



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:20 PM UTC

PDB ID : 3LBM / pdb_00003lbm
Title : D-sialic acid aldolase
Authors : Ko, T.-P.; Chou, C.-Y.; Wang, A.H.-J.
Deposited on : 2010-01-08
Resolution : 1.48 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

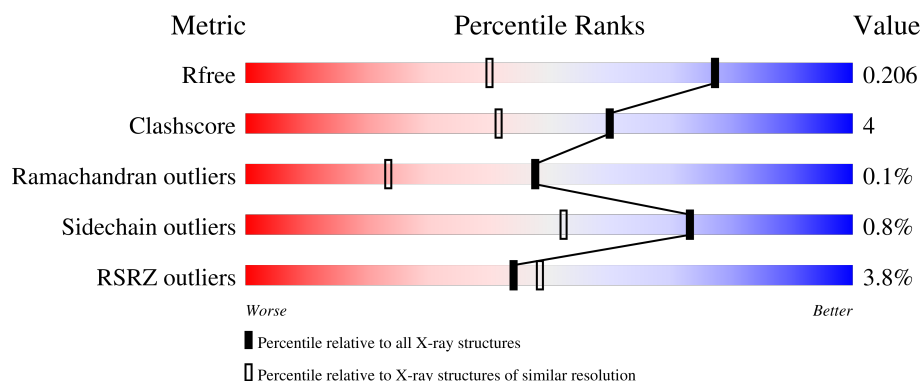
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

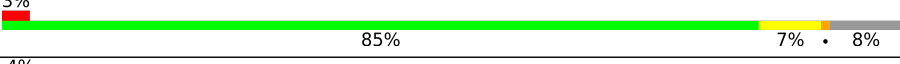
The reported resolution of this entry is 1.48 Å.

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	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	319	
1	B	319	
1	C	319	
1	D	319	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10679 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 N-acetylneuraminate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	73	0	0
			2279	1452	386	431	10			
1	B	295	Total	C	N	O	S	74	0	0
			2279	1452	386	431	10			
1	C	294	Total	C	N	O	S	70	0	0
			2274	1449	385	430	10			
1	D	295	Total	C	N	O	S	54	0	0
			2279	1452	386	431	10			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP P0A6L4
A	-20	GLY	-	expression tag	UNP P0A6L4
A	-19	HIS	-	expression tag	UNP P0A6L4
A	-18	HIS	-	expression tag	UNP P0A6L4
A	-17	HIS	-	expression tag	UNP P0A6L4
A	-16	HIS	-	expression tag	UNP P0A6L4
A	-15	HIS	-	expression tag	UNP P0A6L4
A	-14	HIS	-	expression tag	UNP P0A6L4
A	-13	HIS	-	expression tag	UNP P0A6L4
A	-12	HIS	-	expression tag	UNP P0A6L4
A	-11	HIS	-	expression tag	UNP P0A6L4
A	-10	HIS	-	expression tag	UNP P0A6L4
A	-9	SER	-	expression tag	UNP P0A6L4
A	-8	SER	-	expression tag	UNP P0A6L4
A	-7	GLY	-	expression tag	UNP P0A6L4
A	-6	HIS	-	expression tag	UNP P0A6L4
A	-5	ILE	-	expression tag	UNP P0A6L4
A	-4	GLU	-	expression tag	UNP P0A6L4
A	-3	GLY	-	expression tag	UNP P0A6L4
A	-2	ARG	-	expression tag	UNP P0A6L4
A	-1	HIS	-	expression tag	UNP P0A6L4

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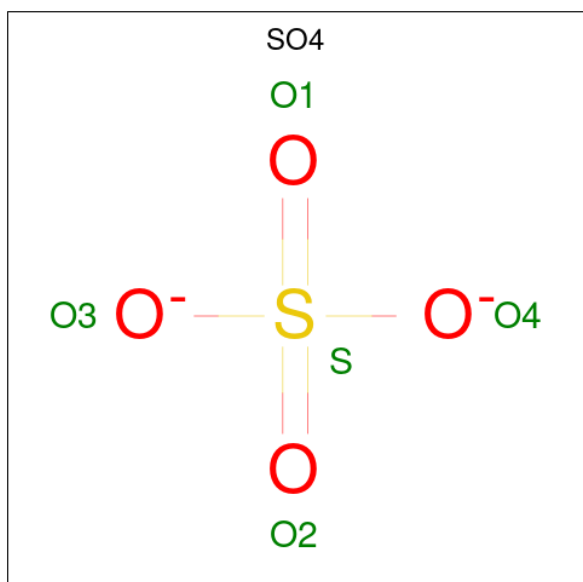
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP P0A6L4
B	-21	MET	-	expression tag	UNP P0A6L4
B	-20	GLY	-	expression tag	UNP P0A6L4
B	-19	HIS	-	expression tag	UNP P0A6L4
B	-18	HIS	-	expression tag	UNP P0A6L4
B	-17	HIS	-	expression tag	UNP P0A6L4
B	-16	HIS	-	expression tag	UNP P0A6L4
B	-15	HIS	-	expression tag	UNP P0A6L4
B	-14	HIS	-	expression tag	UNP P0A6L4
B	-13	HIS	-	expression tag	UNP P0A6L4
B	-12	HIS	-	expression tag	UNP P0A6L4
B	-11	HIS	-	expression tag	UNP P0A6L4
B	-10	HIS	-	expression tag	UNP P0A6L4
B	-9	SER	-	expression tag	UNP P0A6L4
B	-8	SER	-	expression tag	UNP P0A6L4
B	-7	GLY	-	expression tag	UNP P0A6L4
B	-6	HIS	-	expression tag	UNP P0A6L4
B	-5	ILE	-	expression tag	UNP P0A6L4
B	-4	GLU	-	expression tag	UNP P0A6L4
B	-3	GLY	-	expression tag	UNP P0A6L4
B	-2	ARG	-	expression tag	UNP P0A6L4
B	-1	HIS	-	expression tag	UNP P0A6L4
B	0	MET	-	expression tag	UNP P0A6L4
C	-21	MET	-	expression tag	UNP P0A6L4
C	-20	GLY	-	expression tag	UNP P0A6L4
C	-19	HIS	-	expression tag	UNP P0A6L4
C	-18	HIS	-	expression tag	UNP P0A6L4
C	-17	HIS	-	expression tag	UNP P0A6L4
C	-16	HIS	-	expression tag	UNP P0A6L4
C	-15	HIS	-	expression tag	UNP P0A6L4
C	-14	HIS	-	expression tag	UNP P0A6L4
C	-13	HIS	-	expression tag	UNP P0A6L4
C	-12	HIS	-	expression tag	UNP P0A6L4
C	-11	HIS	-	expression tag	UNP P0A6L4
C	-10	HIS	-	expression tag	UNP P0A6L4
C	-9	SER	-	expression tag	UNP P0A6L4
C	-8	SER	-	expression tag	UNP P0A6L4
C	-7	GLY	-	expression tag	UNP P0A6L4
C	-6	HIS	-	expression tag	UNP P0A6L4
C	-5	ILE	-	expression tag	UNP P0A6L4
C	-4	GLU	-	expression tag	UNP P0A6L4
C	-3	GLY	-	expression tag	UNP P0A6L4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	ARG	-	expression tag	UNP P0A6L4
C	-1	HIS	-	expression tag	UNP P0A6L4
C	0	MET	-	expression tag	UNP P0A6L4
D	-21	MET	-	expression tag	UNP P0A6L4
D	-20	GLY	-	expression tag	UNP P0A6L4
D	-19	HIS	-	expression tag	UNP P0A6L4
D	-18	HIS	-	expression tag	UNP P0A6L4
D	-17	HIS	-	expression tag	UNP P0A6L4
D	-16	HIS	-	expression tag	UNP P0A6L4
D	-15	HIS	-	expression tag	UNP P0A6L4
D	-14	HIS	-	expression tag	UNP P0A6L4
D	-13	HIS	-	expression tag	UNP P0A6L4
D	-12	HIS	-	expression tag	UNP P0A6L4
D	-11	HIS	-	expression tag	UNP P0A6L4
D	-10	HIS	-	expression tag	UNP P0A6L4
D	-9	SER	-	expression tag	UNP P0A6L4
D	-8	SER	-	expression tag	UNP P0A6L4
D	-7	GLY	-	expression tag	UNP P0A6L4
D	-6	HIS	-	expression tag	UNP P0A6L4
D	-5	ILE	-	expression tag	UNP P0A6L4
D	-4	GLU	-	expression tag	UNP P0A6L4
D	-3	GLY	-	expression tag	UNP P0A6L4
D	-2	ARG	-	expression tag	UNP P0A6L4
D	-1	HIS	-	expression tag	UNP P0A6L4
D	0	MET	-	expression tag	UNP P0A6L4

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



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

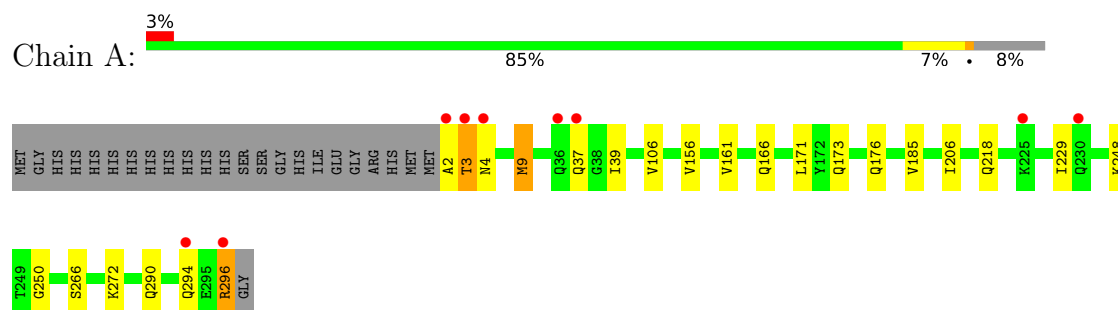
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	389	Total O 389 389	0	0
3	B	409	Total O 409 409	0	0
3	C	375	Total O 375 375	0	0
3	D	375	Total O 375 375	0	0

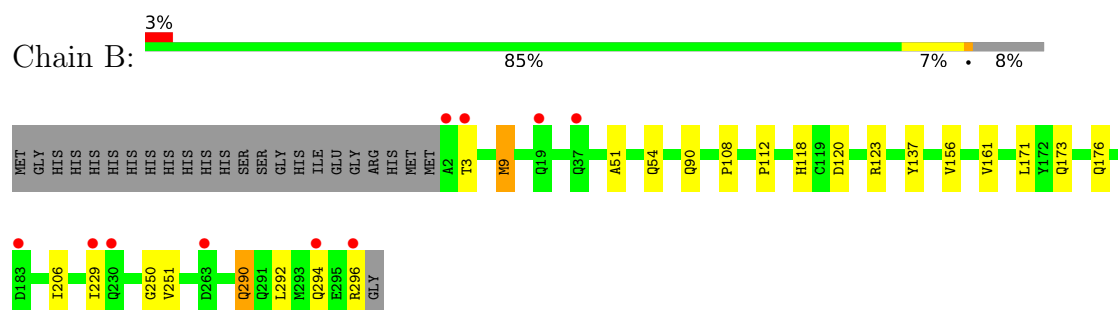
3 Residue-property plots [i](#)

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.

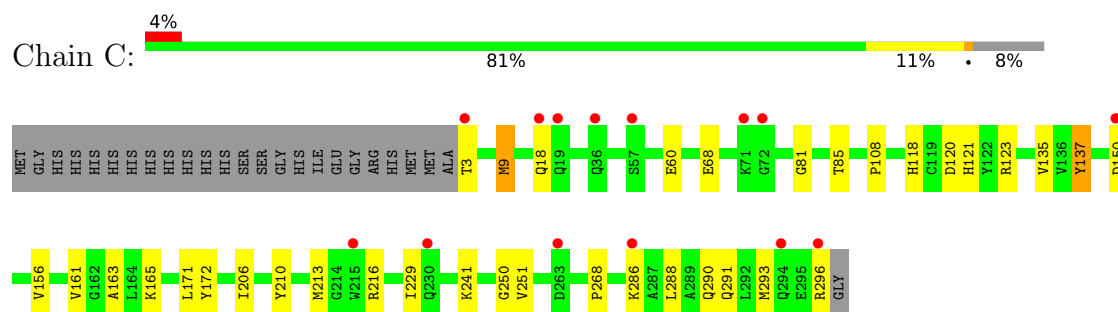
- Molecule 1: N-acetylneuraminate lyase



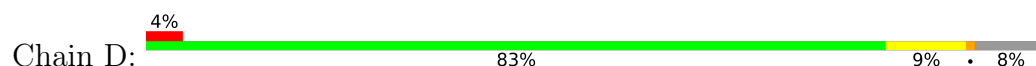
- Molecule 1: N-acetylneuraminate lyase



- Molecule 1: N-acetylneuraminate lyase



- Molecule 1: N-acetylneuraminate lyase





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.01Å 121.01Å 197.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.48 30.00 – 1.48	Depositor EDS
% Data completeness (in resolution range)	91.0 (30.00-1.48) 95.9 (30.00-1.48)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 1.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.186 , 0.203 0.186 , 0.206	Depositor DCC
R_{free} test set	13174 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10679	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: 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	1.02	3/2319 (0.1%)	1.12	3/3139 (0.1%)
1	B	1.07	2/2319 (0.1%)	1.14	4/3139 (0.1%)
1	C	1.10	2/2314 (0.1%)	1.18	6/3132 (0.2%)
1	D	1.08	3/2319 (0.1%)	1.15	4/3139 (0.1%)
All	All	1.07	10/9271 (0.1%)	1.15	17/12549 (0.1%)

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	B	0	1
1	C	0	2
1	D	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	9	MET	SD-CE	-13.45	1.46	1.79
1	B	9	MET	SD-CE	-10.64	1.52	1.79
1	D	262	MET	SD-CE	-8.41	1.58	1.79
1	A	9	MET	CB-CG	7.74	1.75	1.52
1	A	9	MET	CG-SD	-6.76	1.63	1.80
1	C	293	MET	SD-CE	-6.28	1.63	1.79
1	D	9	MET	CB-CG	5.90	1.70	1.52
1	A	106	VAL	CA-CB	5.80	1.59	1.54
1	D	112	PRO	CA-C	5.20	1.59	1.52
1	B	112	PRO	CA-C	5.13	1.58	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	251	VAL	N-CA-C	7.56	117.64	110.53
1	B	9	MET	CG-SD-CE	-7.30	84.85	100.90
1	D	70	ALA	N-CA-C	7.23	124.17	114.12
1	D	172	TYR	N-CA-C	-7.20	103.36	111.14
1	B	251	VAL	N-CA-C	5.97	116.15	110.53
1	D	185	VAL	N-CA-C	-5.82	102.03	109.30
1	C	250	GLY	N-CA-C	-5.79	99.45	113.18
1	C	241	LYS	N-CA-C	-5.68	105.17	111.36
1	B	250	GLY	N-CA-C	-5.53	100.08	113.18
1	A	250	GLY	N-CA-C	-5.49	100.18	113.18
1	D	251	VAL	N-CA-C	5.45	115.54	110.42
1	A	185	VAL	N-CA-C	-5.39	101.72	108.84
1	C	9	MET	CG-SD-CE	-5.23	89.39	100.90
1	A	266	SER	N-CA-C	5.21	116.96	111.28
1	C	172	TYR	N-CA-C	-5.20	105.52	111.14
1	C	81	GLY	N-CA-C	5.17	118.57	111.54
1	B	3	THR	N-CA-C	-5.04	106.87	112.57

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	137	TYR	Sidechain
1	C	137	TYR	Sidechain
1	C	210	TYR	Sidechain
1	D	137	TYR	Sidechain

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	2279	0	2300	19	0
1	B	2279	0	2300	16	0
1	C	2274	0	2295	23	0
1	D	2279	0	2300	24	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	389	0	0	4	0
3	B	409	0	0	3	0
3	C	375	0	0	7	0
3	D	375	0	0	7	0
All	All	10679	0	9195	76	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 (76) 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:9:MET:CB	1:A:9:MET:CG	1.75	1.55
1:C:150:ASP:HB3	3:C:1317:HOH:O	1.48	1.14
1:C:296:ARG:HG2	1:C:296:ARG:HH11	1.19	1.05
1:A:9:MET:CB	1:A:9:MET:SD	2.62	0.87
1:D:2:ALA:N	3:D:970:HOH:O	2.08	0.86
1:B:229:ILE:HD11	1:D:229:ILE:HD11	1.57	0.85
1:B:229:ILE:CD1	1:D:229:ILE:HD11	2.08	0.84
1:D:127:ASP:HB2	3:D:1503:HOH:O	1.79	0.80
1:C:3:THR:HA	3:C:1230:HOH:O	1.83	0.77
1:A:290:GLN:O	1:A:294:GLN:HG2	1.83	0.77
1:C:60:GLU:OE1	3:C:1288:HOH:O	2.04	0.76
1:A:296:ARG:HD2	3:A:1544:HOH:O	1.90	0.72
1:B:229:ILE:HD11	1:D:229:ILE:CD1	2.21	0.70
1:C:296:ARG:HG2	1:C:296:ARG:NH1	1.93	0.70
1:A:2:ALA:O	1:A:3:THR:C	2.34	0.68
1:A:9:MET:CG	1:A:9:MET:CA	2.73	0.66
1:C:68:GLU:HG2	3:C:1299:HOH:O	1.97	0.63
1:C:108:PRO:HD2	1:C:118:HIS:HD2	1.62	0.63
1:D:3:THR:HG23	3:D:374:HOH:O	1.99	0.63
1:B:90:GLN:NE2	3:B:948:HOH:O	2.31	0.62
1:D:108:PRO:HD2	1:D:118:HIS:HD2	1.64	0.62
1:B:173:GLN:HA	1:B:176:GLN:HE21	1.65	0.62
1:D:173:GLN:HA	1:D:176:GLN:HE21	1.65	0.62
1:D:51:ALA:HA	1:D:54:GLN:HE21	1.66	0.61
1:C:296:ARG:NH1	1:C:296:ARG:CG	2.61	0.61
1:A:248:LYS:HE3	3:A:392:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:ASP:CB	3:D:1503:HOH:O	2.43	0.59
1:D:37:GLN:HB3	1:D:296:ARG:CZ	2.32	0.59
1:A:2:ALA:C	1:A:3:THR:O	2.46	0.58
1:A:272:LYS:NZ	3:A:755:HOH:O	2.36	0.58
1:C:288:LEU:HA	1:C:291:GLN:HG2	1.86	0.57
1:B:290:GLN:O	1:B:294:GLN:HG2	2.05	0.57
1:A:173:GLN:HA	1:A:176:GLN:HE21	1.70	0.56
1:B:108:PRO:HD2	1:B:118:HIS:HD2	1.69	0.56
1:A:2:ALA:O	1:A:3:THR:O	2.23	0.55
1:C:85:THR:OG1	1:C:121:HIS:HD2	1.88	0.55
1:C:121:HIS:HE1	3:C:302:HOH:O	1.89	0.54
1:D:3:THR:CG2	1:D:3:THR:O	2.55	0.54
1:A:229:ILE:HD11	1:C:229:ILE:CD1	2.39	0.53
1:B:51:ALA:HA	1:B:54:GLN:HE21	1.72	0.53
1:D:37:GLN:HB3	1:D:296:ARG:NH1	2.24	0.52
1:C:296:ARG:NE	3:C:1271:HOH:O	2.42	0.51
1:B:120:ASP:OD1	1:B:123:ARG:NH1	2.44	0.51
1:D:33:PHE:CZ	1:D:296:ARG:NH1	2.80	0.49
1:B:292:LEU:O	1:B:296:ARG:HG3	2.12	0.48
1:B:123:ARG:NH2	3:B:1034:HOH:O	2.45	0.48
1:C:108:PRO:HD2	1:C:118:HIS:CD2	2.45	0.48
1:C:137:TYR:CE1	1:C:165:LYS:HD3	2.48	0.48
1:D:2:ALA:CA	3:D:970:HOH:O	2.58	0.47
1:A:171:LEU:HD12	1:C:171:LEU:HD12	1.96	0.47
1:A:37:GLN:CD	3:A:468:HOH:O	2.57	0.47
1:D:108:PRO:HD2	1:D:118:HIS:CD2	2.48	0.47
1:A:3:THR:O	1:A:4:ASN:C	2.58	0.46
1:A:218:GLN:HE21	1:A:218:GLN:HA	1.79	0.46
1:B:171:LEU:HD12	1:D:171:LEU:HD12	1.97	0.45
1:D:9:MET:O	1:D:206:ILE:HA	2.17	0.45
1:A:156:VAL:HA	1:A:161:VAL:HG11	1.97	0.44
1:B:156:VAL:HA	1:B:161:VAL:HG11	2.00	0.43
1:D:71:LYS:NZ	3:D:1476:HOH:O	2.52	0.42
1:C:156:VAL:HA	1:C:161:VAL:HG11	2.00	0.42
1:C:213:MET:HB2	1:C:216:ARG:HD2	2.02	0.42
1:D:96:LYS:CD	1:D:130:ASP:HB3	2.50	0.42
1:A:9:MET:O	1:A:206:ILE:HA	2.20	0.42
1:B:108:PRO:HD2	1:B:118:HIS:CD2	2.53	0.41
1:B:118:HIS:HE1	3:B:365:HOH:O	2.02	0.41
1:C:120:ASP:OD1	1:C:123:ARG:NH1	2.52	0.41
1:D:118:HIS:HE1	3:D:316:HOH:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:MET:O	1:C:206:ILE:HA	2.19	0.41
1:B:9:MET:O	1:B:206:ILE:HA	2.21	0.41
1:D:249:THR:HG22	1:D:281:TYR:CG	2.56	0.41
1:A:39:ILE:HD12	1:A:39:ILE:HA	1.93	0.41
1:C:118:HIS:HE1	3:C:391:HOH:O	2.03	0.41
1:C:135:VAL:HG22	1:C:163:ALA:HB3	2.03	0.41
1:D:294:GLN:HE21	1:D:294:GLN:HB3	1.64	0.41
1:D:19:GLN:O	1:D:20:GLN:HB2	2.21	0.40
1:C:286:LYS:O	1:C:290:GLN:HG2	2.21	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	293/319 (92%)	287 (98%)	5 (2%)	1 (0%)	36	17
1	B	293/319 (92%)	290 (99%)	3 (1%)	0	100	100
1	C	292/319 (92%)	289 (99%)	3 (1%)	0	100	100
1	D	293/319 (92%)	289 (99%)	4 (1%)	0	100	100
All	All	1171/1276 (92%)	1155 (99%)	15 (1%)	1 (0%)	48	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	THR

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	232/263 (88%)	230 (99%)	2 (1%)	70	48
1	B	212/263 (81%)	211 (100%)	1 (0%)	81	65
1	C	243/263 (92%)	241 (99%)	2 (1%)	73	52
1	D	243/263 (92%)	241 (99%)	2 (1%)	73	52
All	All	930/1052 (88%)	923 (99%)	7 (1%)	73	52

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	296	ARG
1	B	290	GLN
1	C	18	GLN
1	C	268	PRO
1	D	3	THR
1	D	294	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	34	ASN
1	A	138	ASN
1	A	166	GLN
1	A	173	GLN
1	A	176	GLN
1	A	230	GLN
1	A	290	GLN
1	B	18	GLN
1	B	34	ASN
1	B	54	GLN
1	B	118	HIS
1	B	166	GLN
1	B	173	GLN
1	B	176	GLN
1	B	188	ASN

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Mol	Chain	Res	Type
1	B	211	ASN
1	C	18	GLN
1	C	34	ASN
1	C	118	HIS
1	C	121	HIS
1	C	138	ASN
1	C	166	GLN
1	C	173	GLN
1	C	211	ASN
1	D	34	ASN
1	D	54	GLN
1	D	118	HIS
1	D	176	GLN
1	D	188	ASN
1	D	211	ASN
1	D	230	GLN
1	D	233	GLN
1	D	291	GLN
1	D	294	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	2004	-	4,4,4	0.69	0	6,6,6	0.46	0
2	SO4	C	2006	-	4,4,4	0.48	0	6,6,6	0.24	0
2	SO4	A	2002	-	4,4,4	0.44	0	6,6,6	0.25	0
2	SO4	D	2008	-	4,4,4	0.80	0	6,6,6	0.38	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.

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	295/319 (92%)	0.06	9 (3%)	51 56	8, 18, 28, 49	17 (5%)
1	B	295/319 (92%)	0.16	10 (3%)	48 52	8, 19, 31, 48	17 (5%)
1	C	294/319 (92%)	0.42	14 (4%)	35 39	10, 20, 32, 49	17 (5%)
1	D	295/319 (92%)	0.09	12 (4%)	41 45	9, 18, 29, 46	13 (4%)
All	All	1179/1276 (92%)	0.18	45 (3%)	44 48	8, 19, 30, 49	64 (5%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	THR	8.1
1	C	3	THR	7.8
1	B	2	ALA	7.1
1	A	2	ALA	6.1
1	B	3	THR	4.7
1	D	296	ARG	4.6
1	D	72	GLY	4.5
1	A	296	ARG	4.3
1	D	2	ALA	4.2
1	C	296	ARG	4.0
1	C	294	GLN	3.4
1	B	294	GLN	3.2
1	A	4	ASN	3.2
1	C	19	GLN	3.1
1	A	230	GLN	3.0
1	B	263	ASP	2.9
1	A	37	GLN	2.8
1	D	3	THR	2.8
1	D	294	GLN	2.7
1	A	225	LYS	2.7
1	D	230	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	296	ARG	2.6
1	D	229	ILE	2.5
1	C	36	GLN	2.5
1	D	70	ALA	2.5
1	D	127	ASP	2.5
1	C	57	SER	2.4
1	A	294	GLN	2.4
1	D	71	LYS	2.4
1	B	19	GLN	2.4
1	B	183	ASP	2.3
1	C	286	LYS	2.3
1	C	150	ASP	2.3
1	B	229	ILE	2.3
1	D	291	GLN	2.2
1	C	72	GLY	2.2
1	C	215	TRP	2.2
1	B	37	GLN	2.2
1	D	19	GLN	2.2
1	C	71	LYS	2.1
1	C	18	GLN	2.1
1	C	230	GLN	2.1
1	A	36	GLN	2.1
1	C	263	ASP	2.1
1	B	230	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	2002	5/5	0.99	0.06	17,19,19,20	0
2	SO4	B	2004	5/5	0.99	0.05	17,17,20,21	0
2	SO4	C	2006	5/5	0.99	0.07	19,19,21,21	0
2	SO4	D	2008	5/5	0.99	0.06	17,18,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.