Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2024 – 08:17 PM EDT

PDB ID	:	3FFH
Title	:	The crystal structure of histidinol-phosphate aminotransferase from Listeria innocua Clip11262.
Authors	:	Tan, K.; Gu, M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2008-12-03
Resolution	:	2.31 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:

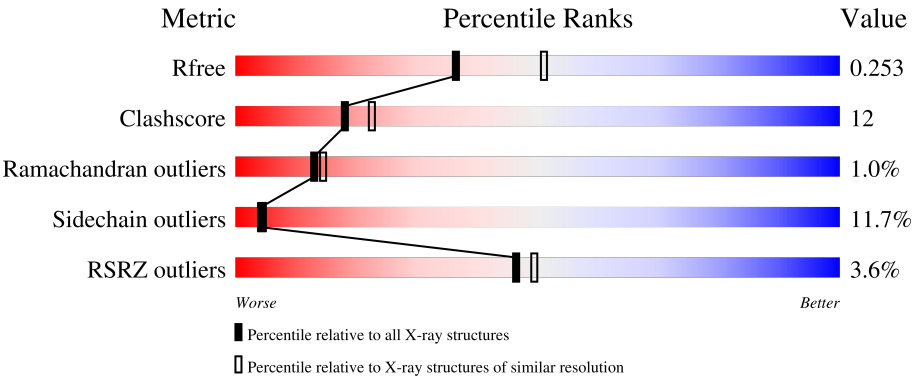
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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}	164625	7250 (2.34-2.30)
Clashscore	180529	8063 (2.34-2.30)
Ramachandran outliers	177936	7993 (2.34-2.30)
Sidechain outliers	177891	7993 (2.34-2.30)
RSRZ outliers	164620	7250 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	363	4% 70% 22% 6%
1	B	363	3% 69% 24%

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	A	361	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5686 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.

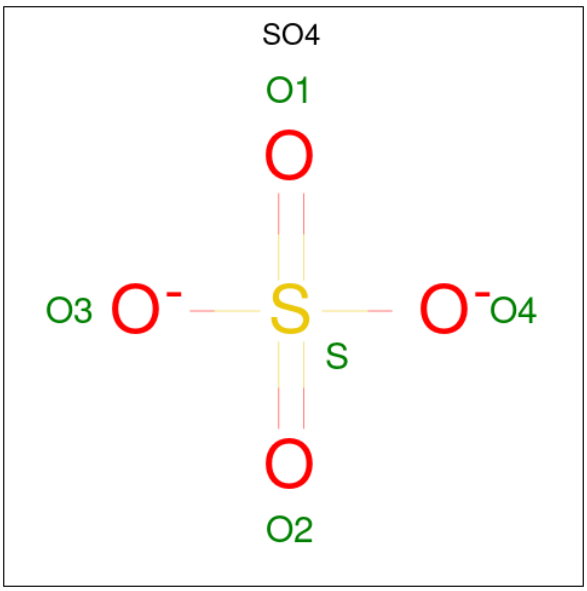
- Molecule 1 is a protein called Histidinol-phosphate aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	Se	0	0	0
			2766	1759	460	541	2	4			
1	B	352	Total	C	N	O	S	Se	0	0	0
			2750	1751	456	537	2	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q92A83
A	-1	ASN	-	expression tag	UNP Q92A83
A	0	ALA	-	expression tag	UNP Q92A83
B	-2	SER	-	expression tag	UNP Q92A83
B	-1	ASN	-	expression tag	UNP Q92A83
B	0	ALA	-	expression tag	UNP Q92A83

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

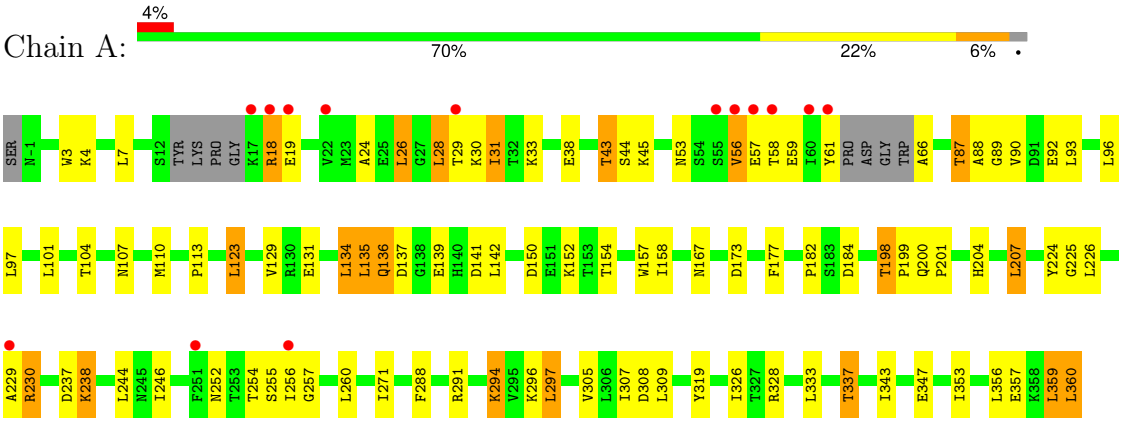
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	59	Total O 59 59	0	0
3	B	66	Total O 66 66	0	0

3 Residue-property plots (i)

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

• Molecule 1: Histidinol-phosphate aminotransferase

Chain A:



• Molecule 1: Histidinol-phosphate aminotransferase

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.46Å 83.67Å 122.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.85 – 2.31 41.85 – 2.31	Depositor EDS
% Data completeness (in resolution range)	95.0 (41.85-2.31) 95.2 (41.85-2.31)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, R_{free}	0.206 , 0.252 0.208 , 0.253	Depositor DCC
R_{free} test set	1712 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	40.5	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5686	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.61	0/2801	0.70	1/3784 (0.0%)
1	B	0.63	0/2786	0.73	0/3766
All	All	0.62	0/5587	0.71	1/7550 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	297	LEU	CA-CB-CG	5.10	127.03	115.30

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	2766	0	2815	82	0
1	B	2750	0	2798	62	0
2	A	20	0	0	4	0
2	B	25	0	0	1	0
3	A	59	0	0	2	0
3	B	66	0	0	4	0
All	All	5686	0	5613	134	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 12.

All (134) 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:238:LYS:HD2	1:A:238:LYS:H	1.14	1.07
1:A:7:LEU:HD11	1:B:100:VAL:HG23	1.42	0.98
1:A:224:TYR:CE1	1:A:271:ILE:HD11	2.08	0.87
1:A:136:GLN:HE21	1:A:136:GLN:HA	1.40	0.87
1:A:7:LEU:HD11	1:B:100:VAL:CG2	2.07	0.83
1:A:238:LYS:H	1:A:238:LYS:CD	1.88	0.82
1:A:319:TYR:CD2	1:A:359:LEU:HD21	2.14	0.81
1:A:319:TYR:CE2	1:A:359:LEU:HD21	2.15	0.81
1:B:29:THR:HG22	1:B:30:LYS:N	1.94	0.79
1:B:29:THR:HG22	1:B:30:LYS:H	1.49	0.78
1:B:87:THR:HG23	1:B:89:GLY:O	1.84	0.77
1:B:66:ALA:HB2	1:B:258:GLN:OE1	1.85	0.75
1:A:129:VAL:HG12	1:A:131:GLU:HG2	1.69	0.75
1:A:88:ALA:HB2	1:A:252:ASN:O	1.90	0.72
1:A:90:VAL:HG12	2:A:361:SO4:O4	1.88	0.72
1:A:87:THR:CG2	1:A:89:GLY:O	2.40	0.70
1:A:7:LEU:CD1	1:B:100:VAL:HG23	2.20	0.69
1:A:319:TYR:CE2	1:A:359:LEU:CD2	2.75	0.69
1:B:31:ILE:HD12	1:B:324:GLY:HA2	1.74	0.69
1:A:224:TYR:HE1	1:A:271:ILE:HD11	1.56	0.69
1:A:18:ARG:HH12	1:A:328:ARG:HH11	1.39	0.68
1:A:307:ILE:HG22	1:A:309:LEU:CD1	2.27	0.65
1:A:230:ARG:NH1	2:A:361:SO4:O2	2.30	0.64
1:B:224:TYR:CE1	1:B:271:ILE:HD11	2.33	0.64
1:A:38:GLU:OE2	1:A:225:GLY:HA2	1.98	0.63
1:A:238:LYS:HD2	1:A:238:LYS:N	1.99	0.63
1:A:58:THR:HB	1:A:254:THR:CG2	2.29	0.62
1:A:139:GLU:HG2	1:A:167:ASN:HD22	1.63	0.61
1:B:50:ILE:HD11	1:B:263:GLU:HG3	1.81	0.61
1:B:60:ILE:HG12	1:B:61:TYR:N	2.15	0.61
1:A:307:ILE:HG22	1:A:309:LEU:HD13	1.83	0.61
1:A:18:ARG:HE	1:A:33:LYS:HE3	1.66	0.61
1:B:87:THR:HG21	1:B:93:LEU:HB2	1.82	0.61
1:A:309:LEU:HD21	1:A:356:LEU:HD22	1.83	0.60
1:A:18:ARG:HD2	1:A:326:ILE:HG21	1.83	0.60
1:A:30:LYS:HG2	1:A:31:ILE:H	1.67	0.59
1:B:253:THR:HG22	1:B:254:THR:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:LEU:O	1:B:359:LEU:HB2	2.03	0.58
1:B:206:LYS:HD2	3:B:421:HOH:O	2.04	0.58
1:B:55:SER:C	1:B:57:GLU:H	2.08	0.57
1:B:87:THR:CG2	1:B:89:GLY:O	2.51	0.57
1:B:4:LYS:HB2	1:B:7:LEU:HG	1.88	0.56
1:A:198:THR:HA	1:A:199:PRO:C	2.26	0.56
1:A:305:VAL:HG13	1:A:343:ILE:HD11	1.87	0.56
1:A:56:VAL:HG21	1:B:256:ILE:HG12	1.87	0.55
1:A:129:VAL:HG12	1:A:131:GLU:CG	2.36	0.55
1:A:182:PRO:C	1:A:184:ASP:H	2.09	0.55
1:B:18:ARG:O	1:B:21:GLU:HB3	2.07	0.55
1:A:308:ASP:OD2	1:A:337:THR:HG22	2.07	0.55
1:B:116:VAL:HG13	3:B:386:HOH:O	2.08	0.54
1:A:59:GLU:HG2	1:A:255:SER:HB3	1.90	0.54
1:A:7:LEU:CD1	1:B:100:VAL:CG2	2.83	0.54
1:A:87:THR:HG22	1:A:89:GLY:O	2.08	0.53
1:B:272:GLY:O	1:B:276:THR:HG23	2.09	0.53
1:B:224:TYR:CD1	1:B:271:ILE:HD11	2.44	0.52
1:A:58:THR:HB	1:A:254:THR:HG21	1.91	0.52
1:A:204:HIS:HB2	1:A:207:LEU:HD22	1.91	0.52
1:B:224:TYR:CE1	1:B:271:ILE:CD1	2.93	0.52
1:B:291:ARG:NH2	1:B:357:GLU:OE2	2.44	0.51
1:A:87:THR:HG21	1:A:93:LEU:HB2	1.94	0.50
1:A:308:ASP:CG	1:A:337:THR:HG22	2.32	0.50
1:A:139:GLU:OE1	1:A:167:ASN:HB3	2.12	0.50
1:B:82:GLU:HG3	3:B:427:HOH:O	2.11	0.50
1:A:307:ILE:CG2	1:A:309:LEU:CD1	2.91	0.49
1:B:91:ASP:HB2	1:B:230:ARG:HH12	1.76	0.49
1:B:7:LEU:HA	1:B:10:LEU:HD21	1.94	0.48
1:B:113:PRO:HD2	1:B:134:LEU:HD12	1.96	0.48
1:A:154:THR:HG22	1:B:2:LYS:HE3	1.95	0.48
1:A:337:THR:HG23	1:A:337:THR:O	2.12	0.48
1:A:158:ILE:HD11	1:A:177:PHE:CE2	2.49	0.47
1:A:229:ALA:HB2	1:A:257:GLY:HA2	1.97	0.47
1:B:129:VAL:HG12	1:B:131:GLU:HG3	1.95	0.47
1:A:43:THR:HG23	1:A:44:SER:O	2.15	0.47
1:A:353:ILE:O	1:A:357:GLU:HG3	2.15	0.47
1:A:28:LEU:HD12	1:A:28:LEU:H	1.79	0.47
1:B:47:VAL:HG11	1:B:226:LEU:HD21	1.97	0.47
1:B:193:TYR:OH	1:B:222:LYS:HE3	2.15	0.46
1:A:113:PRO:HD2	1:A:134:LEU:HD22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:HIS:HD2	3:B:392:HOH:O	1.98	0.46
1:A:328:ARG:NH2	2:A:363:SO4:O3	2.47	0.46
1:A:3:TRP:CD2	1:B:243:GLN:HG2	2.51	0.46
1:A:101:LEU:HD23	1:B:2:LYS:O	2.16	0.46
1:B:269:ALA:O	1:B:273:GLU:HG2	2.16	0.46
1:B:40:PRO:HG2	1:B:343:ILE:O	2.16	0.45
1:A:224:TYR:CE1	1:A:271:ILE:CD1	2.90	0.45
1:A:135:LEU:HD13	1:A:141:ASP:HB2	1.98	0.45
1:B:307:ILE:HG22	1:B:309:LEU:CD1	2.46	0.45
1:A:66:ALA:HB3	3:A:418:HOH:O	2.17	0.45
1:A:137:ASP:OD1	1:A:139:GLU:HB2	2.17	0.45
1:A:296:LYS:HB3	1:A:308:ASP:HB3	1.99	0.45
1:B:71:LYS:HE3	1:B:75:ASP:OD2	2.17	0.45
1:B:226:LEU:O	1:B:229:ALA:O	2.34	0.45
1:B:305:VAL:HG13	1:B:343:ILE:HD11	1.99	0.44
1:B:228:SER:OG	1:B:229:ALA:N	2.51	0.44
1:A:308:ASP:OD1	1:A:337:THR:CG2	2.65	0.44
1:A:150:ASP:HB3	1:A:152:LYS:H	1.82	0.44
1:B:95:GLU:O	1:B:99:ARG:HG3	2.17	0.44
1:A:19:GLU:OE2	1:A:33:LYS:HB2	2.18	0.44
1:A:254:THR:HG22	1:A:256:ILE:H	1.83	0.44
1:A:256:ILE:CD1	1:B:56:VAL:HG11	2.48	0.43
1:B:190:ASP:HA	1:B:217:THR:OG1	2.18	0.43
1:A:288:PHE:HA	1:A:291:ARG:NH2	2.34	0.43
1:A:123:LEU:HD12	1:A:123:LEU:HA	1.89	0.43
1:B:85:ILE:CD1	1:B:244:LEU:HB3	2.49	0.43
1:B:281:GLY:O	1:B:284:GLN:HB2	2.18	0.43
1:B:85:ILE:HD13	1:B:244:LEU:HB3	2.01	0.43
1:A:254:THR:HG22	1:A:255:SER:N	2.34	0.42
1:B:253:THR:CG2	1:B:254:THR:N	2.82	0.42
1:B:248:ARG:NH2	1:B:252:ASN:HD21	2.17	0.42
1:A:246:ILE:HG22	1:B:10:LEU:HD12	2.01	0.42
1:A:129:VAL:CG1	1:A:131:GLU:HG2	2.45	0.42
1:B:45:LYS:N	2:B:365:SO4:O4	2.52	0.42
1:A:110:MSE:HE2	1:A:157:TRP:CD1	2.54	0.42
1:A:328:ARG:HG3	1:A:333:LEU:HD11	2.01	0.42
1:A:90:VAL:HG12	2:A:361:SO4:S	2.61	0.41
1:A:337:THR:O	1:A:337:THR:CG2	2.67	0.41
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.76	0.41
1:A:18:ARG:NH1	1:A:328:ARG:HH11	2.13	0.41
1:B:100:VAL:HG13	1:B:101:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:THR:HG22	1:B:254:THR:O	2.19	0.41
1:A:294:LYS:H	1:A:294:LYS:HG2	1.60	0.41
1:B:135:LEU:HD13	1:B:141:ASP:HB2	2.03	0.41
1:B:7:LEU:O	1:B:10:LEU:HG	2.20	0.41
1:B:29:THR:CG2	1:B:30:LYS:N	2.65	0.41
1:A:24:ALA:C	1:A:26:LEU:H	2.24	0.41
1:B:62:PRO:HG3	1:B:255:SER:HB3	2.03	0.41
1:A:18:ARG:H	1:A:18:ARG:HG2	1.61	0.41
1:A:66:ALA:N	3:A:410:HOH:O	2.54	0.40
1:B:198:THR:HA	1:B:199:PRO:C	2.40	0.40
1:A:136:GLN:HA	1:A:136:GLN:NE2	2.21	0.40
1:A:45:LYS:HD3	1:A:45:LYS:HA	1.82	0.40
1:A:294:LYS:HE3	1:A:360:LEU:HG	2.03	0.40
1:B:66:ALA:CB	1:B:258:GLN:OE1	2.62	0.40
1:A:200:GLN:HA	1:A:201:PRO:HD3	1.87	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	348/363 (96%)	334 (96%)	13 (4%)	1 (0%)	37 46
1	B	346/363 (95%)	330 (95%)	10 (3%)	6 (2%)	7 6
All	All	694/726 (96%)	664 (96%)	23 (3%)	7 (1%)	13 14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	228	SER
1	B	56	VAL
1	A	26	LEU

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Mol	Chain	Res	Type
1	B	29	THR
1	B	207	LEU
1	B	21	GLU
1	B	250	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	300/304 (99%)	265 (88%)	35 (12%)	4 4
1	B	298/304 (98%)	263 (88%)	35 (12%)	4 4
All	All	598/608 (98%)	528 (88%)	70 (12%)	4 4

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	18	ARG
1	A	28	LEU
1	A	29	THR
1	A	31	ILE
1	A	43	THR
1	A	53	ASN
1	A	56	VAL
1	A	57	GLU
1	A	61	TYR
1	A	87	THR
1	A	92	GLU
1	A	96	LEU
1	A	97	LEU
1	A	104	THR
1	A	107	ASN
1	A	123	LEU
1	A	134	LEU
1	A	135	LEU

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Mol	Chain	Res	Type
1	A	136	GLN
1	A	142	LEU
1	A	173	ASP
1	A	198	THR
1	A	207	LEU
1	A	230	ARG
1	A	237	ASP
1	A	238	LYS
1	A	244	LEU
1	A	260	LEU
1	A	294	LYS
1	A	297	LEU
1	A	337	THR
1	A	347	GLU
1	A	359	LEU
1	A	360	LEU
1	B	10	LEU
1	B	19	GLU
1	B	30	LYS
1	B	31	ILE
1	B	38	GLU
1	B	46	LYS
1	B	53	ASN
1	B	58	THR
1	B	60	ILE
1	B	67	SER
1	B	87	THR
1	B	97	LEU
1	B	107	ASN
1	B	112	THR
1	B	123	LEU
1	B	135	LEU
1	B	142	LEU
1	B	143	GLU
1	B	150	ASP
1	B	151	GLU
1	B	206	LYS
1	B	230	ARG
1	B	237	ASP
1	B	238	LYS
1	B	242	ARG
1	B	244	LEU

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Mol	Chain	Res	Type
1	B	255	SER
1	B	260	LEU
1	B	265	ILE
1	B	276	THR
1	B	293	GLU
1	B	345	LYS
1	B	347	GLU
1	B	359	LEU
1	B	360	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	53	ASN
1	A	107	ASN
1	A	136	GLN
1	A	140	HIS
1	A	175	GLN
1	A	252	ASN
1	B	37	ASN
1	B	107	ASN
1	B	140	HIS
1	B	175	GLN
1	B	252	ASN

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)

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	$\#\|Z\| > 2$
2	SO4	B	364	-	4,4,4	0.28	0	6,6,6	0.29	0
2	SO4	B	361	-	4,4,4	0.20	0	6,6,6	0.44	0
2	SO4	A	363	-	4,4,4	0.19	0	6,6,6	0.47	0
2	SO4	A	364	-	4,4,4	0.28	0	6,6,6	0.32	0
2	SO4	A	361	-	4,4,4	0.19	0	6,6,6	0.37	0
2	SO4	A	362	-	4,4,4	0.31	0	6,6,6	0.25	0
2	SO4	B	363	-	4,4,4	0.28	0	6,6,6	0.12	0
2	SO4	B	362	-	4,4,4	0.30	0	6,6,6	0.65	0
2	SO4	B	365	-	4,4,4	0.29	0	6,6,6	0.31	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	363	SO4	1	0
2	A	361	SO4	3	0
2	B	365	SO4	1	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	350/363 (96%)	-0.02	14 (4%)	43	45	16, 29, 56, 83	0
1	B	348/363 (95%)	0.05	11 (3%)	50	53	18, 29, 51, 81	0
All	All	698/726 (96%)	0.02	25 (3%)	46	49	16, 29, 55, 83	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	TYR	4.4
1	A	60	ILE	3.9
1	B	56	VAL	3.5
1	A	17	LYS	3.5
1	A	58	THR	3.2
1	B	61	TYR	3.1
1	A	19	GLU	2.8
1	B	60	ILE	2.7
1	A	18	ARG	2.7
1	A	22	VAL	2.7
1	A	56	VAL	2.7
1	A	229	ALA	2.7
1	A	55	SER	2.6
1	B	24	ALA	2.5
1	A	251	PHE	2.5
1	B	250	PRO	2.5
1	B	58	THR	2.5
1	A	57	GLU	2.4
1	B	22	VAL	2.4
1	B	0	ALA	2.4
1	A	256	ILE	2.3
1	A	29	THR	2.2
1	B	62	PRO	2.2
1	B	252	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	251	PHE	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	364	5/5	0.61	0.20	79,79,79,79	5
2	SO4	B	365	5/5	0.74	0.15	76,76,77,77	5
2	SO4	B	363	5/5	0.86	0.11	80,80,80,80	5
2	SO4	A	363	5/5	0.93	0.10	50,51,52,52	0
2	SO4	B	362	5/5	0.94	0.11	49,50,52,52	0
2	SO4	A	364	5/5	0.94	0.10	66,67,67,67	0
2	SO4	A	362	5/5	0.95	0.09	57,58,58,58	0
2	SO4	A	361	5/5	0.97	0.06	42,42,43,43	0
2	SO4	B	361	5/5	0.97	0.07	42,42,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.