



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:53 PM UTC

PDB ID : 1SHQ / pdb_00001shq
Title : Crystal structure of shrimp alkaline phosphatase with magnesium in M3
Authors : de Backer, M.M.E.; McSweeney, S.; Lindley, P.F.; Hough, E.
Deposited on : 2004-02-26
Resolution : 2.00 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

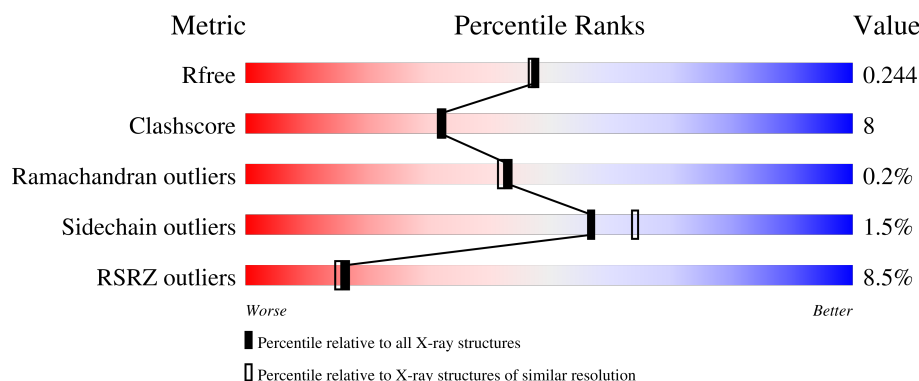
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

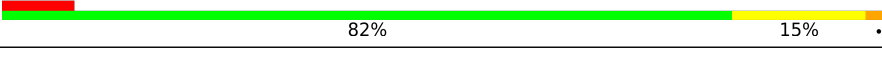
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	478	 9% 79% 17% •
1	B	478	 8% 82% 15% •

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7618 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.

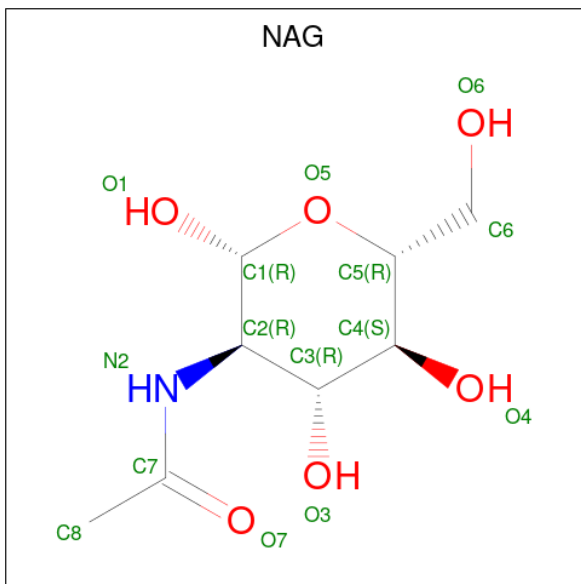
- Molecule 1 is a protein called alkaline phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3731	2333	629	755	14			
1	B	476	Total	C	N	O	S	0	0	0
			3731	2333	629	755	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	-	cloning artifact	UNP Q9BHT8
A	2	GLU	-	cloning artifact	UNP Q9BHT8
A	3	ASP	-	cloning artifact	UNP Q9BHT8
B	1	GLU	-	cloning artifact	UNP Q9BHT8
B	2	GLU	-	cloning artifact	UNP Q9BHT8
B	3	ASP	-	cloning artifact	UNP Q9BHT8

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

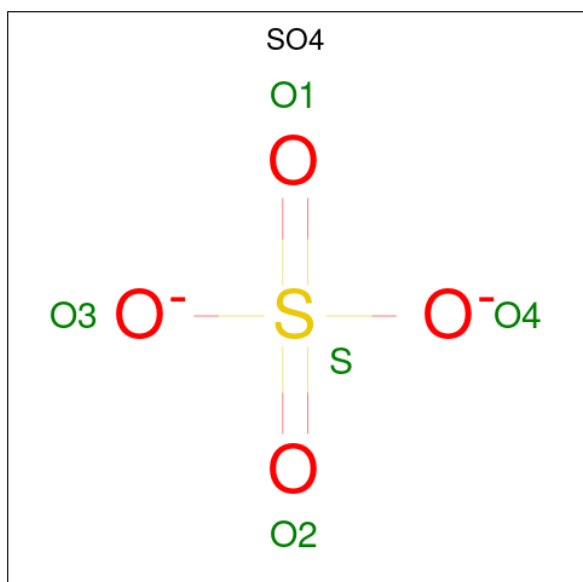
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

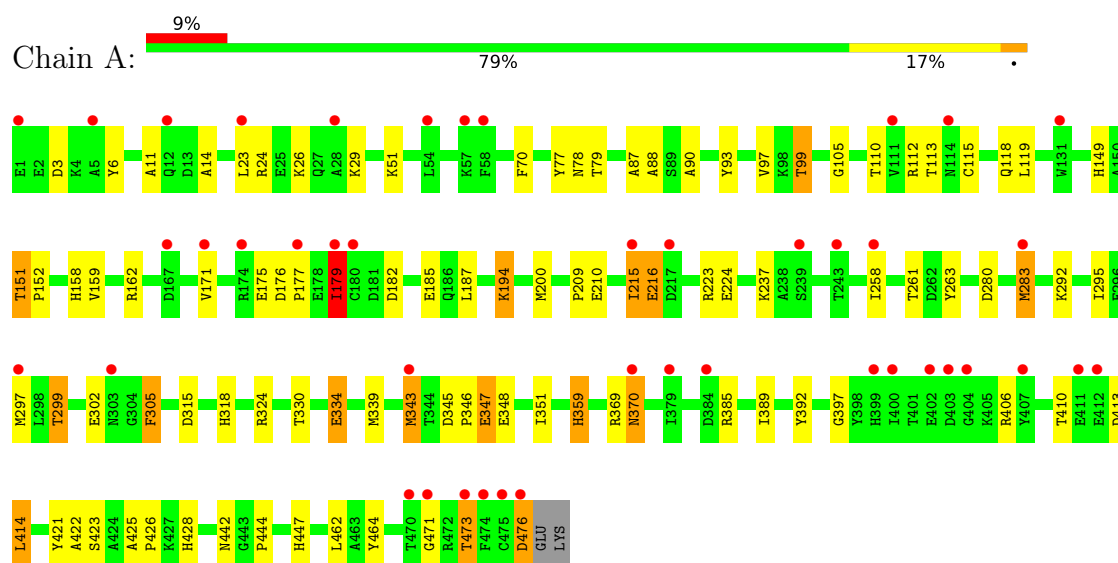
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	51	Total	O	0	0
			51	51		
6	B	51	Total	O	0	0
			51	51		

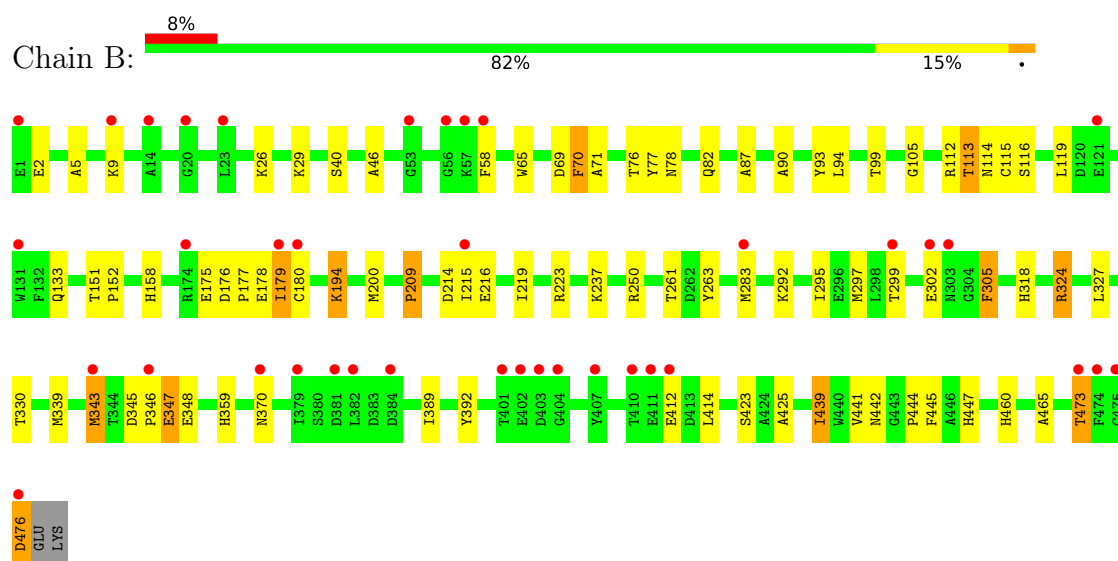
3 Residue-property plots [i](#)

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: alkaline phosphatase



• Molecule 1: alkaline phosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	171.01Å 171.01Å 84.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.53 – 2.00 29.53 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.53-2.00) 98.4 (29.53-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.70 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.215 , 0.238 0.225 , 0.244	Depositor DCC
R_{free} test set	4171 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7618	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8105e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MG, SO4, NAG, ZN

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	1.45	34/3811 (0.9%)	1.25	13/5174 (0.3%)
1	B	1.42	29/3811 (0.8%)	1.23	10/5174 (0.2%)
All	All	1.44	63/7622 (0.8%)	1.24	23/10348 (0.2%)

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	343	MET	SD-CE	-15.82	1.40	1.79
1	A	343	MET	SD-CE	-13.72	1.45	1.79
1	A	263	TYR	CG-CD2	-8.87	1.20	1.39
1	A	339	MET	SD-CE	-8.83	1.57	1.79
1	B	305	PHE	CG-CD2	-8.82	1.20	1.38
1	B	70	PHE	CE2-CZ	-8.60	1.12	1.38
1	B	339	MET	SD-CE	-8.48	1.58	1.79
1	A	70	PHE	CE1-CZ	-8.48	1.13	1.38
1	B	263	TYR	CE1-CZ	-8.38	1.18	1.38
1	A	305	PHE	CE1-CZ	-8.36	1.13	1.38
1	B	263	TYR	CG-CD1	-8.12	1.22	1.39
1	B	263	TYR	CG-CD2	-8.08	1.22	1.39
1	A	70	PHE	CE2-CZ	-7.72	1.15	1.38
1	A	70	PHE	CG-CD1	-7.71	1.22	1.38
1	B	305	PHE	CE2-CZ	-7.65	1.15	1.38
1	A	77	TYR	CG-CD2	-7.59	1.23	1.39
1	A	99	THR	CA-C	-7.54	1.43	1.52
1	A	70	PHE	CG-CD2	-7.51	1.23	1.38
1	A	305	PHE	CE2-CZ	-7.47	1.16	1.38
1	B	305	PHE	CE1-CZ	-7.45	1.16	1.38
1	B	77	TYR	CG-CD1	-7.39	1.23	1.39
1	B	70	PHE	CG-CD2	-7.35	1.23	1.38
1	B	263	TYR	CE2-CZ	-7.33	1.20	1.38
1	A	305	PHE	CG-CD2	-7.23	1.23	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	TYR	CE1-CZ	-7.17	1.21	1.38
1	A	263	TYR	CG-CD1	-7.10	1.24	1.39
1	B	5	ALA	C-O	-7.07	1.15	1.24
1	B	305	PHE	CG-CD1	-6.97	1.24	1.38
1	A	151	THR	N-CA	-6.89	1.41	1.46
1	B	70	PHE	CE1-CZ	-6.83	1.18	1.38
1	B	77	TYR	CE2-CZ	-6.76	1.22	1.38
1	A	263	TYR	CE2-CZ	-6.74	1.22	1.38
1	A	200	MET	SD-CE	-6.74	1.62	1.79
1	B	70	PHE	CG-CD1	-6.71	1.24	1.38
1	B	87	ALA	C-O	-6.63	1.16	1.24
1	A	97	VAL	CA-C	-6.57	1.44	1.52
1	A	305	PHE	CG-CD1	-6.35	1.25	1.38
1	B	46	ALA	CA-CB	-6.34	1.43	1.53
1	A	428	HIS	CA-C	6.32	1.60	1.52
1	A	79	THR	CA-C	-6.27	1.44	1.52
1	A	77	TYR	CE1-CZ	-6.11	1.23	1.38
1	A	77	TYR	CE2-CZ	-5.99	1.23	1.38
1	B	77	TYR	CE1-CZ	-5.91	1.24	1.38
1	B	77	TYR	CG-CD2	-5.88	1.26	1.39
1	B	389	ILE	CA-CB	-5.77	1.48	1.54
1	A	88	ALA	C-O	-5.77	1.17	1.24
1	B	439	ILE	C-O	-5.66	1.18	1.24
1	A	330	THR	C-O	-5.66	1.17	1.24
1	B	113	THR	CA-CB	-5.57	1.46	1.54
1	A	283	MET	SD-CE	-5.53	1.65	1.79
1	B	327	LEU	C-O	-5.47	1.17	1.24
1	A	179	ILE	C-O	-5.46	1.18	1.24
1	B	200	MET	SD-CE	-5.44	1.66	1.79
1	A	187	LEU	C-O	-5.41	1.17	1.24
1	A	351	ILE	CA-CB	-5.35	1.47	1.54
1	B	133	GLN	CA-C	5.29	1.59	1.52
1	B	425	ALA	CA-CB	-5.26	1.47	1.53
1	A	462	LEU	C-O	-5.21	1.18	1.24
1	A	425	ALA	CA-CB	-5.20	1.45	1.53
1	B	465	ALA	CA-CB	-5.18	1.45	1.53
1	A	334	GLU	CA-C	5.10	1.59	1.52
1	A	442	ASN	CG-OD1	-5.07	1.14	1.23
1	A	185	GLU	CA-C	-5.04	1.46	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	9	LYS	N-CA-C	-7.50	103.18	111.36
1	A	426	PRO	CA-C-O	6.91	129.21	121.34
1	B	219	ILE	N-CA-C	-6.82	102.76	108.63
1	A	87	ALA	N-CA-C	6.66	118.33	111.14
1	A	79	THR	N-CA-C	6.65	120.66	112.54
1	B	250	ARG	N-CA-C	6.29	117.80	111.07
1	B	76	THR	N-CA-C	6.24	121.03	113.17
1	A	110	THR	N-CA-C	6.00	118.94	110.23
1	A	14	ALA	N-CA-C	-5.96	104.91	111.82
1	A	215	ILE	N-CA-C	-5.92	101.94	109.58
1	B	209	PRO	N-CA-C	5.78	119.73	111.13
1	A	471	GLY	N-CA-C	-5.65	105.02	112.81
1	A	299	THR	OG1-CB-CG2	-5.62	98.05	109.30
1	B	65	TRP	N-CA-C	-5.57	106.44	113.18
1	A	182	ASP	OD1-CG-OD2	-5.55	109.58	122.90
1	B	412	GLU	N-CA-C	-5.46	105.41	111.36
1	A	422	ALA	N-CA-C	5.39	117.68	110.35
1	A	258	ILE	N-CA-C	5.33	116.06	110.62
1	A	347	GLU	N-CA-C	-5.32	106.74	113.18
1	A	414	LEU	N-CA-C	5.17	118.37	111.75
1	B	324	ARG	CG-CD-NE	-5.07	100.85	112.00
1	B	347	GLU	N-CA-C	-5.07	107.05	113.18
1	B	330	THR	OG1-CB-CG2	-5.05	99.21	109.30

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	3731	0	3517	56	0
1	B	3731	0	3519	62	0
2	A	14	0	13	0	0
2	B	14	0	13	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
6	A	51	0	0	0	0
6	B	51	0	0	2	0
All	All	7618	0	7062	115	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (115) 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:114:ASN:HD21	2:B:483:NAG:C1	1.07	1.65
1:A:292:LYS:HG3	1:A:343:MET:HE1	1.43	0.99
1:B:292:LYS:HG3	1:B:343:MET:HE1	1.43	0.99
1:A:292:LYS:HG3	1:A:343:MET:CE	1.94	0.97
1:B:26:LYS:NZ	1:B:347:GLU:OE1	2.01	0.92
1:B:292:LYS:HG3	1:B:343:MET:CE	2.00	0.92
1:B:114:ASN:HD21	2:B:483:NAG:C2	1.89	0.85
1:A:318:HIS:HB3	1:A:359:HIS:CD2	2.17	0.80
1:A:215:ILE:O	1:A:216:GLU:HB2	1.83	0.77
1:A:23:LEU:HD22	1:A:447:HIS:ND1	2.02	0.75
1:B:114:ASN:CG	2:B:483:NAG:C1	2.58	0.75
1:A:292:LYS:CG	1:A:343:MET:HE1	2.18	0.72
1:A:29:LYS:HE3	1:A:302:GLU:O	1.92	0.70
1:B:158:HIS:HE1	6:B:526:HOH:O	1.74	0.69
1:A:295:ILE:O	1:A:299:THR:HG23	1.94	0.66
1:B:292:LYS:CG	1:B:343:MET:HE1	2.22	0.65
1:B:215:ILE:O	1:B:216:GLU:HB2	1.97	0.65
1:A:113:THR:O	1:A:113:THR:HG22	1.98	0.64
1:B:119:LEU:HD11	1:B:179:ILE:HD11	1.80	0.62
1:A:292:LYS:HG3	1:A:343:MET:HE3	1.81	0.61
1:B:295:ILE:O	1:B:299:THR:HG23	2.00	0.61
1:B:214:ASP:OD2	1:B:215:ILE:O	2.19	0.60
1:A:299:THR:HG22	1:A:305:PHE:CE1	2.36	0.60
1:A:119:LEU:HD11	1:A:179:ILE:HD11	1.83	0.59
1:A:370:ASN:N	1:A:370:ASN:HD22	2.03	0.57
1:A:112:ARG:O	1:A:113:THR:HB	2.03	0.57
1:B:58:PHE:CD2	1:B:370:ASN:OD1	2.57	0.57
1:B:115:CYS:HG	1:B:180:CYS:CB	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:VAL:CG2	1:A:177:PRO:HG3	2.36	0.56
1:B:324:ARG:NH1	1:B:414:LEU:O	2.37	0.56
1:A:119:LEU:CD1	1:A:179:ILE:HD11	2.36	0.56
1:B:119:LEU:CD1	1:B:179:ILE:HD11	2.36	0.56
1:A:299:THR:HG22	1:A:305:PHE:HE1	1.70	0.55
1:A:78:ASN:HB2	1:A:99:THR:O	2.07	0.55
1:B:194:LYS:O	1:B:237:LYS:NZ	2.41	0.54
1:B:115:CYS:HG	1:B:180:CYS:HG	1.53	0.53
1:A:26:LYS:NZ	1:A:347:GLU:OE1	2.31	0.53
1:A:324:ARG:NH1	1:A:414:LEU:O	2.41	0.53
1:B:70:PHE:N	1:B:70:PHE:CD1	2.75	0.53
1:B:261:THR:O	1:B:297:MET:HE1	2.08	0.53
1:B:105:GLY:O	1:B:158:HIS:HD2	1.93	0.52
1:B:26:LYS:HZ2	1:B:347:GLU:HB3	1.74	0.52
1:A:112:ARG:O	1:A:113:THR:CB	2.58	0.52
1:B:70:PHE:CD2	1:B:447:HIS:HA	2.44	0.52
1:B:473:THR:HG22	1:B:476:ASP:H	1.74	0.52
1:B:447:HIS:H	1:B:447:HIS:CD2	2.28	0.52
1:B:151:THR:HB	1:B:152:PRO:CD	2.40	0.51
1:B:112:ARG:O	1:B:113:THR:HB	2.10	0.51
1:B:292:LYS:HG3	1:B:343:MET:HE3	1.89	0.51
1:A:209:PRO:HA	1:A:223:ARG:HB2	1.92	0.51
1:A:315:ASP:OD1	1:A:359:HIS:HE1	1.93	0.51
1:B:78:ASN:HB2	1:B:99:THR:O	2.11	0.51
1:A:473:THR:HG22	1:A:476:ASP:H	1.76	0.50
1:B:29:LYS:HE3	1:B:302:GLU:O	2.12	0.49
1:B:299:THR:HG22	1:B:305:PHE:HE2	1.78	0.49
1:B:90:ALA:HA	1:B:93:TYR:CE2	2.47	0.49
1:A:345:ASP:HB3	1:A:348:GLU:HG2	1.94	0.49
1:A:410:THR:O	1:A:413:ASP:HB2	2.13	0.48
1:A:90:ALA:HA	1:A:93:TYR:CE2	2.48	0.48
1:A:171:VAL:HG22	1:A:177:PRO:HG3	1.96	0.47
1:B:69:ASP:C	1:B:70:PHE:CD1	2.92	0.47
1:B:112:ARG:O	1:B:113:THR:CB	2.63	0.47
1:B:318:HIS:HB3	1:B:359:HIS:CG	2.50	0.47
1:A:473:THR:O	1:A:476:ASP:HB2	2.14	0.47
1:A:369:ARG:HD3	1:B:78:ASN:O	2.14	0.46
1:B:115:CYS:SG	1:B:180:CYS:SG	3.11	0.46
1:B:93:TYR:CD1	1:B:94:LEU:HG	2.50	0.46
1:A:105:GLY:O	1:A:158:HIS:HD2	1.99	0.46
1:B:26:LYS:NZ	1:B:347:GLU:HB3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:GLY:HA3	1:A:421:TYR:O	2.17	0.45
1:A:175:GLU:O	1:A:177:PRO:HD3	2.16	0.45
1:A:151:THR:HB	1:A:152:PRO:CD	2.46	0.45
1:B:392:TYR:O	1:B:423:SER:HA	2.16	0.45
1:B:447:HIS:H	1:B:447:HIS:HD2	1.63	0.45
1:A:194:LYS:O	1:A:237:LYS:NZ	2.50	0.45
1:A:385:ARG:O	1:A:406:ARG:NH2	2.50	0.45
1:B:299:THR:HG22	1:B:305:PHE:CE2	2.52	0.45
1:B:115:CYS:O	1:B:116:SER:C	2.57	0.44
1:A:297:MET:HB3	1:A:297:MET:HE3	1.41	0.44
1:B:114:ASN:OD1	2:B:483:NAG:C1	2.64	0.44
1:B:345:ASP:HB3	1:B:348:GLU:HG2	1.98	0.44
1:B:176:ASP:OD1	1:B:178:GLU:HB2	2.18	0.44
1:A:389:ILE:HD13	1:B:82:GLN:HE22	1.82	0.44
1:A:447:HIS:CD2	1:A:447:HIS:C	2.95	0.43
1:B:40:SER:HB3	1:B:359:HIS:H	1.83	0.43
1:A:176:ASP:OD2	1:A:179:ILE:HG23	2.17	0.43
1:B:209:PRO:HA	1:B:223:ARG:HB2	1.99	0.43
1:B:346:PRO:O	1:B:444:PRO:HD3	2.17	0.43
1:A:24:ARG:HB3	1:A:444:PRO:HA	2.01	0.43
1:A:318:HIS:HB3	1:A:359:HIS:CG	2.54	0.43
1:B:90:ALA:HA	1:B:93:TYR:CZ	2.54	0.43
1:B:113:THR:HG22	1:B:113:THR:O	2.19	0.43
1:A:118:GLN:OE1	1:A:159:VAL:HA	2.19	0.42
1:A:261:THR:O	1:A:297:MET:HE1	2.19	0.42
1:B:71:ALA:O	6:B:490:HOH:O	2.21	0.42
1:A:210:GLU:OE2	1:A:224:GLU:HG2	2.20	0.42
1:B:297:MET:HB3	1:B:297:MET:HE3	1.41	0.42
1:A:3:ASP:O	1:A:6:TYR:HB3	2.20	0.42
1:A:11:ALA:CB	1:B:460:HIS:CD2	3.03	0.42
1:B:71:ALA:HA	1:B:439:ILE:O	2.19	0.42
1:A:280:ASP:CG	1:A:283:MET:HG2	2.45	0.41
1:B:151:THR:HB	1:B:152:PRO:HD3	2.02	0.41
1:A:51:LYS:NZ	1:A:334:GLU:OE2	2.49	0.41
1:A:315:ASP:OD1	1:A:359:HIS:CE1	2.72	0.41
1:A:464:TYR:CD1	1:A:464:TYR:C	2.99	0.41
1:B:58:PHE:CG	1:B:370:ASN:OD1	2.73	0.41
1:B:175:GLU:O	1:B:177:PRO:HD3	2.20	0.41
1:A:93:TYR:OH	1:A:151:THR:HG23	2.21	0.41
1:A:392:TYR:O	1:A:423:SER:HA	2.21	0.41
1:B:473:THR:O	1:B:476:ASP:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ARG:HH11	1:A:162:ARG:HD3	1.72	0.40
1:A:115:CYS:HB3	1:A:175:GLU:OE1	2.21	0.40
1:A:346:PRO:O	1:A:444:PRO:HD3	2.21	0.40
1:B:441:VAL:HG12	1:B:442:ASN:N	2.36	0.40
1:B:445:PHE:HA	1:B:447:HIS:CD2	2.56	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	474/478 (99%)	459 (97%)	14 (3%)	1 (0%)	43	42
1	B	474/478 (99%)	459 (97%)	14 (3%)	1 (0%)	43	42
All	All	948/956 (99%)	918 (97%)	28 (3%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	GLU
1	B	2	GLU

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	394/398 (99%)	387 (98%)	7 (2%)	51	58
1	B	394/398 (99%)	389 (99%)	5 (1%)	61	68
All	All	788/796 (99%)	776 (98%)	12 (2%)	57	64

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
1	A	179	ILE
1	A	194	LYS
1	A	359	HIS
1	A	370	ASN
1	A	473	THR
1	A	476	ASP
1	B	179	ILE
1	B	194	LYS
1	B	283	MET
1	B	473	THR
1	B	476	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	133	GLN
1	A	158	HIS
1	A	228	HIS
1	A	359	HIS
1	A	370	ASN
1	A	399	HIS
1	B	82	GLN
1	B	114	ASN
1	B	133	GLN
1	B	158	HIS
1	B	195	ASN
1	B	228	HIS
1	B	303	ASN
1	B	399	HIS
1	B	418	ASN
1	B	447	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
5	SO4	A	487	-	4,4,4	0.52	0	6,6,6	0.90	0
5	SO4	B	488	-	4,4,4	0.26	0	6,6,6	0.29	0
2	NAG	B	483	1	14,14,15	1.12	2 (14%)	17,19,21	1.80	6 (35%)
2	NAG	A	483	1	14,14,15	1.17	1 (7%)	17,19,21	2.57	6 (35%)
5	SO4	A	486	3	4,4,4	0.26	0	6,6,6	0.69	0
5	SO4	B	487	3	4,4,4	0.41	0	6,6,6	1.19	1 (16%)

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
2	NAG	B	483	1	-	2/6/23/26	0/1/1/1
2	NAG	A	483	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	483	NAG	O5-C1	-3.49	1.37	1.43
2	B	483	NAG	O5-C1	-2.31	1.39	1.43
2	B	483	NAG	C1-C2	-2.27	1.49	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	483	NAG	O5-C1-C2	-6.15	101.77	111.29
2	A	483	NAG	C1-C2-N2	-4.35	103.57	110.43
2	A	483	NAG	C4-C3-C2	-3.88	105.33	111.02
2	A	483	NAG	O3-C3-C4	3.71	119.13	110.38
2	B	483	NAG	C1-C2-N2	-3.31	105.22	110.43
2	B	483	NAG	O6-C6-C5	2.87	121.10	111.33
2	B	483	NAG	C4-C3-C2	-2.81	106.89	111.02
2	A	483	NAG	O7-C7-N2	2.66	126.68	121.98
2	B	483	NAG	C1-O5-C5	2.35	115.33	112.19
2	B	483	NAG	C6-C5-C4	2.35	118.78	113.02
2	B	483	NAG	O3-C3-C4	2.19	115.53	110.38
5	B	487	SO4	O3-S-O2	-2.16	98.27	109.56
2	A	483	NAG	C6-C5-C4	2.06	118.08	113.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	483	NAG	O5-C5-C6-O6
2	A	483	NAG	C4-C5-C6-O6
2	B	483	NAG	C4-C5-C6-O6
2	B	483	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	483	NAG	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	476/478 (99%)	0.56	43 (9%) 15 14	20, 29, 45, 67	0
1	B	476/478 (99%)	0.55	38 (7%) 18 17	19, 29, 45, 67	0
All	All	952/956 (99%)	0.55	81 (8%) 16 15	19, 29, 45, 67	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	179	ILE	4.4
1	A	180	CYS	4.1
1	B	283	MET	4.1
1	A	215	ILE	4.0
1	A	402	GLU	3.9
1	A	476	ASP	3.9
1	B	215	ILE	3.9
1	A	412	GLU	3.9
1	A	303	ASN	3.8
1	A	475	CYS	3.7
1	A	470	THR	3.7
1	A	57	LYS	3.6
1	B	474	PHE	3.6
1	A	403	ASP	3.5
1	A	179	ILE	3.5
1	B	174	ARG	3.4
1	B	382	LEU	3.4
1	B	302	GLU	3.4
1	B	370	ASN	3.3
1	A	283	MET	3.2
1	B	402	GLU	3.1
1	B	412	GLU	3.1
1	A	473	THR	3.0
1	A	474	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	475	CYS	3.0
1	B	411	GLU	2.8
1	A	399	HIS	2.8
1	A	471	GLY	2.8
1	A	54	LEU	2.8
1	B	476	ASP	2.8
1	A	297	MET	2.7
1	B	410	THR	2.7
1	B	404	GLY	2.7
1	B	23	LEU	2.7
1	B	299	THR	2.7
1	B	57	LYS	2.7
1	B	180	CYS	2.6
1	B	303	ASN	2.6
1	A	58	PHE	2.6
1	A	171	VAL	2.6
1	A	131	TRP	2.6
1	A	12	GLN	2.5
1	B	121	GLU	2.5
1	A	411	GLU	2.4
1	A	400	ILE	2.4
1	B	384	ASP	2.4
1	B	401	THR	2.4
1	B	473	THR	2.4
1	B	131	TRP	2.4
1	A	177	PRO	2.4
1	A	370	ASN	2.4
1	B	407	TYR	2.3
1	A	1	GLU	2.3
1	A	174	ARG	2.3
1	A	5	ALA	2.3
1	B	9	LYS	2.3
1	B	1	GLU	2.3
1	A	111	VAL	2.3
1	B	403	ASP	2.3
1	A	404	GLY	2.3
1	B	379	ILE	2.2
1	A	217	ASP	2.2
1	A	239	SER	2.2
1	A	167	ASP	2.2
1	A	343	MET	2.2
1	B	346	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	20	GLY	2.2
1	B	14	ALA	2.1
1	B	381	ASP	2.1
1	B	53	GLY	2.1
1	A	258	ILE	2.1
1	A	379	ILE	2.1
1	A	114	ASN	2.1
1	A	407	TYR	2.1
1	B	56	GLY	2.1
1	B	58	PHE	2.1
1	A	28	ALA	2.1
1	B	343	MET	2.0
1	A	243	THR	2.0
1	A	23	LEU	2.0
1	A	384	ASP	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
5	SO4	B	487	5/5	0.69	0.29	29,33,36,38	5
5	SO4	A	486	5/5	0.75	0.22	26,32,34,37	5
5	SO4	A	487	5/5	0.77	0.23	33,34,38,40	5
5	SO4	B	488	5/5	0.79	0.23	33,37,39,41	5
2	NAG	A	483	14/15	0.83	0.13	35,42,48,49	0
2	NAG	B	483	14/15	0.85	0.14	40,44,55,57	0
4	MG	A	479	1/1	0.86	0.11	30,30,30,30	0
3	ZN	A	485	1/1	0.88	0.22	32,32,32,32	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	B	481	1/1	0.96	0.14	27,27,27,27	1
4	MG	B	482	1/1	0.96	0.10	32,32,32,32	0
3	ZN	B	480	1/1	0.99	0.07	32,32,32,32	0
3	ZN	A	484	1/1	0.99	0.06	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.