



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 8, 2018 – 07:48 AM EST

PDB ID : 6BV3
Title : Crystal structure of porcine aminopeptidase-N with Leucine
Authors : Chen, L.; Lin, Y.-L.; Li, F.
Deposited on : 2017-12-12
Resolution : 2.20 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

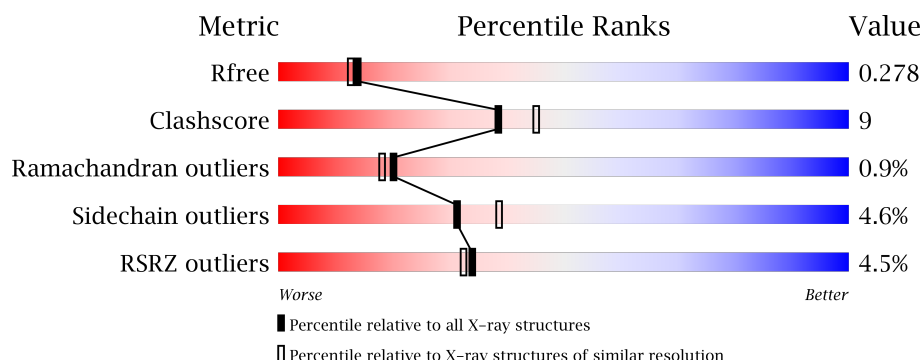
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	902	<div> <div>5%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1004	-	-	-	X
2	NAG	A	1011	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LEU	A	1024	-	-	-	X
4	SO4	A	1025	-	-	X	X
4	SO4	A	1026	-	-	-	X
4	SO4	A	1027	-	-	X	X
4	SO4	A	1028	-	-	-	X
4	SO4	A	1029	-	-	-	X
4	SO4	A	1031	-	-	-	X
4	SO4	A	1032	-	-	-	X
4	SO4	A	1033	-	-	-	X
4	SO4	A	1035	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8376 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.

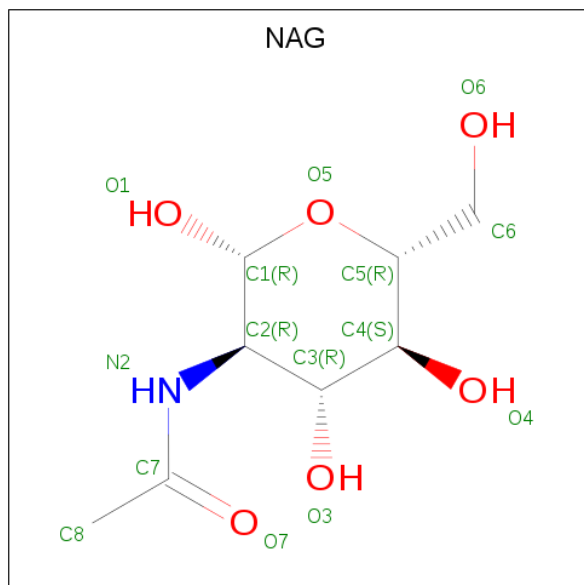
- Molecule 1 is a protein called Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	902	7241	4622	1210	1379	30	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	PHE	LEU	conflict	UNP P15145
A	964	SER	-	expression tag	UNP P15145

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



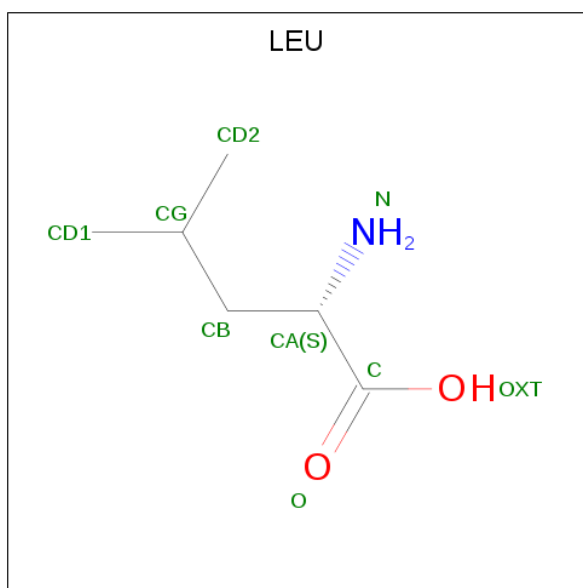
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0

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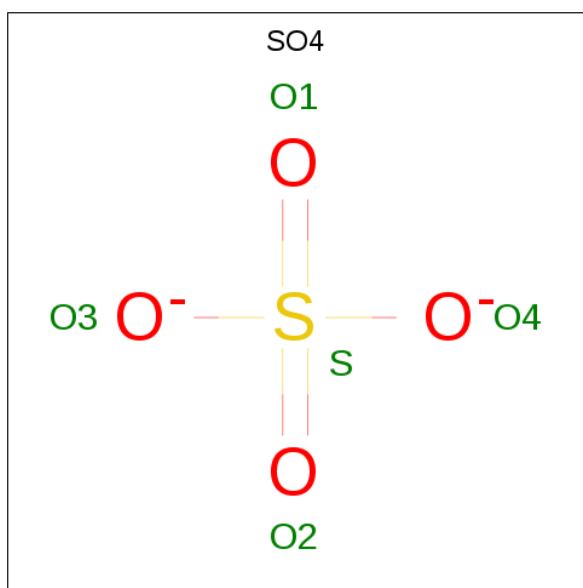
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1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

- Molecule 3 is LEUCINE (three-letter code: LEU) (formula: $C_6H_{13}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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		

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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	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	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

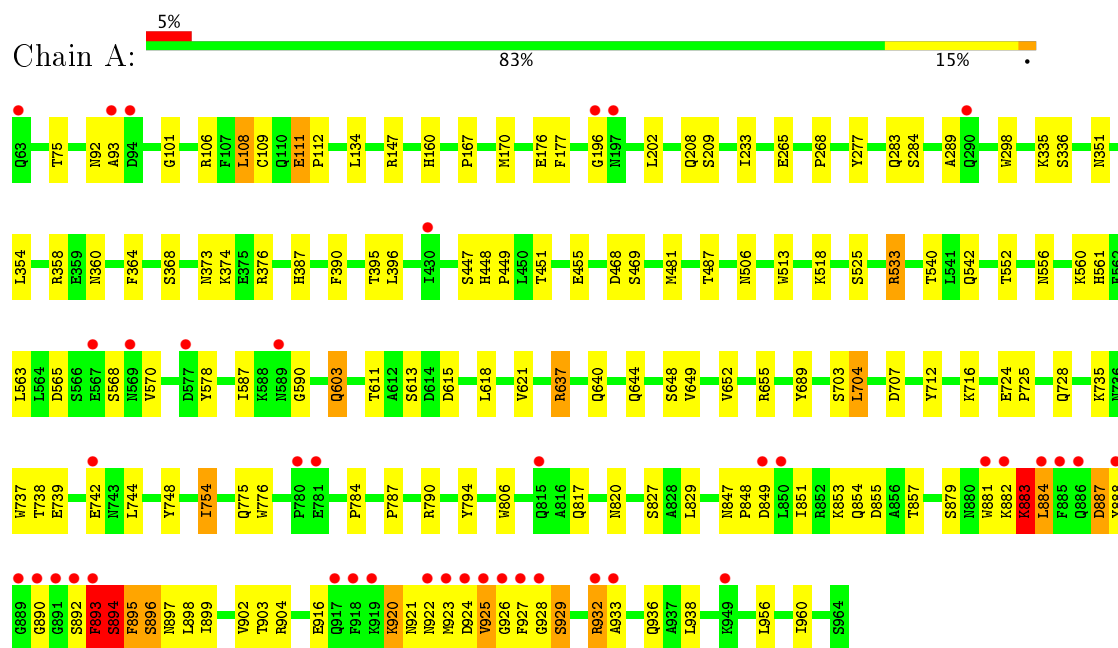
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	748	Total	O	0	0
			748	748		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Aminopeptidase N



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	259.55Å 62.98Å 81.65Å 90.00° 100.38° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 47.67 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-2.20) 98.9 (47.67-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.212 , 0.270 0.215 , 0.278	Depositor DCC
R_{free} test set	3309 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8376	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: ZN, NAG, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.77	2/7429 (0.0%)	0.68	1/10124 (0.0%)

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	A	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	GLU	CD-OE2	5.53	1.31	1.25
1	A	455	GLU	CD-OE1	5.04	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	ARG	NE-CZ-NH1	6.10	123.35	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	883	LYS	Peptide
1	A	887	ASP	Peptide
1	A	894	SER	Peptide
1	A	920	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	A	93	ALA	Peptide

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	7241	0	6994	121	0
2	A	322	0	287	4	0
3	A	9	0	10	2	0
4	A	55	0	0	8	1
5	A	1	0	0	0	0
6	A	748	0	0	34	1
All	All	8376	0	7291	128	1

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 9.

All (128) 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:637:ARG:NH2	1:A:640:GLN:HE22	1.11	1.40
1:A:451:THR:HG22	6:A:1252:HOH:O	1.35	1.25
1:A:637:ARG:NH2	1:A:640:GLN:NE2	1.87	1.21
1:A:637:ARG:HH21	1:A:640:GLN:NE2	1.40	1.20
1:A:637:ARG:HH21	1:A:640:GLN:CD	1.69	0.94
1:A:637:ARG:HH22	1:A:640:GLN:HE22	1.07	0.94
1:A:560:LYS:NZ	6:A:1101:HOH:O	2.00	0.93
1:A:111:GLU:HG2	6:A:1692:HOH:O	1.73	0.88
1:A:817:GLN:NE2	6:A:1104:HOH:O	2.06	0.88
1:A:360:ASN:OD1	4:A:1035:SO4:O4	1.93	0.86
1:A:932:ARG:O	1:A:936:GLN:HG3	1.75	0.86
2:A:1005:NAG:H62	2:A:1006:NAG:H61	1.59	0.84
1:A:883:LYS:HD3	1:A:883:LYS:O	1.78	0.84
1:A:926:GLY:C	1:A:927:PHE:CD1	2.57	0.78
1:A:176:GLU:OE1	6:A:1102:HOH:O	2.02	0.78
1:A:924:ASP:O	1:A:926:GLY:N	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:ASP:HB3	1:A:568:SER:OG	1.85	0.76
1:A:929:SER:HB2	6:A:1578:HOH:O	1.86	0.75
1:A:883:LYS:CD	1:A:883:LYS:O	2.35	0.74
4:A:1026:SO4:O2	6:A:1106:HOH:O	2.06	0.73
4:A:1027:SO4:O2	6:A:1105:HOH:O	2.06	0.72
1:A:374:LYS:HE2	6:A:1144:HOH:O	1.92	0.70
1:A:374:LYS:CE	6:A:1144:HOH:O	2.39	0.69
1:A:283:GLN:OE1	6:A:1107:HOH:O	2.11	0.67
1:A:208:GLN:HG2	3:A:1024:LEU:HG	1.75	0.67
1:A:289:ALA:HB2	6:A:1681:HOH:O	1.94	0.66
1:A:896:SER:OG	1:A:933:ALA:HB2	1.97	0.65
1:A:448:HIS:HD2	1:A:449:PRO:O	1.80	0.65
1:A:533:ARG:NH2	6:A:1103:HOH:O	2.05	0.64
1:A:373:ASN:ND2	6:A:1112:HOH:O	2.29	0.64
1:A:395:THR:O	1:A:506:ASN:HA	1.98	0.64
1:A:921:ASN:ND2	6:A:1116:HOH:O	2.31	0.63
1:A:611:THR:HG21	6:A:1162:HOH:O	1.97	0.63
1:A:929:SER:CB	6:A:1578:HOH:O	2.44	0.63
1:A:884:LEU:HD12	1:A:895:PHE:CE2	2.34	0.62
1:A:742:GLU:HB3	6:A:1122:HOH:O	1.98	0.62
1:A:883:LYS:CD	1:A:883:LYS:C	2.68	0.62
1:A:820:ASN:HB2	6:A:1504:HOH:O	2.01	0.60
4:A:1031:SO4:O2	6:A:1109:HOH:O	2.15	0.60
1:A:92:ASN:HB3	6:A:1150:HOH:O	2.01	0.60
1:A:933:ALA:HA	1:A:936:GLN:OE1	2.02	0.59
1:A:883:LYS:CG	1:A:883:LYS:O	2.50	0.59
1:A:899:ILE:O	1:A:903:THR:HG23	2.02	0.59
1:A:160:HIS:ND1	6:A:1114:HOH:O	2.31	0.58
1:A:108:LEU:HD12	1:A:109:CYS:N	2.18	0.58
1:A:652:VAL:HA	1:A:655:ARG:HG3	1.86	0.58
1:A:806:TRP:CE2	1:A:829:LEU:HD22	2.39	0.57
1:A:896:SER:HB2	6:A:1578:HOH:O	2.05	0.56
1:A:927:PHE:CD1	1:A:927:PHE:N	2.74	0.55
1:A:108:LEU:CD1	1:A:109:CYS:N	2.69	0.55
1:A:724:GLU:HB3	1:A:725:PRO:HD3	1.88	0.55
1:A:533:ARG:NH1	6:A:1103:HOH:O	2.40	0.55
1:A:884:LEU:HD12	1:A:895:PHE:CD2	2.43	0.54
1:A:712:TYR:CE2	1:A:716:LYS:HD2	2.43	0.54
1:A:265:GLU:HG3	6:A:1751:HOH:O	2.09	0.53
1:A:884:LEU:HD22	1:A:925:VAL:O	2.09	0.53
1:A:857:THR:HB	1:A:898:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:SER:OG	1:A:897:ASN:ND2	2.43	0.52
1:A:637:ARG:HD2	1:A:640:GLN:OE1	2.09	0.52
4:A:1025:SO4:O2	6:A:1110:HOH:O	2.18	0.52
1:A:561:HIS:HB2	1:A:578:TYR:HB3	1.92	0.52
1:A:737:TRP:CZ3	1:A:754:ILE:HD11	2.45	0.52
1:A:742:GLU:N	6:A:1122:HOH:O	2.36	0.52
1:A:202:LEU:C	1:A:202:LEU:HD12	2.30	0.52
1:A:396:LEU:O	4:A:1025:SO4:O3	2.28	0.52
1:A:451:THR:HG23	1:A:540:THR:HB	1.92	0.52
1:A:112:PRO:HD3	1:A:167:PRO:HG3	1.92	0.51
1:A:916:GLU:OE2	1:A:938:LEU:HD22	2.10	0.51
1:A:787:PRO:HA	1:A:790:ARG:HD2	1.92	0.51
1:A:728:GLN:HA	1:A:728:GLN:OE1	2.11	0.50
1:A:364:PHE:CZ	1:A:374:LYS:HD2	2.47	0.50
1:A:689:TYR:CD1	1:A:748:TYR:HB3	2.47	0.50
1:A:108:LEU:HD22	1:A:170:MET:HG2	1.93	0.49
1:A:790:ARG:HG2	1:A:794:TYR:CZ	2.47	0.49
1:A:542:GLN:OE1	1:A:578:TYR:HA	2.12	0.49
1:A:351:ASN:HB2	1:A:354:LEU:O	2.13	0.49
1:A:556:ASN:HD22	2:A:1018:NAG:H83	1.78	0.48
1:A:387:HIS:HA	1:A:390:PHE:O	2.13	0.48
1:A:884:LEU:HA	1:A:895:PHE:CE2	2.49	0.48
1:A:108:LEU:C	1:A:108:LEU:HD12	2.35	0.47
1:A:560:LYS:CE	6:A:1101:HOH:O	2.57	0.47
1:A:603:GLN:HB2	1:A:603:GLN:HE21	1.56	0.47
1:A:847:ASN:OD1	1:A:849:ASP:HB2	2.14	0.47
1:A:106:ARG:HG2	1:A:170:MET:CE	2.44	0.47
1:A:368:SER:O	1:A:787:PRO:HB3	2.15	0.47
1:A:704:LEU:HD22	6:A:1496:HOH:O	2.14	0.47
1:A:956:LEU:O	1:A:960:ILE:HG13	2.15	0.47
1:A:106:ARG:HG2	1:A:170:MET:HE1	1.97	0.47
1:A:921:ASN:OD1	1:A:921:ASN:O	2.32	0.46
2:A:1012:NAG:H3	6:A:1449:HOH:O	2.14	0.46
1:A:108:LEU:CD1	1:A:108:LEU:C	2.84	0.46
1:A:881:TRP:O	1:A:883:LYS:N	2.49	0.46
1:A:898:LEU:O	1:A:902:VAL:HG12	2.15	0.46
1:A:587:ILE:HG22	1:A:618:LEU:HB3	1.98	0.45
1:A:289:ALA:CB	6:A:1681:HOH:O	2.61	0.45
1:A:448:HIS:HE1	1:A:468:ASP:OD2	1.99	0.45
1:A:565:ASP:HB3	1:A:568:SER:HG	1.80	0.45
1:A:735:LYS:HG3	1:A:739:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ARG:NH2	4:A:1027:SO4:O1	2.50	0.44
1:A:563:LEU:HD11	1:A:570:VAL:CG2	2.48	0.44
1:A:284:SER:HB3	1:A:298:TRP:CD2	2.53	0.43
1:A:358:ARG:HD3	1:A:376:ARG:NH2	2.33	0.43
1:A:208:GLN:HA	1:A:209:SER:HA	1.82	0.43
1:A:892:SER:O	1:A:893:PHE:CB	2.67	0.43
1:A:590:GLY:HA3	1:A:649:VAL:HG13	2.00	0.42
1:A:196:GLY:N	6:A:1154:HOH:O	2.52	0.42
1:A:552:THR:HB	1:A:611:THR:HG22	2.02	0.42
1:A:883:LYS:HG2	1:A:883:LYS:O	2.20	0.42
1:A:637:ARG:NH2	1:A:640:GLN:OE1	2.47	0.42
3:A:1024:LEU:C	6:A:1257:HOH:O	2.58	0.42
1:A:853:LYS:C	1:A:855:ASP:H	2.23	0.42
1:A:170:MET:HE2	1:A:170:MET:HB3	1.82	0.42
1:A:447:SER:OG	1:A:448:HIS:N	2.52	0.42
1:A:926:GLY:C	1:A:927:PHE:CG	2.93	0.41
1:A:358:ARG:NH2	6:A:1155:HOH:O	2.52	0.41
1:A:481:MET:HB3	1:A:481:MET:HE2	1.95	0.41
1:A:848:PRO:HA	1:A:851:ILE:O	2.21	0.41
1:A:893:PHE:HB3	1:A:895:PHE:CE1	2.55	0.41
1:A:75:THR:HG22	1:A:111:GLU:HB2	2.03	0.41
1:A:108:LEU:HD12	1:A:109:CYS:O	2.20	0.41
1:A:621:VAL:HG11	2:A:1021:NAG:H82	2.01	0.41
1:A:707:ASP:HA	1:A:712:TYR:CG	2.55	0.41
1:A:233:ILE:HD12	4:A:1028:SO4:O1	2.20	0.41
1:A:776:TRP:HB2	1:A:784:PRO:HD2	2.02	0.40
1:A:892:SER:O	1:A:893:PHE:HB2	2.21	0.40
1:A:637:ARG:HA	1:A:637:ARG:HD3	1.75	0.40
1:A:888:TYR:CE2	1:A:928:GLY:HA3	2.57	0.40
1:A:101:GLY:HA3	1:A:177:PHE:CE1	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1029:SO4:O1	6:A:1159:HOH:O[2_556]	1.59	0.61

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	900/902 (100%)	853 (95%)	39 (4%)	8 (1%)	20 18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	882	LYS
1	A	883	LYS
1	A	893	PHE
1	A	895	PHE
1	A	890	GLY
1	A	925	VAL
1	A	487	THR
1	A	894	SER

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	797/797 (100%)	760 (95%)	37 (5%)	31 39

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	134	LEU
1	A	268	PRO

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Mol	Chain	Res	Type
1	A	277	TYR
1	A	335	LYS
1	A	336	SER
1	A	469	SER
1	A	513	TRP
1	A	518	LYS
1	A	525	SER
1	A	533	ARG
1	A	603	GLN
1	A	613	SER
1	A	615	ASP
1	A	637	ARG
1	A	644	GLN
1	A	648	SER
1	A	703	SER
1	A	704	LEU
1	A	738	THR
1	A	744	LEU
1	A	754	ILE
1	A	775	GLN
1	A	827	SER
1	A	854	GLN
1	A	879	SER
1	A	883	LYS
1	A	884	LEU
1	A	887	ASP
1	A	893	PHE
1	A	896	SER
1	A	904	ARG
1	A	920	LYS
1	A	922	ASN
1	A	923	MET
1	A	929	SER
1	A	932	ARG

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

Mol	Chain	Res	Type
1	A	208	GLN
1	A	283	GLN
1	A	448	HIS
1	A	500	HIS

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Mol	Chain	Res	Type
1	A	603	GLN
1	A	640	GLN
1	A	764	GLN
1	A	886	GLN
1	A	897	ASN
1	A	917	GLN
1	A	921	ASN
1	A	922	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 1 is monoatomic - leaving 35 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	$\# Z > 2$
2	NAG	A	1001	1,2	14,14,15	0.88	1 (7%)	15,19,21	1.18	1 (6%)
2	NAG	A	1002	2	14,14,15	0.76	0	15,19,21	1.66	2 (13%)
2	NAG	A	1003	2	14,14,15	1.22	1 (7%)	15,19,21	1.49	2 (13%)
2	NAG	A	1004	1,2	14,14,15	0.51	0	15,19,21	1.35	2 (13%)
2	NAG	A	1005	2	14,14,15	1.02	1 (7%)	15,19,21	1.84	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1006	2	14,14,15	0.93	1 (7%)	15,19,21	1.94	3 (20%)
2	NAG	A	1007	1,2	14,14,15	0.88	0	15,19,21	0.85	0
2	NAG	A	1008	2	14,14,15	0.82	0	15,19,21	1.48	4 (26%)
2	NAG	A	1009	1,2	14,14,15	0.74	0	15,19,21	1.23	2 (13%)
2	NAG	A	1010	2	14,14,15	0.86	0	15,19,21	1.60	4 (26%)
2	NAG	A	1011	1,2	14,14,15	0.60	0	15,19,21	1.40	3 (20%)
2	NAG	A	1012	2	14,14,15	0.79	0	15,19,21	1.84	6 (40%)
2	NAG	A	1013	2	14,14,15	0.92	1 (7%)	15,19,21	1.20	2 (13%)
2	NAG	A	1014	1,2	14,14,15	0.89	1 (7%)	15,19,21	1.25	2 (13%)
2	NAG	A	1015	2	14,14,15	0.78	0	15,19,21	1.34	3 (20%)
2	NAG	A	1016	1,2	14,14,15	0.71	0	15,19,21	1.58	3 (20%)
2	NAG	A	1017	2	14,14,15	0.53	0	15,19,21	1.72	3 (20%)
2	NAG	A	1018	1,2	14,14,15	0.69	0	15,19,21	1.55	3 (20%)
2	NAG	A	1019	2	14,14,15	0.76	0	15,19,21	1.25	1 (6%)
2	NAG	A	1020	1	14,14,15	1.16	1 (7%)	15,19,21	1.83	3 (20%)
2	NAG	A	1021	1,2	14,14,15	0.48	0	15,19,21	0.98	2 (13%)
2	NAG	A	1022	2	14,14,15	0.74	0	15,19,21	1.53	2 (13%)
2	NAG	A	1023	1	14,14,15	0.80	1 (7%)	15,19,21	1.52	1 (6%)
3	LEU	A	1024	-	4,8,8	0.57	0	5,10,10	0.85	0
4	SO4	A	1025	-	4,4,4	1.47	0	6,6,6	1.21	1 (16%)
4	SO4	A	1026	-	4,4,4	1.82	1 (25%)	6,6,6	0.98	0
4	SO4	A	1027	-	4,4,4	1.94	1 (25%)	6,6,6	0.43	0
4	SO4	A	1028	-	4,4,4	1.48	1 (25%)	6,6,6	1.29	1 (16%)
4	SO4	A	1029	-	4,4,4	1.03	0	6,6,6	0.68	0
4	SO4	A	1030	-	4,4,4	1.46	0	6,6,6	0.69	0
4	SO4	A	1031	-	4,4,4	2.12	2 (50%)	6,6,6	0.60	0
4	SO4	A	1032	-	4,4,4	1.69	1 (25%)	6,6,6	0.47	0
4	SO4	A	1033	-	4,4,4	2.06	2 (50%)	6,6,6	0.71	0
4	SO4	A	1034	-	4,4,4	1.69	1 (25%)	6,6,6	0.41	0
4	SO4	A	1035	-	4,4,4	1.05	0	6,6,6	0.27	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
2	NAG	A	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1003	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1004	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1005	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1006	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1007	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1008	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1009	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1010	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1011	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1012	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1013	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1014	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1015	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1016	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1017	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1018	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1019	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1020	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1021	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1022	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1023	1	-	0/6/23/26	0/1/1/1
3	LEU	A	1024	-	-	0/4/8/8	0/0/0/0
4	SO4	A	1025	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1026	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1027	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1028	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1029	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1030	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1031	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1032	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1033	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1034	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1035	-	-	0/0/0/0	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1005	NAG	O5-C1	-2.10	1.40	1.43
2	A	1001	NAG	C2-N2	-2.06	1.42	1.46
2	A	1023	NAG	C1-C2	2.01	1.55	1.52
4	A	1034	SO4	O1-S	2.10	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1033	SO4	O2-S	2.15	1.57	1.45
2	A	1013	NAG	O7-C7	2.19	1.28	1.23
4	A	1028	SO4	O2-S	2.22	1.57	1.45
2	A	1014	NAG	O5-C1	2.29	1.47	1.43
4	A	1032	SO4	O1-S	2.38	1.58	1.45
2	A	1006	NAG	O7-C7	2.40	1.28	1.23
4	A	1031	SO4	O1-S	2.42	1.58	1.45
2	A	1020	NAG	O5-C1	2.44	1.47	1.43
4	A	1026	SO4	O2-S	2.58	1.59	1.45
4	A	1031	SO4	O2-S	2.87	1.61	1.45
4	A	1027	SO4	O2-S	3.08	1.62	1.45
4	A	1033	SO4	O1-S	3.14	1.62	1.45
2	A	1003	NAG	C1-C2	3.45	1.57	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1023	NAG	O5-C1-C2	-5.38	103.99	111.47
2	A	1017	NAG	O5-C1-C2	-4.41	105.33	111.47
2	A	1020	NAG	C1-O5-C5	-3.91	106.78	112.17
2	A	1005	NAG	O3-C3-C4	-3.39	102.98	110.36
2	A	1012	NAG	C1-C2-N2	-3.33	104.79	110.49
2	A	1005	NAG	C2-N2-C7	-3.28	118.15	122.94
2	A	1006	NAG	O3-C3-C4	-3.01	103.80	110.36
2	A	1015	NAG	O5-C1-C2	-2.98	107.32	111.47
2	A	1016	NAG	O5-C1-C2	-2.86	107.49	111.47
2	A	1011	NAG	C2-N2-C7	-2.85	118.78	122.94
2	A	1003	NAG	C1-C2-N2	-2.76	105.78	110.49
2	A	1006	NAG	C6-C5-C4	-2.75	106.56	113.00
2	A	1009	NAG	O4-C4-C3	-2.67	104.54	110.36
2	A	1014	NAG	C1-O5-C5	-2.66	108.50	112.17
2	A	1020	NAG	O5-C1-C2	-2.61	107.84	111.47
2	A	1022	NAG	C4-C3-C2	-2.56	107.27	111.02
2	A	1008	NAG	O5-C1-C2	-2.53	107.96	111.47
2	A	1015	NAG	C4-C3-C2	-2.46	107.42	111.02
2	A	1010	NAG	O7-C7-C8	-2.45	117.60	122.06
2	A	1009	NAG	O7-C7-C8	-2.44	117.62	122.06
2	A	1017	NAG	O7-C7-C8	-2.42	117.65	122.06
2	A	1010	NAG	C3-C4-C5	-2.35	106.08	110.22
2	A	1004	NAG	O5-C1-C2	-2.31	108.25	111.47
2	A	1021	NAG	O7-C7-C8	-2.30	117.87	122.06
2	A	1011	NAG	O4-C4-C3	-2.30	105.35	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1014	NAG	C3-C4-C5	-2.30	106.17	110.22
2	A	1008	NAG	O3-C3-C4	-2.29	105.37	110.36
2	A	1010	NAG	C4-C3-C2	-2.25	107.72	111.02
2	A	1016	NAG	C1-C2-N2	-2.19	106.75	110.49
2	A	1013	NAG	C4-C3-C2	-2.17	107.84	111.02
2	A	1008	NAG	C1-O5-C5	-2.15	109.20	112.17
2	A	1019	NAG	C4-C3-C2	-2.15	107.87	111.02
2	A	1017	NAG	C2-N2-C7	-2.14	119.82	122.94
2	A	1012	NAG	O4-C4-C3	-2.11	105.76	110.36
2	A	1002	NAG	O4-C4-C3	-2.11	105.77	110.36
2	A	1015	NAG	C2-N2-C7	-2.11	119.86	122.94
2	A	1018	NAG	C6-C5-C4	-2.08	108.13	113.00
2	A	1008	NAG	C2-N2-C7	-2.06	119.94	122.94
2	A	1012	NAG	O5-C1-C2	-2.03	108.64	111.47
2	A	1012	NAG	C1-O5-C5	-2.02	109.38	112.17
2	A	1005	NAG	C1-C2-N2	-2.02	107.04	110.49
4	A	1028	SO4	O4-S-O2	2.03	120.43	109.26
2	A	1013	NAG	C3-C4-C5	2.03	113.80	110.22
2	A	1021	NAG	O7-C7-N2	2.31	126.36	121.92
2	A	1001	NAG	C1-O5-C5	2.51	115.62	112.17
4	A	1025	SO4	O4-S-O3	2.63	120.80	108.96
2	A	1011	NAG	C1-C2-N2	2.72	115.13	110.49
2	A	1004	NAG	C2-N2-C7	2.82	127.05	122.94
2	A	1012	NAG	C3-C4-C5	2.90	115.32	110.22
2	A	1018	NAG	C3-C4-C5	2.98	115.47	110.22
2	A	1010	NAG	C1-C2-N2	3.12	115.81	110.49
2	A	1012	NAG	C4-C3-C2	3.38	115.97	111.02
2	A	1018	NAG	C1-O5-C5	3.43	116.89	112.17
2	A	1016	NAG	C1-O5-C5	3.83	117.45	112.17
2	A	1003	NAG	C4-C3-C2	3.86	116.67	111.02
2	A	1022	NAG	C1-O5-C5	3.92	117.58	112.17
2	A	1020	NAG	C2-N2-C7	4.37	129.32	122.94
2	A	1002	NAG	C4-C3-C2	4.51	117.63	111.02
2	A	1006	NAG	C1-O5-C5	5.83	120.21	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1005	NAG	1	0
2	A	1006	NAG	1	0
2	A	1012	NAG	1	0
2	A	1018	NAG	1	0
2	A	1021	NAG	1	0
3	A	1024	LEU	2	0
4	A	1025	SO4	2	0
4	A	1026	SO4	1	0
4	A	1027	SO4	2	0
4	A	1028	SO4	1	0
4	A	1029	SO4	0	1
4	A	1031	SO4	1	0
4	A	1035	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	902/902 (100%)	0.27	41 (4%) 34 32	26, 37, 46, 50	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	885	PHE	8.1
1	A	925	VAL	7.6
1	A	889	GLY	6.8
1	A	888	TYR	6.7
1	A	890	GLY	6.7
1	A	891	GLY	5.8
1	A	923	MET	4.9
1	A	881	TRP	4.6
1	A	93	ALA	4.5
1	A	893	PHE	4.4
1	A	63	GLN	4.3
1	A	926	GLY	4.3
1	A	927	PHE	4.2
1	A	924	ASP	4.1
1	A	932	ARG	3.9
1	A	918	PHE	3.6
1	A	290	GLN	3.6
1	A	882	LYS	3.6
1	A	781	GLU	3.4
1	A	933	ALA	3.2
1	A	197	ASN	3.1
1	A	886	GLN	3.0
1	A	917	GLN	2.8
1	A	569	ASN	2.8
1	A	884	LEU	2.7
1	A	922	ASN	2.7
1	A	919	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	928	GLY	2.6
1	A	850	LEU	2.6
1	A	196	GLY	2.5
1	A	742	GLU	2.4
1	A	892	SER	2.4
1	A	94	ASP	2.4
1	A	567	GLU	2.4
1	A	949	LYS	2.3
1	A	577	ASP	2.3
1	A	815	GLN	2.3
1	A	430	ILE	2.3
1	A	589	ASN	2.2
1	A	849	ASP	2.0
1	A	780	PRO	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	A	1026	5/5	0.89	0.55	35.75	34,39,40,43	0
4	SO4	A	1028	5/5	0.91	0.37	33.99	38,38,43,43	0
4	SO4	A	1032	5/5	0.88	0.50	19.09	38,40,42,43	0
4	SO4	A	1033	5/5	0.82	0.47	16.77	36,37,43,44	0
4	SO4	A	1025	5/5	0.88	0.40	12.89	34,38,42,43	0
4	SO4	A	1031	5/5	0.83	0.47	9.94	36,38,42,43	0
4	SO4	A	1027	5/5	0.81	0.45	8.61	41,42,43,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	A	1035	5/5	0.96	0.27	4.84	40,42,42,42	0
4	SO4	A	1029	5/5	0.94	0.22	3.89	39,41,43,44	0
3	LEU	A	1024	9/9	0.84	0.24	2.77	31,36,39,41	0
2	NAG	A	1011	14/15	0.89	0.18	2.71	34,36,39,40	0
2	NAG	A	1004	14/15	0.94	0.16	2.57	34,35,39,40	0
4	SO4	A	1030	5/5	0.96	0.22	0.96	38,39,40,42	0
2	NAG	A	1001	14/15	0.96	0.12	-1.33	31,35,37,38	0
2	NAG	A	1021	14/15	0.92	0.09	-1.90	34,36,39,41	0
2	NAG	A	1016	14/15	0.94	0.12	-2.06	32,34,35,37	0
2	NAG	A	1007	14/15	0.94	0.11	-2.32	31,34,36,43	0
5	ZN	A	1036	1/1	1.00	0.14	-3.30	28,28,28,28	0
2	NAG	A	1005	14/15	0.82	0.42	-	36,37,43,43	0
2	NAG	A	1013	14/15	0.65	0.49	-	35,38,44,44	0
4	SO4	A	1034	5/5	0.93	0.51	-	40,40,41,43	0
2	NAG	A	1014	14/15	0.78	0.30	-	36,38,41,43	0
2	NAG	A	1018	14/15	0.90	0.25	-	36,37,43,45	0
2	NAG	A	1012	14/15	0.78	0.30	-	35,37,41,42	0
2	NAG	A	1002	14/15	0.88	0.28	-	35,37,43,44	0
2	NAG	A	1008	14/15	0.93	0.26	-	34,37,38,44	0
2	NAG	A	1015	14/15	0.84	0.35	-	35,37,42,44	0
2	NAG	A	1019	14/15	0.85	0.38	-	36,38,43,43	0
2	NAG	A	1006	14/15	0.65	0.47	-	36,38,42,43	0
2	NAG	A	1023	14/15	0.83	0.37	-	35,38,43,43	0
2	NAG	A	1003	14/15	0.73	0.38	-	36,38,43,44	0
2	NAG	A	1009	14/15	0.88	0.15	-	35,36,43,43	0
2	NAG	A	1022	14/15	0.87	0.30	-	35,37,41,43	0
2	NAG	A	1020	14/15	0.65	0.56	-	36,38,44,44	0
2	NAG	A	1017	14/15	0.89	0.16	-	35,36,43,45	0
2	NAG	A	1010	14/15	0.73	0.41	-	36,38,42,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.