



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 10:08 AM UTC

PDB ID : 6RBF / pdb_00006rbf
Title : Mucin 2 D3 domain
Authors : Javitt, G.; Fass, D.
Deposited on : 2019-04-10
Resolution : 2.70 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

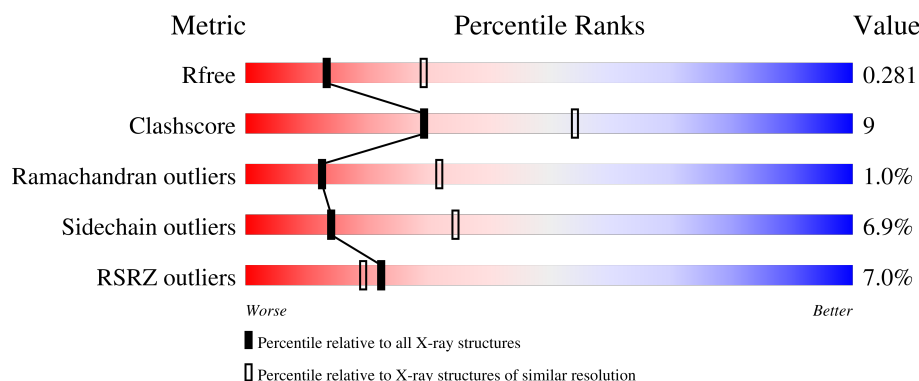
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	410	5% 70% 19% • 9%
1	B	410	3% 68% 20% • 11%
1	C	410	6% 66% 17% • 17%
1	D	410	10% 60% 20% • 17%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20813 atoms, of which 9800 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 Mucin-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	372	Total	C	H	N	O	S	0	1	0
			5357	1752	2544	470	555	36			
1	B	364	Total	C	H	N	O	S	0	0	0
			5286	1724	2520	462	545	35			
1	C	341	Total	C	H	N	O	S	0	1	0
			4948	1626	2352	430	509	31			
1	D	341	Total	C	H	N	O	S	0	2	0
			4905	1621	2318	424	511	31			

There are 32 discrepancies between the modelled and reference sequences:

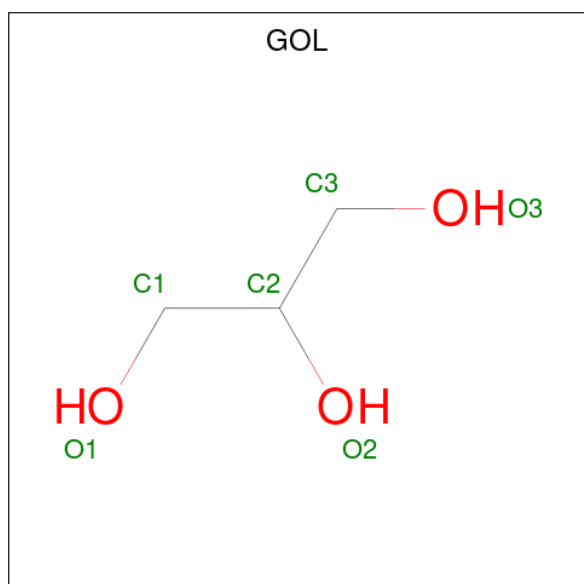
Chain	Residue	Modelled	Actual	Comment	Reference
A	856	ALA	-	expression tag	UNP Q02817
A	857	PRO	-	expression tag	UNP Q02817
A	1260	HIS	-	expression tag	UNP Q02817
A	1261	HIS	-	expression tag	UNP Q02817
A	1262	HIS	-	expression tag	UNP Q02817
A	1263	HIS	-	expression tag	UNP Q02817
A	1264	HIS	-	expression tag	UNP Q02817
A	1265	HIS	-	expression tag	UNP Q02817
B	856	ALA	-	expression tag	UNP Q02817
B	857	PRO	-	expression tag	UNP Q02817
B	1260	HIS	-	expression tag	UNP Q02817
B	1261	HIS	-	expression tag	UNP Q02817
B	1262	HIS	-	expression tag	UNP Q02817
B	1263	HIS	-	expression tag	UNP Q02817
B	1264	HIS	-	expression tag	UNP Q02817
B	1265	HIS	-	expression tag	UNP Q02817
C	856	ALA	-	expression tag	UNP Q02817
C	857	PRO	-	expression tag	UNP Q02817
C	1260	HIS	-	expression tag	UNP Q02817
C	1261	HIS	-	expression tag	UNP Q02817
C	1262	HIS	-	expression tag	UNP Q02817

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1263	HIS	-	expression tag	UNP Q02817
C	1264	HIS	-	expression tag	UNP Q02817
C	1265	HIS	-	expression tag	UNP Q02817
D	856	ALA	-	expression tag	UNP Q02817
D	857	PRO	-	expression tag	UNP Q02817
D	1260	HIS	-	expression tag	UNP Q02817
D	1261	HIS	-	expression tag	UNP Q02817
D	1262	HIS	-	expression tag	UNP Q02817
D	1263	HIS	-	expression tag	UNP Q02817
D	1264	HIS	-	expression tag	UNP Q02817
D	1265	HIS	-	expression tag	UNP Q02817

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

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



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

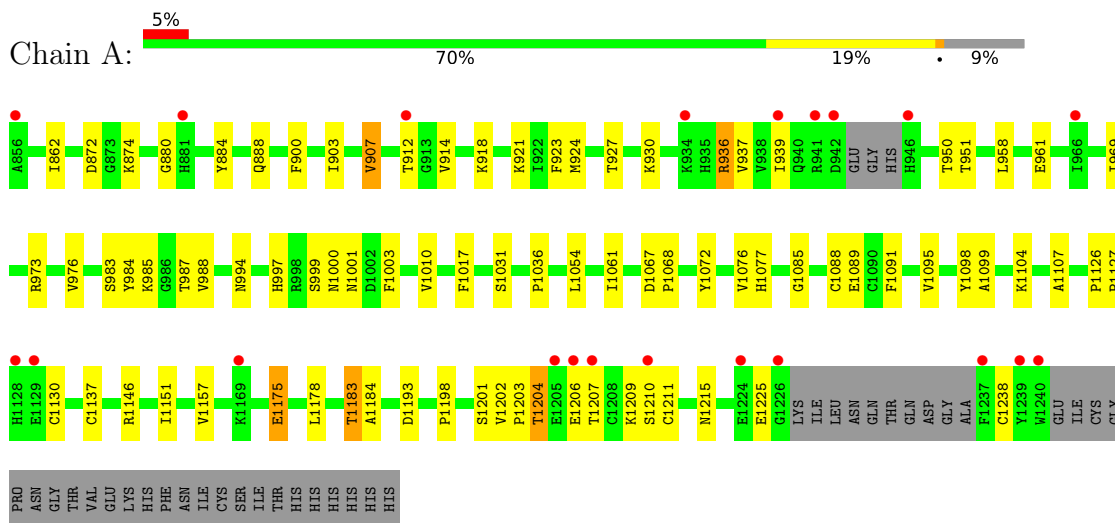
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total	O	0	0
			32	32		
6	B	47	Total	O	0	0
			47	47		
6	C	42	Total	O	0	0
			42	42		
6	D	36	Total	O	0	0
			36	36		

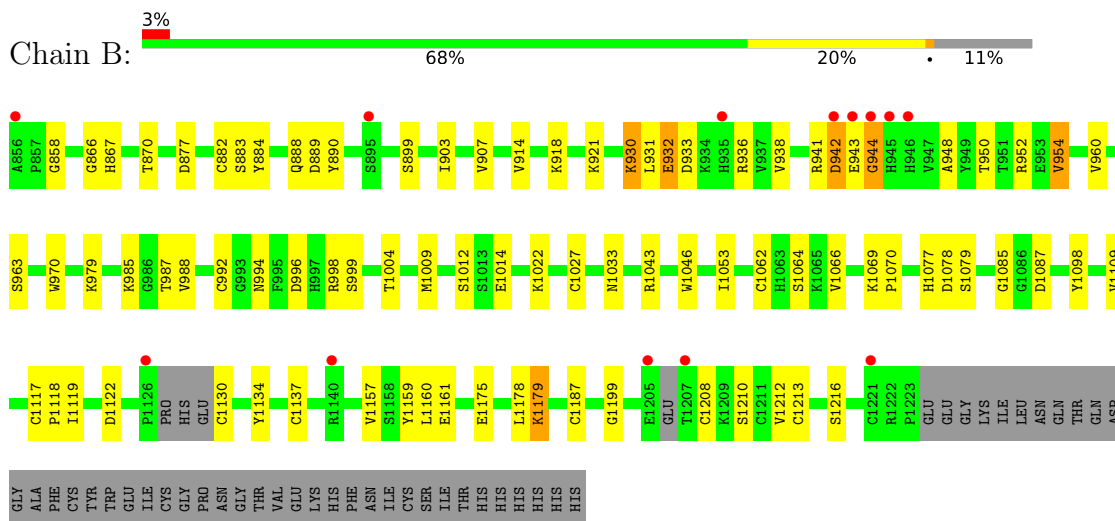
3 Residue-property plots [i](#)

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: Mucin-2

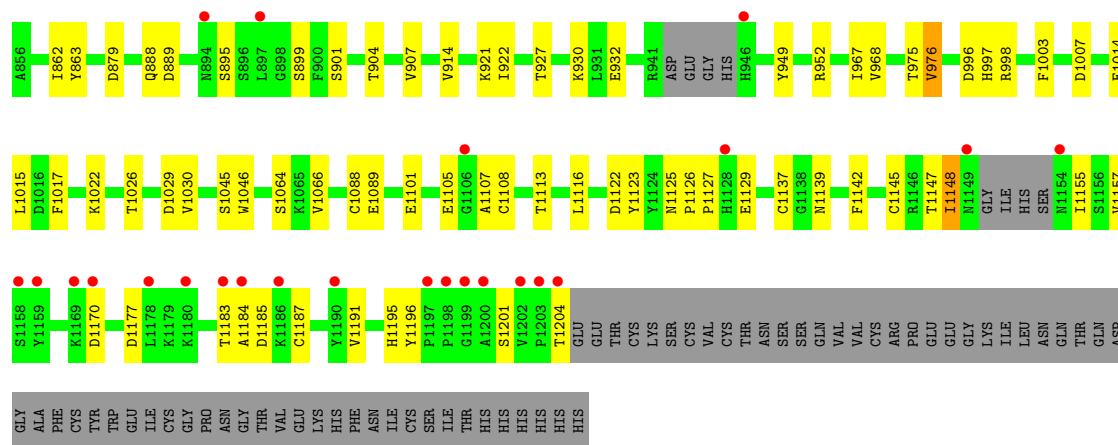


- Molecule 1: Mucin-2

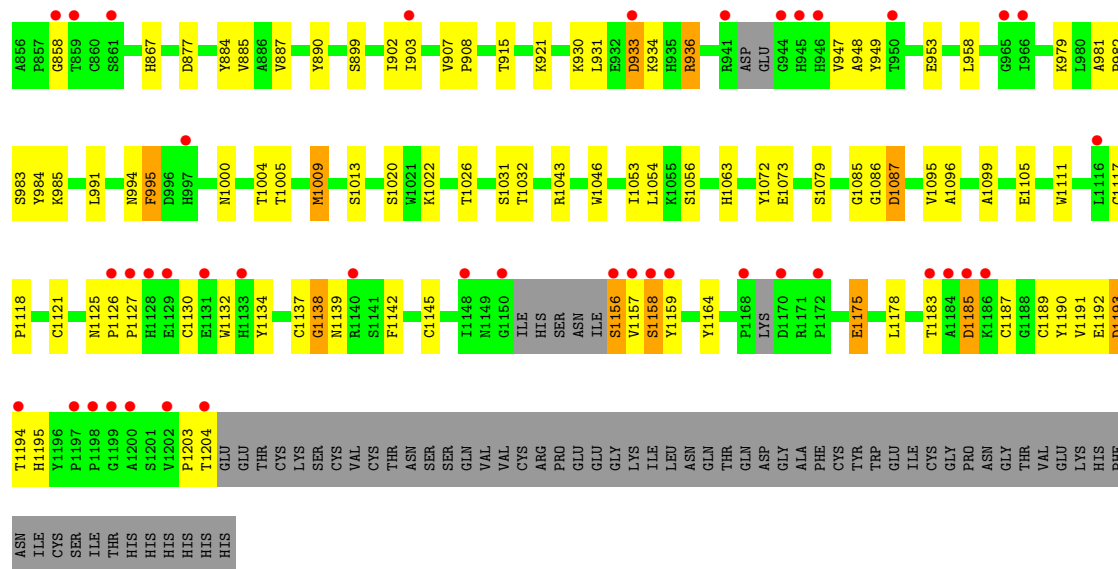


- Molecule 1: Mucin-2





• Molecule 1: Mucin-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	152.46Å 156.93Å 93.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 2.70 48.35 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.35-2.70) 99.8 (48.35-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.217 , 0.283 0.216 , 0.281	Depositor DCC
R_{free} test set	3100 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20813	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: GOL, SO4, CA, 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	0.61	0/2889	0.73	0/3938
1	B	0.63	0/2838	0.76	0/3866
1	C	0.62	0/2670	0.75	0/3641
1	D	0.58	0/2664	0.75	1/3633 (0.0%)
All	All	0.61	0/11061	0.75	1/15078 (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	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	936	ARG	CG-CD-NE	-5.02	100.96	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	1138	GLY	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	2813	2544	2542	44	0
1	B	2766	2520	2517	47	0
1	C	2596	2352	2351	34	0
1	D	2587	2318	2316	57	0
2	A	6	8	8	1	0
2	B	12	16	16	0	0
3	A	14	14	13	3	0
3	B	28	28	26	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	15	0	0	0	0
5	C	5	0	0	1	0
5	D	10	0	0	1	0
6	A	32	0	0	0	0
6	B	47	0	0	1	0
6	C	42	0	0	2	0
6	D	36	0	0	0	0
All	All	11013	9800	9789	178	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 9.

All (178) 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:C:1022:LYS:NZ	1:C:1029:ASP:OD1	2.05	0.90
3:A:1302:NAG:H83	3:A:1302:NAG:H3	1.55	0.85
1:D:1054:LEU:HD21	1:D:1095:VAL:HG22	1.64	0.78
1:B:889:ASP:OD2	1:B:899:SER:HB3	1.87	0.74
1:D:1043:ARG:NH2	1:D:1087:ASP:OD1	2.23	0.72
1:A:914:VAL:HG11	1:A:1077:HIS:CE1	2.32	0.65
1:A:958:LEU:C	1:A:958:LEU:HD23	2.22	0.65
1:A:1175:GLU:OE1	1:A:1178:LEU:HD12	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:862:ILE:HB	1:C:976:VAL:HG12	1.77	0.64
1:C:1015:LEU:HD22	1:C:1030:VAL:CG1	2.27	0.64
3:A:1302:NAG:H3	3:A:1302:NAG:C8	2.28	0.63
1:D:936:ARG:NH2	1:D:1193:ASP:OD2	2.30	0.63
1:A:1088[B]:CYS:HB2	1:C:1088:CYS:SG	2.39	0.62
1:A:930:LYS:HB2	1:A:939:ILE:HD11	1.82	0.62
1:C:1015:LEU:HD22	1:C:1030:VAL:HG12	1.81	0.62
1:A:1061:ILE:HG13	1:A:1107:ALA:HB1	1.82	0.61
1:A:1077:HIS:HB2	2:A:1301:GOL:H12	1.82	0.61
1:B:914:VAL:HG11	1:B:1077:HIS:CE1	2.36	0.60
1:A:907:VAL:HG11	1:A:918:LYS:HD3	1.83	0.59
1:B:1087:ASP:OD2	1:D:1087:ASP:HB2	2.02	0.59
1:D:903:ILE:HB	1:D:921:LYS:HB2	1.85	0.58
1:B:942:ASP:O	1:B:944:GLY:N	2.30	0.58
1:D:1203:PRO:O	1:D:1204:THR:HG23	2.04	0.57
1:A:973:ARG:NH1	1:A:1089:GLU:OE2	2.39	0.56
1:C:1145:CYS:O	1:C:1148:ILE:HG22	2.06	0.56
1:B:1043:ARG:NH1	1:B:1079:SER:O	2.38	0.55
1:D:947:VAL:HG12	1:D:948:ALA:N	2.22	0.55
1:B:914:VAL:HG11	1:B:1077:HIS:HE1	1.72	0.55
1:B:1014:GLU:H	1:B:1014:GLU:CD	2.15	0.55
1:B:930:LYS:HD3	1:B:932:GLU:OE1	2.06	0.54
1:D:1159[A]:TYR:H	1:D:1159[A]:TYR:HD1	1.56	0.54
1:C:889:ASP:OD2	1:C:899:SER:HB3	2.08	0.54
1:D:1054:LEU:HD12	1:D:1072:TYR:HA	1.89	0.53
1:A:1198:PRO:HB3	1:A:1215:ASN:HA	1.91	0.53
1:B:931:LEU:HB3	1:B:970:TRP:CE3	2.45	0.52
1:C:899:SER:OG	6:C:1401:HOH:O	2.17	0.52
1:A:1000:ASN:OD1	1:A:1001:ASN:N	2.43	0.52
1:B:994:ASN:ND2	1:B:996:ASP:OD2	2.43	0.52
1:C:967:ILE:HG21	1:C:1157:VAL:HG11	1.92	0.52
1:C:1183:THR:O	1:C:1185:ASP:N	2.44	0.51
1:B:1212:VAL:HG12	1:B:1213:CYS:H	1.75	0.51
1:B:1199:GLY:N	1:B:1213:CYS:O	2.37	0.51
1:D:984:TYR:O	1:D:985:LYS:C	2.53	0.51
1:D:1156:SER:O	1:D:1156:SER:OG	2.27	0.51
1:D:1117:CYS:N	1:D:1118:PRO:CD	2.73	0.50
1:B:888:GLN:O	1:B:988:VAL:HA	2.11	0.50
1:D:908:PRO:HA	1:D:915:THR:HG22	1.93	0.50
1:C:904:THR:HG23	1:C:904:THR:O	2.12	0.50
1:B:882:CYS:SG	1:B:883:SER:N	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:996:ASP:OD1	1:B:998:ARG:HB2	2.11	0.50
1:B:1087:ASP:OD2	1:D:1087:ASP:CB	2.58	0.50
1:D:931:LEU:HD23	1:D:936:ARG:HB3	1.94	0.50
1:C:1003:PHE:HA	1:C:1017:PHE:CD1	2.47	0.50
1:D:1000:ASN:OD1	1:D:1000:ASN:C	2.54	0.50
1:C:967:ILE:HD11	1:C:1155:ILE:HB	1.93	0.50
1:B:1130:CYS:SG	1:B:1130:CYS:O	2.70	0.49
3:A:1302:NAG:H83	3:A:1302:NAG:C3	2.34	0.49
1:B:1085:GLY:HA3	1:D:1046:TRP:CG	2.46	0.49
1:B:954:VAL:CG2	1:B:1160:LEU:HD12	2.43	0.49
1:A:1146:ARG:NH1	1:A:1193:ASP:OD1	2.46	0.49
1:D:1126:PRO:HB2	1:D:1127:PRO:HD2	1.95	0.49
1:C:922:ILE:HD13	1:C:968:VAL:HG21	1.94	0.48
1:D:1145:CYS:HB3	1:D:1190:TYR:HE2	1.78	0.48
1:D:1139:ASN:OD1	1:D:1142:PHE:HB2	2.13	0.48
1:A:914:VAL:HG11	1:A:1077:HIS:HE1	1.77	0.48
1:C:921:LYS:HD3	5:C:1301:SO4:O3	2.14	0.48
1:B:1062:CYS:SG	1:B:1066:VAL:HB	2.54	0.47
1:A:1126:PRO:CB	1:A:1127:PRO:HD2	2.44	0.47
1:D:1175:GLU:OE2	1:D:1178:LEU:N	2.45	0.47
1:A:1204:THR:C	1:A:1206:GLU:H	2.23	0.47
1:A:969:ILE:O	1:A:976:VAL:HA	2.15	0.47
1:A:985:LYS:O	1:A:987:THR:HG23	2.15	0.47
1:A:1225:GLU:HA	1:A:1238:CYS:O	2.14	0.47
1:B:870:THR:HB	1:B:992:CYS:O	2.15	0.47
1:B:1046:TRP:CG	1:D:1085:GLY:HA3	2.50	0.47
1:A:1126:PRO:HB3	1:A:1127:PRO:HD2	1.96	0.47
1:D:1031:SER:O	1:D:1032:THR:HG23	2.15	0.46
1:C:952:ARG:NH1	1:C:1147:THR:HG21	2.31	0.46
1:C:930:LYS:HD3	1:C:932:GLU:OE2	2.16	0.46
1:D:908:PRO:CA	1:D:915:THR:HG22	2.45	0.46
1:D:1056:SER:O	1:D:1063:HIS:HE1	1.98	0.46
1:A:1000:ASN:OD1	1:A:1001:ASN:HB3	2.15	0.46
1:A:880:GLY:HA3	1:A:884:TYR:OH	2.15	0.45
1:A:1054:LEU:HD12	1:A:1072:TYR:HA	1.97	0.45
1:B:1087:ASP:HB2	1:D:1087:ASP:HB2	1.98	0.45
1:C:1148:ILE:HD11	1:C:1184:ALA:HB1	1.97	0.45
1:D:867:HIS:ND1	1:D:877:ASP:OD1	2.48	0.45
1:A:936:ARG:HD3	1:A:951:THR:OG1	2.16	0.45
1:B:1119:ILE:HG21	1:B:1134:TYR:CD1	2.51	0.45
1:C:1187:CYS:O	1:C:1195:HIS:NE2	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:TYR:O	1:A:903:ILE:HG23	2.16	0.45
1:D:1043:ARG:HH22	1:D:1087:ASP:CG	2.22	0.45
1:A:984:TYR:O	1:A:985:LYS:C	2.58	0.45
1:B:907:VAL:HG22	1:B:918:LYS:HB2	1.98	0.45
1:C:949:TYR:C	1:C:949:TYR:CD1	2.94	0.45
1:B:858:GLY:O	1:B:979:LYS:HA	2.17	0.45
1:B:907:VAL:CG2	1:B:918:LYS:HB2	2.47	0.45
1:D:887:VAL:HG12	1:D:902:ILE:HB	1.99	0.45
1:A:1067:ASP:OD1	1:A:1068:PRO:HD2	2.17	0.45
1:D:1158:SER:HB2	1:D:1159[B]:TYR:CD1	2.52	0.45
1:D:995:PHE:CD1	1:D:995:PHE:O	2.70	0.44
1:D:1121:CYS:SG	1:D:1134:TYR:HB2	2.56	0.44
1:C:888:GLN:HB3	1:C:901:SER:HB2	1.98	0.44
1:C:1204:THR:OG1	6:C:1402:HOH:O	2.20	0.44
1:D:1086:GLY:O	1:D:1087:ASP:C	2.60	0.44
1:C:863:TYR:HB3	1:C:975:THR:HG23	1.98	0.44
1:D:1185:ASP:OD1	1:D:1185:ASP:N	2.51	0.44
1:B:938:VAL:HG11	1:B:941:ARG:HD3	1.99	0.44
1:B:1212:VAL:HG12	1:B:1213:CYS:N	2.33	0.44
1:D:1096:ALA:O	1:D:1099:ALA:N	2.51	0.44
1:D:1190:TYR:CE1	1:D:1195:HIS:CD2	3.05	0.44
1:C:1107:ALA:O	1:C:1108:CYS:C	2.60	0.43
1:B:884:TYR:CD1	1:B:884:TYR:N	2.86	0.43
1:C:879:ASP:OD1	1:C:914:VAL:HA	2.18	0.43
1:A:872:ASP:OD1	1:A:997:HIS:N	2.51	0.43
1:A:912:THR:HG21	1:A:1036:PRO:HB3	1.99	0.43
1:D:1004:THR:HA	1:D:1009:MET:O	2.18	0.43
1:D:1183:THR:O	1:D:1185:ASP:N	2.51	0.43
1:D:994:ASN:O	1:D:995:PHE:HB3	2.18	0.43
1:D:1125:ASN:OD1	1:D:1132:TRP:HB2	2.18	0.43
1:A:961:GLU:O	1:A:1151:ILE:HD12	2.18	0.43
1:A:1085:GLY:HA3	1:C:1046:TRP:CG	2.54	0.43
1:D:931:LEU:HD23	1:D:936:ARG:CB	2.49	0.43
1:D:991:LEU:HA	1:D:991:LEU:HD23	1.86	0.43
1:D:1175:GLU:OE2	1:D:1178:LEU:CB	2.67	0.43
1:D:949:TYR:CD1	1:D:949:TYR:C	2.97	0.43
1:D:953:GLU:OE1	1:D:958:LEU:HD12	2.19	0.43
1:B:866:GLY:O	1:B:877:ASP:HA	2.19	0.42
1:B:903:ILE:HB	1:B:921:LYS:HB2	2.01	0.42
1:C:1116:LEU:C	1:C:1116:LEU:HD23	2.44	0.42
1:A:950:THR:HG21	1:A:1151:ILE:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:884:TYR:HB3	1:D:991:LEU:HD11	2.02	0.42
1:A:1183:THR:O	1:A:1184:ALA:C	2.63	0.42
1:B:932:GLU:O	1:B:933:ASP:C	2.61	0.42
1:C:996:ASP:O	1:C:997:HIS:HB2	2.19	0.42
1:B:994:ASN:CG	1:B:996:ASP:OD2	2.63	0.42
1:A:874:LYS:HE3	1:A:1003:PHE:CE2	2.54	0.42
1:A:903:ILE:HB	1:A:921:LYS:HB2	2.02	0.42
1:A:1091:PHE:O	1:A:1095:VAL:HG23	2.19	0.42
1:B:1178:LEU:O	1:B:1179:LYS:C	2.62	0.42
1:D:981:ALA:O	1:D:983:SER:N	2.53	0.42
1:A:862:ILE:HB	1:A:976:VAL:HG12	2.01	0.42
1:A:1209:LYS:HE2	1:A:1211:CYS:SG	2.60	0.42
1:A:888:GLN:HA	1:A:900:PHE:O	2.20	0.42
1:B:985:LYS:NZ	6:B:1409:HOH:O	2.52	0.42
1:B:1069:LYS:HB3	1:B:1070:PRO:CD	2.50	0.42
1:D:858:GLY:O	1:D:979:LYS:HA	2.20	0.42
1:D:1095:VAL:O	1:D:1096:ALA:C	2.63	0.42
1:C:1122:ASP:O	1:C:1123:TYR:C	2.63	0.41
1:B:948:ALA:HB3	1:B:963:SER:HB3	2.01	0.41
1:C:1015:LEU:HD22	1:C:1030:VAL:HG11	2.02	0.41
1:A:1098:TYR:O	1:A:1099:ALA:C	2.62	0.41
1:B:1022:LYS:NZ	1:B:1027:CYS:O	2.50	0.41
1:A:988:VAL:HG23	1:A:994:ASN:HA	2.02	0.41
1:A:1202:VAL:HA	1:A:1203:PRO:HD3	1.96	0.41
1:B:867:HIS:HE2	1:B:1078:ASP:CG	2.29	0.41
1:B:1046:TRP:CH2	1:B:1087:ASP:HB3	2.56	0.41
1:D:953:GLU:OE1	1:D:958:LEU:HB2	2.20	0.41
1:A:1072:TYR:O	1:A:1076:VAL:HG23	2.21	0.41
1:D:930:LYS:NZ	5:D:1301:SO4:O4	2.43	0.41
1:B:988:VAL:O	1:B:994:ASN:HA	2.20	0.41
1:D:947:VAL:HG12	1:D:948:ALA:H	1.85	0.41
1:D:982:PRO:O	1:D:985:LYS:HG3	2.21	0.41
1:B:1066:VAL:HG12	1:B:1098:TYR:HE1	1.86	0.40
1:D:1053:ILE:HD13	1:D:1053:ILE:HG21	1.83	0.40
1:A:1003:PHE:HA	1:A:1017:PHE:CE1	2.57	0.40
1:C:996:ASP:OD1	1:C:996:ASP:C	2.62	0.40
1:C:1191:VAL:HG12	1:C:1196:TYR:HE2	1.87	0.40
1:A:923:PHE:HA	1:A:927:THR:O	2.21	0.40
1:D:933:ASP:O	1:D:934:LYS:CB	2.70	0.40
1:D:1138:GLY:HA2	1:D:1164:TYR:CE2	2.56	0.40
1:B:994:ASN:OD1	1:B:994:ASN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1004:THR:HA	1:B:1009:MET:O	2.21	0.40
1:D:1111:TRP:CD1	1:D:1111:TRP:H	2.40	0.40
1:B:1117:CYS:N	1:B:1118:PRO:CD	2.85	0.40
1:B:1137:CYS:O	1:B:1159:TYR:HA	2.22	0.40
1:C:1125:ASN:HA	1:C:1126:PRO:HD3	1.98	0.40
1:C:1139:ASN:OD1	1:C:1142:PHE:N	2.53	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	367/410 (90%)	334 (91%)	32 (9%)	1 (0%)	36	60
1	B	358/410 (87%)	327 (91%)	25 (7%)	6 (2%)	7	19
1	C	336/410 (82%)	304 (90%)	30 (9%)	2 (1%)	21	44
1	D	335/410 (82%)	291 (87%)	39 (12%)	5 (2%)	8	22
All	All	1396/1640 (85%)	1256 (90%)	126 (9%)	14 (1%)	12	32

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	942	ASP
1	B	1122	ASP
1	B	943	GLU
1	D	933	ASP
1	B	890	TYR
1	B	944	GLY
1	B	1179	LYS
1	C	1127	PRO
1	D	890	TYR

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Mol	Chain	Res	Type
1	D	1158	SER
1	D	1192	GLU
1	A	1104	LYS
1	C	1170	ASP
1	D	995	PHE

5.3.2 Protein sidechains ⓘ

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	315/366 (86%)	298 (95%)	17 (5%)	20	45
1	B	312/366 (85%)	291 (93%)	21 (7%)	15	36
1	C	289/366 (79%)	269 (93%)	20 (7%)	14	34
1	D	285/366 (78%)	261 (92%)	24 (8%)	10	26
All	All	1201/1464 (82%)	1119 (93%)	82 (7%)	14	35

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	907	VAL
1	A	924	MET
1	A	936	ARG
1	A	937	VAL
1	A	983	SER
1	A	999	SER
1	A	1010	VAL
1	A	1031	SER
1	A	1130	CYS
1	A	1137	CYS
1	A	1157	VAL
1	A	1175	GLU
1	A	1183	THR
1	A	1201	SER
1	A	1204	THR
1	A	1207	THR

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Mol	Chain	Res	Type
1	A	1210	SER
1	B	930	LYS
1	B	932	GLU
1	B	936	ARG
1	B	950	THR
1	B	952	ARG
1	B	954	VAL
1	B	960	VAL
1	B	987	THR
1	B	999	SER
1	B	1012	SER
1	B	1033	ASN
1	B	1053	ILE
1	B	1064	SER
1	B	1109	VAL
1	B	1157	VAL
1	B	1161	GLU
1	B	1175	GLU
1	B	1187	CYS
1	B	1208	CYS
1	B	1210	SER
1	B	1216	SER
1	C	895	SER
1	C	907	VAL
1	C	927	THR
1	C	976	VAL
1	C	998	ARG
1	C	1007	ASP
1	C	1014	GLU
1	C	1026	THR
1	C	1045	SER
1	C	1064	SER
1	C	1066	VAL
1	C	1089	GLU
1	C	1101	GLU
1	C	1105	GLU
1	C	1113	THR
1	C	1129	GLU
1	C	1137	CYS
1	C	1148	ILE
1	C	1177	ASP
1	C	1201	SER

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Mol	Chain	Res	Type
1	D	885	VAL
1	D	899	SER
1	D	907	VAL
1	D	1005	THR
1	D	1009	MET
1	D	1013	SER
1	D	1020	SER
1	D	1022	LYS
1	D	1026	THR
1	D	1073	GLU
1	D	1079	SER
1	D	1087	ASP
1	D	1105	GLU
1	D	1130	CYS
1	D	1137	CYS
1	D	1156	SER
1	D	1157	VAL
1	D	1175	GLU
1	D	1185	ASP
1	D	1187	CYS
1	D	1189	CYS
1	D	1191	VAL
1	D	1193	ASP
1	D	1194	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1149	ASN
1	A	1154	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	C	1301	-	4,4,4	0.40	0	6,6,6	0.17	0
2	GOL	A	1301	-	5,5,5	1.28	1 (20%)	5,5,5	1.07	0
3	NAG	B	1304	1	14,14,15	0.71	1 (7%)	17,19,21	0.80	1 (5%)
5	SO4	B	1306	-	4,4,4	0.33	0	6,6,6	0.45	0
2	GOL	B	1303	-	5,5,5	1.55	1 (20%)	5,5,5	0.87	0
3	NAG	B	1301	1	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
5	SO4	B	1307	-	4,4,4	0.35	0	6,6,6	0.50	0
2	GOL	B	1302	-	5,5,5	2.55	2 (40%)	5,5,5	0.93	0
5	SO4	D	1301	-	4,4,4	0.31	0	6,6,6	0.21	0
5	SO4	B	1305	-	4,4,4	0.23	0	6,6,6	0.32	0
5	SO4	D	1302	-	4,4,4	0.33	0	6,6,6	0.23	0
3	NAG	A	1302	1	14,14,15	0.90	2 (14%)	17,19,21	1.57	3 (17%)

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	GOL	A	1301	-	-	2/4/4/4	-
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
2	GOL	B	1303	-	-	2/4/4/4	-
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
2	GOL	B	1302	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1302	1	-	3/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1302	GOL	C1-C2	3.95	1.66	1.51
2	B	1302	GOL	C3-C2	3.56	1.65	1.51
3	A	1302	NAG	C1-C2	2.53	1.55	1.52
2	B	1303	GOL	C1-C2	2.43	1.61	1.51
3	B	1304	NAG	O5-C1	2.24	1.47	1.43
2	A	1301	GOL	C3-C2	2.10	1.59	1.51
3	A	1302	NAG	O5-C1	-2.00	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1302	NAG	C2-N2-C7	3.89	128.12	122.90
3	A	1302	NAG	C1-C2-N2	3.74	116.33	110.43
3	B	1301	NAG	C1-O5-C5	2.88	116.05	112.19
3	B	1304	NAG	C2-N2-C7	2.04	125.64	122.90
3	A	1302	NAG	O4-C4-C3	-2.00	105.65	110.38

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1302	GOL	O1-C1-C2-C3
2	B	1303	GOL	C1-C2-C3-O3
2	B	1303	GOL	O2-C2-C3-O3
3	B	1304	NAG	C4-C5-C6-O6
3	A	1302	NAG	C8-C7-N2-C2
3	A	1302	NAG	O7-C7-N2-C2
3	B	1304	NAG	O5-C5-C6-O6
2	B	1302	GOL	O1-C1-C2-O2
3	A	1302	NAG	C3-C2-N2-C7
2	A	1301	GOL	O1-C1-C2-C3
2	A	1301	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1301	SO4	1	0
2	A	1301	GOL	1	0
5	D	1301	SO4	1	0
3	A	1302	NAG	3	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	372/410 (90%)	0.41	21 (5%)	30 26	26, 57, 99, 136	1 (0%)
1	B	364/410 (88%)	0.18	13 (3%)	46 42	30, 52, 84, 123	0
1	C	341/410 (83%)	0.35	24 (7%)	22 19	19, 52, 106, 132	1 (0%)
1	D	341/410 (83%)	0.65	41 (12%)	9 7	19, 61, 121, 173	2 (0%)
All	All	1418/1640 (86%)	0.39	99 (6%)	22 19	19, 56, 107, 173	4 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	942	ASP	9.6
1	D	1128	HIS	8.1
1	D	1186	LYS	6.7
1	A	1240	TRP	6.2
1	B	945	HIS	5.8
1	B	943	GLU	5.8
1	D	944	GLY	5.8
1	B	946	HIS	5.1
1	C	894	ASN	5.0
1	D	1127	PRO	4.9
1	B	942	ASP	4.5
1	D	1159[A]	TYR	4.3
1	A	1207	THR	4.3
1	D	1150	GLY	4.1
1	A	1226	GLY	4.0
1	D	1126	PRO	4.0
1	A	941	ARG	4.0
1	B	944	GLY	4.0
1	D	933	ASP	3.9
1	B	856	ALA	3.9
1	D	1156	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	1186	LYS	3.7
1	D	1140	ARG	3.7
1	C	1159	TYR	3.6
1	A	1128	HIS	3.6
1	B	1207	THR	3.6
1	C	1106	GLY	3.6
1	D	945	HIS	3.5
1	D	941	ARG	3.5
1	C	946	HIS	3.5
1	D	1204	THR	3.4
1	D	1170	ASP	3.2
1	D	1158	SER	3.2
1	C	1128	HIS	3.2
1	D	1157	VAL	3.2
1	B	895	SER	3.1
1	D	1198	PRO	3.1
1	D	1183	THR	3.1
1	A	1129	GLU	3.1
1	C	1199	GLY	3.1
1	D	1199	GLY	3.0
1	B	1205	GLU	3.0
1	C	1170	ASP	3.0
1	D	903	ILE	3.0
1	D	859	THR	3.0
1	B	1140	ARG	2.9
1	C	1202	VAL	2.9
1	D	1129	GLU	2.9
1	A	966	ILE	2.9
1	A	1237	PHE	2.9
1	C	1197	PRO	2.8
1	C	1204	THR	2.8
1	D	1184	ALA	2.8
1	A	1224	GLU	2.8
1	D	1172	PRO	2.8
1	C	1149	ASN	2.8
1	C	1169	LYS	2.8
1	D	946	HIS	2.8
1	C	1158	SER	2.8
1	A	1239	TYR	2.8
1	C	1203	PRO	2.7
1	A	856	ALA	2.7
1	A	1206	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	1131	GLU	2.7
1	D	1185	ASP	2.7
1	C	897	LEU	2.6
1	D	966	ILE	2.6
1	A	1205	GLU	2.6
1	C	1183	THR	2.5
1	B	935	HIS	2.4
1	C	1180	LYS	2.4
1	C	1154	ASN	2.4
1	A	1210	SER	2.4
1	D	1168	PRO	2.4
1	A	881	HIS	2.4
1	C	1178	LEU	2.3
1	A	1169	LYS	2.3
1	D	858	GLY	2.3
1	C	1200	ALA	2.3
1	A	934	LYS	2.3
1	D	1197	PRO	2.3
1	D	965	GLY	2.3
1	A	946	HIS	2.3
1	B	1126	PRO	2.2
1	C	1198	PRO	2.2
1	D	1116	LEU	2.2
1	A	912	THR	2.2
1	D	1202	VAL	2.2
1	A	939	ILE	2.1
1	D	861	SER	2.1
1	B	1221	CYS	2.1
1	C	1190	TYR	2.1
1	D	950	THR	2.1
1	D	1200	ALA	2.0
1	D	1194	THR	2.0
1	D	997	HIS	2.0
1	C	1184	ALA	2.0
1	D	1133	HIS	2.0
1	D	1148	ILE	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
5	SO4	D	1302	5/5	0.64	0.16	92,98,126,169	0
5	SO4	B	1307	5/5	0.71	0.15	73,77,101,109	0
5	SO4	D	1301	5/5	0.72	0.12	85,101,114,117	0
3	NAG	A	1302	14/15	0.78	0.13	56,71,83,85	0
2	GOL	B	1302	6/6	0.80	0.21	42,77,117,117	0
5	SO4	C	1301	5/5	0.81	0.12	71,82,95,102	0
2	GOL	B	1303	6/6	0.82	0.19	51,69,89,89	0
2	GOL	A	1301	6/6	0.85	0.15	50,61,68,71	0
3	NAG	B	1301	14/15	0.89	0.11	54,74,100,102	0
3	NAG	B	1304	14/15	0.89	0.11	66,76,91,91	0
5	SO4	B	1305	5/5	0.94	0.14	48,63,67,67	0
5	SO4	B	1306	5/5	0.95	0.08	57,58,68,71	0
4	CA	C	1302	1/1	0.97	0.10	57,57,57,57	0
4	CA	D	1303	1/1	0.97	0.04	83,83,83,83	0
4	CA	A	1303	1/1	0.98	0.04	66,66,66,66	0
4	CA	B	1308	1/1	0.98	0.03	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.