105	0	0	0	1
4	B	96	0	0	1	0
4	C	85	0	0	1	1
4	D	97	0	0	4	0
4	E	29	0	0	1	0
4	F	18	0	0	0	0
All	All	11971	0	11188	276	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (276) 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:F:78[B]:SER:CB	2:F:301:PMS:S	2.34	1.15
1:E:166:PRO:HG2	1:E:169:HIS:CD2	1.82	1.14
1:F:138:GLY:O	1:F:176:THR:OG1	1.65	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78[B]:SER:HB2	2:F:301:PMS:S	1.91	1.07
1:E:166:PRO:HG2	1:E:169:HIS:NE2	1.79	0.96
1:E:166:PRO:CG	1:E:169:HIS:HE2	1.78	0.95
1:F:78[B]:SER:OG	1:F:79:LEU:N	1.92	0.94
1:E:166:PRO:CG	1:E:169:HIS:NE2	2.33	0.92
1:E:106:THR:HB	1:E:110:VAL:HG23	1.54	0.88
1:E:156:MSE:SE	1:E:165:PRO:HD2	2.25	0.87
1:C:4:THR:HG21	1:C:70:GLY:H	1.41	0.86
1:B:156:MSE:SE	1:B:164:MSE:HG3	2.26	0.86
1:E:78[B]:SER:OG	1:E:79:LEU:N	2.06	0.84
1:B:156:MSE:HE2	1:B:170:PHE:CZ	2.14	0.83
1:B:185:MSE:HE2	1:B:190:LEU:HD23	1.61	0.83
1:B:156:MSE:SE	1:B:164:MSE:HE3	2.31	0.81
1:D:104:VAL:HG11	1:D:112:PRO:HB3	1.62	0.81
1:E:166:PRO:CG	1:E:169:HIS:CD2	2.63	0.79
1:E:193:PRO:HG3	1:E:252:ALA:HA	1.64	0.79
1:F:207:ILE:HG13	1:F:211:ARG:HH22	1.48	0.78
1:D:78[B]:SER:OG	1:D:79:LEU:N	2.15	0.76
1:B:78[B]:SER:HA	1:B:103:ALA:HA	1.68	0.76
1:F:207:ILE:HG13	1:F:211:ARG:NH2	2.00	0.75
1:D:163:GLY:N	4:D:402:HOH:O	2.19	0.75
1:F:104:VAL:HA	1:F:213:MSE:SE	2.39	0.73
1:E:7:ILE:HD11	1:E:61:VAL:HG22	1.73	0.71
1:F:53:ASP:OD1	1:F:54:MSE:N	2.22	0.71
1:F:71:GLN:HB3	1:F:96:ALA:HB2	1.72	0.71
1:F:134:PRO:HA	1:F:141:LEU:HD23	1.71	0.70
1:F:143:ALA:HB3	1:F:145:PHE:HE1	1.59	0.68
1:E:122:ASN:HB2	1:E:212:GLN:NE2	2.09	0.68
1:B:156:MSE:HE2	1:B:170:PHE:CE2	2.29	0.67
1:E:205:LEU:CD1	1:E:210:GLN:HG3	2.25	0.66
1:E:150:ARG:O	1:E:154:VAL:HG23	1.96	0.66
1:C:78[B]:SER:OG	1:C:79:LEU:N	2.29	0.66
1:E:107:ALA:O	1:E:110:VAL:HG22	1.96	0.65
1:C:37:ASP:O	4:C:402:HOH:O	2.15	0.64
1:E:9:ILE:HD13	1:E:84:ILE:HG22	1.80	0.64
1:E:94:LYS:H	1:E:94:LYS:HD2	1.63	0.63
1:E:156:MSE:SE	1:E:165:PRO:CD	2.95	0.63
1:E:94:LYS:HD2	1:E:94:LYS:N	2.14	0.63
1:E:89:GLN:OE1	1:E:186:GLU:N	2.24	0.62
1:E:123:ARG:NH1	1:E:212:GLN:OE1	2.32	0.62
1:E:7:ILE:HD11	1:E:36:PRO:HG3	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LEU:HD21	1:C:178:PRO:HG2	1.83	0.61
1:F:114:THR:O	1:F:123:ARG:HD3	1.99	0.61
1:E:189:ALA:O	1:E:192:ILE:HG12	2.00	0.61
1:D:79:LEU:HD21	1:D:178:PRO:HG2	1.83	0.61
1:E:166:PRO:HG3	1:E:169:HIS:HE2	1.64	0.61
1:D:156:MSE:SE	1:D:164:MSE:CE	2.99	0.60
1:F:13:LEU:HA	1:F:171:ILE:HD11	1.83	0.60
1:E:207:ILE:O	1:E:211:ARG:HD2	2.01	0.59
1:C:188:ARG:NH2	1:E:55:GLU:OE1	2.35	0.59
1:E:154:VAL:HG13	1:E:203:VAL:HG23	1.85	0.59
1:E:164:MSE:HB3	1:E:165:PRO:CD	2.33	0.59
1:E:23:VAL:HG23	1:E:24:PRO:HD3	1.83	0.58
1:E:210:GLN:O	1:E:214:GLN:HG3	2.04	0.58
1:D:202:ASP:OD1	1:D:204:VAL:N	2.37	0.58
1:E:8:LEU:O	4:E:401:HOH:O	2.17	0.58
1:E:210:GLN:HA	1:E:213:MSE:CE	2.32	0.58
1:F:149:GLU:O	1:F:153:GLU:HG2	2.03	0.58
1:D:9:ILE:HD12	1:D:84:ILE:HG22	1.86	0.58
1:F:13:LEU:HD22	1:F:174:GLN:HB2	1.85	0.58
1:C:4:THR:HG23	1:C:5:ASP:OD1	2.04	0.57
1:B:9:ILE:HD12	1:B:84:ILE:HG22	1.86	0.57
1:F:3:VAL:HA	1:F:71:GLN:HB2	1.86	0.57
1:F:7:ILE:HD11	1:F:36:PRO:HD3	1.87	0.57
1:F:101:LEU:HD11	1:F:232:PRO:HG2	1.86	0.57
1:A:104:VAL:HG11	1:A:112:PRO:HB3	1.86	0.57
1:F:54:MSE:HE3	1:F:58:THR:HG23	1.87	0.56
1:C:31:TYR:OH	1:C:249:ASP:OD1	2.18	0.56
1:F:199:ALA:HB1	1:F:229:SER:O	2.05	0.56
1:E:144:ASP:OD2	1:E:147:ARG:NH2	2.36	0.55
1:E:10:HIS:C	1:E:10:HIS:CD2	2.84	0.55
1:D:211:ARG:HA	1:D:214:GLN:NE2	2.21	0.55
1:F:192:ILE:HG13	1:F:193:PRO:HD2	1.89	0.55
1:C:158:ASP:OD2	1:C:229:SER:HB2	2.06	0.55
1:A:164:MSE:HB3	1:A:165:PRO:CD	2.37	0.54
1:B:86:TRP:CD1	1:B:184:PRO:HG3	2.43	0.54
1:C:121:PRO:HG2	1:C:212:GLN:NE2	2.22	0.54
1:F:27:GLU:HG3	1:F:33:VAL:HG12	1.89	0.54
1:E:150:ARG:NH1	1:E:153:GLU:OE2	2.39	0.53
1:A:227:PRO:HD2	1:A:236:MSE:SE	2.57	0.53
1:E:89:GLN:HA	1:E:189:ALA:HB2	1.90	0.53
1:F:196:TYR:N	1:F:222:ALA:O	2.34	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78[A]:SER:OG	1:E:79:LEU:N	2.40	0.53
1:C:198:GLU:OE1	1:C:225:SER:OG	2.23	0.53
1:D:229:SER:HB2	4:D:458:HOH:O	2.07	0.53
1:F:84:ILE:HG23	1:F:98:LEU:CD2	2.39	0.53
1:F:105:LEU:H	1:F:213:MSE:SE	2.42	0.52
1:F:195:LEU:HA	1:F:222:ALA:HB3	1.91	0.52
1:E:88:ALA:HB1	1:E:192:ILE:CD1	2.38	0.52
1:E:106:THR:HB	1:E:110:VAL:CG2	2.33	0.52
1:E:154:VAL:HG12	1:E:204:VAL:HG22	1.91	0.52
1:B:55:GLU:OE1	1:B:59:ARG:NH1	2.43	0.52
1:C:89:GLN:HE22	1:C:186:GLU:HG2	1.75	0.52
1:D:156:MSE:SE	1:D:164:MSE:HE2	2.60	0.52
1:A:195:LEU:HD11	1:A:224:VAL:HG13	1.92	0.52
1:C:188:ARG:HH22	1:E:56:HIS:HA	1.74	0.52
1:F:174:GLN:HG3	1:F:175:SER:N	2.24	0.52
1:F:79:LEU:HD21	1:F:178:PRO:HB2	1.92	0.51
1:C:116:VAL:HG12	1:C:117:LEU:HD22	1.92	0.51
1:E:156:MSE:SE	1:E:164:MSE:HB3	2.61	0.51
1:F:205:LEU:HD21	1:F:213:MSE:HE1	1.91	0.51
1:F:111:THR:HG23	1:F:113:GLU:HG2	1.93	0.51
1:C:9:ILE:HD12	1:C:84:ILE:HG22	1.92	0.51
1:E:74:LEU:HD11	1:E:95:VAL:HG21	1.93	0.51
1:E:98:LEU:HD11	1:E:192:ILE:HG13	1.93	0.51
1:E:12:ALA:HB3	2:E:301:PMS:O2S	2.11	0.51
1:C:7:ILE:HG21	1:C:61:VAL:HG13	1.94	0.50
1:F:7:ILE:HG23	1:F:74:LEU:HD23	1.93	0.50
1:F:84:ILE:HG23	1:F:98:LEU:HD23	1.94	0.50
1:E:18:CYS:HA	1:E:169:HIS:ND1	2.25	0.50
1:E:89:GLN:O	1:E:89:GLN:NE2	2.44	0.50
1:B:212:GLN:O	1:B:216:GLU:HG3	2.11	0.50
1:A:113:GLU:HG3	1:A:179:PHE:O	2.11	0.50
1:F:106:THR:HB	1:F:110:VAL:HG12	1.94	0.50
1:F:111:THR:OG1	1:F:112:PRO:HD2	2.12	0.49
1:F:156:MSE:HE2	1:F:170:PHE:CZ	2.47	0.49
1:E:210:GLN:HA	1:E:213:MSE:HE2	1.94	0.49
1:A:89:GLN:HB2	1:A:185:MSE:HA	1.93	0.49
1:B:104:VAL:HG11	1:B:112:PRO:HB3	1.94	0.49
1:E:10:HIS:CE1	1:E:38:LEU:HG	2.47	0.49
1:E:166:PRO:CD	1:E:169:HIS:HE2	2.22	0.49
1:F:58:THR:HG21	1:F:86:TRP:CD1	2.47	0.49
1:C:158:ASP:HB3	1:C:235:SER:HB3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78[B]:SER:CB	2:E:301:PMS:S	2.87	0.49
1:E:58:THR:HB	1:E:87:LEU:HD11	1.94	0.49
1:F:207:ILE:HA	1:F:210:GLN:HE21	1.78	0.48
1:C:97:GLY:HA2	1:C:192:ILE:HG22	1.95	0.48
1:F:6:ILE:HG12	1:F:73:ILE:HB	1.94	0.48
1:C:103:ALA:O	1:C:213:MSE:HE1	2.14	0.48
1:C:106:THR:HB	1:C:110:VAL:HB	1.95	0.48
1:E:15:ARG:HD3	1:E:168:GLU:O	2.13	0.48
1:D:47:GLY:O	1:D:50:SER:OG	2.30	0.48
1:E:166:PRO:CD	1:E:169:HIS:NE2	2.76	0.48
1:F:197:ILE:HG12	1:F:224:VAL:CG1	2.44	0.48
1:B:156:MSE:SE	1:B:164:MSE:CG	3.07	0.48
1:E:193:PRO:CG	1:E:252:ALA:HA	2.40	0.48
1:F:7:ILE:HD12	1:F:34:HIS:O	2.14	0.48
1:B:79:LEU:HD21	1:B:178:PRO:HG2	1.96	0.47
1:E:166:PRO:CD	1:E:169:HIS:CD2	2.97	0.47
1:F:149:GLU:OE1	1:F:152:ARG:NH2	2.46	0.47
1:B:7:ILE:HD13	1:B:61:VAL:HG13	1.97	0.47
1:D:205:LEU:HG	1:D:210:GLN:HG3	1.95	0.47
1:F:86:TRP:CE3	1:F:184:PRO:HG3	2.50	0.47
1:F:119:GLY:C	1:F:120:GLU:HG2	2.39	0.47
1:B:150:ARG:HD2	1:B:153:GLU:OE2	2.14	0.47
1:C:162:GLU:HG3	1:C:162:GLU:O	2.14	0.47
1:F:156:MSE:SE	1:F:164:MSE:CE	3.13	0.47
1:E:229:SER:OG	1:E:230:HIS:N	2.48	0.47
1:E:15:ARG:NH2	1:E:37:ASP:OD2	2.35	0.47
1:E:79:LEU:HD11	1:E:178:PRO:HG2	1.97	0.47
1:F:113:GLU:HB2	1:F:117:LEU:HD12	1.96	0.47
1:A:197:ILE:HG12	1:A:224:VAL:HG22	1.97	0.46
1:E:204:VAL:HG21	1:E:230:HIS:CD2	2.50	0.46
1:E:17:ALA:CB	1:E:168:GLU:HG2	2.46	0.46
1:E:89:GLN:HB2	1:E:185:MSE:HA	1.95	0.46
1:E:121:PRO:C	1:E:212:GLN:HE22	2.22	0.46
1:E:98:LEU:HD13	1:E:194:ARG:HB3	1.98	0.46
1:E:10:HIS:HE1	1:E:38:LEU:H	1.63	0.46
1:F:19:TYR:O	1:F:23:VAL:HG23	2.15	0.46
1:B:185:MSE:HE2	1:B:190:LEU:CD2	2.40	0.46
1:F:115:PHE:CD2	1:F:213:MSE:HG2	2.51	0.46
1:D:39:THR:HB	1:D:57:TYR:HA	1.96	0.46
1:E:37:ASP:HB3	1:E:41:HIS:HB2	1.98	0.46
1:E:39:THR:HG21	1:E:56:HIS:NE2	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:LEU:O	1:F:41:HIS:HB2	2.15	0.46
1:F:119:GLY:O	1:F:120:GLU:HG2	2.14	0.46
1:B:195:LEU:HD11	1:B:224:VAL:HG22	1.97	0.46
1:C:15:ARG:CZ	1:C:43:PRO:HD3	2.46	0.46
1:D:158:ASP:HB3	1:D:235:SER:HB3	1.96	0.46
1:C:115:PHE:CE1	1:C:213:MSE:HG2	2.51	0.46
1:C:4:THR:HG21	1:C:70:GLY:N	2.21	0.45
1:A:41:HIS:HA	1:A:171:ILE:HD13	1.98	0.45
1:B:197:ILE:HG23	1:B:224:VAL:HG23	1.97	0.45
1:F:78[B]:SER:OG	2:F:301:PMS:S	2.06	0.45
1:F:79:LEU:HB2	2:F:301:PMS:O1S	2.17	0.45
1:F:7:ILE:HD11	1:F:36:PRO:HG3	1.99	0.45
1:A:158:ASP:HB3	1:A:235:SER:HB3	1.98	0.45
1:B:152:ARG:HA	1:B:156:MSE:HB2	1.99	0.45
1:D:128:ALA:O	1:D:132:ILE:HG12	2.17	0.45
1:F:54:MSE:HE2	1:F:83:SER:HA	1.99	0.45
1:B:55:GLU:OE2	1:B:59:ARG:HD3	2.16	0.45
1:D:175:SER:O	1:D:178:PRO:HD2	2.16	0.45
1:B:45:ASP:OD2	4:B:401:HOH:O	2.21	0.44
1:C:25:LEU:HD13	1:C:238:GLU:OE2	2.17	0.44
1:E:98:LEU:HD11	1:E:192:ILE:CG1	2.46	0.44
1:E:121:PRO:O	1:E:212:GLN:NE2	2.46	0.44
1:E:10:HIS:CE1	1:E:38:LEU:H	2.36	0.44
1:D:150:ARG:HA	1:D:153:GLU:HG2	1.99	0.44
1:E:39:THR:OG1	1:E:56:HIS:O	2.35	0.44
1:E:77:HIS:HA	1:E:101:LEU:O	2.17	0.44
1:F:7:ILE:HD11	1:F:36:PRO:CD	2.48	0.44
1:F:81:GLY:HA3	1:F:103:ALA:HB1	1.99	0.44
1:F:156:MSE:SE	1:F:164:MSE:HE2	2.67	0.44
1:E:135:VAL:HG12	1:E:140:GLY:C	2.43	0.44
1:A:149:GLU:O	1:A:153:GLU:HG2	2.18	0.44
1:B:205:LEU:HD21	1:B:213:MSE:HE1	1.98	0.44
1:D:173:THR:N	4:D:406:HOH:O	2.44	0.44
1:E:166:PRO:HD2	1:E:169:HIS:NE2	2.33	0.44
1:F:48:HIS:CD2	1:F:48:HIS:H	2.36	0.44
1:F:78[A]:SER:OG	1:F:79:LEU:N	2.51	0.44
1:A:61:VAL:HG11	1:A:87:LEU:HD13	2.00	0.44
1:E:197:ILE:HG23	1:E:224:VAL:HG23	1.99	0.44
1:B:156:MSE:SE	1:B:164:MSE:CE	3.12	0.43
1:C:188:ARG:NH2	1:E:56:HIS:HA	2.34	0.43
1:C:142:GLN:HG3	1:C:172:GLN:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:LEU:O	1:F:171:ILE:HG13	2.18	0.43
1:F:53:ASP:CG	1:F:54:MSE:N	2.77	0.43
1:A:158:ASP:OD2	1:A:229:SER:OG	2.28	0.43
1:D:5:ASP:HB2	1:D:72:SER:OG	2.19	0.43
1:C:60:PRO:O	1:C:64:ILE:HG13	2.18	0.43
1:B:4:THR:HG21	1:B:69:GLU:HG3	2.00	0.43
1:C:134:PRO:HA	1:C:141:LEU:HD23	2.00	0.43
1:E:207:ILE:HG13	1:E:211:ARG:HD2	2.01	0.43
1:E:214:GLN:HG3	1:E:214:GLN:H	1.57	0.43
1:F:95:VAL:O	1:F:192:ILE:HD12	2.19	0.43
1:A:79:LEU:HD21	1:A:178:PRO:HG2	2.00	0.43
1:E:135:VAL:HG12	1:E:140:GLY:O	2.19	0.43
1:C:79:LEU:HD21	1:C:178:PRO:CG	2.47	0.43
1:C:91:HIS:N	1:C:92:PRO:HD3	2.34	0.43
1:D:181:THR:HB	4:D:408:HOH:O	2.18	0.43
1:E:154:VAL:HG12	1:E:204:VAL:CG2	2.48	0.43
1:F:89:GLN:OE1	1:F:186:GLU:N	2.34	0.43
1:C:187:GLY:N	1:C:190:LEU:HD12	2.34	0.43
1:D:129:LEU:HD23	1:D:129:LEU:HA	1.77	0.43
1:E:116:VAL:CG1	1:E:129:LEU:HD21	2.49	0.43
1:D:106:THR:HB	1:D:110:VAL:HB	2.01	0.42
1:E:23:VAL:HG23	1:E:24:PRO:CD	2.47	0.42
1:E:85:SER:O	1:E:185:MSE:SE	2.87	0.42
1:F:59:ARG:HB3	1:F:60:PRO:HD3	2.01	0.42
1:E:15:ARG:CZ	1:E:43:PRO:HD3	2.50	0.42
1:E:17:ALA:HB1	1:E:168:GLU:HG2	2.01	0.42
1:A:54:MSE:HG3	1:A:181:THR:HG21	1.99	0.42
1:B:122:ASN:OD1	1:B:122:ASN:N	2.52	0.42
1:F:4:THR:OG1	1:F:70:GLY:HA3	2.18	0.42
1:D:156:MSE:SE	1:D:164:MSE:HE3	2.69	0.42
1:F:80:GLY:O	1:F:84:ILE:HD13	2.18	0.42
1:E:166:PRO:HD2	1:E:169:HIS:CD2	2.55	0.42
1:E:54:MSE:CE	1:E:83:SER:HA	2.50	0.42
1:B:205:LEU:HD23	1:B:210:GLN:HG2	2.01	0.42
1:F:196:TYR:O	1:F:223:VAL:HA	2.19	0.42
1:E:149:GLU:HG3	1:E:153:GLU:OE1	2.20	0.41
1:F:10:HIS:O	1:F:10:HIS:ND1	2.52	0.41
1:B:79:LEU:HD22	1:B:179:PHE:CE2	2.55	0.41
1:E:166:PRO:HG2	1:E:169:HIS:HD2	1.67	0.41
1:F:74:LEU:O	1:F:98:LEU:HA	2.19	0.41
1:D:93:ASP:N	1:D:93:ASP:OD1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:LEU:HD12	1:F:192:ILE:HG12	2.01	0.41
1:F:164:MSE:HE2	1:F:164:MSE:HB3	1.84	0.41
1:A:39:THR:HB	1:A:57:TYR:HA	2.03	0.41
1:C:115:PHE:CD1	1:C:213:MSE:HG2	2.55	0.41
1:E:152:ARG:HG3	1:E:164:MSE:CG	2.51	0.41
1:E:228:ALA:CB	1:E:232:PRO:HB3	2.50	0.41
1:B:84:ILE:HD12	1:B:98:LEU:HB3	2.02	0.41
1:C:75:LEU:HD12	1:C:99:ILE:HG21	2.01	0.41
1:D:48:HIS:NE2	1:D:136:ASP:OD2	2.47	0.41
1:C:15:ARG:HH21	1:C:42:THR:HG23	1.86	0.41
1:F:79:LEU:N	2:F:301:PMS:S	2.93	0.41
1:E:128:ALA:HB1	2:E:301:PMS:C5	2.51	0.41
1:E:152:ARG:HG3	1:E:164:MSE:HG3	2.02	0.41
1:E:84:ILE:HD11	1:E:100:TYR:CD2	2.56	0.41
1:E:116:VAL:HG13	1:E:129:LEU:HD21	2.03	0.41
1:E:177:VAL:N	1:E:178:PRO:HD2	2.36	0.41
1:F:168:GLU:H	1:F:168:GLU:CD	2.29	0.41
1:D:79:LEU:O	1:D:79:LEU:HG	2.21	0.40
1:E:79:LEU:HD12	1:E:179:PHE:CZ	2.56	0.40
1:F:6:ILE:O	1:F:33:VAL:HA	2.20	0.40
1:E:91:HIS:HA	1:E:94:LYS:HD3	2.04	0.40
1:F:210:GLN:O	1:F:214:GLN:HG3	2.20	0.40
1:E:150:ARG:HA	1:E:150:ARG:HD2	1.94	0.40
1:B:84:ILE:HD11	1:B:100:TYR:CE2	2.56	0.40
1:E:9:ILE:HG23	1:E:38:LEU:HD21	2.03	0.40
1:F:136:ASP:OD1	1:F:139:ARG:CB	2.70	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:449:HOH:O	4:C:479:HOH:O[3_555]	2.17	0.03

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	248/288 (86%)	235 (95%)	13 (5%)	0	100	100
1	B	249/288 (86%)	237 (95%)	12 (5%)	0	100	100
1	C	252/288 (88%)	240 (95%)	12 (5%)	0	100	100
1	D	249/288 (86%)	237 (95%)	12 (5%)	0	100	100
1	E	248/288 (86%)	234 (94%)	14 (6%)	0	100	100
1	F	252/288 (88%)	231 (92%)	21 (8%)	0	100	100
All	All	1498/1728 (87%)	1414 (94%)	84 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	202/220 (92%)	202 (100%)	0	100	100
1	B	202/220 (92%)	201 (100%)	1 (0%)	81	82
1	C	202/220 (92%)	201 (100%)	1 (0%)	81	82
1	D	202/220 (92%)	202 (100%)	0	100	100
1	E	198/220 (90%)	198 (100%)	0	100	100
1	F	191/220 (87%)	187 (98%)	4 (2%)	47	41
All	All	1197/1320 (91%)	1191 (100%)	6 (0%)	81	82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	164	MSE
1	C	254	TYR
1	F	105	LEU
1	F	153	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	225	SER
1	F	229	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	B	14	ASN
1	C	89	GLN
1	C	127	HIS
1	D	122	ASN
1	D	127	HIS
1	D	172	GLN
1	F	127	HIS
1	F	174	GLN
1	F	212	GLN
1	F	214	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	D	302	-	4,4,4	0.17	0	6,6,6	0.24	0
3	SO4	A	302	-	4,4,4	0.25	0	6,6,6	0.19	0
2	PMS	F	301	1	7,10,11	0.88	0	11,12,15	1.04	0
3	SO4	B	302	-	4,4,4	0.25	0	6,6,6	0.24	0
3	SO4	E	302	-	4,4,4	0.25	0	6,6,6	0.22	0
3	SO4	F	302	-	4,4,4	0.24	0	6,6,6	0.34	0
2	PMS	B	301	1	7,10,11	0.47	0	11,12,15	2.58	4 (36%)
3	SO4	C	302	-	4,4,4	0.22	0	6,6,6	0.17	0
2	PMS	D	301	1	7,10,11	0.43	0	11,12,15	2.45	3 (27%)
2	PMS	A	301	1	7,10,11	0.47	0	11,12,15	2.88	4 (36%)
2	PMS	C	301	1	7,10,11	0.73	0	11,12,15	2.14	3 (27%)
2	PMS	E	301	1	7,10,11	0.30	0	11,12,15	1.93	2 (18%)

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
2	PMS	F	301	1	-	0/4/4/5	0/1/1/1
2	PMS	B	301	1	-	2/4/4/5	0/1/1/1
2	PMS	D	301	1	-	2/4/4/5	0/1/1/1
2	PMS	A	301	1	-	2/4/4/5	0/1/1/1
2	PMS	C	301	1	-	4/4/4/5	0/1/1/1
2	PMS	E	301	1	-	2/4/4/5	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	PMS	O2S-S-C	7.01	117.65	105.55
2	D	301	PMS	O2S-S-C	6.13	116.14	105.55
2	A	301	PMS	O1S-S-C	5.98	115.88	105.55
2	A	301	PMS	O2S-S-C	5.86	115.67	105.55
2	C	301	PMS	O2S-S-C	5.17	114.49	105.55
2	E	301	PMS	O2S-S-C	5.01	114.20	105.55
2	D	301	PMS	O1S-S-C	4.08	112.59	105.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	PMS	O1S-S-C	3.64	111.84	105.55
2	A	301	PMS	C1-C-S	3.24	118.90	110.71
2	C	301	PMS	C1-C-S	2.75	117.67	110.71
2	B	301	PMS	C-C1-C6	-2.68	117.64	120.56
2	D	301	PMS	C1-C-S	2.60	117.30	110.71
2	B	301	PMS	O1S-S-C	2.53	109.92	105.55
2	A	301	PMS	C-C1-C6	-2.47	117.86	120.56
2	B	301	PMS	C1-C-S	2.34	116.61	110.71
2	E	301	PMS	C-C1-C2	-2.31	118.04	120.56

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	PMS	S-C-C1-C2
2	A	301	PMS	S-C-C1-C6
2	B	301	PMS	S-C-C1-C2
2	B	301	PMS	S-C-C1-C6
2	C	301	PMS	C1-C-S-O2S
2	C	301	PMS	C1-C-S-O1S
2	D	301	PMS	S-C-C1-C2
2	D	301	PMS	S-C-C1-C6
2	E	301	PMS	S-C-C1-C2
2	E	301	PMS	S-C-C1-C6
2	C	301	PMS	S-C-C1-C2
2	C	301	PMS	S-C-C1-C6

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	PMS	5	0
2	E	301	PMS	3	0

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, 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	245/288 (85%)	0.03	2 (0%) 82 86	13, 27, 41, 60	1 (0%)
1	B	246/288 (85%)	0.16	3 (1%) 76 82	12, 29, 44, 61	1 (0%)
1	C	247/288 (85%)	0.47	8 (3%) 50 56	14, 34, 49, 69	1 (0%)
1	D	246/288 (85%)	0.36	5 (2%) 65 72	15, 30, 45, 60	1 (0%)
1	E	245/288 (85%)	1.72	84 (34%) 1 0	21, 47, 66, 78	1 (0%)
1	F	247/288 (85%)	2.37	142 (57%) 0 0	29, 60, 85, 94	1 (0%)
All	All	1476/1728 (85%)	0.85	244 (16%) 4 4	12, 35, 70, 94	6 (0%)

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	107	ALA	7.7
1	E	135	VAL	6.1
1	F	190	LEU	5.9
1	F	110	VAL	5.7
1	F	86	TRP	5.7
1	F	87	LEU	5.4
1	F	57	TYR	5.3
1	F	135	VAL	5.3
1	F	106	THR	5.1
1	F	254	TYR	4.9
1	F	179	PHE	4.8
1	F	84	ILE	4.8
1	F	80	GLY	4.7
1	F	184	PRO	4.6
1	F	143	ALA	4.6
1	E	221	VAL	4.6
1	F	65	LEU	4.5
1	F	189	ALA	4.5
1	F	140	GLY	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	189	ALA	4.4
1	F	64	ILE	4.4
1	F	61	VAL	4.3
1	F	221	VAL	4.3
1	F	104	VAL	4.3
1	F	188	ARG	4.3
1	E	110	VAL	4.2
1	F	52	VAL	4.2
1	F	139	ARG	4.2
1	F	177	VAL	4.1
1	E	86	TRP	4.1
1	F	82	ALA	4.1
1	F	181	THR	4.1
1	F	217	PHE	4.0
1	E	107	ALA	4.0
1	F	178	PRO	4.0
1	E	141	LEU	4.0
1	F	79	LEU	4.0
1	F	88	ALA	4.0
1	F	171	ILE	4.0
1	F	51	VAL	3.9
1	F	44	GLY	3.9
1	F	105	LEU	3.8
1	F	161	GLY	3.8
1	F	12	ALA	3.8
1	F	192	ILE	3.7
1	F	115	PHE	3.7
1	F	182	PRO	3.7
1	C	163	GLY	3.7
1	F	112	PRO	3.7
1	F	38	LEU	3.7
1	E	70	GLY	3.7
1	E	115	PHE	3.7
1	E	179	PHE	3.7
1	F	183	ASN	3.6
1	F	114	THR	3.6
1	E	62	ALA	3.6
1	E	252	ALA	3.6
1	F	66	ALA	3.6
1	F	95	VAL	3.6
1	E	190	LEU	3.6
1	F	100	TYR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	117	LEU	3.5
1	E	2	THR	3.5
1	D	209	VAL	3.5
1	E	51	VAL	3.5
1	F	98	LEU	3.5
1	F	109	GLY	3.5
1	F	138	GLY	3.5
1	E	84	ILE	3.4
1	E	161	GLY	3.4
1	F	187	GLY	3.4
1	F	209	VAL	3.4
1	F	81	GLY	3.3
1	E	95	VAL	3.3
1	B	161	GLY	3.3
1	F	111	THR	3.3
1	F	108	PRO	3.3
1	E	3	VAL	3.3
1	C	2	THR	3.3
1	F	3	VAL	3.2
1	A	139	ARG	3.2
1	E	192	ILE	3.2
1	F	33	VAL	3.2
1	F	72	SER	3.2
1	E	88	ALA	3.2
1	E	98	LEU	3.2
1	F	129	LEU	3.2
1	F	34	HIS	3.2
1	F	141	LEU	3.1
1	F	175	SER	3.1
1	F	17	ALA	3.1
1	F	36	PRO	3.1
1	F	83	SER	3.1
1	F	97	GLY	3.1
1	F	163	GLY	3.1
1	B	163	GLY	3.1
1	F	74	LEU	3.0
1	F	39	THR	3.0
1	F	167	ALA	3.0
1	F	145	PHE	3.0
1	E	106	THR	3.0
1	F	218	PRO	3.0
1	E	64	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	73	ILE	3.0
1	E	13	LEU	3.0
1	F	47	GLY	3.0
1	E	108	PRO	2.9
1	F	247	PHE	2.9
1	E	96	ALA	2.9
1	F	41	HIS	2.9
1	E	85	SER	2.9
1	E	111	THR	2.9
1	F	176	THR	2.9
1	E	40	GLY	2.9
1	E	209	VAL	2.9
1	F	50	SER	2.9
1	E	38	LEU	2.9
1	E	132	ILE	2.9
1	F	7	ILE	2.8
1	F	220	PRO	2.8
1	F	60	PRO	2.8
1	C	162	GLU	2.8
1	F	193	PRO	2.8
1	C	66	ALA	2.7
1	E	250	ALA	2.7
1	F	173	THR	2.7
1	F	99	ILE	2.7
1	E	182	PRO	2.7
1	E	193	PRO	2.7
1	F	116	VAL	2.7
1	F	76	GLY	2.7
1	E	43	PRO	2.7
1	E	206	PRO	2.7
1	F	6	ILE	2.7
1	E	66	ALA	2.7
1	F	96	ALA	2.7
1	E	254	TYR	2.7
1	F	16	GLY	2.7
1	F	30	GLY	2.7
1	E	125	THR	2.7
1	E	126	PRO	2.7
1	F	89	GLN	2.6
1	F	118	PRO	2.6
1	A	158	ASP	2.6
1	F	28	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	196	TYR	2.6
1	E	90	HIS	2.6
1	E	195	LEU	2.6
1	E	171	ILE	2.6
1	E	138	GLY	2.6
1	F	186	GLU	2.6
1	F	68	ALA	2.6
1	F	56	HIS	2.6
1	F	92	PRO	2.6
1	E	79	LEU	2.6
1	F	13	LEU	2.6
1	F	172	GLN	2.6
1	E	46	GLY	2.6
1	F	180	GLY	2.6
1	D	224	VAL	2.6
1	F	223	VAL	2.6
1	F	85	SER	2.6
1	E	121	PRO	2.5
1	F	134	PRO	2.5
1	F	73	ILE	2.5
1	E	167	ALA	2.5
1	D	223	VAL	2.5
1	E	97	GLY	2.5
1	F	35	ALA	2.5
1	F	162	GLU	2.5
1	F	191	GLU	2.5
1	F	8	LEU	2.5
1	F	75	LEU	2.5
1	F	9	ILE	2.5
1	F	174	GLN	2.5
1	F	117	LEU	2.4
1	E	222	ALA	2.4
1	F	4	THR	2.4
1	F	40	GLY	2.4
1	F	10	HIS	2.4
1	F	49	LEU	2.4
1	B	2	THR	2.4
1	E	4	THR	2.4
1	F	11	GLY	2.4
1	F	169	HIS	2.4
1	F	170	PHE	2.4
1	F	62	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	248	ALA	2.4
1	F	67	ARG	2.3
1	E	57	TYR	2.3
1	F	2	THR	2.3
1	E	248	ALA	2.3
1	E	180	GLY	2.3
1	F	119	GLY	2.3
1	E	72	SER	2.3
1	F	58	THR	2.3
1	E	134	PRO	2.3
1	F	46	GLY	2.3
1	F	207	ILE	2.3
1	E	39	THR	2.3
1	D	115	PHE	2.2
1	E	60	PRO	2.2
1	E	184	PRO	2.2
1	E	99	ILE	2.2
1	E	48	HIS	2.2
1	E	42	THR	2.2
1	E	114	THR	2.2
1	E	105	LEU	2.2
1	F	216	GLU	2.2
1	E	93	ASP	2.2
1	F	90	HIS	2.2
1	C	161	GLY	2.2
1	F	250	ALA	2.2
1	E	247	PHE	2.2
1	C	110	VAL	2.2
1	F	222	ALA	2.2
1	F	252	ALA	2.2
1	F	91	HIS	2.1
1	E	104	VAL	2.1
1	E	140	GLY	2.1
1	E	87	LEU	2.1
1	E	251	PRO	2.1
1	F	241	ALA	2.1
1	E	145	PHE	2.1
1	E	169	HIS	2.1
1	E	143	ALA	2.1
1	F	245	ALA	2.1
1	E	78[A]	SER	2.1
1	C	181	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	42	THR	2.1
1	E	47	GLY	2.1
1	F	70	GLY	2.1
1	E	33	VAL	2.1
1	E	52	VAL	2.1
1	F	224	VAL	2.1
1	E	155	PHE	2.0
1	F	23	VAL	2.0
1	F	251	PRO	2.0
1	C	252	ALA	2.0
1	D	163	GLY	2.0
1	E	81	GLY	2.0
1	F	212	GLN	2.0
1	E	123	ARG	2.0
1	F	59	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PMS	E	301	10/11	0.60	0.22	54,57,60,65	10
2	PMS	F	301	10/11	0.73	0.19	56,60,70,70	10
2	PMS	B	301	10/11	0.88	0.11	23,32,35,42	10
2	PMS	C	301	10/11	0.88	0.12	23,26,34,39	10
2	PMS	D	301	10/11	0.89	0.11	27,33,39,45	10
3	SO4	B	302	5/5	0.89	0.14	34,35,45,46	0
2	PMS	A	301	10/11	0.93	0.10	22,31,35,35	10
3	SO4	D	302	5/5	0.93	0.10	40,41,47,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	F	302	5/5	0.93	0.10	34,38,52,63	0
3	SO4	E	302	5/5	0.95	0.08	35,37,46,46	0
3	SO4	C	302	5/5	0.96	0.07	30,39,45,46	0
3	SO4	A	302	5/5	0.97	0.07	26,32,34,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.