



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:45 PM UTC

PDB ID : 3ACZ / pdb_00003acz
Title : Crystal structure of Entamoeba histolytica methionine gamma-lyase 1
Authors : Karaki, T.; Sato, D.; Shimizu, A.; Nozaki, T.; Harada, S.
Deposited on : 2010-01-13
Resolution : 1.97 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

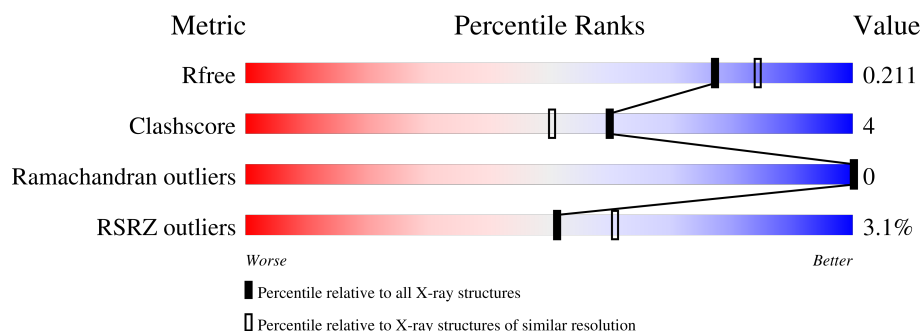
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	389	3% 91% 9% .
1	B	389	3% 91% 8% ..
1	C	389	3% 88% 11% .
1	D	389	3% 88% 10% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12951 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.

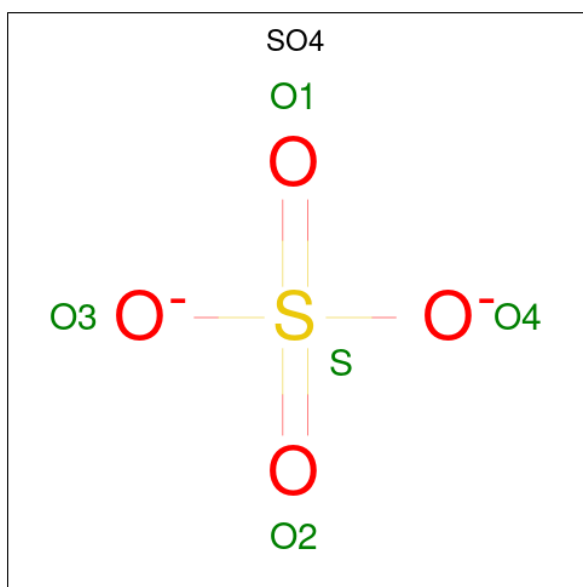
- Molecule 1 is a protein called Methionine gamma-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	P	S	0	3	0
			2975	1892	498	558	1	26			
1	B	386	Total	C	N	O	P	S	0	3	0
			2960	1881	496	556	1	26			
1	C	387	Total	C	N	O	P	S	0	5	0
			2987	1900	499	561	1	26			
1	D	384	Total	C	N	O	P	S	0	4	0
			2952	1877	494	554	1	26			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	308	LEU	SER	SEE REMARK 999	UNP Q86D28
B	808	LEU	SER	SEE REMARK 999	UNP Q86D28
C	1308	LEU	SER	SEE REMARK 999	UNP Q86D28
D	1808	LEU	SER	SEE REMARK 999	UNP Q86D28

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

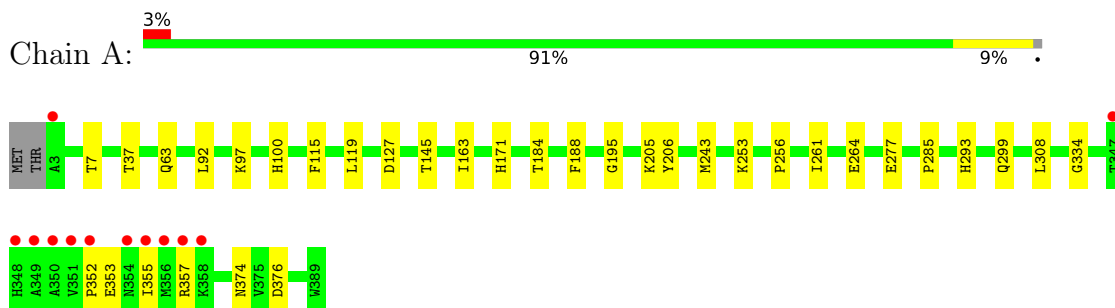
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	320	Total	O	0	0
			320	320		
4	B	197	Total	O	0	0
			197	197		
4	C	317	Total	O	0	0
			317	317		
4	D	171	Total	O	0	0
			171	171		

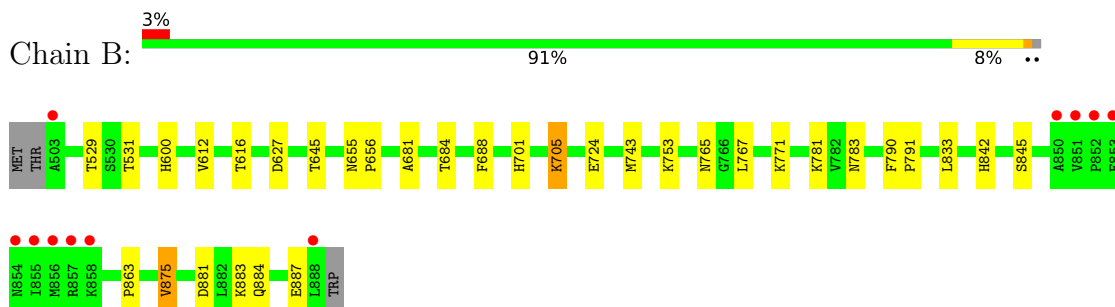
3 Residue-property plots [i](#)

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.

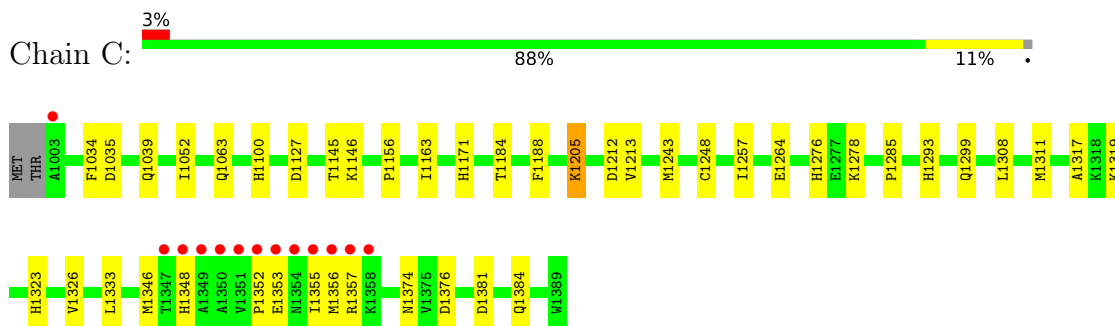
- Molecule 1: Methionine gamma-lyase



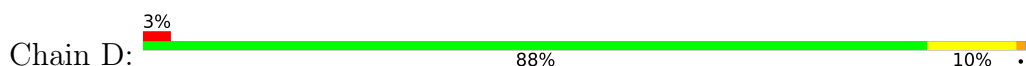
- Molecule 1: Methionine gamma-lyase

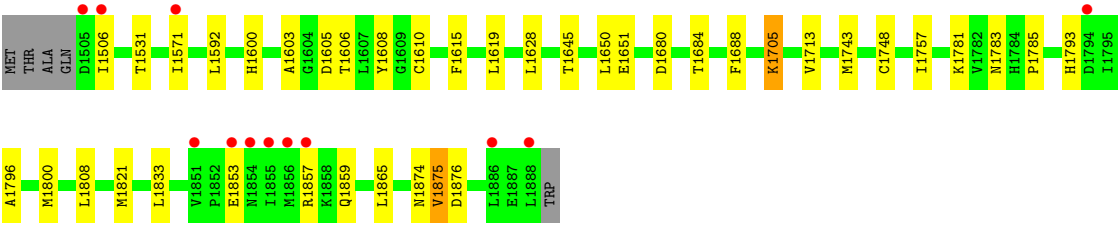


- Molecule 1: Methionine gamma-lyase



- Molecule 1: Methionine gamma-lyase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.28Å 85.34Å 114.62Å 90.00° 101.96° 90.00°	Depositor
Resolution (Å)	39.06 – 1.97 39.06 – 1.97	Depositor EDS
% Data completeness (in resolution range)	97.3 (39.06-1.97) 97.5 (39.06-1.97)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 1.97Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.156 , 0.190 (Not available) , 0.211	Depositor DCC
R_{free} test set	6498 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12951	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: LLP, SO4, GOL

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	0.92	0/3022	0.90	0/4084
1	B	0.79	0/3005	0.87	1/4061 (0.0%)
1	C	0.95	1/3040 (0.0%)	0.88	2/4108 (0.0%)
1	D	0.76	0/3000	0.88	1/4054 (0.0%)
All	All	0.86	1/12067 (0.0%)	0.89	4/16307 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1346	MET	CA-C	9.54	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	875	VAL	CB-CA-C	-7.97	100.41	112.05
1	D	1875	VAL	CB-CA-C	-7.85	101.54	112.14
1	C	1052	ILE	CB-CA-C	-5.65	106.02	111.05
1	C	1326	VAL	N-CA-C	-5.51	106.43	111.67

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	2975	0	2974	26	0
1	B	2960	0	2964	27	0
1	C	2987	0	2988	32	0
1	D	2952	0	2959	30	0
2	A	15	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	6	0	8	0	0
3	C	6	0	8	0	0
4	A	320	0	0	4	0
4	B	197	0	0	1	0
4	C	317	0	0	8	0
4	D	171	0	0	3	0
All	All	12951	0	11901	103	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 4.

All (103) 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:352:PRO:HG2	1:A:355:ILE:HD12	1.57	0.87
1:C:1276:HIS:HD2	1:C:1278:LYS:H	1.30	0.80
1:A:261:ILE:HD11	1:C:1257:ILE:HG12	1.69	0.76
1:C:1352:PRO:HG2	1:C:1355:ILE:HD12	1.68	0.76
1:A:92:LEU:HD21	1:A:119:LEU:HD22	1.68	0.74
1:A:353:GLU:HB3	1:A:357:ARG:HH21	1.52	0.73
1:D:1781:LYS:HE3	1:D:1783:ASN:HD21	1.56	0.70
1:B:842:HIS:HE1	1:B:863:PRO:O	1.76	0.69
1:D:1600:HIS:HD2	1:D:1645:THR:OG1	1.77	0.68
1:B:600:HIS:HD2	1:B:645:THR:OG1	1.76	0.68
1:C:1035:ASP:H	1:C:1039:GLN:NE2	1.92	0.67
1:A:285:PRO:O	1:A:293:HIS:HD2	1.80	0.65
1:B:781:LYS:HD3	1:B:783:ASN:HD21	1.61	0.64
1:D:1592:LEU:HD21	1:D:1619:LEU:HD22	1.81	0.63
1:C:1100:HIS:HD2	1:C:1145:THR:OG1	1.80	0.63
1:C:1063[A]:GLN:HG2	4:C:3564:HOH:O	1.99	0.61
1:B:600:HIS:HE1	1:B:627:ASP:OD2	1.82	0.61
1:D:1705:LLP:HD3	1:D:1833:LEU:HG	1.83	0.61
1:A:100:HIS:HD2	1:A:145:THR:OG1	1.84	0.60
1:B:781:LYS:HD3	1:B:783:ASN:ND2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1243:MET:CE	1:D:1743:MET:HE1	2.31	0.60
1:A:264:GLU:HG3	4:A:3675:HOH:O	2.02	0.60
1:D:1874:ASN:HD21	1:D:1876:ASP:HB2	1.67	0.59
1:C:1100:HIS:HE1	1:C:1127:ASP:OD2	1.85	0.59
1:C:1276:HIS:CD2	1:C:1278:LYS:H	2.15	0.58
1:D:1684:THR:HG22	1:D:1688:PHE:HB2	1.86	0.58
1:C:1319:LYS:O	1:C:1323:HIS:HD2	1.88	0.56
1:A:63:GLN:HG2	4:A:3343:HOH:O	2.04	0.56
1:B:765:ASN:ND2	1:B:875:VAL:HG22	2.21	0.55
1:C:1285:PRO:O	1:C:1293:HIS:HD2	1.90	0.55
1:D:1875:VAL:HG22	4:D:3269:HOH:O	2.06	0.55
1:D:1781:LYS:CE	1:D:1783:ASN:HD21	2.20	0.53
1:A:243:MET:HE3	1:B:743:MET:HE1	1.90	0.53
1:D:1606:THR:HG22	1:D:1859:GLN:HG2	1.89	0.53
1:A:100:HIS:HE1	1:A:127:ASP:OD2	1.93	0.52
1:B:883:LYS:O	1:B:887:GLU:HG3	2.09	0.52
1:D:1651:GLU:HG3	1:D:1680:ASP:HB3	1.90	0.52
1:C:1308:LEU:HB3	4:C:3348:HOH:O	2.10	0.52
1:A:243:MET:CE	1:B:743:MET:HE1	2.40	0.52
1:C:1205:LLP:HD3	1:C:1333:LEU:HG	1.90	0.52
1:C:1243:MET:CE	1:D:1743:MET:CE	2.88	0.52
1:A:261:ILE:CD1	1:C:1257:ILE:HG12	2.40	0.51
1:C:1264:GLU:HG3	4:C:3850:HOH:O	2.10	0.51
4:A:3182:HOH:O	1:D:1531:THR:HG22	2.11	0.50
1:C:1146:LYS:HE3	4:C:3317:HOH:O	2.11	0.50
1:B:743:MET:HE3	1:C:1243:MET:HE3	1.93	0.49
1:A:184:THR:HG22	1:A:188:PHE:HB2	1.94	0.49
1:D:1608:TYR:HE2	1:D:1610:CYS:HB2	1.78	0.49
1:C:1034:PHE:HA	1:C:1039:GLN:HE22	1.77	0.49
1:C:1163:ILE:H	1:C:1299:GLN:HE22	1.60	0.49
1:A:243:MET:HE3	1:B:743:MET:CE	2.43	0.49
1:C:1374:ASN:HD21	1:C:1376:ASP:HB2	1.78	0.49
1:D:1874:ASN:ND2	1:D:1876:ASP:HB2	2.28	0.48
1:A:206:TYR:CE2	1:A:334:GLY:HA2	2.49	0.48
1:C:1184:THR:HG22	1:C:1188:PHE:HB2	1.96	0.48
1:C:1243:MET:HE1	1:D:1743:MET:CE	2.43	0.48
1:B:705:LLP:HD3	1:B:833:LEU:HG	1.95	0.48
1:A:308:LEU:HB3	4:A:3314:HOH:O	2.13	0.48
1:B:881:ASP:O	1:B:884:GLN:HB3	2.13	0.48
1:A:171:HIS:HE1	1:A:195:GLY:O	1.96	0.47
1:D:1650:LEU:HA	4:D:3368:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1615:PHE:HA	1:D:1619:LEU:HG	1.96	0.47
1:D:1757:ILE:HD12	4:D:3208:HOH:O	2.15	0.47
1:A:7:THR:HG22	1:A:256:PRO:HB2	1.97	0.47
1:D:1605:ASP:OD2	1:D:1606:THR:HG23	2.14	0.47
1:B:842:HIS:HD2	1:B:845:SER:OG	1.98	0.47
1:A:37:THR:HG21	1:D:1821:MET:HE3	1.98	0.46
1:B:684:THR:HG22	1:B:688:PHE:HB2	1.97	0.46
1:D:1506:ILE:HG23	1:D:1571:ILE:HD12	1.97	0.46
1:C:1353:GLU:O	1:C:1357:ARG:HG3	2.16	0.46
1:D:1796:ALA:HB1	1:D:1800:MET:HE2	1.97	0.46
1:D:1608:TYR:CE2	1:D:1610:CYS:HB2	2.51	0.45
1:B:681:ALA:HB3	1:B:701:HIS:CE1	2.51	0.45
1:C:1171:HIS:HD2	4:C:3041:HOH:O	1.98	0.45
1:B:705:LLP:O3	1:B:705:LLP:NZ	2.49	0.45
1:D:1785:PRO:O	1:D:1793:HIS:HD2	2.00	0.45
1:B:531:THR:HG22	4:C:3101:HOH:O	2.17	0.45
1:B:600:HIS:CE1	1:B:627:ASP:OD2	2.68	0.45
1:B:612:VAL:O	1:B:616:THR:HB	2.17	0.44
1:C:1311:MET:HG3	1:C:1317:ALA:HA	2.00	0.44
1:A:374:ASN:HD21	1:A:376:ASP:HB2	1.82	0.44
1:A:277:GLU:O	1:A:277:GLU:HG2	2.18	0.43
1:B:753:LYS:NZ	4:B:3848:HOH:O	2.46	0.43
1:D:1713:VAL:HG11	1:D:1748:CYS:SG	2.59	0.43
1:A:115:PHE:HA	1:A:119:LEU:HG	2.01	0.43
1:B:790:PHE:HA	1:B:791:PRO:HD3	1.91	0.43
1:D:1603:ALA:HB3	1:D:1628:LEU:HD22	2.00	0.43
1:D:1808:LEU:HD21	1:D:1865:LEU:HD22	2.01	0.42
1:D:1705:LLP:O3	1:D:1705:LLP:NZ	2.50	0.42
1:D:1853:GLU:HG3	1:D:1857:ARG:HH21	1.85	0.42
1:C:1348:HIS:CD2	4:C:3772:HOH:O	2.72	0.42
1:A:163:ILE:H	1:A:299:GLN:HE22	1.68	0.41
1:C:1213:VAL:HG11	1:C:1248:CYS:SG	2.60	0.41
1:A:243:MET:CE	1:B:743:MET:CE	2.98	0.41
1:B:529:THR:HA	1:C:1212:ASP:HA	2.02	0.41
1:C:1381:ASP:O	1:C:1384:GLN:HG3	2.20	0.41
1:B:767:LEU:O	1:B:771:LYS:HG3	2.20	0.41
1:C:1156:PRO:HD3	1:C:1348:HIS:NE2	2.35	0.41
1:B:655:ASN:HA	1:B:656:PRO:HA	1.83	0.41
1:A:253:LYS:HE3	4:C:3551:HOH:O	2.21	0.41
1:B:724:GLU:H	1:B:724:GLU:CD	2.30	0.40
1:C:1353:GLU:HA	1:C:1356:MET:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LYS:HE2	1:A:97:LYS:HB3	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/389 (100%)	377 (97%)	10 (3%)	0	100	100
1	B	386/389 (99%)	376 (97%)	10 (3%)	0	100	100
1	C	389/389 (100%)	381 (98%)	8 (2%)	0	100	100
1	D	385/389 (99%)	380 (99%)	5 (1%)	0	100	100
All	All	1547/1556 (99%)	1514 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

4 non-standard protein/DNA/RNA residues 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
1	LLP	C	1205	1	23,24,25	1.85	6 (26%)	25,32,34	1.62	5 (20%)
1	LLP	D	1705	1	23,24,25	2.01	5 (21%)	25,32,34	1.80	5 (20%)
1	LLP	A	205	1	23,24,25	1.95	6 (26%)	25,32,34	1.56	4 (16%)
1	LLP	B	705	1	23,24,25	2.17	7 (30%)	25,32,34	1.97	8 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	C	1205	1	-	2/16/17/19	0/1/1/1
1	LLP	D	1705	1	-	4/16/17/19	0/1/1/1
1	LLP	A	205	1	-	5/16/17/19	0/1/1/1
1	LLP	B	705	1	-	4/16/17/19	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	705	LLP	O3-C3	-6.14	1.22	1.36
1	A	205	LLP	O3-C3	-5.95	1.23	1.36
1	D	1705	LLP	O3-C3	-5.53	1.24	1.36
1	C	1205	LLP	O3-C3	-4.81	1.25	1.36
1	D	1705	LLP	C6-N1	3.83	1.42	1.34
1	B	705	LLP	CE-NZ	3.76	1.55	1.46
1	C	1205	LLP	CE-NZ	3.32	1.54	1.46
1	C	1205	LLP	C2-N1	3.16	1.39	1.33
1	B	705	LLP	C4'-NZ	3.14	1.37	1.27
1	D	1705	LLP	C4'-NZ	3.02	1.37	1.27
1	A	205	LLP	C6-N1	3.01	1.40	1.34
1	D	1705	LLP	CE-NZ	2.92	1.53	1.46
1	B	705	LLP	C6-N1	2.79	1.40	1.34
1	D	1705	LLP	C4-C4'	2.77	1.52	1.46
1	C	1205	LLP	C4'-NZ	2.75	1.36	1.27
1	B	705	LLP	C4-C4'	2.70	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	LLP	C2-N1	2.63	1.38	1.33
1	C	1205	LLP	C4-C4'	2.52	1.52	1.46
1	A	205	LLP	C4'-NZ	2.47	1.35	1.27
1	A	205	LLP	CE-NZ	2.37	1.52	1.46
1	B	705	LLP	C2'-C2	2.29	1.54	1.50
1	B	705	LLP	CD-CE	2.15	1.58	1.51
1	A	205	LLP	CD-CE	2.14	1.58	1.51
1	C	1205	LLP	C6-N1	2.11	1.38	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	705	LLP	OP4-C5'-C5	5.48	119.63	109.36
1	C	1205	LLP	OP4-C5'-C5	5.38	119.44	109.36
1	D	1705	LLP	OP4-C5'-C5	5.35	119.39	109.36
1	A	205	LLP	OP4-C5'-C5	4.14	117.11	109.36
1	B	705	LLP	C4-C3-C2	3.99	122.39	120.14
1	B	705	LLP	CD-CE-NZ	3.76	120.78	110.83
1	A	205	LLP	CD-CE-NZ	3.64	120.45	110.83
1	D	1705	LLP	C4-C3-C2	3.62	122.18	120.14
1	D	1705	LLP	C4-C4'-NZ	-2.95	110.44	124.04
1	A	205	LLP	C4-C3-C2	2.66	121.64	120.14
1	C	1205	LLP	CD-CE-NZ	2.52	117.50	110.83
1	A	205	LLP	C4-C4'-NZ	-2.51	112.44	124.04
1	D	1705	LLP	CD-CE-NZ	2.35	117.04	110.83
1	B	705	LLP	C3-C2-N1	-2.34	118.01	120.96
1	C	1205	LLP	OP4-P-OP1	-2.33	100.16	106.44
1	B	705	LLP	C4-C4'-NZ	-2.21	113.86	124.04
1	B	705	LLP	OP4-P-OP1	-2.19	100.52	106.44
1	C	1205	LLP	C5-C6-N1	-2.18	120.28	123.83
1	B	705	LLP	C5-C6-N1	-2.16	120.32	123.83
1	C	1205	LLP	C4-C4'-NZ	-2.15	114.14	124.04
1	D	1705	LLP	C3-C2-N1	-2.13	118.27	120.96
1	B	705	LLP	C2'-C2-N1	2.12	121.64	117.64

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	205	LLP	O-C-CA-CB
1	B	705	LLP	C4-C4'-NZ-CE
1	B	705	LLP	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	C	1205	LLP	O-C-CA-CB
1	D	1705	LLP	C4-C4'-NZ-CE
1	D	1705	LLP	O-C-CA-CB
1	A	205	LLP	C4-C4'-NZ-CE
1	C	1205	LLP	C4-C4'-NZ-CE
1	A	205	LLP	CG-CD-CE-NZ
1	A	205	LLP	CA-CB-CG-CD
1	A	205	LLP	C3-C4-C4'-NZ
1	D	1705	LLP	C3-C4-C4'-NZ
1	B	705	LLP	C3-C4-C4'-NZ
1	B	705	LLP	N-CA-CB-CG
1	D	1705	LLP	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	1205	LLP	1	0
1	D	1705	LLP	2	0
1	B	705	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	2003	-	4,4,4	0.22	0	6,6,6	0.21	0
2	SO4	A	2011	-	4,4,4	0.30	0	6,6,6	0.11	0
2	SO4	D	2008	-	4,4,4	0.23	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	2007	-	4,4,4	0.44	0	6,6,6	0.73	0
2	SO4	C	2009	-	4,4,4	0.23	0	6,6,6	0.25	0
2	SO4	D	2010	-	4,4,4	0.24	0	6,6,6	0.48	0
2	SO4	B	2006	-	4,4,4	0.23	0	6,6,6	0.14	0
3	GOL	C	2014	-	5,5,5	0.39	0	5,5,5	0.38	0
2	SO4	B	2004	-	4,4,4	0.23	0	6,6,6	0.53	0
2	SO4	D	2012	-	4,4,4	0.24	0	6,6,6	0.24	0
2	SO4	A	2001	-	4,4,4	0.41	0	6,6,6	0.99	0
2	SO4	B	2005	-	4,4,4	0.26	0	6,6,6	0.16	0
2	SO4	C	2002	-	4,4,4	0.24	0	6,6,6	0.20	0
3	GOL	A	2013	-	5,5,5	0.43	0	5,5,5	0.27	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
3	GOL	C	2014	-	-	0/4/4/4	-
3	GOL	A	2013	-	-	0/4/4/4	-

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	386/389 (99%)	-0.19	12 (3%)	51	61	12, 19, 38, 65	4 (1%)
1	B	385/389 (98%)	0.02	11 (2%)	53	63	13, 29, 52, 76	4 (1%)
1	C	386/389 (99%)	-0.15	13 (3%)	48	58	11, 19, 37, 67	5 (1%)
1	D	383/389 (98%)	0.11	12 (3%)	51	61	12, 32, 56, 75	4 (1%)
All	All	1540/1556 (98%)	-0.05	48 (3%)	51	61	11, 23, 51, 76	17 (1%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1351	VAL	6.6
1	C	1355	ILE	5.8
1	B	888	LEU	5.6
1	A	355	ILE	5.3
1	C	1350	ALA	5.3
1	A	351	VAL	5.2
1	A	352	PRO	5.1
1	C	1352	PRO	4.6
1	C	1354	ASN	4.5
1	D	1888	LEU	4.3
1	A	348	HIS	4.1
1	C	1349	ALA	4.0
1	A	354	ASN	4.0
1	C	1348	HIS	4.0
1	B	503	ALA	3.6
1	A	350	ALA	3.6
1	D	1855	ILE	3.5
1	A	358	LYS	3.5
1	B	856	MET	3.4
1	A	3	ALA	3.3
1	D	1851	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	855	ILE	3.1
1	A	349	ALA	3.1
1	A	356	MET	3.0
1	C	1356	MET	3.0
1	D	1854	ASN	2.8
1	C	1358	LYS	2.6
1	C	1357	ARG	2.6
1	D	1856	MET	2.6
1	D	1505	ASP	2.5
1	B	858	LYS	2.5
1	C	1353	GLU	2.5
1	B	852	PRO	2.5
1	D	1794	ASP	2.5
1	C	1347	THR	2.4
1	B	854	ASN	2.4
1	B	853	GLU	2.3
1	D	1886	LEU	2.3
1	C	1003	ALA	2.3
1	A	347	THR	2.2
1	B	857	ARG	2.2
1	D	1857	ARG	2.2
1	A	357	ARG	2.1
1	D	1506	ILE	2.1
1	B	851	VAL	2.1
1	D	1853	GLU	2.1
1	D	1571	ILE	2.0
1	B	850	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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($\text{\AA}^2$)	Q<0.9
1	LLP	B	705	24/25	0.95	0.10	15,21,26,29	10
1	LLP	D	1705	24/25	0.95	0.10	17,23,28,29	10
1	LLP	C	1205	24/25	0.97	0.06	14,18,20,21	6
1	LLP	A	205	24/25	0.97	0.07	14,17,20,20	6

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($\text{\AA}^2$)	Q<0.9
2	SO4	A	2011	5/5	0.74	0.27	110,110,111,111	0
2	SO4	B	2005	5/5	0.76	0.23	104,104,104,104	0
2	SO4	C	2002	5/5	0.77	0.22	90,90,91,91	0
2	SO4	D	2008	5/5	0.77	0.24	106,106,106,106	0
2	SO4	B	2006	5/5	0.82	0.11	73,73,74,74	0
2	SO4	D	2012	5/5	0.83	0.11	73,73,73,74	0
3	GOL	A	2013	6/6	0.84	0.14	45,47,48,49	0
2	SO4	C	2009	5/5	0.87	0.11	61,61,62,63	0
2	SO4	A	2003	5/5	0.89	0.10	62,63,63,64	0
2	SO4	B	2004	5/5	0.90	0.18	46,47,49,52	0
3	GOL	C	2014	6/6	0.91	0.11	40,45,46,48	0
2	SO4	D	2010	5/5	0.92	0.15	44,46,47,50	0
2	SO4	C	2007	5/5	0.95	0.12	30,32,35,40	0
2	SO4	A	2001	5/5	0.96	0.10	28,31,33,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.