



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:51 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 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

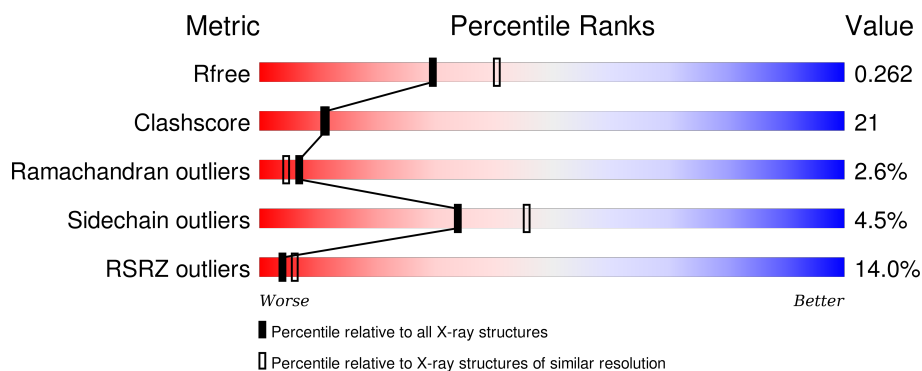
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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. 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	362	
1	B	362	

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	1	-	-	-	X
2	NAG	A	2	-	-	-	X
3	NAG	A	1384	-	-	-	X
3	NAG	A	1385	X	-	-	-
4	GOL	A	1386	-	-	-	X
4	GOL	A	1399	-	-	-	X
4	GOL	B	1385	-	-	X	X
5	SO4	A	1394	-	-	X	X
6	NAG	B	-1	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6374 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 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		

- 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		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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: O₄S).

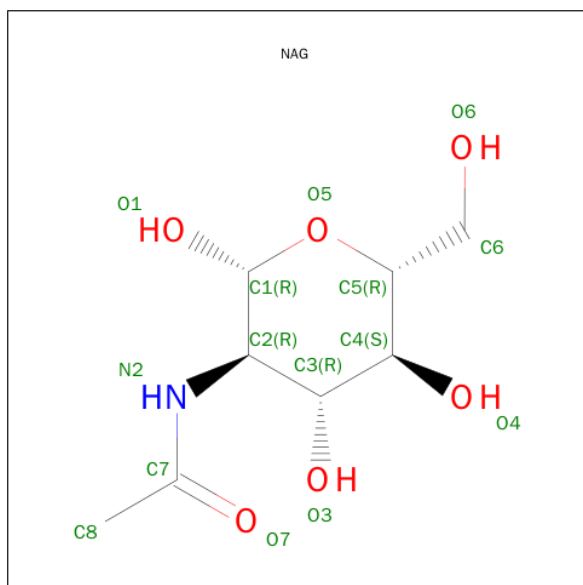


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- 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		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

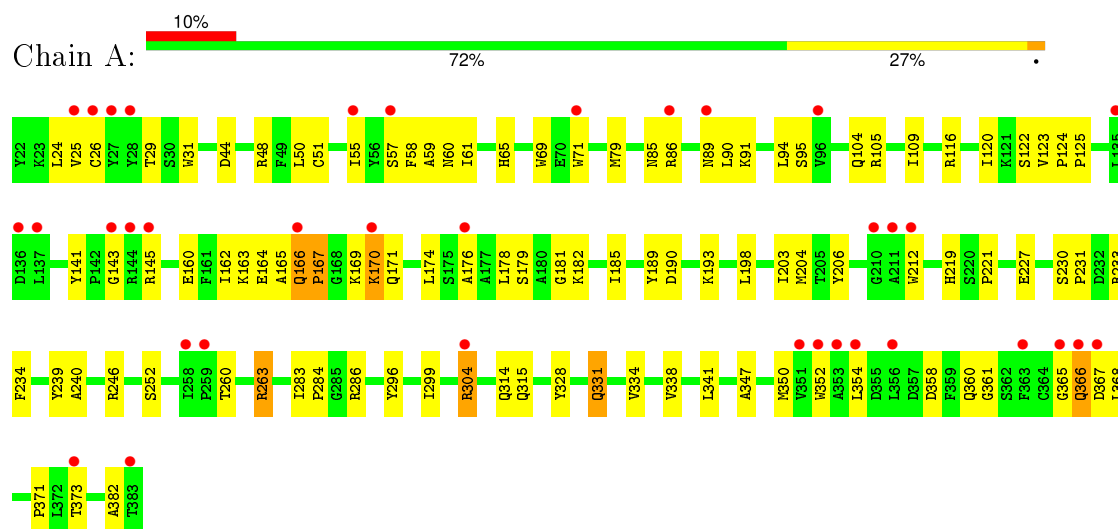
- Molecule 8 is water.

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

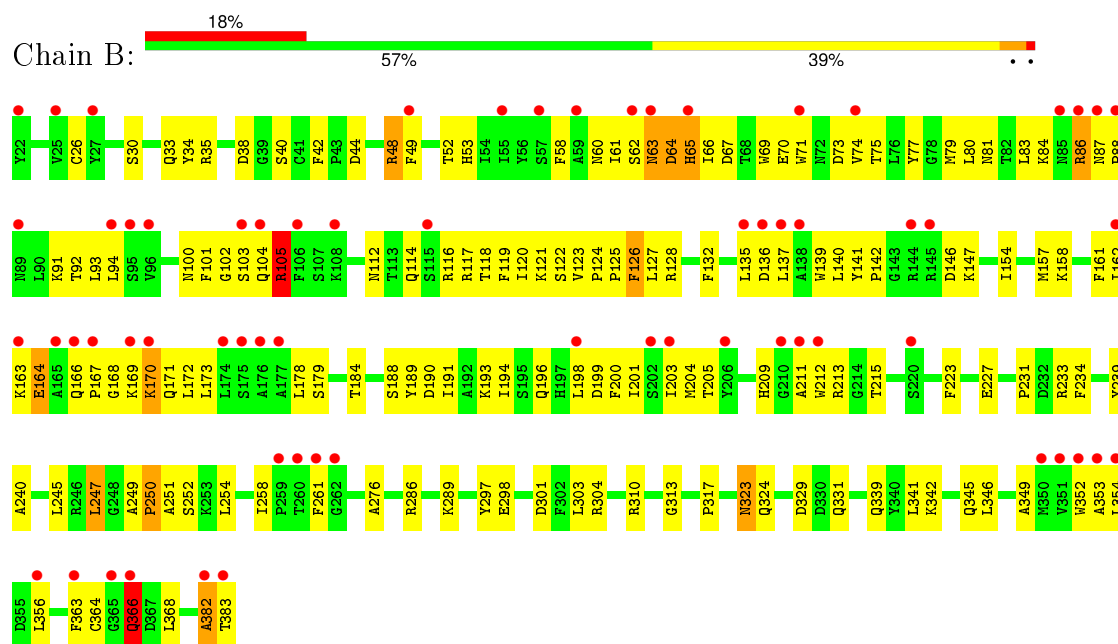
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 0.224 , 0.262	Depositor DCC
R_{free} test set	611 reflections (1.55%)	DCC
Wilson B-factor (Å ²)	58.2	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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 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	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

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 21.

All (245) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:TRP:CH2	6:B:-1:NAG:H3	2.37	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	Interatomic distance (Å)	Clash overlap (Å)
5:A:1394:SO4:O2	5:A:1394:SO4:O2[8_565]	2.19	0.01

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	362/362 (100%)	345 (95%)	12 (3%)	5 (1%)	14	13
1	B	369/362 (102%)	316 (86%)	39 (11%)	14 (4%)	4	2
All	All	731/724 (101%)	661 (90%)	51 (7%)	19 (3%)	7	4

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
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%)	48	65
1	B	311/302 (103%)	289 (93%)	22 (7%)	18	23
All	All	615/604 (102%)	584 (95%)	31 (5%)	34	41

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 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 ⓘ

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	14,14,15	0.87	1 (7%)	15,19,21	1.08	2 (13%)
2	NAG	A	-2	2	14,14,15	0.89	0	15,19,21	0.89	0
2	NAG	A	-3	2	14,14,15	0.63	0	15,19,21	0.68	1 (6%)
2	NAG	A	-4	2	14,14,15	0.97	1 (7%)	15,19,21	0.59	0
2	NAG	A	1	2	14,14,15	0.72	0	15,19,21	1.07	1 (6%)
3	NAG	A	1384	1,3	14,14,15	0.72	0	15,19,21	0.87	1 (6%)
3	NAG	A	1385	3	14,14,15	0.91	1 (7%)	15,19,21	0.63	0
2	NAG	A	2	2	15,15,15	0.67	0	17,21,21	0.82	1 (5%)
6	NAG	B	-1	6	14,14,15	0.81	0	15,19,21	1.23	2 (13%)
6	NAG	B	-2	6	14,14,15	0.73	0	15,19,21	0.81	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	-3	6	14,14,15	0.71	0	15,19,21	0.62	0
6	NAG	B	1	6	14,14,15	0.63	0	15,19,21	0.83	1 (6%)
6	NAG	B	2	6	15,15,15	0.70	0	17,21,21	0.75	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
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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	-1	NAG	C1-C2	2.14	1.55	1.52
3	A	1385	NAG	C1-C2	2.27	1.55	1.52
2	A	-4	NAG	C1-C2	2.49	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	C2-N2-C7	-3.06	119.11	123.04
6	B	-1	NAG	C2-N2-C7	-3.01	119.17	123.04
2	A	-1	NAG	C2-N2-C7	-2.84	119.39	123.04
6	B	1	NAG	C2-N2-C7	-2.35	120.01	123.04
3	A	1384	NAG	C2-N2-C7	-2.22	120.19	123.04
6	B	-2	NAG	C2-N2-C7	-2.12	120.31	123.04
2	A	-3	NAG	C2-N2-C7	-2.01	120.46	123.04
2	A	2	NAG	C4-C3-C2	2.43	113.79	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	-1	NAG	C1-O5-C5	2.49	115.41	112.25
6	B	-1	NAG	C1-O5-C5	2.91	115.94	112.25

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.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	-1	NAG	5	0
2	A	-2	NAG	1	0
2	A	-3	NAG	1	0
2	A	-4	NAG	1	0
2	A	1	NAG	2	0
6	B	-1	NAG	7	0
6	B	-2	NAG	2	0
6	B	-3	NAG	2	0
6	B	1	NAG	1	0

5.6 Ligand geometry [i](#)

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	0.40	0	5,5,5	0.28	0
4	GOL	A	1387	-	5,5,5	0.39	0	5,5,5	0.18	0
4	GOL	A	1388	-	5,5,5	0.31	0	5,5,5	0.24	0
4	GOL	A	1389	-	5,5,5	0.39	0	5,5,5	0.33	0
5	SO4	A	1392	-	4,4,4	0.22	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	A	1394	-	4,4,4	0.22	0	6,6,6	0.15	0
5	SO4	A	1396	-	4,4,4	0.19	0	6,6,6	0.10	0
4	GOL	A	1399	-	5,5,5	0.36	0	5,5,5	0.20	0
7	NAG	B	1383	1	14,14,15	0.53	0	15,19,21	0.59	0
4	GOL	B	1384	-	5,5,5	0.43	0	5,5,5	0.22	0
4	GOL	B	1385	-	5,5,5	0.56	0	5,5,5	0.29	0
5	SO4	B	1386	-	4,4,4	0.17	0	6,6,6	0.12	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 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1387	GOL	2	0
4	A	1389	GOL	2	0
5	A	1394	SO4	1	1
4	B	1384	GOL	2	0
4	B	1385	GOL	4	0

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%)	0.31	36 (9%) 9 14	41, 56, 80, 99	0
1	B	362/362 (100%)	0.79	65 (17%) 2 3	37, 75, 113, 125	0
All	All	724/724 (100%)	0.55	101 (13%) 4 6	37, 61, 108, 125	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	65[A]	HIS	7.5
1	B	212	TRP	6.3
1	B	365	GLY	5.2
1	B	145	ARG	5.1
1	B	259	PRO	4.8
1	B	177	ALA	4.5
1	B	166	GLN	4.5
1	B	137	LEU	4.5
1	A	166	GLN	4.5
1	A	86	ARG	4.5
1	B	95	SER	4.2
1	B	63[A]	ASN	4.1
1	B	351	VAL	4.1
1	B	352	TRP	4.1
1	B	176	ALA	4.1
1	B	162	ILE	4.0
1	B	27	TYR	3.9
1	B	94	LEU	3.9
1	A	135	LEU	3.8
1	B	135	LEU	3.8
1	B	211	ALA	3.7
1	A	351	VAL	3.7
1	B	260	THR	3.6
1	B	55	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	96	VAL	3.6
1	A	365	GLY	3.5
1	B	382	ALA	3.5
1	B	86	ARG	3.4
1	B	261	PHE	3.4
1	A	144	ARG	3.3
1	B	262	GLY	3.3
1	A	354	LEU	3.3
1	A	55	ILE	3.3
1	B	144	ARG	3.3
1	B	87	ASN	3.2
1	A	383	THR	3.2
1	A	27	TYR	3.2
1	B	59	ALA	3.2
1	B	210	GLY	3.2
1	B	356	LEU	3.2
1	B	103	SER	3.1
1	A	96	VAL	3.0
1	A	145	ARG	3.0
1	B	202	SER	3.0
1	A	212	TRP	2.9
1	B	57[A]	SER	2.9
1	B	366	GLN	2.9
1	B	169	LYS	2.9
1	B	170	LYS	2.9
1	B	85	ASN	2.9
1	B	136	ASP	2.9
1	A	26	CYS	2.9
1	B	383	THR	2.8
1	A	25	VAL	2.8
1	B	167	PRO	2.8
1	B	62	SER	2.8
1	A	352	TRP	2.8
1	B	89	ASN	2.7
1	B	220	SER	2.7
1	B	175	SER	2.7
1	B	108	LYS	2.7
1	A	71	TRP	2.7
1	A	176	ALA	2.6
1	B	25	VAL	2.6
1	B	104[A]	GLN	2.6
1	B	88	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	74	VAL	2.5
1	A	259	PRO	2.5
1	B	138	ALA	2.5
1	A	356	LEU	2.5
1	B	203	ILE	2.5
1	B	350	MET	2.4
1	A	367	ASP	2.4
1	B	363	PHE	2.4
1	B	165	ALA	2.4
1	A	363	PHE	2.3
1	B	353	ALA	2.3
1	A	258	ILE	2.3
1	B	354	LEU	2.3
1	A	353	ALA	2.3
1	A	210	GLY	2.2
1	A	366	GLN	2.2
1	A	137	LEU	2.2
1	A	57	SER	2.2
1	A	89	ASN	2.2
1	A	143	GLY	2.2
1	B	198	LEU	2.2
1	A	373	THR	2.2
1	B	163	LYS	2.1
1	A	28	TYR	2.1
1	A	136	ASP	2.1
1	B	174	LEU	2.1
1	A	170[A]	LYS	2.1
1	B	115	SER	2.1
1	B	49	PHE	2.1
1	B	106	PHE	2.0
1	B	206	TYR	2.0
1	B	71	TRP	2.0
1	A	304	ARG	2.0
1	A	211	ALA	2.0
1	B	22	TYR	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	2	15/15	0.92	0.22	3.77	73,80,83,84	0
3	NAG	A	1384	14/15	0.90	0.25	3.73	85,90,95,101	0
2	NAG	A	1	14/15	0.93	0.22	3.24	71,78,84,87	0
6	NAG	B	-3	14/15	0.88	0.22	1.03	87,90,92,94	0
6	NAG	B	2	15/15	0.83	0.23	0.60	89,96,99,99	0
2	NAG	A	-2	14/15	0.90	0.16	0.06	59,68,71,73	0
6	NAG	B	-2	14/15	0.82	0.16	-0.78	67,81,84,86	0
6	NAG	B	1	14/15	0.85	0.14	-0.83	79,85,89,90	0
2	NAG	A	-1	14/15	0.91	0.13	-0.88	55,63,65,68	0
6	NAG	B	-1	14/15	0.89	0.13	-1.43	64,76,78,79	0
3	NAG	A	1385	14/15	0.81	0.38	-	105,107,109,109	0
2	NAG	A	-3	14/15	0.92	0.21	-	73,81,89,90	0
2	NAG	A	-4	14/15	0.69	0.41	-	96,98,101,101	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	A	1399	6/6	0.49	0.45	18.08	122,122,123,124	0
5	SO4	A	1394	5/5	0.82	0.34	8.69	155,156,156,156	0
4	GOL	B	1385	6/6	0.79	0.31	6.85	101,103,103,104	0
4	GOL	A	1386	6/6	0.87	0.38	2.10	92,95,95,96	0
5	SO4	B	1386	5/5	0.83	0.20	1.92	163,164,164,164	0
7	NAG	B	1383	14/15	0.87	0.24	0.85	102,104,106,106	0
5	SO4	A	1392	5/5	0.94	0.11	-2.09	110,110,111,111	0
4	GOL	A	1389	6/6	0.78	0.32	-	87,89,89,90	0
4	GOL	B	1384	6/6	0.86	0.21	-	85,87,87,89	0
5	SO4	A	1396	5/5	0.86	0.19	-	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	A	1387	6/6	0.75	0.25	-	95,99,99,100	0
4	GOL	A	1388	6/6	0.90	0.14	-	83,85,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.