



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:30 pm BST

PDB ID : 1PG8
Title : Crystal Structure of L-methionine alpha-, gamma-lyase
Authors : Allen, T.W.; Sridhar, V.; Prasad, G.S.; Han, Q.; Xu, M.; Tan, Y.; Hoffman, R.M.; Ramaswamy, S.
Deposited on : 2003-05-28
Resolution : 2.68 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 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	:	2.11
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)	:	2.11

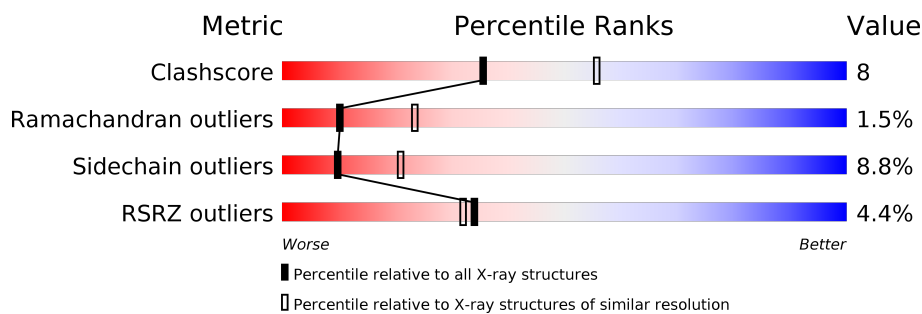
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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))
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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 on 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	398	<div> <div>5%</div> <div>77%</div> <div>20%</div> <div>..</div> </div>
1	B	398	<div> <div>5%</div> <div>80%</div> <div>16%</div> <div>.</div> </div>
1	C	398	<div> <div>5%</div> <div>82%</div> <div>14%</div> <div>..</div> </div>
1	D	398	<div> <div>4%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>

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	B	1138	-	-	X	-
3	PLP	A	1399	-	-	X	-
4	PEG	A	1002	-	-	X	-
4	PEG	A	1003	-	-	-	X
4	PEG	A	1004	-	-	-	X
4	PEG	A	1005	-	-	-	X
4	PEG	A	1008	-	-	X	-
4	PEG	B	1006	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12557 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 Methionine gamma-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			2994	1889	532	555	18			
1	B	398	Total	C	N	O	S	0	0	0
			2994	1889	532	555	18			
1	C	398	Total	C	N	O	S	0	0	0
			2994	1889	532	555	18			
1	D	398	Total	C	N	O	S	0	0	0
			2994	1889	532	555	18			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



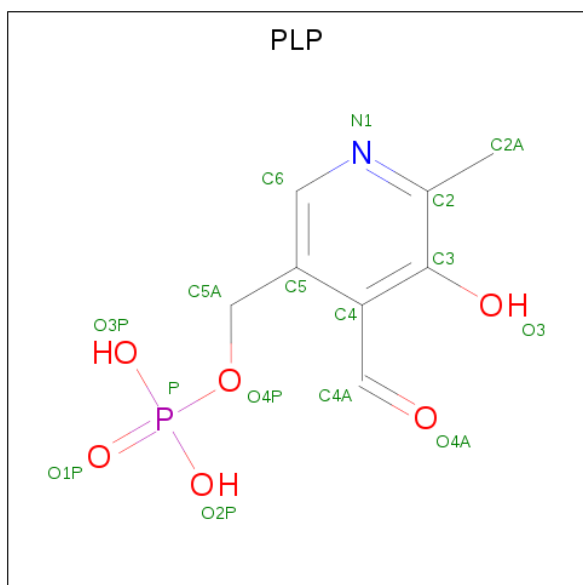
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	137	Total	O	0	0
			137	137		

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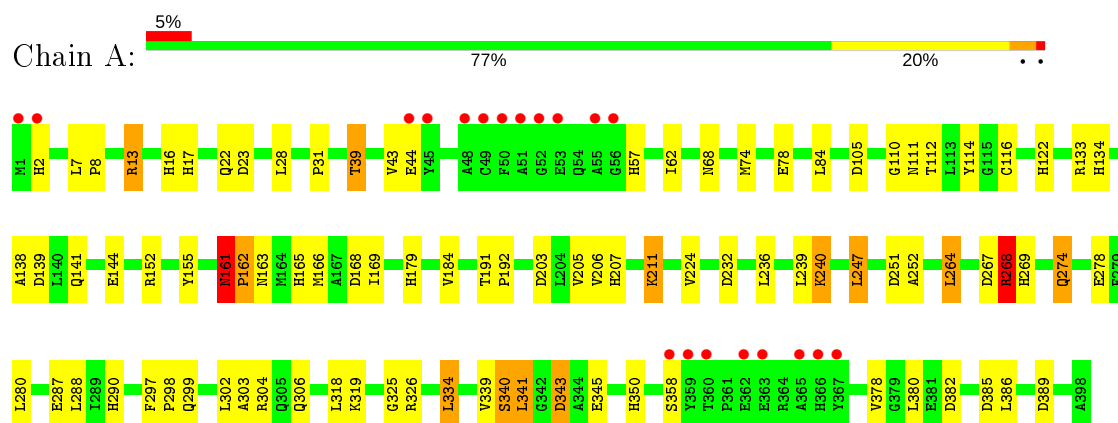
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	72	Total 72	O 72	0	0
5	C	107	Total 107	O 107	0	0
5	D	108	Total 108	O 108	0	0

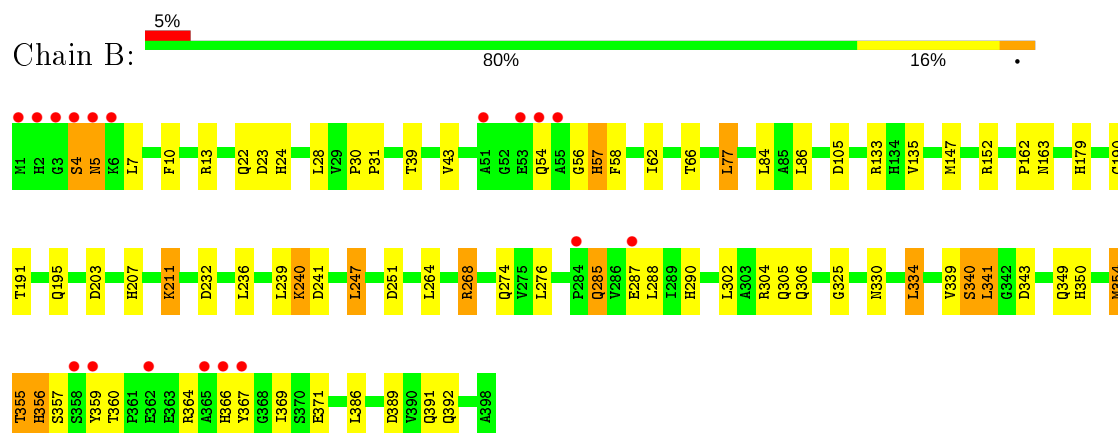
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

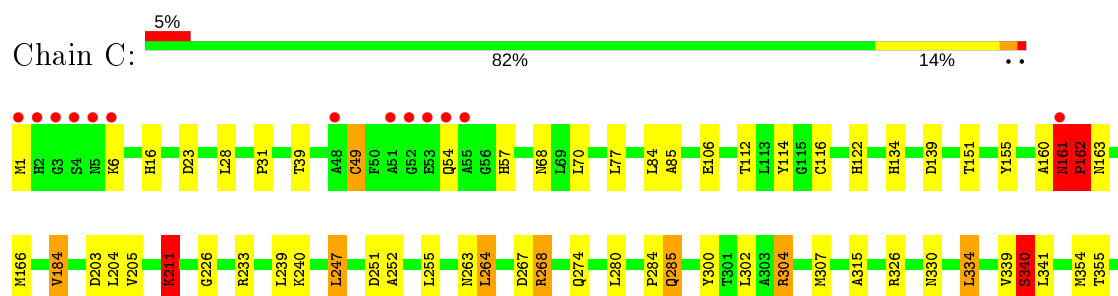
• Molecule 1: Methionine gamma-lyase

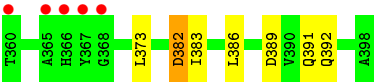


• Molecule 1: Methionine gamma-lyase

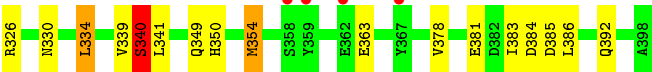
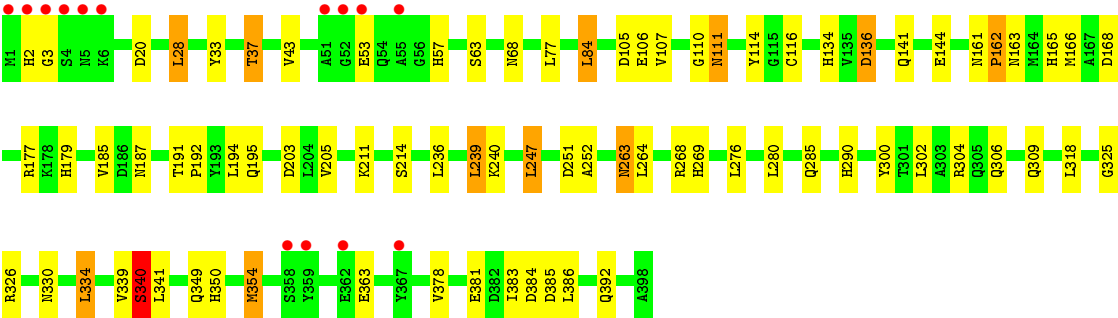
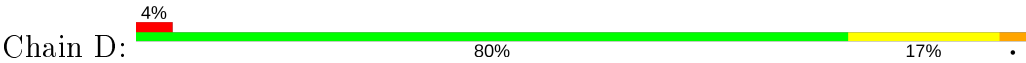


• Molecule 1: Methionine gamma-lyase





● Molecule 1: Methionine gamma-lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	152.83Å 154.64Å 80.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.68 19.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.68) 99.3 (19.99-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.182 , 0.236 0.182 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12557	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: PEG, SO4, PLP

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	0.78	1/3059 (0.0%)	0.95	15/4152 (0.4%)
1	B	0.71	1/3059 (0.0%)	0.88	9/4152 (0.2%)
1	C	0.71	0/3059	0.94	15/4152 (0.4%)
1	D	0.78	1/3059 (0.0%)	0.94	10/4152 (0.2%)
All	All	0.74	3/12236 (0.0%)	0.93	49/16608 (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	1
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	354	MET	SD-CE	-7.06	1.38	1.77
1	A	74	MET	SD-CE	-5.25	1.48	1.77
1	B	354	MET	SD-CE	-5.22	1.48	1.77

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	162	PRO	CA-N-CD	-13.50	92.60	111.50
1	D	268	ARG	NE-CZ-NH2	-12.33	114.14	120.30
1	C	161	ASN	C-N-CD	-10.77	96.92	120.60
1	A	268	ARG	NE-CZ-NH2	-9.65	115.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	ASP	CB-CG-OD2	9.21	126.59	118.30
1	B	251	ASP	CB-CG-OD2	8.87	126.28	118.30
1	A	343	ASP	CB-CG-OD2	8.84	126.26	118.30
1	A	139	ASP	CB-CG-OD2	8.67	126.11	118.30
1	A	268	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	C	162	PRO	CA-C-N	-8.42	98.67	117.20
1	B	268	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	A	23	ASP	CB-CG-OD2	8.05	125.55	118.30
1	A	267	ASP	CB-CG-OD2	8.04	125.54	118.30
1	B	203	ASP	CB-CG-OD2	7.97	125.47	118.30
1	D	268	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	C	268	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	A	203	ASP	CB-CG-OD2	7.41	124.97	118.30
1	C	23	ASP	CB-CG-OD2	7.25	124.82	118.30
1	C	139	ASP	CB-CG-OD2	7.20	124.78	118.30
1	C	267	ASP	CB-CG-OD2	7.13	124.72	118.30
1	D	251	ASP	CB-CG-OD2	7.08	124.67	118.30
1	B	343	ASP	CB-CG-OD2	7.00	124.60	118.30
1	A	105	ASP	CB-CG-OD2	6.97	124.58	118.30
1	C	382	ASP	CB-CG-OD2	6.96	124.57	118.30
1	B	232	ASP	CB-CG-OD2	6.59	124.23	118.30
1	D	105	ASP	CB-CG-OD2	6.51	124.16	118.30
1	D	168	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	105	ASP	CB-CG-OD2	6.47	124.12	118.30
1	C	162	PRO	N-CA-CB	6.27	110.83	103.30
1	D	20	ASP	CB-CG-OD2	6.22	123.90	118.30
1	C	268	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	C	389	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	251	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	13	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	D	385	ASP	CB-CG-OD2	5.98	123.68	118.30
1	C	203	ASP	CB-CG-OD2	5.96	123.67	118.30
1	C	162	PRO	O-C-N	5.78	131.95	122.70
1	B	13	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	385	ASP	CB-CG-OD2	5.38	123.14	118.30
1	D	136	ASP	CB-CG-OD2	5.36	123.13	118.30
1	A	168	ASP	CB-CG-OD2	5.30	123.07	118.30
1	D	384	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	241	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	389	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	233	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	382	ASP	CB-CG-OD2	5.08	122.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	251	ASP	CB-CG-OD2	5.07	122.87	118.30
1	A	389	ASP	CB-CG-OD2	5.04	122.84	118.30
1	D	203	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ASN	Peptide
1	B	207	HIS	Peptide

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	2994	0	2967	61	0
1	B	2994	0	2967	53	0
1	C	2994	0	2967	44	0
1	D	2994	0	2967	47	0
2	A	5	0	0	0	0
2	B	5	0	0	2	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	15	0	6	7	0
3	B	15	0	6	4	0
3	C	15	0	6	2	0
3	D	15	0	6	4	0
4	A	49	0	70	12	0
4	B	14	0	20	7	0
4	C	14	0	20	3	0
5	A	137	0	0	9	0
5	B	72	0	0	2	0
5	C	107	0	0	5	0
5	D	108	0	0	2	0
All	All	12557	0	12002	191	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 8.

All (191) 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:D:166:MET:CE	1:D:166:MET:SD	2.04	1.44
1:C:211:LYS:HZ2	3:C:1199:PLP:C4A	1.36	1.33
1:A:211:LYS:HZ1	3:A:1399:PLP:C4A	1.39	1.27
1:D:211:LYS:HZ1	3:D:1599:PLP:C4A	1.58	1.09
1:B:211:LYS:HZ1	3:B:1799:PLP:C4A	1.64	1.07
1:A:211:LYS:HZ2	3:A:1399:PLP:C4A	1.58	1.01
1:B:211:LYS:HZ2	3:B:1799:PLP:C4A	1.68	0.93
1:D:211:LYS:HZ2	3:D:1599:PLP:C4A	1.69	0.92
1:C:211:LYS:HZ1	3:C:1199:PLP:C4A	1.75	0.91
1:A:17:HIS:ND1	4:A:1002:PEG:H42	1.87	0.90
1:A:161:ASN:O	1:A:161:ASN:ND2	2.04	0.90
1:B:43:VAL:H	1:D:330:ASN:HD21	1.18	0.89
1:A:116:CYS:SG	1:C:240:LYS:NZ	2.47	0.87
1:A:43:VAL:H	1:C:330:ASN:HD21	1.26	0.84
1:B:66:THR:HA	4:B:1006:PEG:H42	1.67	0.77
1:B:57:HIS:HA	5:B:1811:HOH:O	1.85	0.76
1:D:163:ASN:HD22	1:D:290:HIS:CD2	2.02	0.76
1:C:211:LYS:HG3	1:C:341:LEU:HG	1.69	0.74
1:A:290:HIS:ND1	5:A:1520:HOH:O	2.20	0.74
1:B:23:ASP:C	1:B:24:HIS:HD2	1.91	0.74
1:D:263:ASN:H	1:D:263:ASN:HD22	1.35	0.73
1:B:163:ASN:HD22	1:B:290:HIS:CD2	2.07	0.73
1:B:24:HIS:HE1	4:B:1006:PEG:C2	2.01	0.73
1:D:349:GLN:HA	1:D:354:MET:HE1	1.71	0.72
1:A:211:LYS:HZ2	3:A:1399:PLP:C4	2.03	0.71
1:A:57:HIS:HE1	1:A:68:ASN:OD1	1.73	0.70
1:A:161:ASN:C	1:A:161:ASN:ND2	2.47	0.67
1:A:111:ASN:H	4:A:1008:PEG:H42	1.58	0.67
1:D:211:LYS:CE	3:D:1599:PLP:C4A	2.73	0.67
1:A:211:LYS:CE	3:A:1399:PLP:C4A	2.71	0.67
1:B:285:GLN:H	1:B:285:GLN:HE21	1.42	0.66
1:B:330:ASN:HD21	1:D:43:VAL:H	1.42	0.66
1:B:24:HIS:HE1	4:B:1006:PEG:H21	1.59	0.66
1:D:136:ASP:OD1	1:D:165:HIS:HE1	1.78	0.66
1:C:161:ASN:OD1	1:C:161:ASN:O	2.13	0.65
1:A:166:MET:HE1	1:A:303:ALA:HB2	1.79	0.65
1:A:169:ILE:H	1:A:306:GLN:HE22	1.44	0.65
1:A:122:HIS:NE2	1:A:134:HIS:HE1	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LEU:HD13	1:A:252:ALA:HB2	1.80	0.64
1:D:325:GLY:HA3	1:D:350:HIS:CE1	2.34	0.63
1:C:85:ALA:HB1	1:C:247:LEU:HD12	1.80	0.63
1:C:122:HIS:NE2	1:C:134:HIS:HE1	1.96	0.62
1:B:23:ASP:C	1:B:24:HIS:CD2	2.73	0.62
1:D:349:GLN:HA	1:D:354:MET:CE	2.29	0.62
1:A:162:PRO:HD2	5:A:1438:HOH:O	2.00	0.62
1:C:382:ASP:HA	4:C:1009:PEG:H21	1.80	0.62
1:A:325:GLY:HA3	1:A:350:HIS:NE2	2.16	0.61
1:B:30:PRO:HB2	4:B:1006:PEG:H41	1.83	0.60
1:B:339:VAL:O	1:D:37:THR:HG21	2.01	0.60
1:A:112:THR:O	4:A:1008:PEG:H11	2.01	0.60
1:A:155:TYR:CD1	1:A:184:VAL:HG22	2.36	0.60
1:A:211:LYS:NZ	3:A:1399:PLP:O3	2.35	0.60
1:B:43:VAL:HG21	1:D:326:ARG:HG2	1.83	0.60
1:C:247:LEU:HD13	1:C:252:ALA:HB2	1.83	0.60
1:B:23:ASP:O	1:B:24:HIS:HD2	1.85	0.59
1:A:206:VAL:HG12	1:A:224:VAL:HG22	1.85	0.58
1:D:57:HIS:HE1	1:D:68:ASN:OD1	1.85	0.58
1:A:110:GLY:HA3	4:A:1008:PEG:H22	1.84	0.58
1:A:269:HIS:HE1	5:A:1441:HOH:O	1.85	0.58
1:D:263:ASN:HD22	1:D:263:ASN:N	2.00	0.58
1:B:23:ASP:O	1:B:24:HIS:CD2	2.57	0.58
1:A:325:GLY:HA3	1:A:350:HIS:CD2	2.39	0.58
1:C:160:ALA:C	1:C:162:PRO:HD2	2.23	0.58
1:C:274:GLN:HG2	5:C:1254:HOH:O	2.03	0.57
1:B:211:LYS:CE	3:B:1799:PLP:C4A	2.81	0.57
1:C:166:MET:HE1	1:C:307:MET:SD	2.44	0.57
1:D:269:HIS:HE1	5:D:1691:HOH:O	1.86	0.57
1:C:160:ALA:O	1:C:162:PRO:N	2.38	0.56
1:C:204:LEU:HD23	1:C:226:GLY:HA3	1.87	0.56
1:C:382:ASP:HB2	5:C:1212:HOH:O	2.04	0.56
1:A:211:LYS:NZ	3:A:1399:PLP:C4	2.60	0.56
1:C:300:TYR:CZ	1:C:304:ARG:HD2	2.40	0.56
1:C:161:ASN:O	1:C:161:ASN:CG	2.43	0.56
1:A:144:GLU:OE2	1:A:179:HIS:HE1	1.88	0.56
1:C:112:THR:OG1	1:C:162:PRO:HG3	2.06	0.55
1:C:339:VAL:O	1:C:340:SER:CB	2.53	0.55
1:C:334:LEU:HD13	1:C:386:LEU:HD23	1.89	0.55
1:A:299:GLN:HG2	5:A:1427:HOH:O	2.06	0.54
1:A:39:THR:HG22	1:B:22:GLN:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:LEU:HD13	1:A:386:LEU:HD23	1.90	0.54
1:A:297:PHE:O	4:A:1007:PEG:H21	2.08	0.54
1:A:16:HIS:HD2	5:A:1498:HOH:O	1.90	0.54
1:B:86:LEU:O	1:B:247:LEU:HG	2.08	0.54
1:D:269:HIS:HD2	1:D:378:VAL:O	1.91	0.54
1:B:43:VAL:N	1:D:330:ASN:HD21	1.99	0.53
1:B:285:GLN:NE2	1:B:285:GLN:H	2.06	0.53
1:D:191:THR:HB	1:D:192:PRO:HD2	1.89	0.53
1:D:350:HIS:H	1:D:354:MET:HE3	1.72	0.53
1:A:298:PRO:O	4:A:1007:PEG:H12	2.08	0.53
1:B:24:HIS:HE1	4:B:1006:PEG:H22	1.74	0.53
1:A:144:GLU:OE2	1:A:179:HIS:CE1	2.62	0.53
1:A:191:THR:HB	1:A:192:PRO:HD2	1.90	0.53
1:C:114:TYR:CE2	1:C:116:CYS:HB2	2.44	0.53
1:A:339:VAL:O	1:A:340:SER:CB	2.56	0.53
1:D:350:HIS:H	1:D:354:MET:CE	2.21	0.53
1:A:114:TYR:CE2	1:A:116:CYS:HB2	2.44	0.52
1:A:325:GLY:HA3	1:A:350:HIS:HE2	1.74	0.52
1:A:269:HIS:HD2	1:A:378:VAL:O	1.92	0.52
1:B:195:GLN:HE21	1:B:306:GLN:HB3	1.75	0.51
1:A:16:HIS:HE1	1:D:381:GLU:OE2	1.94	0.51
1:B:366:HIS:ND1	1:B:366:HIS:O	2.43	0.51
1:C:166:MET:HE3	5:C:1244:HOH:O	2.11	0.51
1:B:147:MET:HB3	1:B:179:HIS:CD2	2.47	0.50
1:B:364:ARG:NH1	1:B:371:GLU:OE2	2.44	0.50
1:A:162:PRO:HD2	1:A:163:ASN:H	1.76	0.50
1:C:31:PRO:HG3	1:D:33:TYR:CE2	2.48	0.49
1:B:339:VAL:O	1:B:340:SER:CB	2.60	0.49
1:B:330:ASN:HD21	1:D:43:VAL:N	2.08	0.49
1:C:57:HIS:HE1	1:C:68:ASN:OD1	1.96	0.49
1:C:16:HIS:HD2	5:C:1291:HOH:O	1.95	0.49
1:D:334:LEU:HD13	1:D:386:LEU:HD23	1.93	0.49
1:A:264:LEU:HD22	5:A:1449:HOH:O	2.13	0.48
1:C:160:ALA:O	1:C:162:PRO:CD	2.61	0.48
1:C:383:ILE:CG2	4:C:1009:PEG:H31	2.43	0.48
1:B:349:GLN:HA	1:B:354:MET:HE1	1.96	0.48
1:D:114:TYR:HE2	1:D:116:CYS:HB2	1.79	0.47
1:A:13:ARG:HG2	4:A:1002:PEG:H31	1.96	0.47
1:D:300:TYR:CZ	1:D:304:ARG:HD2	2.49	0.47
1:C:263:ASN:ND2	1:C:264:LEU:HD13	2.29	0.47
1:A:165:HIS:ND1	4:A:1008:PEG:H31	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:HIS:CE1	4:B:1006:PEG:H22	2.50	0.46
1:C:162:PRO:HB2	1:C:163:ASN:OD1	2.15	0.46
1:D:187:ASN:HD21	1:D:195:GLN:HB3	1.79	0.46
1:B:367:TYR:HB2	1:B:369:ILE:HD12	1.97	0.46
1:D:339:VAL:O	1:D:340:SER:HB2	2.15	0.46
1:B:356:HIS:ND1	1:B:356:HIS:N	2.64	0.46
1:A:274:GLN:NE2	1:A:278:GLU:OE2	2.49	0.46
1:A:345:GLU:HG2	1:D:28:LEU:HD11	1.98	0.46
1:A:240:LYS:NZ	5:A:1472:HOH:O	2.45	0.45
1:B:24:HIS:CE1	4:B:1006:PEG:C2	2.92	0.45
1:D:185:VAL:O	1:D:205:VAL:HA	2.17	0.45
1:D:247:LEU:HD13	1:D:252:ALA:HB2	1.98	0.45
1:A:287:GLU:HB2	1:A:319:LYS:HG3	1.96	0.45
1:D:211:LYS:HZ2	3:D:1599:PLP:C4	2.28	0.45
1:D:161:ASN:HB3	1:D:162:PRO:HD3	1.98	0.45
1:B:349:GLN:HA	1:B:354:MET:CE	2.46	0.45
1:B:211:LYS:HZ2	3:B:1799:PLP:C4	2.28	0.45
1:B:350:HIS:H	1:B:354:MET:CE	2.30	0.45
1:C:70:LEU:HD21	1:C:255:LEU:HD23	1.99	0.45
1:D:84:LEU:HD21	1:D:239:LEU:HD12	1.98	0.45
1:C:263:ASN:HD21	1:C:264:LEU:HD13	1.82	0.45
1:B:10:PHE:CZ	1:B:77:LEU:HG	2.52	0.44
1:C:161:ASN:N	1:C:162:PRO:HD2	2.33	0.44
1:A:13:ARG:HG2	4:A:1002:PEG:C3	2.47	0.44
1:B:366:HIS:O	1:B:366:HIS:CG	2.70	0.44
1:C:106:GLU:OE2	1:C:151:THR:OG1	2.34	0.44
1:A:211:LYS:HD2	1:A:341:LEU:HG	1.99	0.44
1:B:62:ILE:HG13	1:B:240:LYS:HG3	1.99	0.44
1:C:166:MET:CE	5:C:1244:HOH:O	2.65	0.44
1:C:382:ASP:HA	4:C:1009:PEG:C2	2.48	0.44
1:A:78:GLU:OE2	1:A:207:HIS:NE2	2.47	0.43
1:A:162:PRO:CD	1:A:163:ASN:H	2.31	0.43
1:D:110:GLY:O	1:D:134:HIS:HD2	2.01	0.43
1:D:114:TYR:CE2	1:D:116:CYS:HB2	2.54	0.43
1:D:195:GLN:HE21	1:D:306:GLN:HG3	1.84	0.43
1:A:211:LYS:NZ	3:A:1399:PLP:C3	2.82	0.43
1:D:194:LEU:HD22	1:D:309:GLN:HB2	2.00	0.43
1:D:339:VAL:O	1:D:340:SER:CB	2.67	0.43
1:B:349:GLN:HG2	5:B:1828:HOH:O	2.18	0.43
1:C:155:TYR:CD1	1:C:184:VAL:HG22	2.54	0.43
1:D:195:GLN:HG3	1:D:306:GLN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:PRO:HB2	1:B:31:PRO:HB2	2.01	0.43
1:A:44:GLU:OE2	1:C:326:ARG:HD3	2.19	0.43
1:B:341:LEU:HD23	2:B:1138:SO4:O2	2.19	0.43
1:A:138:ALA:HB2	1:A:166:MET:O	2.18	0.42
1:B:350:HIS:N	1:B:354:MET:CE	2.82	0.42
1:D:111:ASN:HB2	5:D:1701:HOH:O	2.19	0.42
4:A:1008:PEG:H21	5:A:1431:HOH:O	2.20	0.42
1:B:334:LEU:HD13	1:B:386:LEU:HD23	2.01	0.42
1:A:17:HIS:ND1	4:A:1002:PEG:C4	2.73	0.42
1:A:8:PRO:HG2	4:A:1002:PEG:H32	2.02	0.42
1:B:339:VAL:HB	2:B:1138:SO4:O4	2.20	0.42
1:C:315:ALA:HB1	1:C:373:LEU:HD11	2.00	0.42
1:B:163:ASN:ND2	1:B:290:HIS:NE2	2.67	0.42
1:D:111:ASN:HD22	1:D:134:HIS:HB3	1.85	0.42
1:B:350:HIS:H	1:B:354:MET:HE3	1.84	0.42
1:C:211:LYS:N	1:C:211:LYS:CD	2.83	0.42
1:C:284:PRO:HD2	1:C:285:GLN:NE2	2.35	0.42
1:A:62:ILE:HG13	1:A:240:LYS:HG3	2.01	0.41
1:B:4:SER:O	1:B:5:ASN:C	2.58	0.41
1:B:190:CYS:C	1:B:191:THR:HG23	2.40	0.41
1:A:268:ARG:HD3	5:A:1451:HOH:O	2.20	0.41
1:D:141:GLN:HE21	1:D:141:GLN:HB3	1.65	0.41
1:B:355:THR:HB	1:B:356:HIS:ND1	2.36	0.41
1:C:339:VAL:O	1:C:340:SER:HB2	2.21	0.40
1:D:144:GLU:OE1	1:D:179:HIS:CE1	2.74	0.40
1:A:269:HIS:CE1	1:A:380:LEU:HD21	2.56	0.40
1:B:325:GLY:HA3	1:B:350:HIS:NE2	2.36	0.40
1:C:354:MET:O	1:C:355:THR:C	2.59	0.40
1:C:161:ASN:OD1	1:C:161:ASN:C	2.60	0.40
1:B:354:MET:SD	1:D:43:VAL:HG12	2.61	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	396/398 (100%)	377 (95%)	14 (4%)	5 (1%)	12	27
1	B	396/398 (100%)	362 (91%)	24 (6%)	10 (2%)	5	12
1	C	396/398 (100%)	372 (94%)	18 (4%)	6 (2%)	10	23
1	D	396/398 (100%)	378 (96%)	15 (4%)	3 (1%)	19	40
All	All	1584/1592 (100%)	1489 (94%)	71 (4%)	24 (2%)	10	23

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	162	PRO
1	B	5	ASN
1	C	161	ASN
1	C	162	PRO
1	B	54	GLN
1	B	287	GLU
1	B	360	THR
1	C	49	CYS
1	C	54	GLN
1	C	340	SER
1	D	162	PRO
1	A	211	LYS
1	A	340	SER
1	B	340	SER
1	D	340	SER
1	A	161	ASN
1	B	4	SER
1	C	211	LYS
1	B	57	HIS
1	B	211	LYS
1	D	3	GLY
1	B	162	PRO
1	B	56	GLY

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	307/307 (100%)	280 (91%)	27 (9%)	10	21
1	B	307/307 (100%)	277 (90%)	30 (10%)	8	17
1	C	307/307 (100%)	285 (93%)	22 (7%)	14	31
1	D	307/307 (100%)	278 (91%)	29 (9%)	8	18
All	All	1228/1228 (100%)	1120 (91%)	108 (9%)	10	21

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	22	GLN
1	A	28	LEU
1	A	39	THR
1	A	84	LEU
1	A	133	ARG
1	A	141	GLN
1	A	152	ARG
1	A	161	ASN
1	A	205	VAL
1	A	236	LEU
1	A	239	LEU
1	A	240	LYS
1	A	247	LEU
1	A	264	LEU
1	A	268	ARG
1	A	274	GLN
1	A	280	LEU
1	A	288	LEU
1	A	302	LEU
1	A	304	ARG
1	A	318	LEU
1	A	326	ARG
1	A	334	LEU
1	A	341	LEU
1	A	343	ASP
1	A	358	SER
1	B	7	LEU
1	B	28	LEU
1	B	39	THR

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Mol	Chain	Res	Type
1	B	58	PHE
1	B	77	LEU
1	B	84	LEU
1	B	133	ARG
1	B	135	VAL
1	B	152	ARG
1	B	236	LEU
1	B	239	LEU
1	B	240	LYS
1	B	247	LEU
1	B	264	LEU
1	B	268	ARG
1	B	274	GLN
1	B	276	LEU
1	B	285	GLN
1	B	288	LEU
1	B	302	LEU
1	B	304	ARG
1	B	305	GLN
1	B	334	LEU
1	B	341	LEU
1	B	355	THR
1	B	356	HIS
1	B	357	SER
1	B	359	TYR
1	B	391	GLN
1	B	392	GLN
1	C	1	MET
1	C	6	LYS
1	C	28	LEU
1	C	39	THR
1	C	49	CYS
1	C	77	LEU
1	C	84	LEU
1	C	184	VAL
1	C	205	VAL
1	C	211	LYS
1	C	239	LEU
1	C	247	LEU
1	C	264	LEU
1	C	268	ARG
1	C	280	LEU

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Mol	Chain	Res	Type
1	C	285	GLN
1	C	302	LEU
1	C	304	ARG
1	C	334	LEU
1	C	340	SER
1	C	391	GLN
1	C	392	GLN
1	D	2	HIS
1	D	28	LEU
1	D	37	THR
1	D	53	GLU
1	D	63	SER
1	D	77	LEU
1	D	84	LEU
1	D	106	GLU
1	D	107	VAL
1	D	111	ASN
1	D	177	ARG
1	D	214	SER
1	D	236	LEU
1	D	239	LEU
1	D	240	LYS
1	D	247	LEU
1	D	263	ASN
1	D	264	LEU
1	D	276	LEU
1	D	280	LEU
1	D	285	GLN
1	D	302	LEU
1	D	318	LEU
1	D	334	LEU
1	D	340	SER
1	D	341	LEU
1	D	363	GLU
1	D	383	ILE
1	D	392	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	57	HIS

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Mol	Chain	Res	Type
1	A	134	HIS
1	A	179	HIS
1	A	269	HIS
1	A	290	HIS
1	A	306	GLN
1	B	24	HIS
1	B	134	HIS
1	B	163	ASN
1	B	165	HIS
1	B	179	HIS
1	B	187	ASN
1	B	195	GLN
1	B	269	HIS
1	B	274	GLN
1	B	285	GLN
1	B	309	GLN
1	B	330	ASN
1	C	16	HIS
1	C	24	HIS
1	C	57	HIS
1	C	134	HIS
1	C	141	GLN
1	C	187	ASN
1	C	195	GLN
1	C	274	GLN
1	C	285	GLN
1	C	330	ASN
1	C	356	HIS
1	C	392	GLN
1	D	5	ASN
1	D	57	HIS
1	D	111	ASN
1	D	134	HIS
1	D	141	GLN
1	D	163	ASN
1	D	165	HIS
1	D	179	HIS
1	D	187	ASN
1	D	195	GLN
1	D	263	ASN
1	D	269	HIS
1	D	285	GLN

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Mol	Chain	Res	Type
1	D	330	ASN
1	D	356	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

19 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	$\# Z > 2$
4	PEG	B	1006	-	6,6,6	0.66	0	5,5,5	0.68	0
4	PEG	A	1004	-	6,6,6	0.52	0	5,5,5	0.71	0
3	PLP	B	1799	1	15,15,16	1.92	4 (26%)	20,22,23	1.93	7 (35%)
4	PEG	A	1001	-	6,6,6	0.64	0	5,5,5	0.61	0
4	PEG	A	1008	-	6,6,6	0.49	0	5,5,5	0.68	0
2	SO4	D	1147	-	4,4,4	0.24	0	6,6,6	0.38	0
4	PEG	C	1012	-	6,6,6	0.66	0	5,5,5	0.50	0
4	PEG	A	1002	-	6,6,6	0.84	0	5,5,5	1.17	1 (20%)
4	PEG	A	1003	-	6,6,6	0.59	0	5,5,5	0.30	0
4	PEG	A	1007	-	6,6,6	0.95	0	5,5,5	0.99	0
4	PEG	C	1009	-	6,6,6	0.54	0	5,5,5	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	1138	-	4,4,4	0.29	0	6,6,6	0.31	0
3	PLP	C	1199	1	15,15,16	2.00	4 (26%)	20,22,23	1.96	5 (25%)
4	PEG	B	1010	-	6,6,6	0.66	0	5,5,5	0.52	0
4	PEG	A	1005	-	6,6,6	0.53	0	5,5,5	0.21	0
3	PLP	A	1399	1	15,15,16	1.91	4 (26%)	20,22,23	1.37	2 (10%)
2	SO4	C	1146	-	4,4,4	0.18	0	6,6,6	0.33	0
3	PLP	D	1599	1	15,15,16	1.82	2 (13%)	20,22,23	1.59	4 (20%)
2	SO4	A	1124	-	4,4,4	0.35	0	6,6,6	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	B	1006	-	-	2/4/4/4	-
4	PEG	A	1004	-	-	2/4/4/4	-
3	PLP	B	1799	1	-	0/6/6/8	0/1/1/1
4	PEG	A	1001	-	-	1/4/4/4	-
4	PEG	A	1008	-	-	3/4/4/4	-
4	PEG	A	1005	-	-	2/4/4/4	-
4	PEG	C	1012	-	-	0/4/4/4	-
4	PEG	A	1002	-	-	4/4/4/4	-
4	PEG	A	1007	-	-	2/4/4/4	-
4	PEG	C	1009	-	-	2/4/4/4	-
3	PLP	C	1199	1	-	0/6/6/8	0/1/1/1
4	PEG	B	1010	-	-	4/4/4/4	-
3	PLP	A	1399	1	-	0/6/6/8	0/1/1/1
4	PEG	A	1003	-	-	2/4/4/4	-
3	PLP	D	1599	1	-	0/6/6/8	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1799	PLP	O3-C3	-5.70	1.23	1.37
3	D	1599	PLP	O3-C3	-5.63	1.23	1.37
3	C	1199	PLP	O3-C3	-5.58	1.24	1.37
3	A	1399	PLP	O3-C3	-5.38	1.24	1.37
3	D	1599	PLP	C6-N1	2.85	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1199	PLP	P-O2P	-2.82	1.44	1.54
3	B	1799	PLP	C2-N1	2.81	1.39	1.33
3	B	1799	PLP	C6-N1	2.58	1.39	1.34
3	A	1399	PLP	C2-N1	2.58	1.38	1.33
3	A	1399	PLP	C6-N1	2.57	1.39	1.34
3	C	1199	PLP	C2-N1	2.43	1.38	1.33
3	C	1199	PLP	C6-N1	2.27	1.39	1.34
3	B	1799	PLP	P-O3P	-2.07	1.46	1.54
3	A	1399	PLP	P-O3P	-2.05	1.47	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1799	PLP	O4P-C5A-C5	5.39	119.63	109.35
3	C	1199	PLP	C4A-C4-C5	-4.97	115.81	120.94
3	C	1199	PLP	O4P-C5A-C5	3.74	116.48	109.35
3	A	1399	PLP	O4P-C5A-C5	3.49	115.99	109.35
3	B	1799	PLP	C4A-C4-C5	-3.42	117.41	120.94
3	D	1599	PLP	C4A-C4-C5	-3.15	117.69	120.94
3	D	1599	PLP	C2A-C2-C3	2.61	124.12	120.89
3	A	1399	PLP	C4A-C4-C5	-2.54	118.32	120.94
3	D	1599	PLP	O4P-C5A-C5	2.50	114.11	109.35
3	B	1799	PLP	O3P-P-O2P	2.36	116.65	107.64
3	C	1199	PLP	O2P-P-O4P	-2.34	100.50	106.73
4	A	1002	PEG	O2-C3-C4	2.31	120.21	110.07
3	D	1599	PLP	C3-C4-C5	2.26	121.18	118.74
3	B	1799	PLP	C6-C5-C4	2.19	119.88	118.16
3	B	1799	PLP	C5-C6-N1	-2.13	120.28	123.82
3	B	1799	PLP	O4P-P-O1P	-2.11	100.56	106.47
3	B	1799	PLP	O3P-P-O4P	-2.10	101.15	106.73
3	C	1199	PLP	O4P-P-O1P	-2.07	100.67	106.47
3	C	1199	PLP	C3-C4-C5	2.03	120.93	118.74

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1009	PEG	O2-C3-C4-O4
4	B	1010	PEG	O1-C1-C2-O2
4	A	1008	PEG	O2-C3-C4-O4
4	A	1002	PEG	O1-C1-C2-O2
4	B	1006	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	1001	PEG	O2-C3-C4-O4
4	A	1002	PEG	O2-C3-C4-O4
4	C	1009	PEG	O1-C1-C2-O2
4	A	1005	PEG	O1-C1-C2-O2
4	A	1008	PEG	O1-C1-C2-O2
4	A	1003	PEG	O2-C3-C4-O4
4	B	1010	PEG	O2-C3-C4-O4
4	A	1004	PEG	O2-C3-C4-O4
4	B	1006	PEG	O2-C3-C4-O4
4	A	1003	PEG	C4-C3-O2-C2
4	A	1004	PEG	C4-C3-O2-C2
4	B	1010	PEG	C4-C3-O2-C2
4	A	1002	PEG	C1-C2-O2-C3
4	A	1007	PEG	O2-C3-C4-O4
4	A	1007	PEG	C4-C3-O2-C2
4	B	1010	PEG	C1-C2-O2-C3
4	A	1008	PEG	C4-C3-O2-C2
4	A	1005	PEG	C1-C2-O2-C3
4	A	1002	PEG	C4-C3-O2-C2

There are no ring outliers.

10 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1006	PEG	7	0
3	B	1799	PLP	4	0
4	A	1008	PEG	5	0
4	A	1002	PEG	5	0
4	A	1007	PEG	2	0
4	C	1009	PEG	3	0
2	B	1138	SO4	2	0
3	C	1199	PLP	2	0
3	A	1399	PLP	7	0
3	D	1599	PLP	4	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	398/398 (100%)	-0.49	20 (5%) 28 26	17, 31, 78, 89	0
1	B	398/398 (100%)	-0.24	18 (4%) 33 31	21, 42, 81, 98	0
1	C	398/398 (100%)	-0.41	18 (4%) 33 31	22, 35, 72, 104	0
1	D	398/398 (100%)	-0.52	14 (3%) 44 43	21, 32, 69, 98	0
All	All	1592/1592 (100%)	-0.41	70 (4%) 34 32	17, 35, 74, 104	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	10.1
1	C	3	GLY	8.5
1	C	2	HIS	8.5
1	D	4	SER	8.4
1	B	2	HIS	8.3
1	B	1	MET	7.9
1	C	4	SER	7.6
1	B	5	ASN	7.3
1	B	3	GLY	7.2
1	D	2	HIS	7.1
1	C	5	ASN	7.0
1	A	1	MET	6.2
1	D	1	MET	6.2
1	A	55	ALA	5.9
1	D	5	ASN	5.9
1	B	4	SER	5.3
1	B	55	ALA	5.1
1	C	55	ALA	4.9
1	D	358	SER	4.8
1	B	366	HIS	4.7
1	B	54	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	55	ALA	4.5
1	A	362	GLU	4.5
1	B	362	GLU	4.4
1	C	368	GLY	4.3
1	A	51	ALA	4.2
1	D	6	LYS	3.9
1	B	359	TYR	3.9
1	D	3	GLY	3.8
1	C	366	HIS	3.7
1	B	53	GLU	3.7
1	B	6	LYS	3.7
1	D	51	ALA	3.7
1	C	51	ALA	3.7
1	B	367	TYR	3.6
1	D	53	GLU	3.6
1	C	6	LYS	3.6
1	A	44	GLU	3.4
1	A	53	GLU	3.4
1	A	2	HIS	3.4
1	D	52	GLY	3.4
1	A	56	GLY	3.3
1	B	365	ALA	3.3
1	A	52	GLY	3.2
1	C	54	GLN	3.2
1	A	363	GLU	3.1
1	C	367	TYR	3.1
1	C	365	ALA	3.1
1	A	358	SER	3.0
1	A	366	HIS	2.9
1	A	367	TYR	2.8
1	B	51	ALA	2.7
1	D	367	TYR	2.7
1	C	48	ALA	2.6
1	D	359	TYR	2.6
1	B	358	SER	2.6
1	A	50	PHE	2.5
1	A	365	ALA	2.5
1	D	362	GLU	2.4
1	A	359	TYR	2.3
1	B	284	PRO	2.3
1	C	360	THR	2.3
1	B	287	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	161	ASN	2.2
1	A	48	ALA	2.2
1	A	360	THR	2.2
1	C	53	GLU	2.2
1	A	49	CYS	2.1
1	A	45	TYR	2.1
1	C	52	GLY	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 carbohydrates 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
4	PEG	A	1005	7/7	0.47	0.54	89,91,93,93	0
4	PEG	A	1003	7/7	0.51	0.42	70,74,77,77	0
4	PEG	A	1004	7/7	0.56	0.42	82,84,85,85	0
4	PEG	C	1012	7/7	0.56	0.36	70,71,72,72	0
4	PEG	A	1001	7/7	0.71	0.32	65,67,68,68	0
4	PEG	A	1007	7/7	0.76	0.34	60,65,67,67	0
4	PEG	B	1006	7/7	0.77	0.25	53,56,61,61	0
4	PEG	B	1010	7/7	0.79	0.32	54,57,64,65	0
4	PEG	A	1002	7/7	0.85	0.26	40,42,45,47	0
4	PEG	C	1009	7/7	0.86	0.38	68,70,71,71	0
4	PEG	A	1008	7/7	0.88	0.25	38,42,45,46	0
2	SO4	B	1138	5/5	0.96	0.16	30,30,32,33	5
2	SO4	D	1147	5/5	0.97	0.17	24,24,25,26	5
2	SO4	C	1146	5/5	0.97	0.13	23,23,26,26	5
3	PLP	C	1199	15/16	0.98	0.10	22,29,35,38	0
3	PLP	D	1599	15/16	0.98	0.09	21,26,29,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	A	1124	5/5	0.98	0.27	2,4,5,6	5
3	PLP	A	1399	15/16	0.99	0.07	19,22,26,27	0
3	PLP	B	1799	15/16	0.99	0.10	31,34,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.