



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:22 AM UTC

PDB ID : 1K7H / pdb_00001k7h
Title : CRYSTAL STRUCTURE OF SHRIMP ALKALINE PHOSPHATASE
Authors : De Backer, M.E.; Mc Sweeney, S.; Rasmussen, H.B.; Riise, B.W.; Lindley, P.;
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Deposited on : 2001-10-19
Resolution : 1.92 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

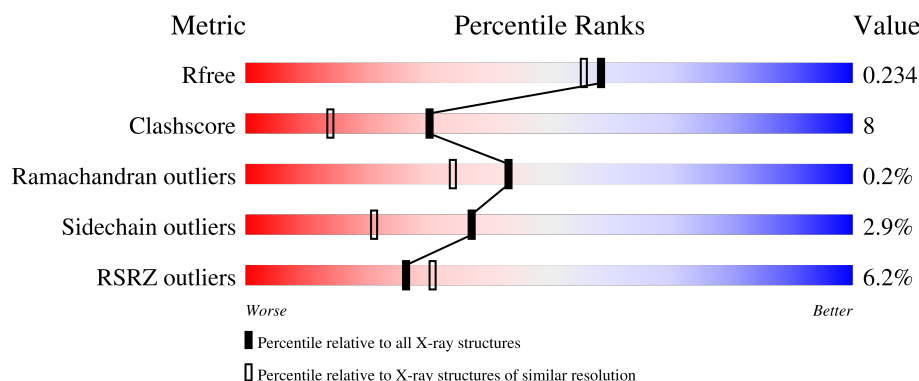
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	476	7% 81% 16% .
1	B	476	6% 83% 14% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8100 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
			3732	2333	629	756	14			
1	B	476	Total	C	N	O	S	0	0	0
			3732	2333	629	756	14			

There are 10 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
A	259	ALA	ARG	conflict	UNP Q9BHT8
A	430	ALA	VAL	conflict	UNP Q9BHT8
B	1	GLU	-	cloning artifact	UNP Q9BHT8
B	2	GLU	-	cloning artifact	UNP Q9BHT8
B	3	ASP	-	cloning artifact	UNP Q9BHT8
B	259	ALA	ARG	conflict	UNP Q9BHT8
B	430	ALA	VAL	conflict	UNP Q9BHT8

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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).

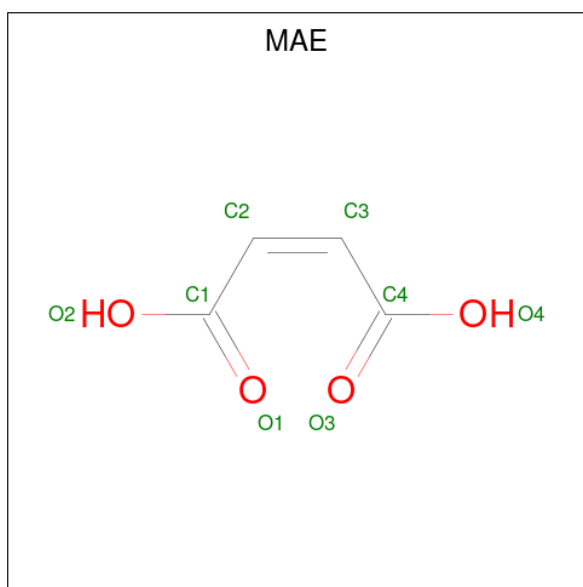
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Zn	0	0
			3	3		
3	B	3	Total	Zn	0	0
			3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is MALEIC ACID (CCD ID: MAE) (formula: C₄H₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	4	4		
5	A	1	Total	C	O	0	0
			8	4	4		
5	B	1	Total	C	O	0	0
			8	4	4		

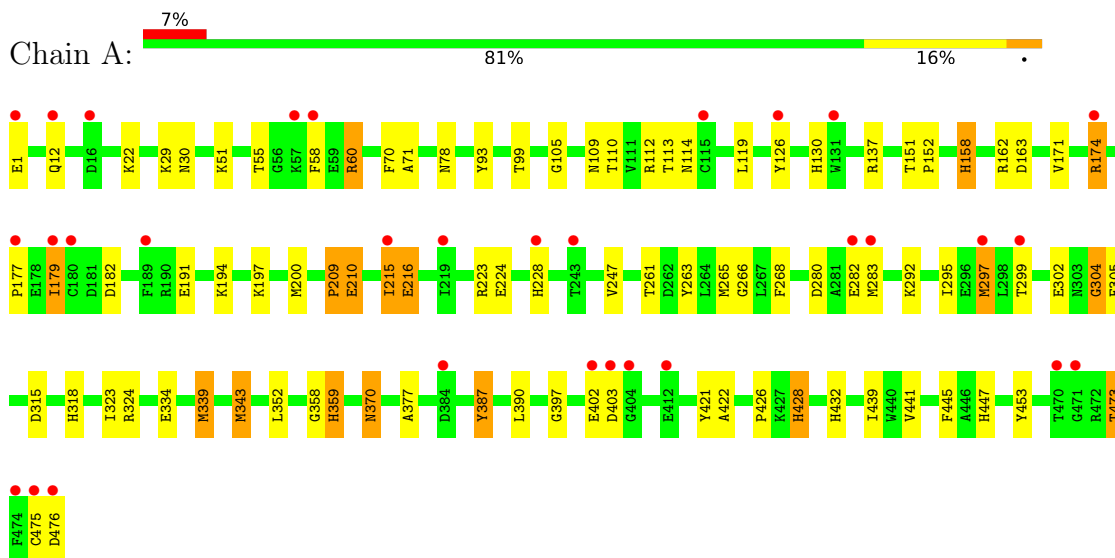
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	294	Total	O	0	0
			294	294		
6	B	254	Total	O	0	0
			254	254		

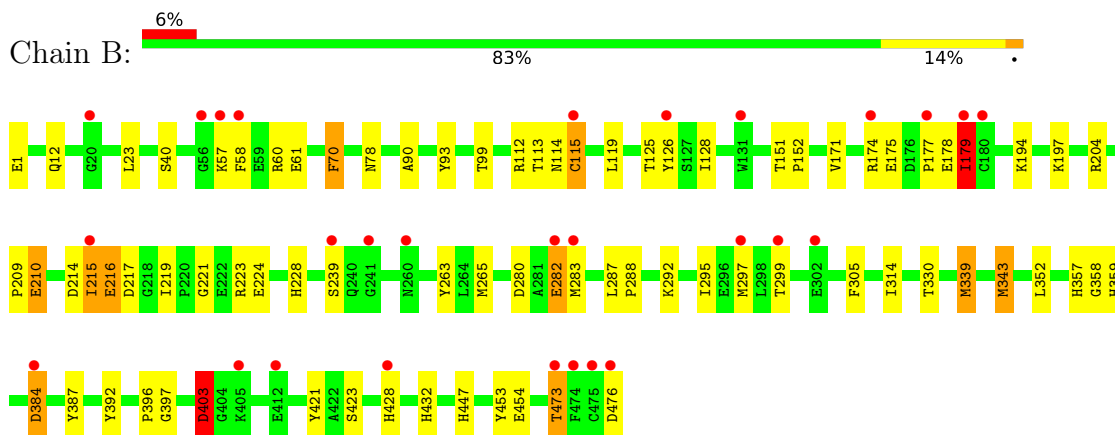
3 Residue-property plots [i](#)

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	171.17Å 171.17Å 84.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.50 – 1.92 119.50 – 1.92	Depositor EDS
% Data completeness (in resolution range)	96.9 (119.50-1.92) 96.9 (119.50-1.92)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.198 , 0.227 0.207 , 0.234	Depositor DCC
R_{free} test set	5156 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8100	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 27.99 % 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 1.9929e-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

5.1 Standard geometry

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

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	1.32	28/3812 (0.7%)	1.20	16/5174 (0.3%)
1	B	1.34	27/3812 (0.7%)	1.20	10/5174 (0.2%)
All	All	1.33	55/7624 (0.7%)	1.20	26/10348 (0.3%)

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	60	ARG	CZ-NH1	-13.55	1.13	1.32
1	B	343	MET	SD-CE	-11.74	1.50	1.79
1	A	60	ARG	CZ-NH1	-11.34	1.16	1.32
1	B	453	TYR	CG-CD2	-10.36	1.17	1.39
1	B	453	TYR	CE1-CZ	-10.11	1.14	1.38
1	A	387	TYR	CG-CD2	-9.58	1.19	1.39
1	A	70	PHE	CE2-CZ	-9.22	1.10	1.38
1	B	70	PHE	CE2-CZ	-9.21	1.11	1.38
1	B	453	TYR	CE2-CZ	-9.21	1.16	1.38
1	A	263	TYR	CE1-CZ	-9.12	1.16	1.38
1	A	126	TYR	CG-CD1	-9.04	1.20	1.39
1	A	343	MET	SD-CE	-8.99	1.57	1.79
1	A	70	PHE	CG-CD1	-8.92	1.20	1.38
1	B	263	TYR	CG-CD1	-8.83	1.20	1.39
1	A	387	TYR	CE1-CZ	-8.79	1.17	1.38
1	A	70	PHE	CG-CD2	-8.55	1.21	1.38
1	A	453	TYR	CG-CD1	-8.43	1.21	1.39
1	A	70	PHE	CE1-CZ	-8.37	1.13	1.38
1	B	70	PHE	CG-CD1	-8.32	1.21	1.38
1	B	70	PHE	CE1-CZ	-8.31	1.13	1.38
1	B	263	TYR	CE1-CZ	-8.30	1.18	1.38
1	B	387	TYR	CE1-CZ	-8.24	1.18	1.38
1	B	263	TYR	CG-CD2	-8.23	1.22	1.39
1	B	453	TYR	CG-CD1	-8.03	1.22	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	TYR	CE2-CZ	-8.01	1.19	1.38
1	A	263	TYR	CG-CD1	-7.95	1.22	1.39
1	B	126	TYR	CG-CD2	-7.95	1.22	1.39
1	A	126	TYR	CE2-CZ	-7.86	1.19	1.38
1	B	126	TYR	CE2-CZ	-7.85	1.19	1.38
1	A	453	TYR	CE2-CZ	-7.81	1.19	1.38
1	A	126	TYR	CE1-CZ	-7.79	1.19	1.38
1	B	387	TYR	CG-CD1	-7.74	1.23	1.39
1	B	339	MET	SD-CE	-7.67	1.60	1.79
1	A	339	MET	SD-CE	-7.66	1.60	1.79
1	A	126	TYR	CG-CD2	-7.57	1.23	1.39
1	A	263	TYR	CG-CD2	-7.53	1.23	1.39
1	A	453	TYR	CG-CD2	-7.42	1.23	1.39
1	B	387	TYR	CE2-CZ	-7.30	1.20	1.38
1	B	126	TYR	CG-CD1	-7.13	1.24	1.39
1	B	387	TYR	CG-CD2	-7.03	1.24	1.39
1	B	70	PHE	CG-CD2	-7.00	1.24	1.38
1	B	126	TYR	CE1-CZ	-6.94	1.21	1.38
1	A	200	MET	SD-CE	-6.70	1.62	1.79
1	A	387	TYR	CG-CD1	-6.45	1.25	1.39
1	A	453	TYR	CE1-CZ	-6.40	1.22	1.38
1	A	265	MET	SD-CE	-6.38	1.63	1.79
1	A	263	TYR	CE2-CZ	-6.16	1.23	1.38
1	A	60	ARG	CZ-NH2	-6.13	1.25	1.33
1	A	387	TYR	CE2-CZ	-5.71	1.24	1.38
1	B	128	ILE	N-CA	-5.56	1.39	1.46
1	A	109	ASN	CA-C	-5.19	1.45	1.52
1	B	60	ARG	CZ-NH2	-5.12	1.26	1.33
1	B	215	ILE	C-O	5.11	1.30	1.24
1	A	428	HIS	CA-C	5.03	1.59	1.52
1	B	454	GLU	N-CA	-5.01	1.40	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	ARG	NE-CZ-NH2	15.20	132.88	119.20
1	A	60	ARG	NE-CZ-NH2	12.22	130.20	119.20
1	B	60	ARG	NH1-CZ-NH2	-9.05	107.53	119.30
1	A	60	ARG	NH1-CZ-NH2	-8.14	108.72	119.30
1	B	174	ARG	CG-CD-NE	7.31	128.09	112.00
1	A	432	HIS	N-CA-C	-6.25	102.72	110.41
1	B	403	ASP	CB-CA-C	-6.00	98.72	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	ARG	CG-CD-NE	5.85	124.86	112.00
1	B	115	CYS	N-CA-C	5.73	117.53	111.28
1	B	297	MET	N-CA-C	5.67	117.26	111.14
1	A	441	VAL	N-CA-C	5.64	116.80	108.45
1	A	209	PRO	N-CA-C	5.64	119.11	111.22
1	A	422	ALA	N-CA-C	5.61	117.97	110.35
1	A	182	ASP	OD1-CG-OD2	-5.53	109.63	122.90
1	A	158	HIS	CB-CG-ND1	5.48	130.91	122.70
1	A	304	GLY	CA-C-O	-5.46	118.52	122.45
1	A	426	PRO	CA-C-O	5.44	127.05	121.23
1	A	268	PHE	N-CA-C	5.31	119.45	112.92
1	A	215	ILE	N-CA-C	-5.22	102.11	109.63
1	A	158	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	A	110	THR	N-CA-C	5.18	117.82	110.10
1	B	174	ARG	NE-CZ-NH2	5.14	123.82	119.20
1	A	297	MET	N-CA-C	5.08	116.63	111.14
1	B	384	ASP	N-CA-C	5.06	119.03	112.86
1	B	179	ILE	CB-CA-C	5.04	115.59	110.65
1	B	125	THR	N-CA-C	-5.03	101.67	109.72

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	3732	0	3522	66	0
1	B	3732	0	3523	54	0
2	A	14	0	13	2	0
2	B	14	0	13	2	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	15	0	0	1	0
4	B	15	0	0	0	0
5	A	16	0	4	2	0
5	B	8	0	2	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	294	0	0	10	0
6	B	254	0	0	3	0
All	All	8100	0	7077	121	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 (121) 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:114:ASN:HD21	2:A:480:NAG:C1	1.05	1.59
1:B:114:ASN:HD21	2:B:480:NAG:C1	1.29	1.43
5:A:487:MAE:O2	6:A:1018:HOH:O	1.52	1.25
1:B:339:MET:SD	1:B:343:MET:HE3	2.14	0.87
1:A:339:MET:SD	1:A:343:MET:HE3	2.15	0.86
1:A:295:ILE:O	1:A:299:THR:HG23	1.78	0.83
1:A:171:VAL:HG23	1:A:177:PRO:HG3	1.62	0.81
1:B:339:MET:SD	1:B:343:MET:CE	2.72	0.78
1:A:299:THR:HG22	1:A:305:PHE:CE1	2.21	0.74
1:B:204:ARG:HD2	5:B:488:MAE:O2	1.88	0.73
1:A:58:PHE:HE1	6:A:904:HOH:O	1.73	0.71
1:A:339:MET:SD	1:A:343:MET:CE	2.78	0.71
1:A:171:VAL:CG2	1:A:177:PRO:HG3	2.20	0.71
1:B:214:ASP:OD2	1:B:215:ILE:O	2.09	0.70
1:A:137:ARG:HD2	6:A:935:HOH:O	1.92	0.70
1:B:23:LEU:HD22	1:B:447:HIS:CD2	2.27	0.69
1:B:23:LEU:HD22	1:B:447:HIS:HD2	1.58	0.69
1:B:171:VAL:HG23	1:B:177:PRO:HG3	1.74	0.68
1:A:318:HIS:HB3	1:A:359:HIS:CD2	2.28	0.67
1:B:295:ILE:O	1:B:299:THR:HG23	1.95	0.67
1:B:209:PRO:HD3	1:B:228:HIS:CD2	2.30	0.65
1:B:209:PRO:HD3	1:B:228:HIS:HD2	1.62	0.64
1:A:370:ASN:N	1:A:370:ASN:HD22	1.95	0.64
1:A:119:LEU:CD1	1:A:179:ILE:HD11	2.29	0.63
1:B:299:THR:HG22	1:B:305:PHE:CE2	2.33	0.63
1:A:445:PHE:CD1	1:A:447:HIS:HE1	2.18	0.62
1:A:55:THR:HB	6:A:741:HOH:O	2.00	0.61
1:B:119:LEU:CD1	1:B:179:ILE:HD11	2.30	0.61
1:A:292:LYS:HG3	1:A:343:MET:HE1	1.83	0.61
1:A:299:THR:HG22	1:A:305:PHE:HE1	1.66	0.61
1:B:209:PRO:CD	1:B:228:HIS:CD2	2.84	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ILE:O	1:B:216:GLU:HB2	2.01	0.60
1:A:377:ALA:HB3	1:A:387:TYR:CE1	2.37	0.60
1:A:119:LEU:HD11	1:A:179:ILE:HD11	1.82	0.60
1:B:171:VAL:CG2	1:B:177:PRO:HG3	2.31	0.60
1:B:58:PHE:HD1	6:B:802:HOH:O	1.85	0.60
1:B:119:LEU:HD11	1:B:179:ILE:HD11	1.84	0.59
1:A:105:GLY:O	1:A:158:HIS:HD2	1.87	0.58
1:B:299:THR:HG22	1:B:305:PHE:HE2	1.69	0.58
1:A:58:PHE:CE1	6:A:904:HOH:O	2.52	0.58
1:A:215:ILE:O	1:A:216:GLU:HB2	2.04	0.57
1:A:197:LYS:HE2	6:A:956:HOH:O	2.05	0.56
1:B:209:PRO:HA	1:B:223:ARG:HB2	1.87	0.56
1:B:473:THR:HG22	1:B:476:ASP:H	1.70	0.56
1:B:292:LYS:HG3	1:B:343:MET:HE1	1.87	0.56
1:A:428:HIS:HD2	1:A:428:HIS:O	1.89	0.55
1:A:292:LYS:HG3	1:A:343:MET:CE	2.38	0.54
1:A:209:PRO:CD	1:A:228:HIS:CD2	2.91	0.53
1:A:114:ASN:CG	2:A:480:NAG:C1	2.74	0.53
1:A:358:GLY:HA3	6:A:641:HOH:O	2.08	0.53
1:A:209:PRO:HA	1:A:223:ARG:HB2	1.89	0.53
1:B:210:GLU:OE2	1:B:224:GLU:HG2	2.10	0.52
1:A:473:THR:HG22	1:A:476:ASP:H	1.74	0.51
1:B:280:ASP:OD1	1:B:282:GLU:HB2	2.10	0.51
1:B:209:PRO:HG2	1:B:228:HIS:HE2	1.76	0.50
1:B:403:ASP:OD1	1:B:403:ASP:N	2.44	0.50
1:A:93:TYR:OH	1:A:151:THR:HG23	2.12	0.50
1:A:22:LYS:O	6:A:774:HOH:O	2.20	0.49
1:B:292:LYS:HG3	1:B:343:MET:CE	2.42	0.49
1:A:352:LEU:C	1:A:352:LEU:HD23	2.38	0.48
1:B:397:GLY:HA3	1:B:421:TYR:O	2.13	0.48
1:B:93:TYR:OH	1:B:151:THR:HG23	2.13	0.47
1:B:428:HIS:C	1:B:428:HIS:CD2	2.92	0.47
1:A:29:LYS:HE2	1:A:302:GLU:O	2.14	0.47
1:B:392:TYR:O	1:B:423:SER:HA	2.13	0.47
1:A:280:ASP:CG	1:A:283:MET:HG3	2.40	0.47
1:A:428:HIS:C	1:A:428:HIS:CD2	2.91	0.47
1:A:210:GLU:OE2	1:A:224:GLU:HG2	2.14	0.47
1:A:51:LYS:NZ	1:A:334:GLU:OE2	2.44	0.47
1:A:209:PRO:HD3	1:A:228:HIS:CD2	2.50	0.46
1:A:445:PHE:CD1	1:A:447:HIS:CE1	3.01	0.46
1:A:402:GLU:HG3	4:A:482:SO4:O2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ASP:CG	1:B:283:MET:HG3	2.40	0.46
1:B:115:CYS:HB3	1:B:175:GLU:OE1	2.15	0.46
1:B:210:GLU:HA	1:B:221:GLY:O	2.17	0.45
1:A:473:THR:O	1:A:476:ASP:HB2	2.17	0.45
1:A:297:MET:HE3	1:A:297:MET:HB3	1.87	0.45
1:B:78:ASN:HB2	1:B:99:THR:O	2.16	0.45
1:B:352:LEU:HD23	1:B:352:LEU:C	2.42	0.44
1:B:217:ASP:HB2	1:B:219:ILE:HG13	2.00	0.44
1:A:171:VAL:CG2	1:A:177:PRO:CG	2.94	0.44
1:A:209:PRO:CD	1:A:228:HIS:HD2	2.30	0.43
1:A:119:LEU:HD13	1:A:179:ILE:HD11	2.00	0.43
1:A:209:PRO:HD3	1:A:228:HIS:HD2	1.83	0.43
1:B:40:SER:HB3	1:B:359:HIS:H	1.84	0.43
1:B:473:THR:O	1:B:476:ASP:HB2	2.18	0.43
1:B:358:GLY:HA3	6:B:676:HOH:O	2.17	0.43
1:B:396:PRO:HG3	1:B:428:HIS:O	2.18	0.43
1:A:215:ILE:HG13	5:A:487:MAE:C4	2.49	0.43
1:B:112:ARG:O	1:B:113:THR:HB	2.19	0.42
1:B:90:ALA:HA	1:B:93:TYR:CE2	2.55	0.42
1:B:70:PHE:CD2	1:B:447:HIS:HA	2.54	0.42
1:B:112:ARG:O	1:B:113:THR:CB	2.65	0.42
1:A:280:ASP:OD1	1:A:282:GLU:HB2	2.19	0.42
1:B:209:PRO:CG	1:B:228:HIS:CD2	3.03	0.42
1:A:162:ARG:HG3	1:A:163:ASP:N	2.34	0.42
1:A:315:ASP:OD1	1:A:359:HIS:HE1	2.01	0.42
1:A:292:LYS:CG	1:A:343:MET:HE1	2.49	0.42
1:A:112:ARG:O	1:A:113:THR:HB	2.20	0.42
1:A:261:THR:O	1:A:297:MET:HE1	2.20	0.42
1:A:71:ALA:HA	1:A:439:ILE:O	2.20	0.41
1:A:113:THR:O	1:A:113:THR:HG22	2.20	0.41
1:A:130:HIS:ND1	1:A:191:GLU:OE1	2.46	0.41
1:B:114:ASN:CG	2:B:480:NAG:C1	2.89	0.41
1:A:30:ASN:OD1	1:A:304:GLY:HA2	2.20	0.41
1:A:324:ARG:NH2	6:A:728:HOH:O	2.53	0.41
1:B:119:LEU:HD13	1:B:179:ILE:HD11	2.00	0.41
1:B:314:ILE:HD11	1:B:330:THR:HA	2.02	0.41
1:A:315:ASP:OD1	1:A:359:HIS:CE1	2.74	0.41
1:A:151:THR:HB	1:A:152:PRO:CD	2.51	0.41
1:A:397:GLY:HA3	1:A:421:TYR:O	2.21	0.41
1:B:57:LYS:HD2	1:B:61:GLU:OE1	2.21	0.41
1:B:151:THR:HB	1:B:152:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:HIS:NE2	1:B:432:HIS:CE1	2.89	0.41
1:A:78:ASN:HB2	1:A:99:THR:O	2.21	0.40
1:B:197:LYS:HE2	6:B:931:HOH:O	2.21	0.40
1:A:247:VAL:O	1:A:266:GLY:HA2	2.21	0.40
1:A:323:ILE:HG12	1:A:390:LEU:HD13	2.03	0.40
1:A:359:HIS:HD2	6:A:501:HOH:O	2.04	0.40
1:A:473:THR:HG22	1:A:475:CYS:N	2.36	0.40
1:B:287:LEU:N	1:B:288:PRO:CD	2.84	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	474/476 (100%)	460 (97%)	13 (3%)	1 (0%)	43	34
1	B	474/476 (100%)	460 (97%)	13 (3%)	1 (0%)	43	34
All	All	948/952 (100%)	920 (97%)	26 (3%)	2 (0%)	43	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	GLU
1	B	216	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	394/394 (100%)	383 (97%)	11 (3%)	38	22
1	B	394/394 (100%)	382 (97%)	12 (3%)	36	20
All	All	788/788 (100%)	765 (97%)	23 (3%)	37	21

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	12	GLN
1	A	60	ARG
1	A	174	ARG
1	A	179	ILE
1	A	194	LYS
1	A	210	GLU
1	A	359	HIS
1	A	370	ASN
1	A	403	ASP
1	A	473	THR
1	B	1	GLU
1	B	12	GLN
1	B	178	GLU
1	B	179	ILE
1	B	194	LYS
1	B	210	GLU
1	B	239	SER
1	B	265	MET
1	B	282	GLU
1	B	384	ASP
1	B	403	ASP
1	B	473	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	158	HIS
1	A	303	ASN
1	A	359	HIS
1	A	370	ASN

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Mol	Chain	Res	Type
1	A	428	HIS
1	A	447	HIS
1	B	82	GLN
1	B	114	ASN
1	B	133	GLN
1	B	303	ASN
1	B	418	ASN
1	B	428	HIS
1	B	447	HIS

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](#)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	$\# Z > 2$
4	SO4	A	481	-	4,4,4	0.27	0	6,6,6	0.48	0
5	MAE	A	489	-	7,7,7	1.93	3 (42%)	8,8,8	2.14	3 (37%)
5	MAE	A	487	-	7,7,7	1.94	3 (42%)	8,8,8	2.14	3 (37%)
4	SO4	A	482	-	4,4,4	0.27	0	6,6,6	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAE	B	488	-	7,7,7	1.94	3 (42%)	8,8,8	2.14	3 (37%)
2	NAG	B	480	1	14,14,15	0.62	0	17,19,21	1.40	4 (23%)
4	SO4	B	485	-	4,4,4	0.29	0	6,6,6	0.71	0
4	SO4	B	484	-	4,4,4	0.34	0	6,6,6	0.37	0
2	NAG	A	480	1	14,14,15	1.09	1 (7%)	17,19,21	1.96	4 (23%)
4	SO4	B	486	-	4,4,4	0.39	0	6,6,6	0.26	0
4	SO4	A	483	-	4,4,4	0.31	0	6,6,6	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAE	A	489	-	-	0/5/5/5	-
5	MAE	A	487	-	-	0/5/5/5	-
5	MAE	B	488	-	-	0/5/5/5	-
2	NAG	A	480	1	-	0/6/23/26	0/1/1/1
2	NAG	B	480	1	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	480	NAG	O5-C1	-2.81	1.39	1.43
5	B	488	MAE	O2-C1	-2.68	1.23	1.30
5	A	489	MAE	O2-C1	-2.68	1.23	1.30
5	A	487	MAE	O2-C1	-2.66	1.23	1.30
5	A	487	MAE	O4-C4	-2.57	1.23	1.30
5	A	489	MAE	O4-C4	-2.52	1.24	1.30
5	B	488	MAE	O4-C4	-2.51	1.24	1.30
5	B	488	MAE	C3-C4	-2.30	1.42	1.48
5	A	487	MAE	C3-C4	-2.27	1.42	1.48
5	A	489	MAE	C3-C4	-2.25	1.42	1.48

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	480	NAG	O6-C6-C5	4.05	125.14	111.33
5	A	487	MAE	O2-C1-O1	-3.77	115.03	122.70
5	B	488	MAE	O2-C1-O1	-3.76	115.05	122.70
5	A	489	MAE	O2-C1-O1	-3.74	115.08	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	480	NAG	C1-C2-N2	-3.69	104.62	110.43
2	A	480	NAG	O3-C3-C4	3.62	118.91	110.38
5	B	488	MAE	O4-C4-O3	-3.54	115.49	122.70
5	A	487	MAE	O4-C4-O3	-3.53	115.51	122.70
5	A	489	MAE	O4-C4-O3	-3.53	115.52	122.70
2	B	480	NAG	C1-O5-C5	3.07	116.31	112.19
2	A	480	NAG	C6-C5-C4	2.95	120.26	113.02
2	B	480	NAG	C6-C5-C4	2.56	119.31	113.02
2	B	480	NAG	O6-C6-C5	2.47	119.74	111.33
5	A	489	MAE	O1-C1-C2	2.34	128.23	121.06
5	A	487	MAE	O1-C1-C2	2.33	128.21	121.06
5	B	488	MAE	O1-C1-C2	2.32	128.18	121.06
2	B	480	NAG	O3-C3-C4	2.12	115.39	110.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	487	MAE	2	0
4	A	482	SO4	1	0
5	B	488	MAE	1	0
2	B	480	NAG	2	0
2	A	480	NAG	2	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	476/476 (100%)	0.49	31 (6%) 25 29	19, 27, 40, 59	0
1	B	476/476 (100%)	0.51	28 (5%) 28 32	18, 27, 40, 59	0
All	All	952/952 (100%)	0.50	59 (6%) 26 31	18, 27, 40, 59	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	476	ASP	5.3
1	A	215	ILE	4.9
1	B	179	ILE	4.9
1	A	179	ILE	4.5
1	A	470	THR	4.2
1	A	474	PHE	4.0
1	A	476	ASP	3.8
1	B	239	SER	3.7
1	A	471	GLY	3.6
1	B	474	PHE	3.6
1	A	131	TRP	3.5
1	A	12	GLN	3.4
1	A	403	ASP	3.3
1	A	174	ARG	3.3
1	B	215	ILE	3.2
1	A	177	PRO	3.2
1	A	1	GLU	3.2
1	B	299	THR	3.1
1	B	302	GLU	3.0
1	B	180	CYS	2.9
1	B	384	ASP	2.9
1	B	428	HIS	2.9
1	B	126	TYR	2.9
1	A	412	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	126	TYR	2.8
1	B	177	PRO	2.8
1	B	58	PHE	2.7
1	B	475	CYS	2.6
1	B	20	GLY	2.6
1	A	16	ASP	2.6
1	B	174	ARG	2.6
1	A	404	GLY	2.6
1	A	180	CYS	2.6
1	A	283	MET	2.6
1	A	58	PHE	2.5
1	B	282	GLU	2.5
1	B	57	LYS	2.5
1	A	57	LYS	2.5
1	B	473	THR	2.5
1	A	228	HIS	2.5
1	B	241	GLY	2.4
1	A	282	GLU	2.4
1	B	260	ASN	2.4
1	A	115	CYS	2.4
1	B	405	LYS	2.4
1	B	56	GLY	2.4
1	A	297	MET	2.4
1	A	384	ASP	2.3
1	A	402	GLU	2.3
1	B	283	MET	2.3
1	A	475	CYS	2.3
1	B	412	GLU	2.3
1	B	297	MET	2.3
1	B	115	CYS	2.3
1	B	131	TRP	2.2
1	A	189	PHE	2.2
1	A	219	ILE	2.1
1	A	243	THR	2.0
1	A	299	THR	2.0

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

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
4	SO4	B	486	5/5	0.72	0.14	63,64,64,66	0
4	SO4	A	483	5/5	0.76	0.15	58,62,64,64	0
2	NAG	B	480	14/15	0.76	0.16	46,48,54,57	0
4	SO4	A	482	5/5	0.79	0.19	51,54,54,55	0
5	MAE	B	488	8/8	0.79	0.23	67,69,74,79	0
2	NAG	A	480	14/15	0.81	0.16	36,41,47,48	0
4	SO4	B	484	5/5	0.81	0.16	45,48,54,54	0
5	MAE	A	487	8/8	0.82	0.23	67,69,74,79	0
4	SO4	B	485	5/5	0.85	0.16	50,50,52,54	0
5	MAE	A	489	8/8	0.89	0.18	67,69,74,79	0
4	SO4	A	481	5/5	0.90	0.10	48,48,52,53	0
3	ZN	A	477	1/1	0.99	0.05	23,23,23,23	0
3	ZN	A	479	1/1	0.99	0.05	27,27,27,27	1
3	ZN	B	477	1/1	0.99	0.04	22,22,22,22	0
3	ZN	A	478	1/1	1.00	0.02	23,23,23,23	0
3	ZN	B	478	1/1	1.00	0.01	22,22,22,22	0
3	ZN	B	479	1/1	1.00	0.09	28,28,28,28	1

6.5 Other polymers [i](#)

There are no such residues in this entry.