



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 01:44 PM GMT

PDB ID : 1HJW
Title : Crystal structure of hcgp-39 in complex with chitin octamer
Authors : Houston, D.R.; Recklies, A.D.; Krupa, J.C.; Van Aalten, D.M.F.
Deposited on : 2003-02-28
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

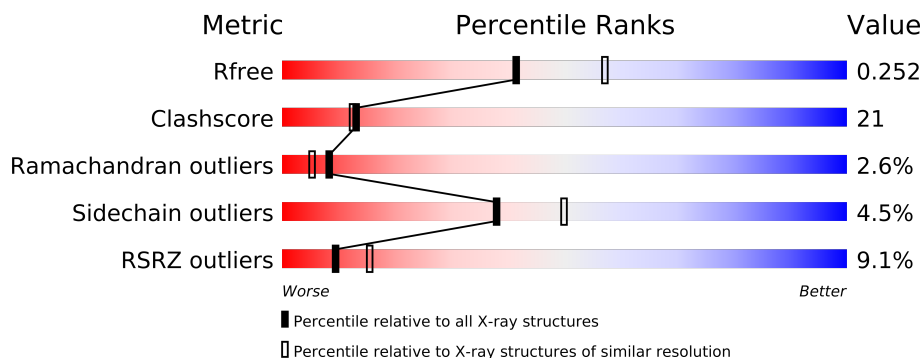
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	362	
1	B	362	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	A	1386	-	X
4	GOL	A	1388	-	X
4	GOL	A	1389	-	X
4	GOL	A	1399	-	X
4	GOL	B	1385	-	X
5	SO4	A	1394	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6374 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CHITINASE-3 LIKE PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	2	0
			2873	1835	497	530	11			
1	B	362	Total	C	N	O	S	0	9	0
			2904	1852	504	537	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	ILE	THR	VARIANT	UNP P36222
B	311	ILE	THR	VARIANT	UNP P36222

- Molecule 2 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	6	Total	C	N	O	0	0
			85	48	6	31		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	ILE	THR	VARIANT	UNP P36222

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	ILE	THR	VARIANT	UNP P36222

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

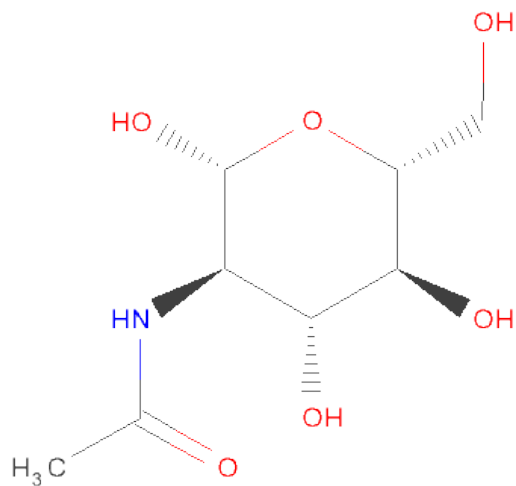
- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	5	Total	C	N	O	0	0
			71	40	5	26		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	311	ILE	THR	VARIANT	UNP P36222

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

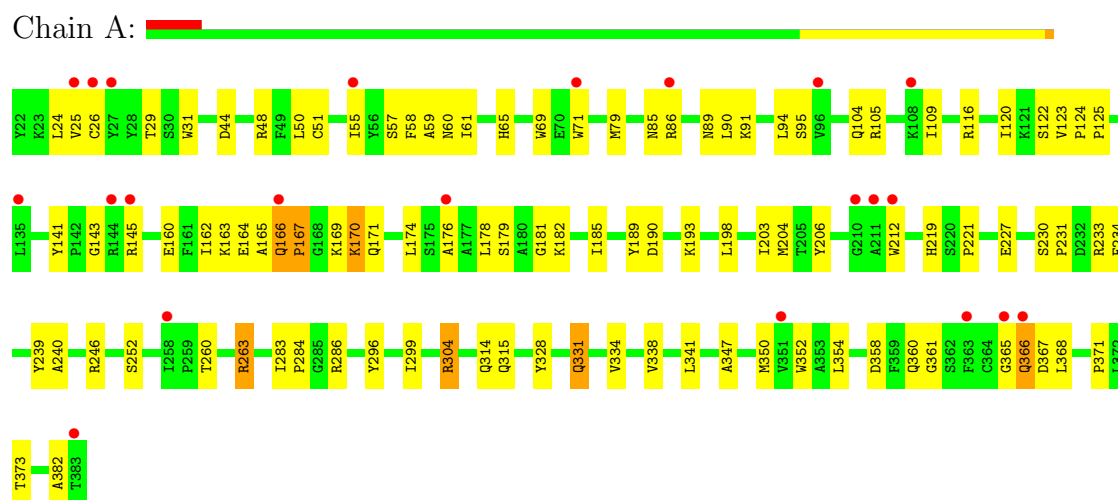
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	178	Total	O	0	0
			178	178		
8	B	159	Total	O	0	0
			159	159		

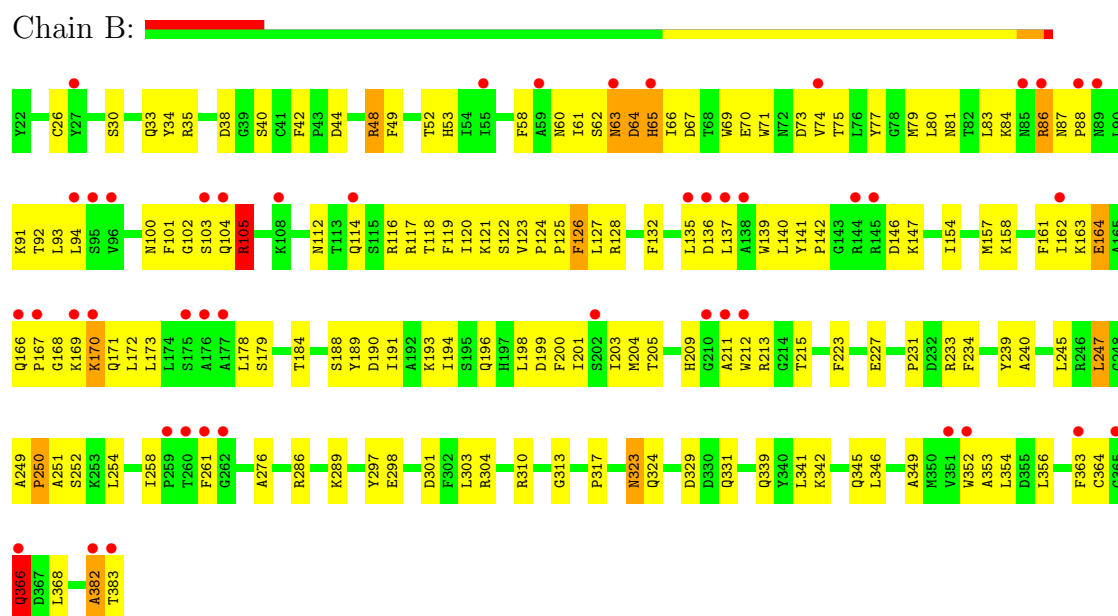
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: CHITINASE-3 LIKE PROTEIN 1



• Molecule 1: CHITINASE-3 LIKE PROTEIN 1



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.48Å 123.63Å 136.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.88 – 2.30 25.03 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.7 (24.88-2.30) 95.8 (25.03-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.31Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.257 0.209 , 0.252	Depositor DCC
R_{free} test set	611 reflections (1.58%)	DCC
Wilson B-factor (Å ²)	58.2	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 39383 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6374	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.57	0/2957	0.73	0/4003
1	B	0.49	0/3019	0.71	0/4086
All	All	0.53	0/5976	0.72	0/8089

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	1
3	A	1	0
All	All	1	1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1385	NAG	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2873	0	2799	85	0
1	B	2904	0	2816	156	0
2	A	85	0	75	8	0
3	A	28	0	25	0	0
4	A	30	0	40	4	0
4	B	12	0	16	6	0
5	A	15	0	0	1	1
5	B	5	0	0	0	0
6	B	71	0	63	11	0
7	B	14	0	13	0	0
8	A	178	0	0	16	0
8	B	159	0	0	14	0
All	All	6374	0	5847	245	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (245) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:366:GLN:HG3	1:A:367:ASP:H	1.35	0.88
1:B:103:SER:HB2	8:B:2028:HOH:O	1.73	0.88
1:A:204:MET:HE2	2:A:1:NAG:H62	1.55	0.87
1:B:86:ARG:NH1	1:B:86:ARG:HB3	1.89	0.86
1:A:48:ARG:HH21	1:A:86:ARG:H	1.22	0.85
1:B:86:ARG:HH11	1:B:86:ARG:HB3	1.42	0.84
1:B:105:ARG:HB3	1:B:105:ARG:HH11	1.42	0.82
1:B:117:ARG:HB2	8:B:2031:HOH:O	1.82	0.79
1:B:44:ASP:HB2	1:B:79:MET:CE	2.14	0.78
1:A:204:MET:CE	2:A:1:NAG:H62	2.14	0.77
1:B:162:ILE:HA	1:B:171:GLN:NE2	2.00	0.77
1:B:162:ILE:HA	1:B:171:GLN:HE21	1.50	0.76
1:A:145:ARG:HG2	8:A:2068:HOH:O	1.85	0.75
1:B:196:GLN:HG3	8:B:2055:HOH:O	1.87	0.74
1:A:203:ILE:HD11	1:A:240:ALA:HB1	1.71	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:147[B]:LYS:HE3	1:B:189:TYR:O	1.88	0.72
1:A:162:ILE:HA	1:A:171:GLN:NE2	2.03	0.72
6:B:-3:NAG:H62	4:B:1385:GOL:H12	1.70	0.72
1:A:331:GLN:HE22	1:A:371:PRO:HB2	1.55	0.72
1:B:117:ARG:HH22	1:B:121:LYS:HD3	1.53	0.72
1:B:48[B]:ARG:HB3	1:B:83:LEU:HB3	1.71	0.71
1:B:123:VAL:HB	1:B:124:PRO:HD3	1.72	0.71
1:B:128:ARG:HH21	1:B:172:LEU:HG	1.56	0.71
1:A:331:GLN:HB2	8:A:2152:HOH:O	1.91	0.70
1:B:105:ARG:HB3	1:B:105:ARG:NH1	2.07	0.69
1:B:127:LEU:HD12	1:B:172:LEU:HD13	1.73	0.69
1:B:117:ARG:NH2	4:B:1384:GOL:H12	2.07	0.69
1:B:167:PRO:HD2	1:B:169:LYS:NZ	2.08	0.68
1:B:112:ASN:OD1	1:B:114:GLN:HG2	1.94	0.67
1:B:209:HIS:HE1	1:B:213:ARG:HH21	1.40	0.67
1:B:35:ARG:HE	4:B:1385:GOL:H32	1.61	0.66
1:B:65[A]:HIS:HB2	1:B:122:SER:CB	2.26	0.66
1:B:352:TRP:CE2	6:B:-1:NAG:H5	2.31	0.65
1:B:139:TRP:O	1:B:142:PRO:HD3	1.95	0.65
1:A:368:LEU:HD12	8:A:2166:HOH:O	1.97	0.65
1:B:141:TYR:HH	6:B:1:NAG:HO6	1.44	0.64
1:B:352:TRP:CZ2	6:B:-1:NAG:H3	2.32	0.64
1:A:163:LYS:O	1:A:166:GLN:HB2	1.98	0.64
1:B:382:ALA:HA	8:B:2156:HOH:O	1.97	0.64
1:B:128:ARG:NH2	1:B:172:LEU:HG	2.11	0.64
1:B:341:LEU:HD12	1:B:342:LYS:N	2.13	0.64
1:A:166:GLN:HB3	1:A:167:PRO:HD3	1.79	0.63
1:B:69:TRP:HD1	1:B:70:GLU:HG3	1.63	0.63
1:B:158:LYS:O	1:B:162:ILE:HG13	1.99	0.63
1:B:163:LYS:O	1:B:166:GLN:HG2	1.99	0.62
1:B:44:ASP:HB2	1:B:79:MET:HE2	1.81	0.62
1:A:71:TRP:NE1	4:A:1389:GOL:H2	2.15	0.62
1:A:105:ARG:O	1:A:109:ILE:HG13	1.99	0.62
1:B:135:LEU:HG	1:B:136:ASP:N	2.14	0.62
1:B:117:ARG:NH2	1:B:121:LYS:HD3	2.14	0.61
1:B:213:ARG:HB2	8:B:2060:HOH:O	1.99	0.61
1:A:170[B]:LYS:HE3	8:A:2078:HOH:O	2.01	0.61
1:B:204:MET:HE3	6:B:-1:NAG:C7	2.30	0.61
1:A:162:ILE:HA	1:A:171:GLN:HE21	1.65	0.60
1:B:213:ARG:NE	8:B:2062:HOH:O	2.34	0.60
1:B:233:ARG:HG2	1:B:233:ARG:HH11	1.67	0.60
1:B:352:TRP:CH2	6:B:-1:NAG:H3	2.37	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:44:ASP:H	1:A:79:MET:HE2	1.68	0.58
1:A:204:MET:HG2	1:A:206:TYR:OH	2.03	0.58
1:A:212:TRP:NE1	4:A:1387:GOL:H2	2.19	0.58
1:B:166:GLN:CG	1:B:167:PRO:HD3	2.34	0.57
2:A:-4:NAG:H83	2:A:-3:NAG:H61	1.85	0.57
1:B:368:LEU:HD23	8:B:2133:HOH:O	2.03	0.57
1:B:173:LEU:HA	1:B:199:ASP:OD2	2.04	0.57
1:A:304:ARG:HB2	1:A:304:ARG:HH11	1.69	0.57
1:B:154:ILE:HD12	1:B:198:LEU:HD21	1.87	0.57
1:B:65[B]:HIS:CD2	1:B:122:SER:HB3	2.41	0.56
1:B:301[A]:ASP:OD1	8:B:2106:HOH:O	2.18	0.56
1:A:61:ILE:HG21	1:A:109:ILE:HD13	1.86	0.56
1:A:182:LYS:HE3	5:A:1394:SO4:O4	2.06	0.56
6:B:-3:NAG:C7	6:B:-2:NAG:H62	2.37	0.55
1:B:167:PRO:HD2	1:B:169:LYS:HZ2	1.69	0.55
1:A:181:GLY:O	1:A:185:ILE:HG13	2.06	0.55
1:B:191:ILE:HG13	1:B:247:LEU:HD13	1.88	0.55
1:A:65:HIS:HB2	8:A:2029:HOH:O	2.07	0.55
1:B:137:LEU:HD12	1:B:154:ILE:CD1	2.37	0.54
1:A:366:GLN:HG3	1:A:367:ASP:N	2.15	0.54
1:B:141:TYR:CE1	1:B:179:SER:HB2	2.43	0.54
1:B:128:ARG:NH1	1:B:169:LYS:HD2	2.23	0.54
1:B:63[B]:ASN:OD1	1:B:65[B]:HIS:ND1	2.41	0.54
1:A:176:ALA:HB1	8:A:2064:HOH:O	2.07	0.54
1:B:366:GLN:NE2	1:B:366:GLN:H	2.05	0.54
1:A:233:ARG:HB2	8:A:2098:HOH:O	2.08	0.53
1:B:48[A]:ARG:HD3	1:B:49:PHE:CE2	2.43	0.53
1:B:298:GLU:O	1:B:301[A]:ASP:HB2	2.08	0.53
1:B:67:ASP:HA	1:B:126:PHE:HE2	1.73	0.53
1:B:128:ARG:NH1	1:B:169:LYS:CD	2.72	0.52
1:A:212:TRP:CE2	4:A:1387:GOL:H2	2.43	0.52
1:B:137:LEU:HD12	1:B:154:ILE:HD13	1.92	0.52
1:B:310:ARG:HG3	8:B:2037:HOH:O	2.09	0.52
1:A:252:SER:O	1:A:347:ALA:HB2	2.10	0.52
1:A:178:LEU:HD22	1:A:189:TYR:CE1	2.44	0.52
1:A:165:ALA:HA	1:A:169:LYS:HB2	1.91	0.51
1:B:44:ASP:HB2	1:B:79:MET:HE1	1.90	0.51
1:A:233:ARG:HG2	8:A:2105:HOH:O	2.09	0.51
1:B:84:LYS:HE2	1:B:92:THR:HG23	1.92	0.51
1:A:122:SER:O	1:A:125:PRO:HG2	2.10	0.51
1:B:166:GLN:HG2	1:B:167:PRO:HD3	1.93	0.51
1:B:140:LEU:HD22	1:B:141:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:209:HIS:CE1	1:B:213:ARG:HH21	2.26	0.51
1:B:233:ARG:NH1	1:B:233:ARG:HG2	2.25	0.51
1:B:53:HIS:HA	1:B:91:LYS:O	2.11	0.51
1:B:304[A]:ARG:HD3	8:B:2110:HOH:O	2.11	0.51
1:A:116:ARG:O	1:A:120:ILE:HG13	2.10	0.50
1:B:184:THR:O	1:B:188:SER:HB2	2.11	0.50
1:B:66:ILE:HG23	1:B:126:PHE:CD2	2.47	0.50
1:B:66:ILE:HB	1:B:119:PHE:HE1	1.77	0.50
1:B:48[A]:ARG:HD2	1:B:49:PHE:H	1.76	0.50
1:B:170:LYS:HD2	1:B:170:LYS:H	1.77	0.50
1:A:143:GLY:HA3	8:A:2068:HOH:O	2.12	0.50
1:B:139:TRP:CZ2	1:B:142:PRO:HA	2.47	0.49
1:B:382:ALA:O	1:B:383:THR:HB	2.11	0.49
1:B:204:MET:CE	6:B:-1:NAG:C7	2.91	0.49
1:B:200:PHE:C	1:B:200:PHE:CD1	2.85	0.49
1:A:204:MET:CE	2:A:-1:NAG:C1	2.90	0.49
1:B:204:MET:HE3	6:B:-1:NAG:C8	2.42	0.49
1:A:190:ASP:CG	1:A:193:LYS:HG3	2.33	0.49
1:B:366:GLN:CD	1:B:366:GLN:H	2.15	0.49
1:B:35:ARG:HG2	4:B:1385:GOL:H32	1.95	0.49
1:B:178:LEU:O	1:B:204:MET:HG3	2.12	0.49
1:B:42:PHE:C	1:B:44:ASP:N	2.66	0.49
1:A:25:VAL:O	1:A:350:MET:HA	2.12	0.49
1:B:35:ARG:O	1:B:40:SER:HB2	2.13	0.48
1:A:141:TYR:CE1	1:A:179:SER:HB2	2.48	0.48
1:A:334:VAL:O	1:A:338:VAL:HG23	2.13	0.48
1:A:90:LEU:HD12	1:A:91:LYS:N	2.29	0.47
1:B:116:ARG:O	1:B:120:ILE:HG13	2.14	0.47
1:A:85:ASN:ND2	8:A:2043:HOH:O	2.47	0.47
1:B:139:TRP:CH2	1:B:146:ASP:HB3	2.49	0.47
1:B:48[A]:ARG:HB3	1:B:83:LEU:HB3	1.95	0.47
1:B:26:CYS:HB3	1:B:354:LEU:HG	1.97	0.47
1:A:50:LEU:HD21	1:A:373:THR:HB	1.97	0.47
1:B:209:HIS:CE1	8:B:2062:HOH:O	2.67	0.47
1:A:57:SER:HA	1:A:58:PHE:HA	1.53	0.47
1:B:86:ARG:O	1:B:88:PRO:HD3	2.14	0.47
1:B:65[A]:HIS:HB2	1:B:122:SER:HB2	1.97	0.46
1:A:61:ILE:HG21	1:A:109:ILE:CD1	2.45	0.46
1:B:157:MET:SD	1:B:161:PHE:CE1	3.08	0.46
1:B:167:PRO:HG2	1:B:169:LYS:HZ1	1.80	0.46
1:B:74:VAL:HG23	1:B:75:THR:N	2.31	0.46
1:A:260:THR:O	1:A:296:TYR:HB2	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:122:SER:O	1:B:125:PRO:HG2	2.15	0.46
1:A:55:ILE:CG2	1:A:95:SER:HB2	2.46	0.46
1:A:352:TRP:CE2	2:A:-1:NAG:H5	2.51	0.46
1:B:298:GLU:O	1:B:301[B]:ASP:HB3	2.16	0.46
1:B:93:LEU:HD12	1:B:93:LEU:N	2.31	0.46
1:A:160:GLU:OE1	1:A:160:GLU:HA	2.15	0.46
1:A:60:ASN:HB2	1:A:69:TRP:HE3	1.80	0.46
1:A:44:ASP:HB3	1:A:79:MET:HE3	1.97	0.45
1:B:77:TYR:O	1:B:81:ASN:ND2	2.49	0.45
1:A:219:HIS:CB	1:A:263:ARG:HG3	2.47	0.45
1:A:124:PRO:N	1:A:125:PRO:HD2	2.31	0.45
1:B:223:PHE:HB2	1:B:313:GLY:O	2.16	0.45
1:A:246:ARG:NH2	8:A:2111:HOH:O	2.47	0.45
1:B:30:SER:O	1:B:33:GLN:HG2	2.17	0.45
1:A:190:ASP:OD1	1:A:193:LYS:HG3	2.17	0.45
1:A:328:TYR:N	1:A:328:TYR:CD1	2.84	0.45
1:B:157:MET:O	1:B:161:PHE:CD1	2.70	0.45
1:A:24:LEU:O	1:A:51:CYS:HB3	2.17	0.45
1:A:104:GLN:HG2	8:A:2050:HOH:O	2.16	0.45
1:B:215:THR:HA	1:B:276:ALA:O	2.17	0.44
1:B:48[A]:ARG:HD3	1:B:49:PHE:CD2	2.52	0.44
1:B:94:LEU:HB2	1:B:132:PHE:CD2	2.52	0.44
1:A:358:ASP:HB3	1:A:371:PRO:CD	2.48	0.44
1:B:301[A]:ASP:OD1	1:B:304[A]:ARG:NH2	2.51	0.44
1:B:84:LYS:HA	1:B:87:ASN:O	2.17	0.44
1:B:38:ASP:N	1:B:38:ASP:OD2	2.51	0.44
1:B:139:TRP:CE2	1:B:142:PRO:HA	2.53	0.44
1:A:352:TRP:CZ3	2:A:-1:NAG:H83	2.52	0.44
1:B:100:ASN:HD22	6:B:-2:NAG:H62	1.81	0.44
1:B:203:ILE:HD11	1:B:240:ALA:HB1	2.00	0.44
1:A:26:CYS:HB3	1:A:354:LEU:HG	1.98	0.44
1:A:59:ALA:HB2	1:A:94:LEU:HD21	1.99	0.44
1:B:139:TRP:O	1:B:141:TYR:HA	2.18	0.44
1:A:304:ARG:HH11	1:A:304:ARG:CB	2.31	0.44
1:A:219:HIS:CG	1:A:263:ARG:HG3	2.52	0.44
1:B:245:LEU:HA	1:B:249:ALA:HB3	2.00	0.43
1:A:71:TRP:CE2	4:A:1389:GOL:H2	2.53	0.43
1:A:124:PRO:HB3	1:A:164:GLU:HG3	1.99	0.43
1:B:178:LEU:CD1	1:B:201:ILE:HD13	2.49	0.43
1:B:65[B]:HIS:CE1	1:B:118:THR:CG2	3.02	0.43
1:A:221:PRO:HB2	1:A:314:GLN:HB3	2.01	0.43
1:A:162:ILE:HG12	1:A:171:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:139:TRP:CD1	1:B:139:TRP:C	2.91	0.43
1:A:170[B]:LYS:HD2	8:A:2079:HOH:O	2.18	0.43
1:A:174:LEU:HG	1:A:198:LEU:HD23	2.00	0.43
1:B:52:THR:OG1	1:B:53:HIS:HD2	2.01	0.43
1:B:124:PRO:HB3	1:B:164:GLU:HG3	2.01	0.42
1:A:338:VAL:O	1:A:341:LEU:HG	2.19	0.42
1:B:234:PHE:CD2	1:B:239:TYR:CZ	3.07	0.42
1:A:204:MET:HE2	2:A:-1:NAG:C1	2.50	0.42
1:B:117:ARG:HH21	4:B:1384:GOL:H31	1.84	0.42
1:B:166:GLN:HG3	1:B:167:PRO:HD3	2.02	0.42
1:B:61:ILE:O	1:B:61:ILE:HG22	2.20	0.42
1:A:29:THR:HB	1:A:31:TRP:CE3	2.55	0.42
1:A:91:LYS:HD2	8:A:2042:HOH:O	2.20	0.42
1:A:246:ARG:NE	8:A:2111:HOH:O	2.43	0.42
1:B:258:ILE:HD12	1:B:349:ALA:HB1	2.02	0.42
1:A:361:GLY:HA2	1:A:368:LEU:O	2.19	0.42
1:B:80:LEU:HD23	1:B:132:PHE:HE1	1.84	0.42
1:B:190:ASP:OD2	1:B:193:LYS:HB3	2.20	0.42
1:A:91:LYS:HE3	1:A:170[A]:LYS:HE3	2.01	0.42
1:B:383:THR:HG22	1:B:383:THR:OXT	2.18	0.42
1:B:303:LEU:HA	1:B:303:LEU:HD23	1.85	0.42
1:A:283:ILE:HA	1:A:284:PRO:HD3	1.95	0.42
1:B:352:TRP:HA	1:B:353:ALA:HA	1.79	0.41
1:B:60:ASN:HB2	1:B:69:TRP:HE3	1.85	0.41
1:A:190:ASP:OD1	1:A:193:LYS:CG	2.68	0.41
1:B:331:GLN:NE2	8:B:2134:HOH:O	2.52	0.41
1:B:254:LEU:HB3	1:B:346:LEU:HD22	2.02	0.41
1:B:103:SER:HB3	1:B:139:TRP:HE1	1.84	0.41
1:B:35:ARG:CG	4:B:1385:GOL:H32	2.50	0.41
1:B:323:ASN:ND2	1:B:324:GLN:HE21	2.18	0.41
1:A:299:ILE:HD13	1:A:328:TYR:CG	2.55	0.41
1:B:166:GLN:N	1:B:167:PRO:CD	2.84	0.41
2:A:-2:NAG:H82	2:A:-1:NAG:H61	2.02	0.41
1:B:193:LYS:HG3	1:B:196:GLN:HE22	1.86	0.41
1:B:297:TYR:HB2	1:B:363:PHE:CG	2.56	0.41
1:B:33:GLN:HG3	1:B:34:TYR:CD1	2.55	0.41
1:B:135:LEU:HG	1:B:136:ASP:H	1.85	0.41
1:B:249:ALA:HA	1:B:250:PRO:HD3	1.75	0.41
1:B:140:LEU:HA	1:B:141:TYR:HA	1.77	0.41
1:B:178:LEU:HD11	1:B:201:ILE:HD13	2.03	0.41
1:B:261:PHE:HB3	1:B:356:LEU:HD13	2.02	0.41
1:B:190:ASP:O	1:B:194:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:233:ARG:HG2	8:B:2072:HOH:O	2.19	0.41
1:B:190:ASP:N	8:B:2053:HOH:O	2.54	0.40
1:B:251:ALA:HB1	1:B:345:GLN:O	2.21	0.40
1:B:352:TRP:NE1	6:B:-1:NAG:H5	2.37	0.40
1:B:163:LYS:HA	1:B:166:GLN:OE1	2.21	0.40
1:B:126:PHE:C	1:B:126:PHE:CD1	2.95	0.40
1:A:123:VAL:HB	1:A:124:PRO:HD3	2.03	0.40
1:A:315:GLN:NE2	8:A:2145:HOH:O	2.53	0.40
1:A:230:SER:HA	1:A:231:PRO:HD3	1.92	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	Distance(Å)	Clash(Å)
5:A:1394:SO4:O2	5:A:1394:SO4:O2[8_565]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	362/362 (100%)	345 (95%)	12 (3%)	5 (1%)	16	15
1	B	369/362 (102%)	316 (86%)	39 (11%)	14 (4%)	5	2
All	All	731/724 (101%)	661 (90%)	51 (7%)	19 (3%)	8	5

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	PRO
1	B	64	ASP
1	A	365	GLY
1	A	366	GLN
1	B	101	PHE
1	B	105	ARG
1	B	211	ALA

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Mol	Chain	Res	Type
1	B	231	PRO
1	B	366	GLN
1	A	382	ALA
1	B	102	GLY
1	B	168	GLY
1	B	289	LYS
1	B	71	TRP
1	B	382	ALA
1	B	164	GLU
1	B	364	CYS
1	A	166	GLN
1	B	250	PRO

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	304/302 (101%)	295 (97%)	9 (3%)	53	70
1	B	311/302 (103%)	289 (93%)	22 (7%)	21	26
All	All	615/604 (102%)	584 (95%)	31 (5%)	38	45

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	170[A]	LYS
1	A	170[B]	LYS
1	A	227	GLU
1	A	234	PHE
1	A	263	ARG
1	A	304	ARG
1	A	331	GLN
1	A	360	GLN
1	B	48[A]	ARG
1	B	48[B]	ARG
1	B	63[A]	ASN
1	B	63[B]	ASN

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Mol	Chain	Res	Type
1	B	65[A]	HIS
1	B	65[B]	HIS
1	B	73	ASP
1	B	86	ARG
1	B	105	ARG
1	B	126	PHE
1	B	170	LYS
1	B	205	THR
1	B	212	TRP
1	B	227	GLU
1	B	247	LEU
1	B	252	SER
1	B	286	ARG
1	B	317	PRO
1	B	323	ASN
1	B	329	ASP
1	B	339	GLN
1	B	366	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	85	ASN
1	A	89	ASN
1	A	104	GLN
1	A	130	HIS
1	A	171	GLN
1	A	196	GLN
1	A	209	HIS
1	A	331	GLN
1	B	53	HIS
1	B	85	ASN
1	B	100	ASN
1	B	130	HIS
1	B	171	GLN
1	B	196	GLN
1	B	209	HIS
1	B	323	ASN
1	B	366	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

13 carbohydrates are modelled in this entry.

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	-1	2	12,14,15	0.66	0	15,19,21	0.76	1 (6%)
2	NAG	A	-2	2	12,14,15	0.57	0	15,19,21	0.75	0
2	NAG	A	-3	2	12,14,15	0.66	0	15,19,21	0.63	0
2	NAG	A	-4	2	12,14,15	0.70	0	15,19,21	0.58	0
2	NAG	A	1	2	12,14,15	0.72	0	15,19,21	0.98	1 (6%)
3	NAG	A	1384	1,3	12,14,15	0.66	0	15,19,21	0.83	0
3	NAG	A	1385	3	12,14,15	0.66	0	15,19,21	0.64	0
2	NAG	A	2	2	15,15,15	0.65	0	21,21,21	0.99	2 (9%)
6	NAG	B	-1	6	12,14,15	0.69	0	15,19,21	0.95	1 (6%)
6	NAG	B	-2	6	12,14,15	0.58	0	15,19,21	0.70	0
6	NAG	B	-3	6	12,14,15	0.61	0	15,19,21	0.67	0
6	NAG	B	1	6	12,14,15	0.59	0	15,19,21	0.78	0
6	NAG	B	2	6	15,15,15	0.69	0	21,21,21	0.67	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	-1	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	-2	2	-	0/6/23/26	0/1/1/1
2	NAG	A	-3	2	-	0/6/23/26	0/1/1/1
2	NAG	A	-4	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1384	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1385	3	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/6/26/26	0/1/1/1
6	NAG	B	-1	6	-	0/6/23/26	0/1/1/1
6	NAG	B	-2	6	-	0/6/23/26	0/1/1/1
6	NAG	B	-3	6	-	0/6/23/26	0/1/1/1
6	NAG	B	1	6	-	0/6/23/26	0/1/1/1
6	NAG	B	2	6	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	C2-N2-C7	-2.37	119.11	123.09
2	A	2	NAG	C4-C3-C2	2.36	113.79	110.44
6	B	-1	NAG	C2-N2-C7	-2.34	119.17	123.09
2	A	2	NAG	C1-C2-N2	-2.23	108.25	110.85
2	A	-1	NAG	C2-N2-C7	-2.20	119.39	123.09

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1385	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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	GOL	A	1386	-	5,5,5	0.36	0	5,5,5	0.32	0
4	GOL	A	1387	-	5,5,5	0.36	0	5,5,5	0.25	0
4	GOL	A	1388	-	5,5,5	0.28	0	5,5,5	0.29	0
4	GOL	A	1389	-	5,5,5	0.35	0	5,5,5	0.36	0
5	SO4	A	1392	-	4,4,4	0.26	0	6,6,6	0.13	0
5	SO4	A	1394	-	4,4,4	0.26	0	6,6,6	0.14	0
5	SO4	A	1396	-	4,4,4	0.23	0	6,6,6	0.10	0
4	GOL	A	1399	-	5,5,5	0.33	0	5,5,5	0.26	0
7	NAG	B	1383	1	12,14,15	0.55	0	15,19,21	0.49	0
4	GOL	B	1384	-	5,5,5	0.40	0	5,5,5	0.27	0
4	GOL	B	1385	-	5,5,5	0.51	0	5,5,5	0.37	0
5	SO4	B	1386	-	4,4,4	0.21	0	6,6,6	0.11	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
4	GOL	A	1386	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1387	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1388	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1389	-	-	0/4/4/4	0/0/0/0
5	SO4	A	1392	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1394	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1396	-	-	0/0/0/0	0/0/0/0
4	GOL	A	1399	-	-	0/4/4/4	0/0/0/0
7	NAG	B	1383	1	-	0/6/23/26	0/1/1/1
4	GOL	B	1384	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1385	-	-	0/4/4/4	0/0/0/0
5	SO4	B	1386	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	362/362 (100%)	0.15	22 (6%) 21 29	41, 56, 80, 99	0
1	B	362/362 (100%)	0.56	46 (12%) 4 7	37, 75, 113, 125	0
All	All	724/724 (100%)	0.36	68 (9%) 9 14	37, 61, 108, 125	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	65[A]	HIS	6.9
1	B	212	TRP	5.7
1	B	166	GLN	4.6
1	B	177	ALA	4.0
1	A	86	ARG	3.9
1	B	365	GLY	3.9
1	B	94	LEU	3.8
1	A	166	GLN	3.7
1	B	63[A]	ASN	3.7
1	B	145	ARG	3.5
1	B	259	PRO	3.4
1	A	383	THR	3.4
1	B	176	ALA	3.3
1	B	137	LEU	3.3
1	B	95	SER	3.3
1	A	365	GLY	3.2
1	B	135	LEU	3.2
1	B	103	SER	3.1
1	B	351	VAL	3.0
1	B	27	TYR	3.0
1	B	352	TRP	2.9
1	B	144	ARG	2.9
1	B	169	LYS	2.9
1	A	96	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	144	ARG	2.8
1	B	55	ILE	2.8
1	B	162	ILE	2.8
1	B	382	ALA	2.8
1	B	86	ARG	2.7
1	A	55	ILE	2.7
1	B	96	VAL	2.6
1	A	210	GLY	2.6
1	B	202	SER	2.6
1	B	108	LYS	2.6
1	B	59	ALA	2.6
1	A	135	LEU	2.6
1	A	363	PHE	2.5
1	A	351	VAL	2.5
1	B	211	ALA	2.5
1	A	145	ARG	2.5
1	B	383	THR	2.5
1	B	260	THR	2.5
1	B	136	ASP	2.5
1	B	89	ASN	2.5
1	B	210	GLY	2.5
1	A	176	ALA	2.5
1	B	167	PRO	2.4
1	A	212	TRP	2.4
1	B	363	PHE	2.4
1	B	88	PRO	2.4
1	A	71	TRP	2.4
1	B	170	LYS	2.4
1	B	114	GLN	2.4
1	B	175	SER	2.4
1	A	211	ALA	2.3
1	B	85	ASN	2.3
1	A	25	VAL	2.2
1	B	262	GLY	2.2
1	A	108	LYS	2.2
1	A	27	TYR	2.2
1	B	138	ALA	2.2
1	A	26	CYS	2.2
1	B	104[A]	GLN	2.1
1	B	261	PHE	2.1
1	A	366	GLN	2.1
1	B	366	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	74	VAL	2.0
1	A	258	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 ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	-4	14/15	0.36	10.49	96,98,101,101	0
3	NAG	A	1384	14/15	0.24	4.33	85,90,95,101	0
2	NAG	A	-3	14/15	0.17	2.26	73,81,89,90	0
2	NAG	A	1	14/15	0.18	2.23	71,78,84,87	0
2	NAG	A	2	15/15	0.17	1.86	73,80,83,84	0
6	NAG	B	2	15/15	0.24	0.88	89,96,99,99	0
6	NAG	B	-3	14/15	0.17	0.42	87,90,92,94	0
2	NAG	A	-2	14/15	0.15	0.21	59,68,71,73	0
6	NAG	B	1	14/15	0.12	-0.74	79,85,89,90	0
6	NAG	B	-2	14/15	0.14	-0.79	67,81,84,86	0
2	NAG	A	-1	14/15	0.11	-1.11	55,63,65,68	0
6	NAG	B	-1	14/15	0.12	-1.42	64,76,78,79	0
3	NAG	A	1385	14/15	0.32	-	105,107,109,109	0

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	A	1399	6/6	0.40	17.39	122,122,123,124	0
5	SO4	A	1394	5/5	0.32	8.30	155,156,156,156	0
4	GOL	B	1385	6/6	0.31	5.24	101,103,103,104	0
4	GOL	A	1388	6/6	0.13	3.11	83,85,86,86	0
4	GOL	A	1386	6/6	0.41	2.60	92,95,95,96	0
4	GOL	A	1389	6/6	0.33	2.56	87,89,89,90	0
5	SO4	B	1386	5/5	0.20	1.75	163,164,164,164	0
7	NAG	B	1383	14/15	0.23	1.61	102,104,106,106	0
5	SO4	A	1396	5/5	0.20	0.86	146,146,146,146	0
4	GOL	B	1384	6/6	0.23	-0.06	85,87,87,89	0
5	SO4	A	1392	5/5	0.11	-1.56	110,110,111,111	0
4	GOL	A	1387	6/6	0.24	-	95,99,99,100	0

6.5 Other polymers ⓘ

There are no such residues in this entry.