



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 02:56 AM EDT

PDB ID : 3BM5
Title : Crystal structure of O-acetyl-serine sulfhydrylase from *Entamoeba histolytica* in complex with cysteine
Authors : Krishna, C.; Kumar, M.; Kumar, S.; Gourinath, S.
Deposited on : 2007-12-12
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

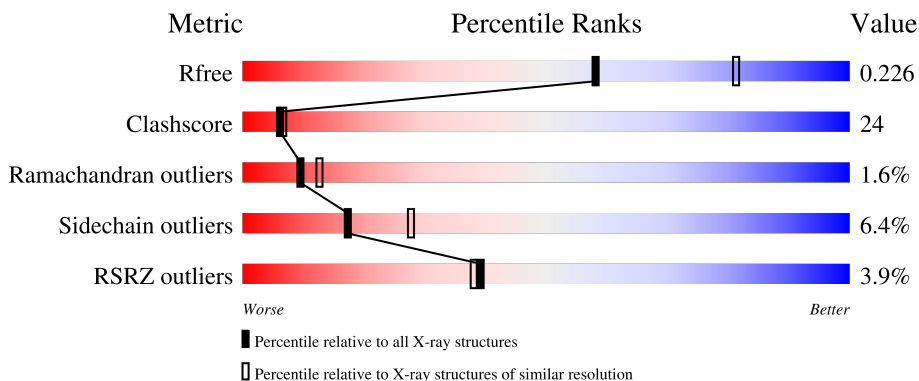
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	338	 68% 28%
1	B	338	 7% 60% 33%

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
4	CYS	B	402	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5442 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 Cysteine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	338	2578	1636	437	491	14	0	0	0
1	B	335	2533	1608	427	484	14	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

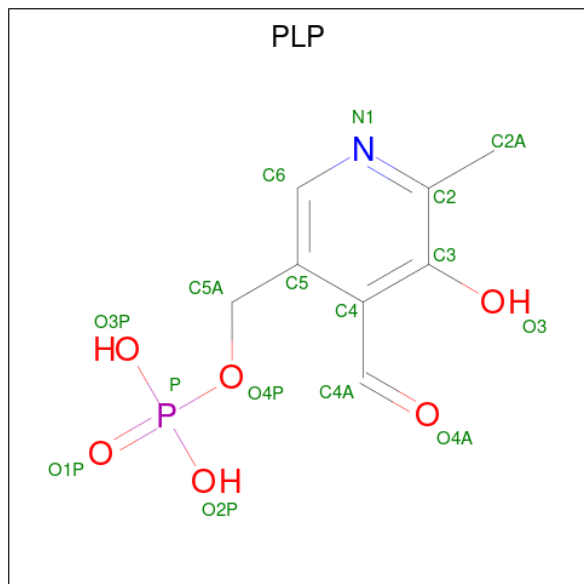
Chain	Residue	Modelled	Actual	Comment	Reference
A	338	HIS	-	expression tag	UNP O15570
A	339	HIS	-	expression tag	UNP O15570
B	338	HIS	-	expression tag	UNP O15570
B	339	HIS	-	expression tag	UNP O15570

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



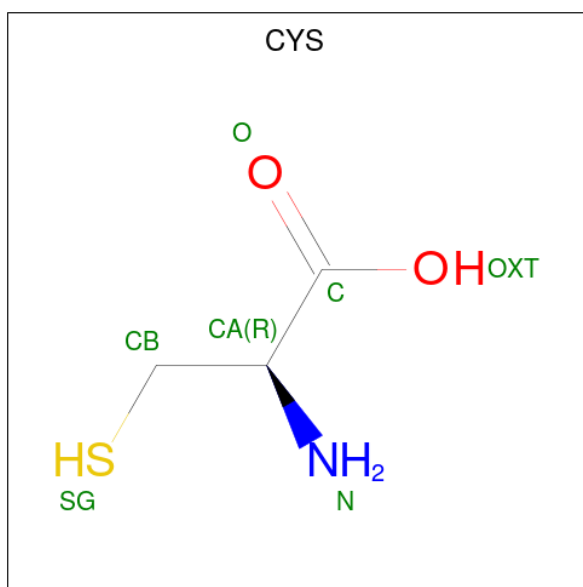
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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		

- Molecule 4 is CYSTEINE (three-letter code: CYS) (formula: C₃H₇NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	7	3	1	2	1	0	0

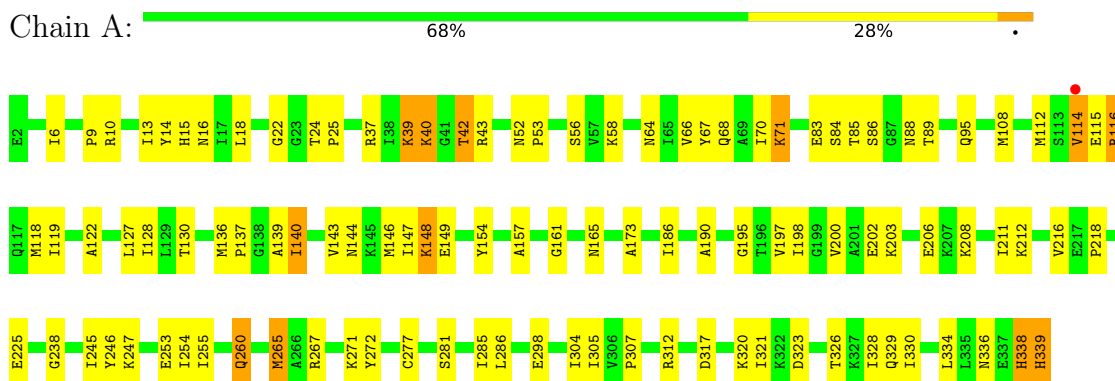
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	141	Total	O	0	0
			141	141		
5	B	123	Total	O	0	0
			123	123		

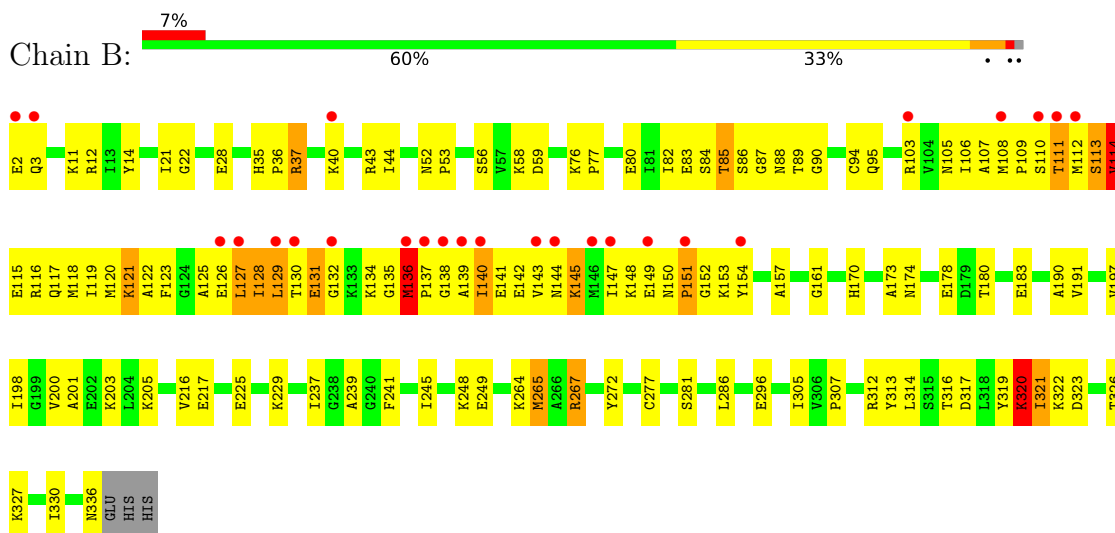
3 Residue-property plots [i](#)

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: Cysteine synthase



- Molecule 1: Cysteine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	80.36Å 80.36Å 111.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.88 – 2.40 45.88 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.3 (45.88-2.40) 94.3 (45.88-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.39Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.193 , 0.231 0.187 , 0.226	Depositor DCC
R_{free} test set	1352 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtrriage
Anisotropy	0.053	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.052 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5442	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.33	0/2622	0.63	2/3535 (0.1%)
1	B	0.34	0/2575	0.64	0/3476
All	All	0.34	0/5197	0.63	2/7011 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ARG	N-CA-C	-7.33	91.21	111.00
1	A	114	VAL	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2578	0	2623	100	0
1	B	2533	0	2569	161	0
2	A	15	0	0	1	0
2	B	15	0	0	1	0
3	A	15	0	6	0	0
3	B	15	0	6	4	0
4	B	7	0	4	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	141	0	0	6	0
5	B	123	0	0	4	0
All	All	5442	0	5208	253	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 24.

All (253) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:LYS:HZ2	3:B:343:PLP:C4A	1.44	1.21
1:B:58:LYS:HZ3	3:B:343:PLP:C4A	1.44	1.14
1:A:317:ASP:HA	1:A:320:LYS:HG3	1.34	1.08
1:B:121:LYS:H	1:B:121:LYS:HE2	0.95	1.08
1:B:136:MET:HG2	1:B:137:PRO:HD3	1.37	1.07
1:B:265:MET:HG3	1:B:286:LEU:HB2	1.40	1.03
1:B:149:GLU:O	1:B:151:PRO:HD3	1.59	1.02
1:A:40:LYS:H	1:A:40:LYS:HD2	1.25	1.02
1:B:110:SER:HB3	1:B:129:LEU:HD11	1.37	1.00
1:B:317:ASP:HA	1:B:320:LYS:HD2	1.40	1.00
1:B:134:LYS:O	1:B:137:PRO:HD2	1.60	0.99
1:B:121:LYS:H	1:B:121:LYS:CE	1.76	0.98
1:B:86:SER:OG	4:B:402:CYS:HB2	1.64	0.97
1:B:121:LYS:HE2	1:B:121:LYS:N	1.79	0.96
1:B:136:MET:CG	1:B:137:PRO:HD3	2.01	0.90
3:B:343:PLP:C4A	4:B:402:CYS:N	2.37	0.88
1:B:87:GLY:HA2	1:B:108:MET:HE1	1.54	0.87
1:B:86:SER:CB	4:B:402:CYS:HB2	2.06	0.85
1:B:138:GLY:O	1:B:142:GLU:HG2	1.76	0.85
1:A:43:ARG:HD2	5:A:379:HOH:O	1.76	0.84
1:B:53:PRO:HB2	1:B:95:GLN:HE22	1.40	0.84
1:B:110:SER:HB3	1:B:129:LEU:CD1	2.08	0.83
1:A:67:TYR:CE2	1:A:71:LYS:HE2	2.14	0.82
1:B:107:ALA:HA	1:B:128:ILE:O	1.80	0.82
1:B:143:VAL:O	1:B:147:ILE:HG13	1.79	0.82
1:B:264:LYS:HA	1:B:267:ARG:NH1	1.94	0.81
1:B:58:LYS:HE2	1:B:89:THR:OG1	1.81	0.81
1:A:115:GLU:HG2	1:A:118:MET:SD	2.21	0.81
1:A:39:LYS:HB2	5:A:371:HOH:O	1.81	0.80
1:A:88:ASN:ND2	1:A:312:ARG:HH11	1.80	0.79
1:A:39:LYS:H	1:A:39:LYS:HD3	1.48	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LYS:H	1:A:40:LYS:CD	1.95	0.79
1:B:110:SER:CB	1:B:129:LEU:HD11	2.13	0.78
1:A:130:THR:HG21	1:A:139:ALA:HA	1.65	0.78
1:B:110:SER:HB3	1:B:129:LEU:HD21	1.66	0.77
1:B:82:ILE:HG13	1:B:105:ASN:HB2	1.67	0.76
1:B:83:GLU:HG3	1:B:84:SER:N	2.01	0.76
1:B:127:LEU:O	1:B:128:ILE:HG13	1.86	0.75
1:A:118:MET:HE3	1:B:319:TYR:HB2	1.69	0.75
1:B:150:ASN:HB3	1:B:154:TYR:HE2	1.52	0.75
1:A:265:MET:HG3	1:A:286:LEU:HB2	1.69	0.73
1:B:114:VAL:O	1:B:118:MET:HG3	1.88	0.73
1:A:39:LYS:HG2	1:A:42:THR:HG22	1.69	0.73
1:A:198:ILE:CD1	1:A:246:TYR:HA	2.18	0.72
1:B:87:GLY:HA2	1:B:108:MET:CE	2.21	0.70
1:A:22:GLY:H	1:A:52:ASN:HD21	1.38	0.70
1:B:110:SER:CB	1:B:129:LEU:HD21	2.23	0.69
1:B:86:SER:HB3	4:B:402:CYS:HB2	1.74	0.69
1:B:141:GLU:O	1:B:144:ASN:HB2	1.93	0.69
1:A:84:SER:HB3	1:A:143:VAL:HG21	1.75	0.68
1:B:88:ASN:ND2	1:B:312:ARG:HH11	1.95	0.65
1:A:37:ARG:NH2	5:A:471:HOH:O	2.30	0.64
1:B:110:SER:HB3	1:B:129:LEU:CD2	2.28	0.64
1:B:116:ARG:NH2	1:B:313:TYR:CE1	2.66	0.63
1:A:137:PRO:O	1:A:140:ILE:HG22	1.98	0.63
1:B:201:ALA:O	1:B:205:LYS:HG2	1.99	0.63
1:B:136:MET:SD	1:B:137:PRO:HD3	2.39	0.63
1:B:180:THR:O	1:B:183:GLU:HG3	1.99	0.62
1:B:86:SER:HB3	4:B:402:CYS:CB	2.28	0.62
1:B:151:PRO:O	1:B:153:LYS:N	2.22	0.62
3:B:343:PLP:C4A	4:B:402:CYS:OXT	2.48	0.62
1:B:264:LYS:HA	1:B:267:ARG:HH12	1.63	0.62
1:A:115:GLU:OE1	1:B:314:LEU:HB3	2.00	0.62
1:A:339:HIS:HD1	1:A:339:HIS:C	2.03	0.61
1:B:117:GLN:O	1:B:121:LYS:HE3	2.00	0.61
1:A:339:HIS:C	1:A:339:HIS:ND1	2.54	0.61
1:A:326:THR:HG23	1:A:328:ILE:HG22	1.83	0.60
1:B:150:ASN:HB3	1:B:154:TYR:CE2	2.36	0.60
1:B:316:THR:O	1:B:320:LYS:HE3	2.02	0.60
1:B:321:ILE:HG13	1:B:322:LYS:N	2.15	0.60
1:A:22:GLY:H	1:A:52:ASN:ND2	1.99	0.60
1:B:83:GLU:HG3	1:B:84:SER:H	1.64	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:MET:HE2	1:B:319:TYR:HD2	1.67	0.59
1:B:134:LYS:O	1:B:136:MET:N	2.33	0.59
1:A:39:LYS:HG2	1:A:42:THR:CG2	2.32	0.59
1:B:58:LYS:HZ3	4:B:402:CYS:N	2.01	0.59
1:A:53:PRO:HB2	1:A:95:GLN:HE22	1.66	0.59
1:A:67:TYR:CD2	1:A:71:LYS:HE2	2.38	0.59
1:B:84:SER:HB3	1:B:139:ALA:C	2.24	0.58
1:B:94:CYS:SG	1:B:125:ALA:HB2	2.43	0.58
1:A:16:ASN:OD1	1:A:18:LEU:HB2	2.04	0.58
1:A:118:MET:CE	1:B:319:TYR:HB2	2.34	0.57
1:B:84:SER:HB3	1:B:139:ALA:O	2.04	0.57
1:B:136:MET:H	1:B:137:PRO:HD2	1.68	0.57
1:A:40:LYS:HD2	1:A:40:LYS:N	2.08	0.57
1:A:173:ALA:HB2	1:A:200:VAL:HA	1.87	0.57
1:B:121:LYS:HG2	1:B:122:ALA:N	2.19	0.57
1:B:85:THR:HG21	1:B:90:GLY:CA	2.34	0.57
1:B:110:SER:HB3	1:B:129:LEU:CG	2.34	0.56
1:A:39:LYS:HE3	1:A:298:GLU:HB2	1.86	0.56
1:B:85:THR:HG21	1:B:90:GLY:N	2.19	0.56
1:B:326:THR:O	1:B:330:ILE:HG13	2.04	0.56
1:A:83:GLU:CD	1:A:157:ALA:HB3	2.25	0.56
1:A:317:ASP:HA	1:A:320:LYS:CG	2.23	0.56
1:B:22:GLY:H	1:B:52:ASN:HD21	1.53	0.56
1:B:22:GLY:H	1:B:52:ASN:ND2	2.03	0.56
1:A:197:VAL:HG13	1:A:198:ILE:HG13	1.88	0.56
1:B:129:LEU:HD23	1:B:129:LEU:C	2.26	0.56
1:B:119:ILE:N	1:B:121:LYS:HE3	2.21	0.55
1:B:115:GLU:O	1:B:119:ILE:HG13	2.06	0.55
1:A:277:CYS:HB2	1:A:281:SER:CB	2.37	0.55
1:A:86:SER:HB3	1:A:108:MET:HB2	1.88	0.55
1:B:103:ARG:NH1	1:B:126:GLU:OE1	2.40	0.55
1:A:10:ARG:HD3	1:A:14:TYR:OH	2.06	0.54
1:B:35:HIS:ND1	1:B:37:ARG:HG2	2.21	0.54
1:B:58:LYS:HZ3	4:B:402:CYS:CA	2.20	0.54
1:B:136:MET:HG2	1:B:137:PRO:CD	2.24	0.54
1:A:144:ASN:HD22	1:A:147:ILE:HD11	1.72	0.54
1:B:136:MET:H	1:B:137:PRO:CD	2.21	0.54
1:B:141:GLU:C	1:B:145:LYS:HE3	2.28	0.53
1:A:198:ILE:HD13	1:A:246:TYR:HA	1.90	0.53
1:A:260:GLN:HG3	5:A:436:HOH:O	2.08	0.53
1:A:326:THR:CG2	1:A:328:ILE:HG22	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:HIS:CE1	1:B:37:ARG:HG2	2.43	0.53
1:A:128:ILE:HD13	1:A:146:MET:SD	2.49	0.52
1:A:198:ILE:O	1:A:202:GLU:HG3	2.10	0.52
1:B:117:GLN:O	1:B:121:LYS:CE	2.57	0.52
1:A:115:GLU:HB3	1:B:314:LEU:HD13	1.90	0.52
1:B:147:ILE:HG23	1:B:154:TYR:HB2	1.92	0.52
1:A:139:ALA:O	1:A:143:VAL:HG23	2.10	0.52
1:A:272:TYR:OH	1:A:330:ILE:HD12	2.09	0.51
1:B:121:LYS:HG2	1:B:122:ALA:H	1.73	0.51
1:B:82:ILE:HG12	1:B:143:VAL:CG2	2.40	0.51
1:A:6:ILE:HB	1:B:21:ILE:O	2.11	0.51
1:A:148:LYS:HG3	1:A:149:GLU:N	2.26	0.51
1:A:198:ILE:HD11	1:A:246:TYR:CD1	2.45	0.51
1:B:82:ILE:CD1	1:B:143:VAL:HG23	2.41	0.51
1:A:271:LYS:NZ	5:A:474:HOH:O	2.43	0.51
1:B:130:THR:HG21	1:B:138:GLY:O	2.10	0.51
1:B:136:MET:CE	1:B:241:PHE:HD2	2.24	0.50
1:B:136:MET:HE3	1:B:239:ALA:O	2.12	0.50
1:A:147:ILE:HG22	1:A:154:TYR:HB2	1.92	0.50
1:A:115:GLU:HG2	1:A:118:MET:CB	2.42	0.50
1:B:134:LYS:O	1:B:137:PRO:CD	2.48	0.50
1:B:85:THR:OG1	1:B:86:SER:N	2.42	0.50
1:B:121:LYS:NZ	1:B:121:LYS:HB3	2.26	0.50
1:B:173:ALA:HB2	1:B:200:VAL:HA	1.94	0.50
1:B:118:MET:C	1:B:121:LYS:HE3	2.33	0.49
1:B:35:HIS:HE1	1:B:37:ARG:HD3	1.77	0.49
1:A:218:PRO:HG2	1:A:238:GLY:HA3	1.95	0.49
1:B:190:ALA:HA	1:B:216:VAL:HB	1.93	0.49
1:B:110:SER:OG	1:B:129:LEU:HD21	2.13	0.49
1:A:277:CYS:HB2	1:A:281:SER:HB2	1.95	0.48
1:B:141:GLU:O	1:B:145:LYS:HE3	2.13	0.48
1:A:186:ILE:HG12	1:A:212:LYS:HB3	1.95	0.48
1:B:136:MET:HE2	1:B:241:PHE:HD2	1.78	0.48
1:A:326:THR:HA	2:A:341:SO4:O1	2.13	0.48
1:B:82:ILE:HG12	1:B:143:VAL:HG23	1.95	0.48
1:B:113:SER:HB3	1:B:116:ARG:HE	1.78	0.48
1:B:132:GLY:C	1:B:134:LYS:H	2.17	0.48
1:B:44:ILE:N	1:B:44:ILE:HD12	2.29	0.48
1:B:83:GLU:CG	1:B:84:SER:N	2.73	0.48
1:B:37:ARG:NH2	2:B:342:SO4:O1	2.47	0.48
1:B:248:LYS:HG2	5:B:466:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LYS:CG	1:B:122:ALA:H	2.27	0.47
1:B:121:LYS:H	1:B:121:LYS:CD	2.24	0.47
1:A:165:ASN:OD1	1:A:195:GLY:HA3	2.14	0.47
1:A:198:ILE:CD1	1:A:247:LYS:H	2.26	0.47
1:B:141:GLU:O	1:B:142:GLU:C	2.52	0.47
1:A:253:GLU:OE2	1:A:255:ILE:HD11	2.14	0.47
1:B:53:PRO:HB2	1:B:95:GLN:NE2	2.20	0.47
1:B:120:MET:HB2	1:B:127:LEU:HD11	1.97	0.47
1:B:120:MET:O	1:B:125:ALA:HB3	2.14	0.47
1:B:249:GLU:H	1:B:249:GLU:CD	2.17	0.47
1:A:136:MET:N	1:A:137:PRO:CD	2.78	0.47
1:B:106:ILE:HG22	1:B:107:ALA:N	2.30	0.46
1:B:37:ARG:HG2	1:B:37:ARG:H	1.41	0.46
1:A:115:GLU:HA	1:A:118:MET:H	1.80	0.46
1:B:174:ASN:O	1:B:178:GLU:HG2	2.15	0.46
1:B:267:ARG:NH1	1:B:323:ASP:OD2	2.49	0.46
1:A:39:LYS:HG3	1:A:298:GLU:HG3	1.97	0.46
1:B:35:HIS:ND1	1:B:36:PRO:HD2	2.30	0.46
1:B:83:GLU:CG	1:B:84:SER:H	2.29	0.46
1:A:267:ARG:HD2	1:A:323:ASP:OD2	2.16	0.46
1:B:94:CYS:HB3	1:B:123:PHE:CB	2.46	0.46
1:B:110:SER:O	1:B:111:THR:HB	2.16	0.46
1:B:161:GLY:HA2	1:B:245:ILE:HG23	1.98	0.46
1:A:39:LYS:HD3	1:A:39:LYS:N	2.25	0.45
1:A:265:MET:HE2	1:A:265:MET:HA	1.98	0.45
1:B:121:LYS:CG	1:B:122:ALA:N	2.78	0.45
1:A:338:HIS:N	1:A:338:HIS:CD2	2.84	0.45
1:A:161:GLY:HA2	1:A:245:ILE:HG23	1.98	0.45
1:A:84:SER:HB3	1:A:143:VAL:CG2	2.44	0.45
1:B:116:ARG:NH1	5:B:451:HOH:O	2.48	0.45
1:B:142:GLU:O	1:B:145:LYS:HG2	2.16	0.45
1:A:58:LYS:HE2	1:A:89:THR:OG1	2.16	0.45
1:B:136:MET:C	1:B:138:GLY:N	2.70	0.45
1:A:39:LYS:H	1:A:39:LYS:CD	2.16	0.45
1:B:84:SER:CB	1:B:139:ALA:O	2.66	0.44
1:B:277:CYS:HB2	1:B:281:SER:CB	2.47	0.44
1:A:190:ALA:HA	1:A:216:VAL:HB	1.98	0.44
1:B:136:MET:HE1	1:B:229:LYS:HD2	2.00	0.44
1:B:121:LYS:HB3	1:B:121:LYS:HZ3	1.82	0.44
1:A:88:ASN:HD21	1:A:312:ARG:HH11	1.62	0.44
1:B:108:MET:HG2	1:B:109:PRO:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:GLU:OE2	1:B:142:GLU:HA	2.16	0.44
1:A:66:VAL:O	1:A:70:ILE:HG13	2.17	0.43
1:A:68:GLN:HG3	5:A:375:HOH:O	2.18	0.43
1:A:317:ASP:OD1	1:A:320:LYS:HE2	2.17	0.43
1:B:272:TYR:CE2	1:B:327:LYS:HG3	2.53	0.43
1:A:305:ILE:O	1:A:307:PRO:HD3	2.19	0.43
1:B:132:GLY:C	1:B:134:LYS:N	2.72	0.43
1:B:296:GLU:OE2	1:B:296:GLU:N	2.38	0.43
1:A:9:PRO:HG2	1:B:178:GLU:HG3	2.00	0.43
1:A:64:ASN:O	1:A:68:GLN:HB2	2.19	0.43
1:A:13:ILE:HG21	1:B:43:ARG:NH2	2.34	0.43
1:B:147:ILE:O	1:B:150:ASN:N	2.51	0.43
1:B:80:GLU:OE1	1:B:103:ARG:HD3	2.19	0.43
1:B:121:LYS:N	1:B:121:LYS:CD	2.82	0.43
1:B:53:PRO:HG2	1:B:59:ASP:OD2	2.18	0.42
1:A:203:LYS:O	1:A:206:GLU:HB2	2.18	0.42
1:B:94:CYS:HB3	1:B:123:PHE:HB3	2.02	0.42
1:B:197:VAL:HG13	1:B:198:ILE:N	2.34	0.42
1:A:114:VAL:O	1:A:114:VAL:HG23	2.19	0.42
1:B:76:LYS:HB2	1:B:77:PRO:HD2	2.02	0.42
1:B:142:GLU:O	1:B:145:LYS:CG	2.67	0.42
1:B:108:MET:O	1:B:129:LEU:HA	2.18	0.42
1:B:150:ASN:O	1:B:151:PRO:O	2.37	0.42
1:A:39:LYS:HE3	1:A:298:GLU:CA	2.50	0.42
1:B:136:MET:HB2	1:B:140:ILE:HD12	2.00	0.42
1:B:267:ARG:HH11	1:B:267:ARG:HB2	1.84	0.42
1:A:13:ILE:HG21	1:B:43:ARG:HH22	1.83	0.42
1:B:145:LYS:HG2	1:B:145:LYS:H	1.46	0.42
1:A:24:THR:HB	1:A:25:PRO:HD2	2.02	0.41
1:B:12:ARG:HD3	1:B:14:TYR:CE1	2.55	0.41
1:B:136:MET:C	1:B:138:GLY:H	2.22	0.41
1:A:173:ALA:CB	1:A:203:LYS:HB3	2.50	0.41
1:A:328:ILE:HD12	1:A:328:ILE:HA	1.86	0.41
1:B:170:HIS:HB3	1:B:203:LYS:HE3	2.03	0.41
1:A:119:ILE:O	1:A:122:ALA:HB3	2.20	0.41
1:A:281:SER:O	1:A:285:ILE:HG13	2.19	0.41
1:A:285:ILE:HA	1:A:304:ILE:HD13	2.01	0.41
1:B:83:GLU:CD	1:B:157:ALA:HB3	2.41	0.41
1:B:191:VAL:O	1:B:237:ILE:HB	2.21	0.41
1:A:118:MET:CE	5:B:457:HOH:O	2.69	0.41
1:A:326:THR:HG23	1:A:329:GLN:H	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:MET:CA	1:B:121:LYS:HE3	2.49	0.41
1:A:115:GLU:O	1:A:119:ILE:HG13	2.20	0.41
1:A:143:VAL:O	1:A:147:ILE:HG12	2.21	0.41
1:A:15:HIS:HA	1:B:28:GLU:OE1	2.20	0.41
1:A:225:GLU:HG3	1:A:254:ILE:HG21	2.03	0.41
1:B:136:MET:O	1:B:140:ILE:N	2.54	0.41
1:A:265:MET:HG2	1:A:334:LEU:HD13	2.02	0.40
1:B:58:LYS:NZ	4:B:402:CYS:N	2.67	0.40
1:B:130:THR:HG21	1:B:142:GLU:CG	2.51	0.40
1:B:147:ILE:HG13	1:B:147:ILE:H	1.63	0.40
1:A:144:ASN:HD22	1:A:144:ASN:HA	1.65	0.40
1:A:208:LYS:HG2	1:A:211:ILE:HD11	2.04	0.40
1:B:131:GLU:O	1:B:134:LYS:CB	2.68	0.40
1:B:217:GLU:OE2	1:B:225:GLU:OE1	2.40	0.40
1:B:305:ILE:O	1:B:307:PRO:HD3	2.21	0.40
1:B:336:ASN:C	5:B:447:HOH:O	2.58	0.40
1:A:267:ARG:NH2	1:A:321:ILE:HD12	2.37	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	336/338 (99%)	322 (96%)	14 (4%)	0	100	100
1	B	333/338 (98%)	300 (90%)	22 (7%)	11 (3%)	4	3
All	All	669/676 (99%)	622 (93%)	36 (5%)	11 (2%)	9	13

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	111	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	136	MET
1	B	140	ILE
1	B	148	LYS
1	B	151	PRO
1	B	114	VAL
1	B	135	GLY
1	B	152	GLY
1	B	112	MET
1	B	320	LYS
1	B	128	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/278 (99%)	260 (94%)	16 (6%)	20	32
1	B	269/278 (97%)	250 (93%)	19 (7%)	14	23
All	All	545/556 (98%)	510 (94%)	35 (6%)	17	28

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	40	LYS
1	A	42	THR
1	A	56	SER
1	A	71	LYS
1	A	85	THR
1	A	112	MET
1	A	116	ARG
1	A	127	LEU
1	A	140	ILE
1	A	148	LYS
1	A	260	GLN
1	A	265	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	336	ASN
1	A	338	HIS
1	A	339	HIS
1	B	2	GLU
1	B	3	GLN
1	B	11	LYS
1	B	37	ARG
1	B	40	LYS
1	B	56	SER
1	B	85	THR
1	B	113	SER
1	B	114	VAL
1	B	121	LYS
1	B	127	LEU
1	B	129	LEU
1	B	131	GLU
1	B	136	MET
1	B	145	LYS
1	B	265	MET
1	B	267	ARG
1	B	320	LYS
1	B	321	ILE

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	52	ASN
1	A	88	ASN
1	A	95	GLN
1	A	144	ASN
1	A	260	GLN
1	A	336	ASN
1	A	338	HIS
1	B	52	ASN
1	B	88	ASN
1	B	95	GLN
1	B	117	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	PLP	A	342	1	15,15,16	1.13	0	20,22,23	1.88	4 (20%)
2	SO4	B	341	-	4,4,4	0.27	0	6,6,6	0.07	0
2	SO4	A	340	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	B	340	-	4,4,4	0.21	0	6,6,6	0.12	0
2	SO4	A	341	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	B	342	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	A	1	-	4,4,4	0.29	0	6,6,6	0.04	0
4	CYS	B	402	-	5,6,6	0.94	0	5,7,7	1.72	1 (20%)
3	PLP	B	343	1	15,15,16	1.32	2 (13%)	20,22,23	1.70	3 (15%)

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	PLP	A	342	1	-	0/6/6/8	0/1/1/1
3	PLP	B	343	1	-	0/6/6/8	0/1/1/1
4	CYS	B	402	-	-	1/6/6/6	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	343	PLP	C5-C4	2.53	1.43	1.40
3	B	343	PLP	C6-C5	2.04	1.42	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	342	PLP	O4P-C5A-C5	4.73	118.36	109.35
3	B	343	PLP	O4P-C5A-C5	4.46	117.86	109.35
3	A	342	PLP	C5A-C5-C6	3.42	124.99	119.37
4	B	402	CYS	OXT-C-CA	2.89	123.23	113.38
3	B	343	PLP	C5A-C5-C6	2.88	124.10	119.37
3	A	342	PLP	C5-C6-N1	-2.70	119.33	123.82
3	B	343	PLP	C5-C6-N1	-2.35	119.91	123.82
3	A	342	PLP	C6-C5-C4	2.15	119.85	118.16

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	402	CYS	N-CA-CB-SG

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	341	SO4	1	0
2	B	342	SO4	1	0
4	B	402	CYS	9	0
3	B	343	PLP	4	0

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	338/338 (100%)	-0.37	1 (0%) 94 93	21, 37, 66, 88	0
1	B	335/338 (99%)	-0.04	25 (7%) 14 13	20, 35, 96, 103	0
All	All	673/676 (99%)	-0.21	26 (3%) 39 38	20, 36, 83, 103	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	ILE	6.6
1	B	138	GLY	6.4
1	B	139	ALA	5.5
1	B	137	PRO	5.5
1	B	143	VAL	5.0
1	B	136	MET	4.6
1	B	127	LEU	4.4
1	B	110	SER	4.4
1	B	132	GLY	4.4
1	B	130	THR	4.2
1	B	2	GLU	4.1
1	B	112	MET	3.7
1	B	111	THR	3.6
1	B	144	ASN	3.4
1	B	147	ILE	3.4
1	B	154	TYR	3.1
1	B	149	GLU	3.1
1	B	129	LEU	3.0
1	B	103	ARG	2.9
1	B	40	LYS	2.6
1	B	108	MET	2.6
1	B	151	PRO	2.5
1	B	126	GLU	2.2
1	B	146	MET	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	3	GLN	2.1
1	A	114	VAL	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	B	340	5/5	0.79	0.23	93,94,95,95	0
4	CYS	B	402	7/7	0.79	0.23	59,60,61,64	0
2	SO4	A	340	5/5	0.85	0.20	92,92,93,93	0
2	SO4	A	341	5/5	0.87	0.20	91,92,92,92	0
2	SO4	A	1	5/5	0.90	0.19	85,85,85,87	0
2	SO4	B	341	5/5	0.93	0.10	88,88,89,90	0
3	PLP	B	343	15/16	0.95	0.17	24,29,34,35	0
2	SO4	B	342	5/5	0.95	0.22	77,77,78,78	0
3	PLP	A	342	15/16	0.96	0.13	24,28,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.