



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 07:22 PM BST

PDB ID : 1SHQ  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

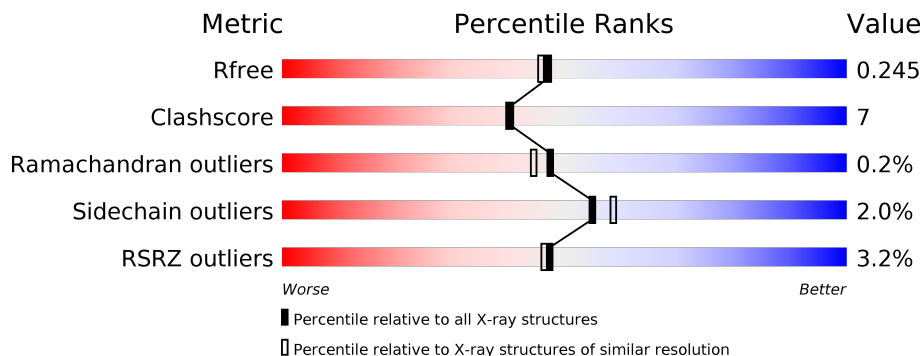
# 1 Overall quality at a glance

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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	B	478	

## 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.

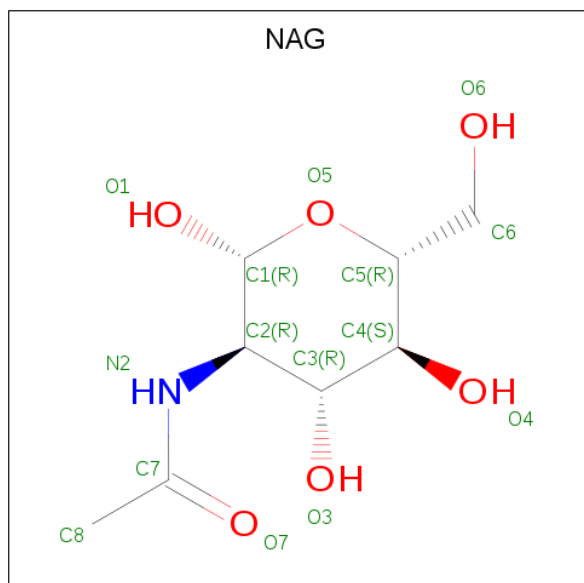
- Molecule 1 is a protein called alkaline phosphatase.

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

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 (three-letter code: 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		

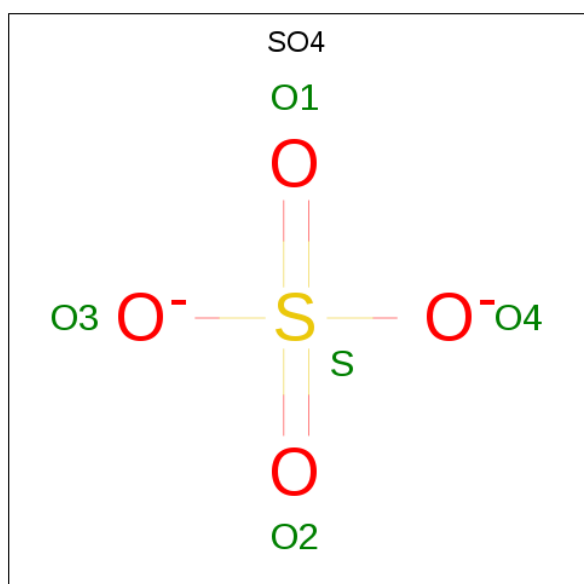
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

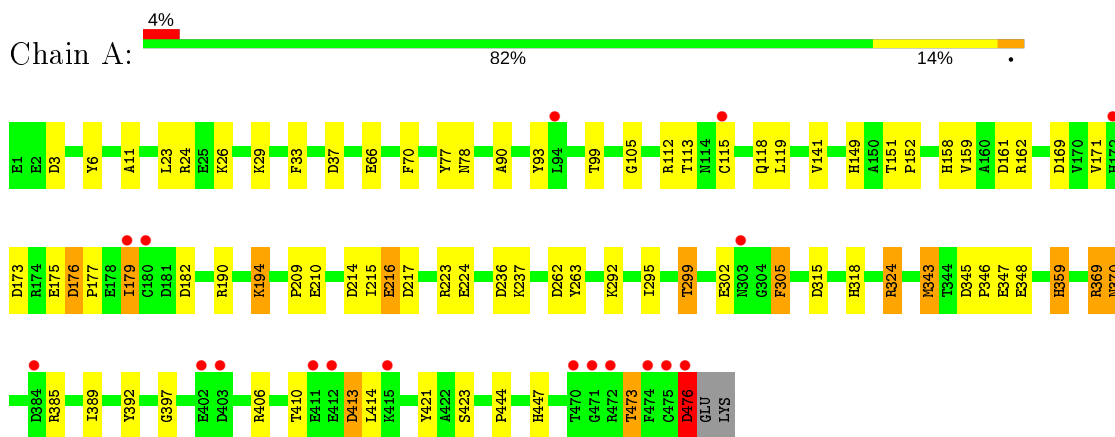
- Molecule 6 is water.

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

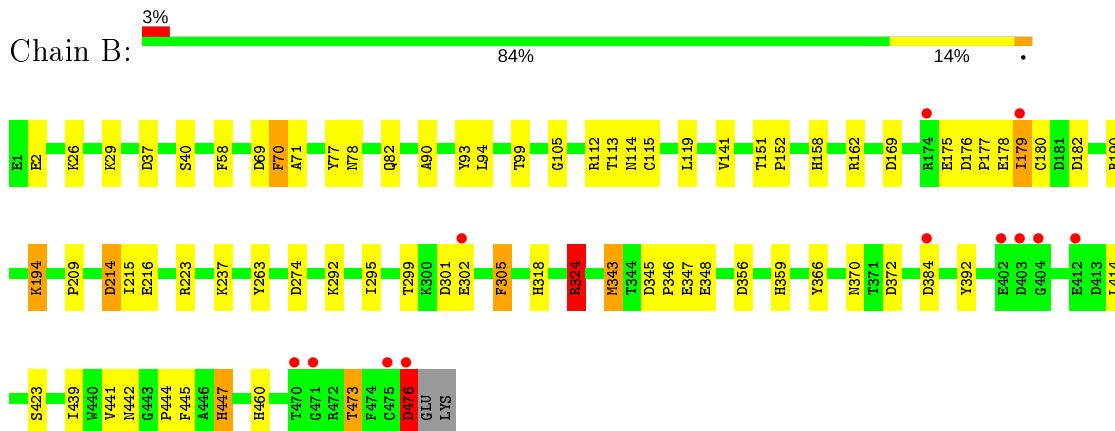
### 3 Residue-property plots [i](#)

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: 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, $\alpha$ , $\beta$ , $\gamma$	171.01Å 171.01Å 84.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.53 – 2.00 29.71 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.53-2.00) 98.5 (29.71-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.70 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.215 , 0.238 0.225 , 0.245	Depositor DCC
$R_{free}$ test set	4171 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtrriage
Anisotropy	0.015	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 39.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7618	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

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

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	1.28	19/3811 (0.5%)	1.12	25/5174 (0.5%)
1	B	1.27	19/3811 (0.5%)	1.11	19/5174 (0.4%)
All	All	1.28	38/7622 (0.5%)	1.11	44/10348 (0.4%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	TYR	CE1-CZ	-15.69	1.18	1.38
1	A	263	TYR	CG-CD2	-14.18	1.20	1.39
1	B	263	TYR	CE2-CZ	-13.76	1.20	1.38
1	A	263	TYR	CE1-CZ	-13.47	1.21	1.38
1	B	263	TYR	CG-CD1	-12.97	1.22	1.39
1	B	263	TYR	CG-CD2	-12.90	1.22	1.39
1	B	70	PHE	CE2-CZ	-12.89	1.12	1.37
1	A	70	PHE	CE1-CZ	-12.71	1.13	1.37
1	B	77	TYR	CE2-CZ	-12.70	1.22	1.38
1	A	263	TYR	CE2-CZ	-12.68	1.22	1.38
1	A	305	PHE	CE1-CZ	-12.52	1.13	1.37
1	B	305	PHE	CG-CD2	-12.29	1.20	1.38
1	A	77	TYR	CG-CD2	-12.11	1.23	1.39
1	B	77	TYR	CG-CD1	-11.78	1.23	1.39
1	A	77	TYR	CE1-CZ	-11.52	1.23	1.38
1	A	70	PHE	CE2-CZ	-11.50	1.15	1.37
1	B	305	PHE	CE2-CZ	-11.39	1.15	1.37
1	A	263	TYR	CG-CD1	-11.31	1.24	1.39
1	A	77	TYR	CE2-CZ	-11.30	1.23	1.38
1	B	77	TYR	CE1-CZ	-11.14	1.24	1.38
1	A	305	PHE	CE2-CZ	-11.12	1.16	1.37
1	B	305	PHE	CE1-CZ	-11.08	1.16	1.37
1	A	70	PHE	CG-CD1	-10.73	1.22	1.38
1	A	70	PHE	CG-CD2	-10.45	1.23	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	PHE	CG-CD2	-10.23	1.23	1.38
1	B	70	PHE	CE1-CZ	-10.11	1.18	1.37
1	A	305	PHE	CG-CD2	-10.05	1.23	1.38
1	B	305	PHE	CG-CD1	-9.70	1.24	1.38
1	B	77	TYR	CG-CD2	-9.35	1.26	1.39
1	B	70	PHE	CG-CD1	-9.32	1.24	1.38
1	A	305	PHE	CG-CD1	-8.83	1.25	1.38
1	A	77	TYR	CG-CD1	-7.80	1.29	1.39
1	B	343	MET	SD-CE	-6.76	1.40	1.77
1	A	343	MET	SD-CE	-5.82	1.45	1.77
1	B	141	VAL	CB-CG2	-5.71	1.40	1.52
1	A	66	GLU	CD-OE1	5.43	1.31	1.25
1	B	366	TYR	CE1-CZ	-5.15	1.31	1.38
1	A	141	VAL	CB-CG2	-5.10	1.42	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	ASP	CB-CG-OD2	9.46	126.82	118.30
1	A	182	ASP	CB-CG-OD2	8.92	126.33	118.30
1	B	182	ASP	CB-CG-OD2	7.51	125.06	118.30
1	A	182	ASP	OD1-CG-OD2	-7.22	109.58	123.30
1	A	169	ASP	CB-CG-OD2	7.14	124.73	118.30
1	A	214	ASP	CB-CG-OD2	6.72	124.34	118.30
1	B	356	ASP	CB-CG-OD1	6.67	124.30	118.30
1	A	176	ASP	CB-CG-OD2	6.65	124.29	118.30
1	B	476	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	182	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	263	TYR	CB-CG-CD1	6.07	124.64	121.00
1	A	70	PHE	CB-CG-CD2	5.93	124.95	120.80
1	A	305	PHE	CB-CG-CD1	5.93	124.95	120.80
1	A	190	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	274	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	37	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	77	TYR	CZ-CE2-CD2	5.86	125.07	119.80
1	B	77	TYR	CD1-CE1-CZ	5.85	125.06	119.80
1	A	217	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	77	TYR	CB-CG-CD1	5.71	124.43	121.00
1	B	214	ASP	CB-CG-OD2	5.64	123.37	118.30
1	A	161	ASP	CB-CG-OD2	5.63	123.36	118.30
1	B	182	ASP	OD1-CG-OD2	-5.50	112.85	123.30
1	B	384	ASP	CB-CG-OD2	5.50	123.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	A	305	PHE	CD1-CG-CD2	-5.47	111.19	118.30
1	B	37	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	262	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	190	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	263	TYR	CZ-CE2-CD2	5.40	124.66	119.80
1	A	173	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	236	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	413	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	77	TYR	CD1-CG-CD2	-5.29	112.08	117.90
1	A	476	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	263	TYR	CD1-CG-CD2	-5.29	112.08	117.90
1	A	369	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	B	324	ARG	CG-CD-NE	-5.22	100.85	111.80
1	A	299	THR	OG1-CB-CG2	-5.19	98.05	110.00
1	B	263	TYR	CB-CG-CD1	5.13	124.08	121.00
1	B	324	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	70	PHE	CD1-CG-CD2	-5.10	111.67	118.30
1	B	301	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	372	ASP	CB-CG-OD2	5.06	122.86	118.30

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	49	0
1	B	3731	0	3519	58	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
4	B	1	0	0	0	0
5	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	104	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 7.

All (104) 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:HE3	1.33	1.07
1:A:292:LYS:HG3	1:A:343:MET:CE	1.94	0.97
1:B:292:LYS:HG3	1:B:343:MET:HE3	1.47	0.96
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:A:29:LYS:HE3	1:A:302:GLU:O	1.92	0.70
1:B:114:ASN:CG	2:B:483:NAG:C1	2.58	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: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: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:B:292:LYS:HG3	1:B:343:MET:HE1	1.83	0.58
1:A:112:ARG:O	1:A:113:THR:HB	2.03	0.57
1:A:370:ASN:HD22	1:A:370:ASN:N	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:324:ARG:NH1	1:A:414:LEU:O	2.41	0.53
1:A:26:LYS:NZ	1:A:347:GLU:OE1	2.31	0.53
1:B:70:PHE:N	1:B:70:PHE:CD1	2.75	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:THR:HG22	1:B:305:PHE:CE2	2.52	0.45
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: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:318:HIS:HB3	1:A:359:HIS:CG	2.54	0.43
1:A:24:ARG:HB3	1:A:444:PRO:HA	2.01	0.43
1:B:113:THR:O	1:B:113:THR:HG22	2.19	0.43
1:B:90:ALA:HA	1:B:93:TYR:CZ	2.54	0.43
1:A:118:GLN:OE1	1:A:159:VAL:HA	2.19	0.42
1:B:69:ASP:C	1:B:70:PHE:CD1	2.92	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:A:292:LYS:HG3	1:A:343:MET:HE1	1.94	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:B:151:THR:HB	1:B:152:PRO:HD3	2.02	0.41
1:A:315:ASP:OD1	1:A:359:HIS:CE1	2.72	0.41
1:B:175:GLU:O	1:B:177:PRO:HD3	2.20	0.41
1:B:58:PHE:CG	1:B:370:ASN:OD1	2.73	0.41
1:A:392:TYR:O	1:A:423:SER:HA	2.21	0.41
1:A:93:TYR:OH	1:A:151:THR:HG23	2.21	0.41
1:B:441:VAL:HG12	1:B:442:ASN:N	2.36	0.41
1:B:473:THR:O	1:B:476:ASP:HB2	2.20	0.40
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: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%)	47	44
1	B	474/478 (99%)	459 (97%)	14 (3%)	1 (0%)	47	44
All	All	948/956 (99%)	918 (97%)	28 (3%)	2 (0%)	47	44

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%)	385 (98%)	9 (2%)	50	53
1	B	394/398 (99%)	387 (98%)	7 (2%)	59	63
All	All	788/796 (99%)	772 (98%)	16 (2%)	55	58

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	PHE
1	A	149	HIS
1	A	179	ILE
1	A	194	LYS

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Mol	Chain	Res	Type
1	A	324	ARG
1	A	359	HIS
1	A	370	ASN
1	A	473	THR
1	A	476	ASP
1	B	162	ARG
1	B	179	ILE
1	B	194	LYS
1	B	324	ARG
1	B	447	HIS
1	B	473	THR
1	B	476	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	133	GLN
1	A	158	HIS
1	A	195	ASN
1	A	322	GLN
1	A	359	HIS
1	A	370	ASN
1	B	82	GLN
1	B	114	ASN
1	B	133	GLN
1	B	158	HIS
1	B	195	ASN
1	B	322	GLN
1	B	418	ASN
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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	B	488	-	4,4,4	0.19	0	6,6,6	0.30	0
5	SO4	A	487	-	4,4,4	0.45	0	6,6,6	0.90	0
2	NAG	B	483	1	14,14,15	1.11	2 (14%)	17,19,21	1.80	6 (35%)
5	SO4	A	486	3	4,4,4	0.22	0	6,6,6	0.74	0
2	NAG	A	483	1	14,14,15	1.21	1 (7%)	17,19,21	2.54	6 (35%)
5	SO4	B	487	3	4,4,4	0.33	0	6,6,6	1.17	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	-3.68	1.37	1.43
2	B	483	NAG	O5-C1	-2.45	1.39	1.43
2	B	483	NAG	C1-C2	-2.06	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	-6.03	101.77	111.29
2	A	483	NAG	C1-C2-N2	-4.05	103.57	110.49
2	A	483	NAG	C4-C3-C2	-3.88	105.33	111.02
2	A	483	NAG	O3-C3-C4	3.80	119.13	110.35
2	B	483	NAG	C1-C2-N2	-3.08	105.22	110.49
2	B	483	NAG	O6-C6-C5	2.86	121.10	111.29
2	B	483	NAG	C4-C3-C2	-2.81	106.89	111.02
2	A	483	NAG	O7-C7-N2	2.57	126.68	121.95
2	B	483	NAG	C6-C5-C4	2.46	118.78	113.00
2	B	483	NAG	C1-O5-C5	2.32	115.33	112.19
2	B	483	NAG	O3-C3-C4	2.24	115.53	110.35
2	A	483	NAG	C6-C5-C4	2.17	118.08	113.00
5	B	487	SO4	O3-S-O2	-2.11	98.27	109.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	483	NAG	C4-C5-C6-O6
2	A	483	NAG	O5-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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	476/478 (99%)	0.13	18 (3%) 40 39	20, 29, 45, 67	0
1	B	476/478 (99%)	0.17	12 (2%) 57 56	19, 29, 45, 67	0
All	All	952/956 (99%)	0.15	30 (3%) 47 46	19, 29, 45, 67	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	475	CYS	6.7
1	A	476	ASP	5.7
1	B	402	GLU	4.5
1	A	402	GLU	4.2
1	B	475	CYS	4.1
1	A	470	THR	3.7
1	B	403	ASP	3.7
1	B	179	ILE	3.6
1	B	302	GLU	3.2
1	B	476	ASP	3.1
1	A	303	ASN	3.0
1	A	412	GLU	3.0
1	A	474	PHE	2.8
1	A	384	ASP	2.8
1	A	403	ASP	2.8
1	B	412	GLU	2.7
1	A	180	CYS	2.6
1	B	384	ASP	2.5
1	B	471	GLY	2.4
1	A	172	HIS	2.4
1	B	174	ARG	2.4
1	A	115	CYS	2.3
1	B	404	GLY	2.3
1	A	94	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	472	ARG	2.3
1	A	471	GLY	2.3
1	B	470	THR	2.2
1	A	415	LYS	2.1
1	A	411	GLU	2.1
1	A	179	ILE	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 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	MG	A	479	1/1	0.66	0.11	30,30,30,30	0
5	SO4	A	487	5/5	0.81	0.21	33,34,38,40	5
5	SO4	B	487	5/5	0.83	0.34	29,33,36,38	5
2	NAG	A	483	14/15	0.86	0.22	35,42,48,49	0
2	NAG	B	483	14/15	0.88	0.20	40,44,55,57	0
5	SO4	B	488	5/5	0.91	0.18	33,37,39,41	5
5	SO4	A	486	5/5	0.95	0.18	26,32,34,37	5
3	ZN	A	485	1/1	0.95	0.17	32,32,32,32	1
4	MG	B	482	1/1	0.97	0.04	32,32,32,32	0
3	ZN	A	484	1/1	0.99	0.03	33,33,33,33	0
3	ZN	B	481	1/1	0.99	0.11	27,27,27,27	1
3	ZN	B	480	1/1	1.00	0.03	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.