



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:20 AM GMT

PDB ID : 2WR2
Title : STRUCTURE OF INFLUENZA H2 AVIAN HEMAGGLUTININ WITH AVIAN RECEPTOR
Authors : Liu, J.; Stevens, D.J.; Haire, L.F.; Walker, P.A.; Coombs, P.J.; Russell, R.J.; Gamblin, S.J.; Skehel, J.J.
Deposited on : 2009-08-29
Resolution : 2.40 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

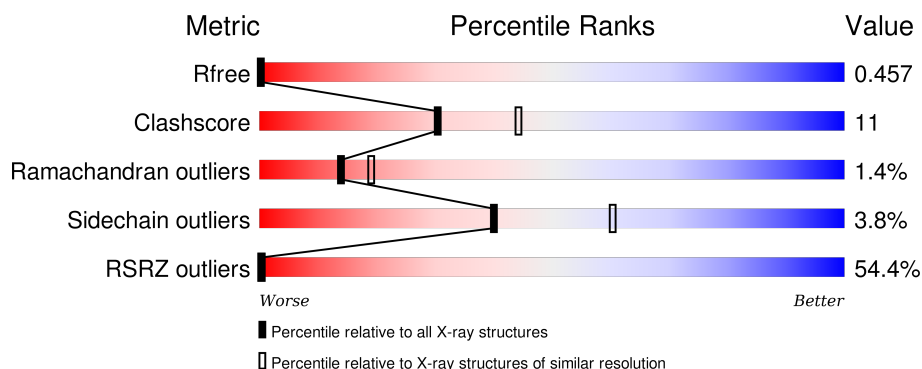
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	509	
1	B	509	
1	C	509	

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	C	1500	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12274 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 HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	4	0	0
			3882	2436	671	753	22			
1	B	490	Total	C	N	O	S	0	1	0
			3887	2438	672	755	22			
1	C	485	Total	C	N	O	S	0	0	0
			3844	2413	664	745	22			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			13	8	1	4		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	3	Total	C	N	O	0	0
			46	25	2	19		
3	C	3	Total	C	N	O	0	0
			46	25	2	19		

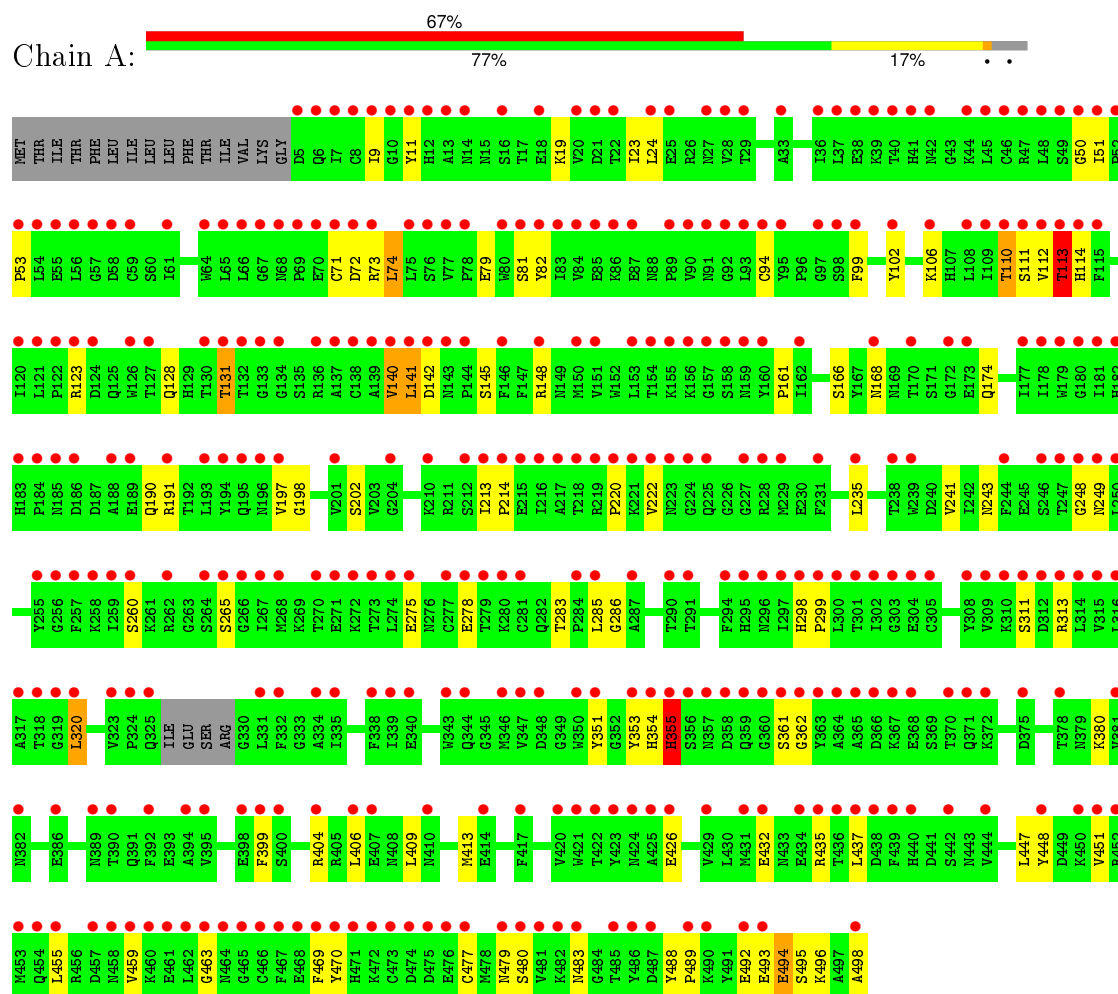
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	185	Total	O	0	0
			185	185		
4	B	169	Total	O	0	0
			169	169		
4	C	174	Total	O	0	0
			174	174		

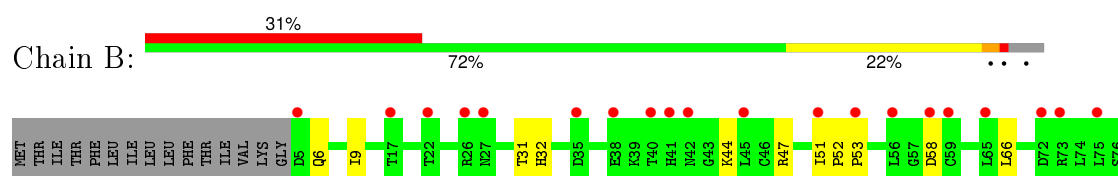
3 Residue-property plots

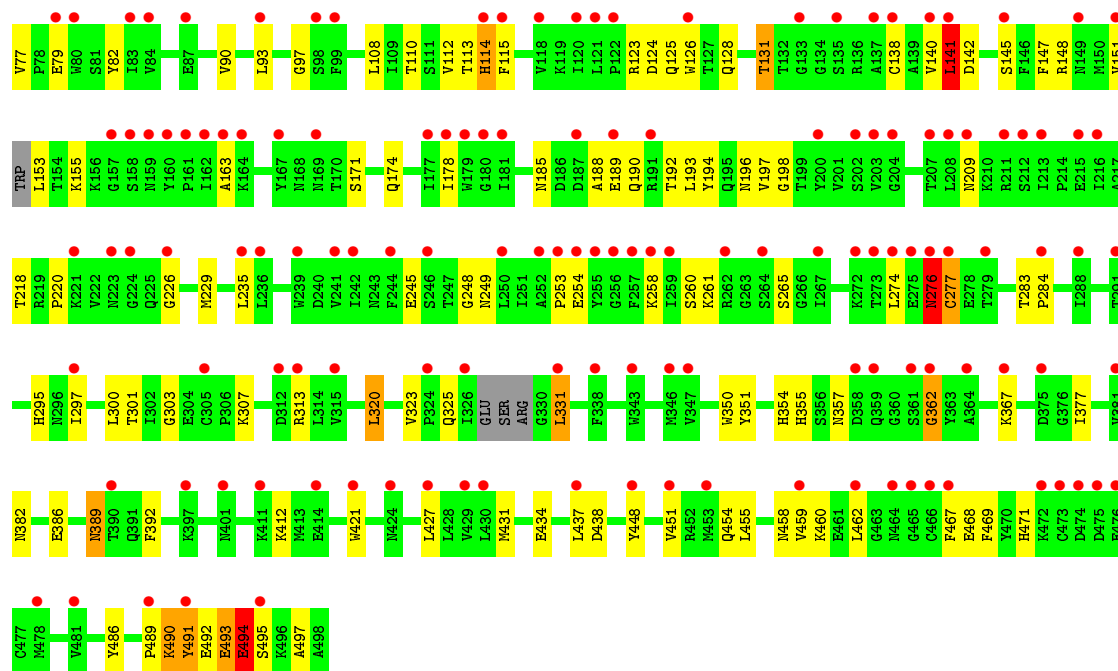
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: HEMAGGLUTININ

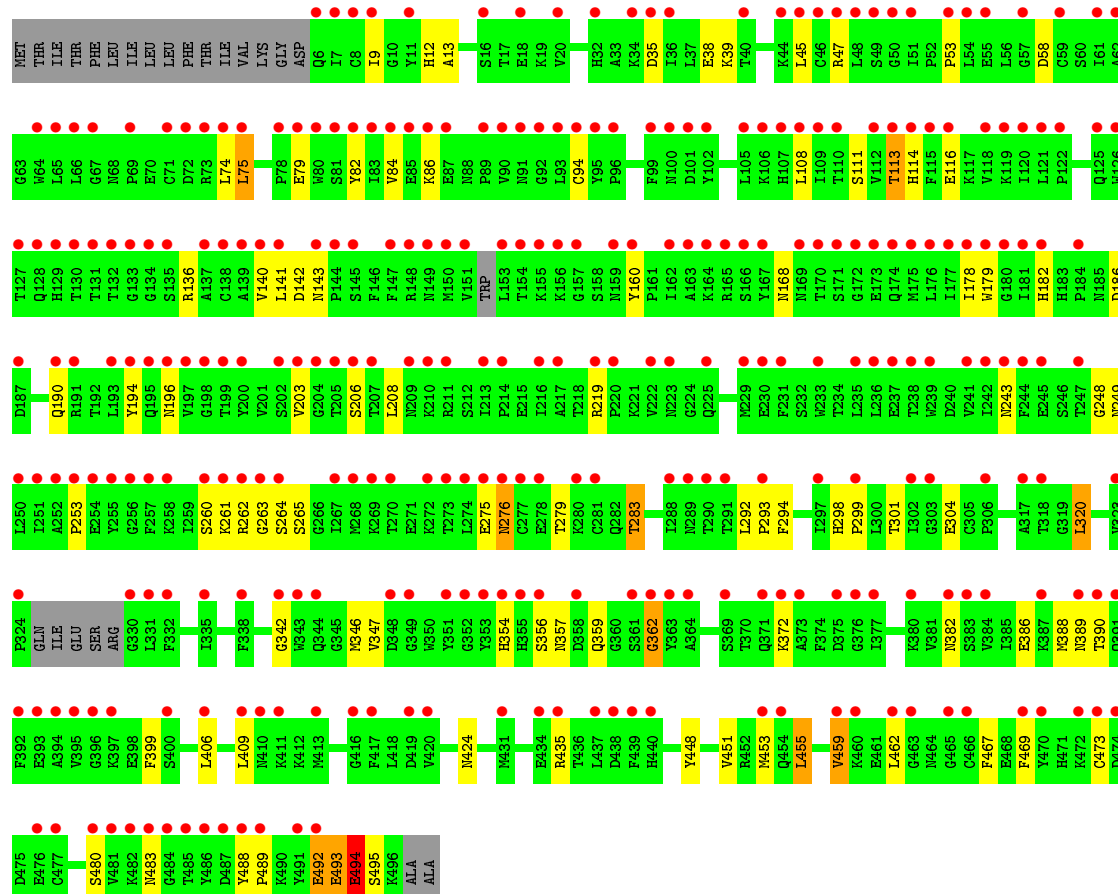
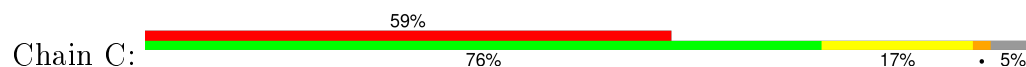


• Molecule 1: HEMAGGLUTININ





• Molecule 1: HEMAGGLUTININ



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.88Å 142.72Å 199.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 2.40 29.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.94-2.40) 99.9 (29.94-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.210 , 0.248 0.446 , 0.457	Depositor DCC
R_{free} test set	3954 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 78792 reflections	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	12274	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, GAL, 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	0.33	0/3968	0.51	0/5372
1	B	0.33	0/3970	0.53	0/5372
1	C	0.33	0/3927	0.51	0/5313
All	All	0.33	0/11865	0.52	0/16057

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3882	0	3742	85	2
1	B	3887	0	3756	109	2
1	C	3844	0	3718	67	0
2	A	27	0	25	7	0
2	C	14	0	13	3	0
3	B	46	0	40	2	0
3	C	46	0	40	0	0
4	A	185	0	0	5	0
4	B	169	0	0	9	0
4	C	174	0	0	2	0
All	All	12274	0	11334	254	2

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 11.

All (254) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLN:NE2	4:B:2109:HOH:O	1.62	1.27
1:A:283:THR:HG22	1:A:285:LEU:H	1.18	1.05
1:A:148:ARG:HG2	1:A:148:ARG:HH11	1.32	0.94
1:B:325:GLN:HB3	4:B:2110:HOH:O	1.65	0.93
1:A:361:SER:HB3	1:A:362:GLY:HA3	1.49	0.92
1:C:114:HIS:H	1:C:260:SER:HB2	1.35	0.91
1:B:140:VAL:O	1:B:141:LEU:HB2	1.72	0.89
1:B:459:VAL:HG22	1:B:469:PHE:HA	1.55	0.89
1:B:276:ASN:HA	1:B:277:CYS:O	1.73	0.89
1:B:459:VAL:HG11	1:B:467:PHE:HB3	1.54	0.88
1:A:110:THR:CG2	1:A:265:SER:H	1.86	0.88
1:C:168:ASN:HD21	2:C:1500:NAG:C1	1.89	0.84
1:B:47:ARG:HE	1:B:276:ASN:HB2	1.42	0.84
1:C:141:LEU:N	1:C:142:ASP:HA	1.95	0.82
1:A:110:THR:HG21	1:A:265:SER:H	1.44	0.82
1:B:141:LEU:N	1:B:142:ASP:HA	1.97	0.79
1:A:114:HIS:H	1:A:260:SER:HB2	1.45	0.79
1:B:110:THR:CG2	1:B:265:SER:H	1.95	0.78
1:B:32:HIS:CD2	4:B:2124:HOH:O	2.37	0.78
1:C:114:HIS:N	1:C:260:SER:HB2	1.98	0.77
1:A:479:ASN:HB3	2:A:1499:NAG:H81	1.64	0.77
1:B:113:THR:HB	1:B:114:HIS:HB3	1.66	0.77
1:A:168:ASN:HD21	2:A:1500:NAG:C5	1.97	0.77
1:A:190:GLN:HE22	1:A:249:ASN:HD21	1.33	0.77
1:A:174:GLN:HE21	1:A:235:LEU:HD13	1.51	0.76
1:B:455:LEU:HD13	1:B:459:VAL:HG21	1.66	0.75
1:B:458:ASN:OD1	1:B:494:GLU:HG2	1.86	0.74
1:A:493:GLU:O	1:A:494:GLU:HB3	1.88	0.73
1:A:174:GLN:NE2	1:A:235:LEU:HD13	2.04	0.73
1:C:190:GLN:HE22	1:C:249:ASN:HD21	1.36	0.73
1:A:283:THR:HG22	1:A:285:LEU:N	1.99	0.73
1:A:320:LEU:H	1:A:320:LEU:HD23	1.53	0.72
1:A:283:THR:HB	1:A:286:GLY:O	1.89	0.72
1:A:166:SER:HB3	1:A:243:ASN:ND2	2.05	0.72
1:B:354:HIS:HA	1:B:362:GLY:O	1.90	0.72
1:B:140:VAL:HG12	1:B:141:LEU:HD13	1.73	0.70
1:C:74:LEU:O	1:C:75:LEU:HB2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:THR:HG23	1:B:265:SER:H	1.57	0.69
1:A:313:ARG:HA	4:A:2015:HOH:O	1.93	0.69
1:A:380:LYS:HE3	1:A:432:GLU:OE1	1.93	0.68
1:C:320:LEU:HD23	1:C:320:LEU:H	1.58	0.68
1:A:493:GLU:O	1:A:494:GLU:CB	2.43	0.67
1:A:168:ASN:ND2	2:A:1500:NAG:C1	2.58	0.66
1:B:490:LYS:O	1:B:490:LYS:HG2	1.93	0.66
1:B:295:HIS:HD2	1:B:297:ILE:H	1.44	0.66
1:B:188:ALA:O	1:B:192:THR:HG22	1.95	0.66
1:C:354:HIS:HA	1:C:362:GLY:O	1.94	0.66
1:A:114:HIS:N	1:A:260:SER:HB2	2.09	0.65
1:C:275:GLU:O	1:C:276:ASN:HB3	1.96	0.65
1:B:459:VAL:HG13	1:B:468:GLU:O	1.96	0.65
1:C:79:GLU:HG3	1:C:113:THR:HB	1.78	0.64
1:C:357:ASN:HB3	1:C:359:GLN:H	1.62	0.64
1:C:262:ARG:HG3	1:C:263:GLY:H	1.63	0.64
1:C:168:ASN:ND2	2:C:1500:NAG:C1	2.59	0.63
1:A:168:ASN:HD21	2:A:1500:NAG:C1	2.12	0.63
1:C:459:VAL:HG23	1:C:469:PHE:HA	1.80	0.62
1:A:283:THR:CG2	1:A:285:LEU:H	2.05	0.62
1:B:350:TRP:NE1	4:B:2124:HOH:O	2.27	0.62
1:B:113:THR:HB	1:B:114:HIS:CB	2.29	0.61
1:A:140:VAL:HG23	1:A:145:SER:HB2	1.81	0.61
1:A:455:LEU:HD23	1:A:459:VAL:HG21	1.81	0.61
1:A:50:GLY:HA2	1:A:278:GLU:OE2	2.00	0.61
1:C:111:SER:HB2	1:C:265:SER:HB2	1.83	0.61
1:A:191:ARG:HD2	4:A:2085:HOH:O	2.00	0.61
1:A:248:GLY:C	1:A:249:ASN:HD22	2.04	0.60
1:A:470:TYR:HB3	1:A:495:SER:HA	1.83	0.60
1:A:353:TYR:OH	1:A:447:LEU:HD11	2.01	0.60
1:B:320:LEU:HD23	1:B:320:LEU:H	1.66	0.60
1:A:435:ARG:NH1	1:C:435:ARG:NH1	2.49	0.60
1:C:459:VAL:HG21	1:C:467:PHE:HB3	1.84	0.59
1:B:190:GLN:HE22	1:B:249:ASN:HD21	1.49	0.59
1:B:454:GLN:NE2	1:B:486:TYR:H	2.00	0.58
1:A:72:ASP:OD1	1:A:73:ARG:N	2.36	0.58
1:B:123:ARG:HB2	1:B:254:GLU:OE2	2.03	0.58
1:B:492:GLU:HA	1:B:493:GLU:C	2.23	0.58
1:B:171:SER:HB2	1:B:258:LYS:HD2	1.85	0.58
1:B:325:GLN:CB	4:B:2110:HOH:O	2.38	0.57
1:C:58:ASP:HB3	1:C:86:LYS:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:THR:HG23	1:C:113:THR:O	2.03	0.57
1:B:110:THR:HG21	1:B:265:SER:H	1.68	0.57
1:A:111:SER:HB2	1:A:265:SER:HB2	1.85	0.57
1:A:148:ARG:CG	1:A:148:ARG:HH11	2.10	0.56
1:C:488:TYR:HB3	1:C:489:PRO:HD3	1.87	0.56
1:C:53:PRO:HG3	1:C:82:TYR:CZ	2.41	0.56
1:B:493:GLU:O	1:B:494:GLU:HB2	2.05	0.56
1:B:112:VAL:HG11	1:B:115:PHE:HB2	1.86	0.56
1:A:298:HIS:ND1	1:A:299:PRO:HD2	2.20	0.56
1:A:9:ILE:HD11	1:A:451:VAL:HG21	1.88	0.56
1:B:44:LYS:HD3	1:B:277:CYS:SG	2.46	0.56
1:B:140:VAL:C	1:B:142:ASP:HA	2.25	0.56
1:C:179:TRP:CE2	1:C:203:VAL:HG21	2.41	0.56
1:A:11:TYR:HB2	1:A:320:LEU:HD11	1.87	0.55
1:C:283:THR:HG22	1:C:301:THR:HG22	1.87	0.55
1:B:492:GLU:OE2	1:B:495:SER:N	2.39	0.55
1:C:47:ARG:O	1:C:279:THR:HG22	2.06	0.55
1:B:193:LEU:HD21	3:B:1499:SIA:O10	2.06	0.55
1:C:493:GLU:C	1:C:494:GLU:HG3	2.27	0.55
1:C:114:HIS:H	1:C:260:SER:CB	2.14	0.55
1:C:45:LEU:HD11	1:C:84:VAL:HG21	1.88	0.54
1:A:72:ASP:OD2	1:A:148:ARG:HD2	2.07	0.54
1:B:283:THR:HG22	1:B:301:THR:HG22	1.89	0.54
1:B:382:ASN:O	1:B:386:GLU:HG2	2.07	0.54
1:B:9:ILE:HD11	1:B:451:VAL:HG21	1.89	0.54
1:A:148:ARG:NH1	1:A:148:ARG:HG2	2.11	0.54
1:A:110:THR:HG23	1:A:265:SER:HB3	1.90	0.54
1:B:138:CYS:O	1:B:145:SER:HB3	2.08	0.53
1:C:114:HIS:CE1	1:C:116:GLU:HB2	2.43	0.53
1:B:124:ASP:OD1	1:B:125:GLN:HG3	2.08	0.53
1:C:424:ASN:ND2	4:C:2149:HOH:O	2.42	0.53
1:B:492:GLU:CD	1:B:495:SER:H	2.12	0.52
1:A:110:THR:CG2	1:A:265:SER:N	2.66	0.52
1:B:53:PRO:HG3	1:B:82:TYR:CZ	2.45	0.52
1:B:355:HIS:CE1	1:B:362:GLY:HA2	2.44	0.52
1:C:357:ASN:OD1	1:C:473:CYS:O	2.28	0.52
1:B:490:LYS:HB2	4:B:2167:HOH:O	2.09	0.52
1:C:262:ARG:HG3	1:C:263:GLY:N	2.24	0.52
1:A:495:SER:HB2	4:A:2177:HOH:O	2.10	0.52
1:C:304:GLU:HB3	1:C:390:THR:HG22	1.90	0.51
1:B:490:LYS:C	1:B:492:GLU:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:SER:CB	1:A:362:GLY:HA3	2.29	0.51
1:B:491:TYR:O	1:B:494:GLU:HB2	2.09	0.51
1:A:19:LYS:O	1:A:313:ARG:NH2	2.44	0.51
1:B:126:TRP:HZ3	1:B:163:ALA:HB1	1.76	0.51
1:B:490:LYS:C	1:B:492:GLU:N	2.63	0.51
1:A:113:THR:O	1:A:113:THR:HG23	2.10	0.51
1:A:355:HIS:CE1	1:A:361:SER:HB2	2.46	0.50
1:B:492:GLU:OE1	1:B:492:GLU:HA	2.11	0.50
1:C:492:GLU:HG2	1:C:492:GLU:O	2.11	0.50
1:C:143:ASN:N	1:C:143:ASN:HD22	2.10	0.50
1:C:262:ARG:NH1	4:C:2029:HOH:O	2.44	0.50
1:A:213:ILE:HD12	1:A:214:PRO:O	2.12	0.50
1:A:141:LEU:O	1:A:141:LEU:HG	2.12	0.49
1:B:53:PRO:HD2	1:B:274:LEU:HD22	1.94	0.49
1:B:491:TYR:O	1:B:494:GLU:CB	2.61	0.49
1:B:495:SER:C	1:B:497:ALA:N	2.65	0.49
1:B:357:ASN:HB2	4:B:2126:HOH:O	2.12	0.49
1:A:479:ASN:O	1:A:483:ASN:HB2	2.13	0.49
1:A:140:VAL:HG12	1:A:141:LEU:HD12	1.93	0.49
1:A:413:MET:HE1	1:B:412:LYS:HE3	1.93	0.49
1:B:31:THR:C	1:B:32:HIS:CD2	2.86	0.49
1:B:126:TRP:CZ3	1:B:163:ALA:HB1	2.48	0.49
1:B:113:THR:HG22	1:B:114:HIS:HB2	1.96	0.48
1:C:248:GLY:O	1:C:249:ASN:HB2	2.13	0.48
1:B:123:ARG:HG2	1:B:131:THR:HG21	1.94	0.48
1:C:168:ASN:HD21	2:C:1500:NAG:C2	2.26	0.48
1:C:160:TYR:CZ	1:C:248:GLY:HA2	2.48	0.48
1:A:361:SER:HB3	1:A:362:GLY:CA	2.33	0.48
1:C:113:THR:C	1:C:260:SER:HB2	2.34	0.48
1:A:51:ILE:HB	1:A:81:SER:HB3	1.96	0.47
1:B:31:THR:OG1	1:B:32:HIS:HD2	1.98	0.47
1:A:354:HIS:O	1:A:355:HIS:CD2	2.67	0.47
1:B:471:HIS:HD2	1:B:494:GLU:OE2	1.98	0.47
1:B:459:VAL:CG1	1:B:460:LYS:N	2.77	0.47
1:A:102:TYR:CZ	1:A:106:LYS:HD3	2.50	0.47
1:B:331:LEU:HD22	1:B:438:ASP:OD2	2.14	0.47
1:B:218:THR:HA	4:B:2072:HOH:O	2.14	0.46
1:A:248:GLY:O	1:A:249:ASN:HB2	2.16	0.46
1:B:459:VAL:HG12	1:B:460:LYS:N	2.30	0.46
1:B:189:GLU:HA	1:B:192:THR:HG22	1.97	0.46
1:A:399:PHE:CE1	1:A:406:LEU:HG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1499:SIA:H6	3:B:1499:SIA:O1A	2.16	0.46
1:C:13:ALA:HB2	1:C:342:GLY:HA3	1.96	0.46
1:B:491:TYR:C	1:B:494:GLU:HB2	2.36	0.46
1:C:480:SER:HA	1:C:483:ASN:OD1	2.16	0.46
1:B:155:LYS:HE2	1:B:192:THR:O	2.16	0.45
1:C:9:ILE:HG13	1:C:448:TYR:HA	1.98	0.45
2:A:1500:NAG:C1	2:A:1500:NAG:C5	2.95	0.45
1:C:455:LEU:HD23	1:C:459:VAL:HG11	1.99	0.45
1:A:220:PRO:HD3	1:C:243:ASN:HD22	1.81	0.45
1:C:12:HIS:HD2	1:C:346:MET:O	1.99	0.45
1:B:51:ILE:HG23	1:B:79:GLU:HG2	1.99	0.45
1:B:276:ASN:HA	1:B:277:CYS:C	2.35	0.45
1:A:9:ILE:HG13	1:A:448:TYR:HA	1.98	0.45
1:B:114:HIS:HB3	1:B:260:SER:HB2	1.98	0.45
1:A:498:ALA:C	4:A:2177:HOH:O	2.55	0.44
1:B:459:VAL:CG1	1:B:467:PHE:HB3	2.38	0.44
1:B:248:GLY:O	1:B:249:ASN:HB2	2.17	0.44
1:B:197:VAL:HG22	1:B:198:GLY:H	1.82	0.44
1:C:140:VAL:C	1:C:142:ASP:HA	2.38	0.44
1:C:182:HIS:CD2	1:C:194:TYR:OH	2.70	0.44
1:B:178:ILE:O	1:B:253:PRO:HG3	2.18	0.44
1:B:174:GLN:OE1	1:B:235:LEU:HD13	2.18	0.44
1:C:390:THR:O	1:C:390:THR:HG22	2.17	0.44
1:B:108:LEU:HD11	1:B:261:LYS:HE2	1.99	0.44
1:A:128:GLN:HB3	1:A:161:PRO:HG2	1.99	0.44
1:B:131:THR:HG23	1:B:131:THR:O	2.18	0.44
1:C:38:GLU:HB2	1:C:292:LEU:HD12	2.00	0.44
1:A:99:PHE:HB3	1:A:102:TYR:HB2	1.99	0.44
1:B:303:GLY:HA2	1:B:392:PHE:CE1	2.53	0.44
1:B:295:HIS:CD2	1:B:297:ILE:H	2.32	0.43
1:A:123:ARG:HG2	1:A:131:THR:HG21	2.00	0.43
1:B:113:THR:HB	1:B:260:SER:HB2	2.00	0.43
1:A:220:PRO:HD3	1:C:243:ASN:ND2	2.34	0.43
1:B:389:ASN:HD22	1:B:389:ASN:HA	1.68	0.43
1:B:66:LEU:O	1:B:147:PHE:HB3	2.18	0.43
1:B:151:VAL:HG12	1:B:153:LEU:HD12	1.99	0.43
1:B:493:GLU:O	1:B:494:GLU:CB	2.66	0.43
1:B:112:VAL:CG1	1:B:115:PHE:HB2	2.48	0.43
1:B:9:ILE:HG13	1:B:448:TYR:HA	2.01	0.43
1:C:9:ILE:HD11	1:C:451:VAL:HG21	2.00	0.43
1:A:71:CYS:O	1:A:74:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:SER:HA	1:A:483:ASN:HB3	2.01	0.43
1:B:458:ASN:OD1	1:B:491:TYR:HA	2.19	0.43
1:C:494:GLU:OE2	1:C:495:SER:N	2.42	0.43
1:A:74:LEU:O	1:A:74:LEU:HD23	2.18	0.43
1:B:185[B]:ASN:OD1	1:B:226:GLY:C	2.56	0.43
1:A:23:ILE:HG23	1:A:24:LEU:HG	2.01	0.43
1:B:194:TYR:O	1:B:196:ASN:N	2.47	0.43
1:A:112:VAL:C	1:A:113:THR:HG22	2.39	0.43
1:C:320:LEU:HD23	1:C:320:LEU:N	2.30	0.42
1:B:209:ASN:OD1	1:C:219:ARG:NH1	2.50	0.42
1:B:307:LYS:HA	1:B:307:LYS:HD3	1.90	0.42
1:A:110:THR:HG23	1:A:265:SER:H	1.77	0.42
1:B:189:GLU:HA	1:B:192:THR:CG2	2.48	0.42
1:A:197:VAL:HG12	1:A:198:GLY:N	2.33	0.42
1:A:492:GLU:O	4:A:2177:HOH:O	2.22	0.42
1:B:320:LEU:N	1:B:320:LEU:HD23	2.33	0.42
1:A:140:VAL:HG23	1:A:145:SER:CB	2.48	0.42
1:C:108:LEU:O	1:C:261:LYS:HD2	2.18	0.42
1:B:471:HIS:CD2	1:B:494:GLU:OE2	2.72	0.42
1:C:178:ILE:O	1:C:253:PRO:HG3	2.19	0.42
1:C:399:PHE:CE1	1:C:406:LEU:HG	2.55	0.42
1:A:311:SER:HB3	1:A:426:GLU:OE1	2.20	0.42
1:C:293:PRO:HG2	1:C:294:PHE:CD2	2.55	0.42
1:A:463:GLY:HA2	1:C:453:MET:CE	2.49	0.42
1:B:307:LYS:HE2	1:B:421:TRP:NE1	2.35	0.42
1:A:53:PRO:HB3	1:A:82:TYR:CE2	2.55	0.42
1:B:459:VAL:HG13	1:B:468:GLU:C	2.39	0.41
1:B:458:ASN:HA	1:B:494:GLU:CG	2.49	0.41
1:A:488:TYR:N	1:A:489:PRO:CD	2.83	0.41
1:C:388:MET:HE2	1:C:388:MET:HB2	1.85	0.41
1:A:409:LEU:HD21	1:C:409:LEU:HD22	2.02	0.41
1:B:367:LYS:HA	1:B:367:LYS:HD3	1.64	0.41
1:A:459:VAL:HG12	1:A:469:PHE:HA	2.02	0.41
1:B:52:PRO:HA	1:B:53:PRO:HD3	1.86	0.41
1:C:298:HIS:ND1	1:C:299:PRO:HD2	2.35	0.41
1:A:141:LEU:O	1:A:141:LEU:CG	2.68	0.41
1:B:163:ALA:O	1:B:245:GLU:HA	2.21	0.41
1:B:113:THR:CB	1:B:114:HIS:CB	2.98	0.41
1:A:241:VAL:HG23	2:A:1500:NAG:H61	2.03	0.41
1:A:79:GLU:HG3	1:A:113:THR:HA	2.02	0.41
1:C:143:ASN:N	1:C:143:ASN:ND2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:ASN:O	1:C:386:GLU:HB2	2.21	0.41
1:B:97:GLY:HA3	1:B:229:MET:O	2.21	0.41
1:B:323:VAL:HG12	4:B:2108:HOH:O	2.21	0.41
1:B:427:LEU:O	1:B:431:MET:HG3	2.20	0.41
1:A:222:VAL:HG22	1:C:206:SER:HB2	2.03	0.41
1:B:495:SER:C	1:B:497:ALA:H	2.24	0.40
1:C:35:ASP:OD2	1:C:39:LYS:NZ	2.54	0.40
1:A:241:VAL:HB	1:B:220:PRO:HG3	2.03	0.40
1:C:372:LYS:HA	1:C:372:LYS:HD2	1.91	0.40
1:B:6:GLN:HB2	1:B:467:PHE:O	2.22	0.40
1:A:168:ASN:ND2	2:A:1500:NAG:C5	2.75	0.40
1:B:284:PRO:HD3	1:B:300:LEU:O	2.21	0.40

All (2) 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)
1:A:141:LEU:CD1	1:B:128:GLN:OE1[1_655]	1.82	0.38
1:A:141:LEU:CD2	1:B:128:GLN:OE1[1_655]	2.03	0.17

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	486/509 (96%)	459 (94%)	21 (4%)	6 (1%)	16	23
1	B	485/509 (95%)	456 (94%)	20 (4%)	9 (2%)	10	12
1	C	479/509 (94%)	457 (95%)	16 (3%)	6 (1%)	15	21
All	All	1450/1527 (95%)	1372 (95%)	57 (4%)	21 (1%)	14	19

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	THR
1	A	494	GLU
1	B	277	CYS
1	B	490	LYS
1	B	494	GLU
1	C	113	THR
1	B	114	HIS
1	B	141	LEU
1	B	276	ASN
1	C	276	ASN
1	B	362	GLY
1	C	362	GLY
1	C	492	GLU
1	C	494	GLU
1	A	496	LYS
1	B	489	PRO
1	C	75	LEU
1	A	140	VAL
1	B	313	ARG
1	A	74	LEU
1	A	355	HIS

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	427/447 (96%)	413 (97%)	14 (3%)	45	66
1	B	429/447 (96%)	410 (96%)	19 (4%)	35	53
1	C	425/447 (95%)	409 (96%)	16 (4%)	40	60
All	All	1281/1341 (96%)	1232 (96%)	49 (4%)	40	60

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	CYS
1	A	110	THR

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Mol	Chain	Res	Type
1	A	113	THR
1	A	131	THR
1	A	141	LEU
1	A	142	ASP
1	A	202	SER
1	A	275	GLU
1	A	320	LEU
1	A	351	TYR
1	A	355	HIS
1	A	404	ARG
1	A	437	LEU
1	A	477	CYS
1	B	58	ASP
1	B	77	VAL
1	B	90	VAL
1	B	93	LEU
1	B	131	THR
1	B	141	LEU
1	B	148	ARG
1	B	276	ASN
1	B	320	LEU
1	B	331	LEU
1	B	351	TYR
1	B	377	ILE
1	B	389	ASN
1	B	434	GLU
1	B	437	LEU
1	B	462	LEU
1	B	491	TYR
1	B	493	GLU
1	B	494	GLU
1	C	94	CYS
1	C	136	ARG
1	C	186	ASP
1	C	196	ASN
1	C	208	LEU
1	C	264	SER
1	C	283	THR
1	C	320	LEU
1	C	347	VAL
1	C	356	SER
1	C	389	ASN

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Mol	Chain	Res	Type
1	C	455	LEU
1	C	459	VAL
1	C	462	LEU
1	C	493	GLU
1	C	494	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	A	114	HIS
1	A	168	ASN
1	A	174	GLN
1	A	182	HIS
1	A	243	ASN
1	A	249	ASN
1	A	295	HIS
1	A	483	ASN
1	B	27	ASN
1	B	32	HIS
1	B	114	HIS
1	B	182	HIS
1	B	249	ASN
1	B	295	HIS
1	B	382	ASN
1	B	391	GLN
1	B	408	ASN
1	B	454	GLN
1	C	12	HIS
1	C	15	ASN
1	C	32	HIS
1	C	91	ASN
1	C	100	ASN
1	C	114	HIS
1	C	125	GLN
1	C	143	ASN
1	C	168	ASN
1	C	174	GLN
1	C	182	HIS
1	C	243	ASN
1	C	249	ASN
1	C	389	ASN

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Mol	Chain	Res	Type
1	C	408	ASN
1	C	454	GLN
1	C	479	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 ⓘ

6 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	$\# Z > 2$
3	SIA	B	1499	3	16,20,21	0.59	0	18,28,31	0.81	0
3	GAL	B	1500	3	11,11,12	0.75	0	14,15,17	0.81	1 (7%)
3	NAG	B	1501	3	15,15,15	0.89	0	17,21,21	0.74	0
3	SIA	C	1497	3	16,20,21	0.67	0	18,28,31	0.78	0
3	GAL	C	1498	3	11,11,12	0.60	0	14,15,17	1.21	2 (14%)
3	NAG	C	1499	3	15,15,15	0.88	0	17,21,21	1.16	1 (5%)

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
3	SIA	B	1499	3	-	0/14/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GAL	B	1500	3	-	0/2/19/22	0/1/1/1
3	NAG	B	1501	3	-	0/6/26/26	0/1/1/1
3	SIA	C	1497	3	-	0/14/34/38	0/1/1/1
3	GAL	C	1498	3	-	0/2/19/22	0/1/1/1
3	NAG	C	1499	3	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1498	GAL	O3-C3-C2	-2.03	106.33	110.00
3	B	1500	GAL	C1-C2-C3	2.31	112.27	109.54
3	C	1499	NAG	C3-C4-C5	2.84	115.16	110.20
3	C	1498	GAL	C1-C2-C3	3.81	114.05	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1499	SIA	2	0

5.6 Ligand geometry ⓘ

3 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
2	NAG	A	1499	-	14,14,15	0.44	0	15,19,21	0.75	0
2	NAG	A	1500	-	12,12,15	0.45	0	12,15,21	0.97	1 (8%)
2	NAG	C	1500	-	14,14,15	0.55	0	15,19,21	0.85	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	1499	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1500	-	-	0/15/15/26	0/0/0/1
2	NAG	C	1500	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	NAG	C1-C2-N2	-2.20	107.11	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1499	NAG	1	0
2	A	1500	NAG	6	0
2	C	1500	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	490/509 (96%)	2.96	341 (69%) 0 0	33, 54, 94, 134	1 (0%)
1	B	490/509 (96%)	1.70	157 (32%) 1 1	35, 55, 95, 159	0
1	C	485/509 (95%)	2.84	299 (61%) 0 0	36, 55, 87, 134	0
All	All	1465/1527 (95%)	2.50	797 (54%) 0 0	33, 55, 92, 159	1 (0%)

All (797) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	196	ASN	13.1
1	A	362	GLY	10.6
1	A	141	LEU	9.9
1	C	473	CYS	9.9
1	B	157	GLY	9.8
1	C	128	GLN	9.5
1	C	376	GLY	9.5
1	A	280	LYS	8.7
1	A	140	VAL	8.7
1	C	44	LYS	8.5
1	C	222	VAL	8.4
1	C	235	LEU	8.2
1	A	361	SER	8.0
1	B	277	CYS	7.9
1	A	42	ASN	7.9
1	C	138	CYS	7.9
1	C	191	ARG	7.9
1	A	90	VAL	7.8
1	A	224	GLY	7.8
1	C	151	VAL	7.8
1	C	127	THR	7.8
1	C	291	THR	7.7
1	C	484	GLY	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	493	GLU	7.6
1	C	51	ILE	7.5
1	A	138	CYS	7.5
1	C	194	TYR	7.3
1	C	9	ILE	7.3
1	C	120	ILE	7.3
1	C	141	LEU	7.1
1	C	49	SER	7.0
1	C	166	SER	7.0
1	A	50	GLY	6.9
1	B	114	HIS	6.9
1	A	469	PHE	6.8
1	A	78	PRO	6.8
1	A	229	MET	6.6
1	C	140	VAL	6.5
1	A	89	PRO	6.4
1	A	475	ASP	6.4
1	C	372	LYS	6.4
1	C	288	ILE	6.4
1	A	18	GLU	6.4
1	C	241	VAL	6.3
1	A	277	CYS	6.3
1	A	480	SER	6.3
1	C	264	SER	6.3
1	C	159	ASN	6.2
1	C	489	PRO	6.1
1	A	49	SER	6.1
1	B	262	ARG	6.1
1	A	9	ILE	6.1
1	B	162	ILE	6.0
1	C	113	THR	6.0
1	C	176	LEU	6.0
1	A	12	HIS	5.9
1	C	198	GLY	5.9
1	A	323	VAL	5.9
1	C	129	HIS	5.9
1	C	172	GLY	5.8
1	A	8	CYS	5.8
1	C	131	THR	5.8
1	A	153	LEU	5.8
1	B	159	ASN	5.8
1	A	95	TYR	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	189	GLU	5.8
1	C	66	LEU	5.8
1	B	160	TYR	5.8
1	A	316	LEU	5.7
1	C	154	THR	5.7
1	B	158	SER	5.7
1	C	91	ASN	5.7
1	A	59	CYS	5.7
1	A	358	ASP	5.7
1	C	187	ASP	5.7
1	C	121	LEU	5.7
1	C	79	GLU	5.6
1	A	58	ASP	5.6
1	A	363	TYR	5.6
1	A	470	TYR	5.6
1	C	387	LYS	5.6
1	A	109	ILE	5.5
1	C	118	VAL	5.5
1	A	13	ALA	5.5
1	A	371	GLN	5.5
1	C	147	PHE	5.5
1	A	114	HIS	5.4
1	C	239	TRP	5.4
1	B	491	TYR	5.4
1	C	126	TRP	5.4
1	A	73	ARG	5.4
1	A	157	GLY	5.4
1	A	297	ILE	5.4
1	A	91	ASN	5.3
1	A	45	LEU	5.3
1	A	136	ARG	5.3
1	B	213	ILE	5.2
1	A	353	TYR	5.2
1	C	92	GLY	5.2
1	A	350	TRP	5.2
1	A	302	ILE	5.2
1	C	274	LEU	5.2
1	A	431	MET	5.2
1	A	325	GLN	5.2
1	A	61	ILE	5.1
1	A	486	TYR	5.1
1	C	143	ASN	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	375	ASP	5.1
1	C	352	GLY	5.1
1	C	225	GLN	5.1
1	C	115	PHE	5.1
1	C	8	CYS	5.1
1	A	184	PRO	5.1
1	C	184	PRO	5.1
1	B	17	THR	5.1
1	A	298	HIS	5.1
1	C	65	LEU	5.1
1	A	177	ILE	5.0
1	A	392	PHE	5.0
1	A	134	GLY	5.0
1	C	223	ASN	5.0
1	C	153	LEU	5.0
1	A	422	THR	5.0
1	A	389	ASN	5.0
1	A	463	GLY	5.0
1	A	375	ASP	5.0
1	C	160	TYR	5.0
1	A	84	VAL	4.9
1	C	155	LYS	4.9
1	C	330	GLY	4.9
1	A	124	ASP	4.9
1	B	167	TYR	4.9
1	A	55	GLU	4.9
1	A	278	GLU	4.9
1	A	75	LEU	4.8
1	A	498	ALA	4.8
1	C	258	LYS	4.8
1	B	75	LEU	4.8
1	A	69	PRO	4.8
1	A	80	TRP	4.8
1	B	141	LEU	4.8
1	C	7	ILE	4.8
1	C	162	ILE	4.8
1	C	470	TYR	4.8
1	A	6	GLN	4.8
1	A	451	VAL	4.8
1	A	318	THR	4.8
1	A	367	LYS	4.8
1	A	219	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	206	SER	4.8
1	A	489	PRO	4.7
1	A	455	LEU	4.7
1	C	85	GLU	4.7
1	C	87	GLU	4.7
1	A	7	ILE	4.7
1	A	454	GLN	4.7
1	C	156	LYS	4.7
1	A	472	LYS	4.6
1	C	89	PRO	4.6
1	A	216	ILE	4.6
1	A	386	GLU	4.6
1	C	82	TYR	4.6
1	C	122	PRO	4.6
1	C	269	LYS	4.6
1	C	276	ASN	4.6
1	C	293	PRO	4.5
1	C	34	LYS	4.5
1	C	256	GLY	4.5
1	B	118	VAL	4.5
1	B	411	LYS	4.5
1	C	238	THR	4.5
1	A	214	PRO	4.5
1	A	459	VAL	4.5
1	A	225	GLN	4.5
1	C	116	GLU	4.5
1	A	5	ASP	4.5
1	C	171	SER	4.5
1	A	287	ALA	4.5
1	A	458	ASN	4.5
1	C	109	ILE	4.4
1	A	239	TRP	4.4
1	C	463	GLY	4.4
1	C	130	THR	4.4
1	A	262	ARG	4.4
1	B	203	VAL	4.4
1	A	186	ASP	4.3
1	C	93	LEU	4.3
1	C	397	LYS	4.3
1	C	78	PRO	4.3
1	C	267	ILE	4.3
1	C	244	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	70	GLU	4.3
1	C	74	LEU	4.3
1	A	265	SER	4.3
1	C	83	ILE	4.3
1	C	434	GLU	4.2
1	C	67	GLY	4.2
1	A	56	LEU	4.2
1	C	364	ALA	4.2
1	A	348	ASP	4.2
1	B	120	ILE	4.2
1	A	477	CYS	4.2
1	A	196	ASN	4.2
1	A	487	ASP	4.2
1	A	450	LYS	4.1
1	A	40	THR	4.1
1	C	59	CYS	4.1
1	A	457	ASP	4.1
1	A	36	ILE	4.1
1	A	260	SER	4.1
1	B	274	LEU	4.1
1	C	180	GLY	4.1
1	C	173	GLU	4.1
1	C	481	VAL	4.1
1	A	52	PRO	4.1
1	C	95	TYR	4.1
1	A	156	LYS	4.1
1	A	247	THR	4.1
1	A	407	GLU	4.1
1	A	417	PHE	4.1
1	B	275	GLU	4.1
1	C	193	LEU	4.1
1	A	146	PHE	4.1
1	C	135	SER	4.1
1	C	302	ILE	4.0
1	B	79	GLU	4.0
1	A	181	ILE	4.0
1	A	274	LEU	4.0
1	C	250	LEU	4.0
1	A	94	CYS	4.0
1	C	175	MET	4.0
1	A	301	THR	4.0
1	C	361	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	144	PRO	4.0
1	A	77	VAL	4.0
1	A	92	GLY	4.0
1	C	394	ALA	4.0
1	A	215	GLU	4.0
1	C	178	ILE	4.0
1	C	237	GLU	3.9
1	C	80	TRP	3.9
1	A	27	ASN	3.9
1	A	29	THR	3.9
1	C	62	ALA	3.9
1	C	253	PRO	3.9
1	C	262	ARG	3.9
1	C	251	ILE	3.9
1	A	332	PHE	3.9
1	C	257	PHE	3.9
1	C	406	LEU	3.9
1	A	53	PRO	3.9
1	B	140	VAL	3.9
1	A	122	PRO	3.9
1	C	181	ILE	3.9
1	B	276	ASN	3.8
1	B	347	VAL	3.8
1	B	291	THR	3.8
1	C	362	GLY	3.8
1	C	72	ASP	3.8
1	C	417	PHE	3.8
1	C	50	GLY	3.8
1	C	243	ASN	3.8
1	A	93	LEU	3.8
1	C	170	THR	3.8
1	B	235	LEU	3.8
1	A	231	PHE	3.8
1	B	381	VAL	3.8
1	C	270	THR	3.8
1	A	143	ASN	3.8
1	A	324	PRO	3.7
1	B	478	MET	3.7
1	C	466	CYS	3.7
1	A	82	TYR	3.7
1	A	366	ASP	3.7
1	C	474	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	64	TRP	3.7
1	A	14	ASN	3.7
1	C	219	ARG	3.7
1	A	85	GLU	3.7
1	A	51	ILE	3.7
1	A	270	THR	3.7
1	B	200	TYR	3.7
1	A	97	GLY	3.7
1	A	172	GLY	3.7
1	C	134	GLY	3.7
1	C	242	ILE	3.7
1	A	39	LYS	3.7
1	A	210	LYS	3.7
1	B	207	THR	3.7
1	C	252	ALA	3.7
1	C	108	LEU	3.7
1	A	467	PHE	3.7
1	B	73	ARG	3.7
1	B	221	LYS	3.7
1	A	250	LEU	3.7
1	A	390	THR	3.6
1	C	318	THR	3.6
1	B	51	ILE	3.6
1	A	10	GLY	3.6
1	A	355	HIS	3.6
1	A	115	PHE	3.6
1	A	334	ALA	3.6
1	A	351	TYR	3.6
1	C	488	TYR	3.6
1	C	272	LYS	3.6
1	A	364	ALA	3.6
1	C	177	ILE	3.6
1	A	195	GLN	3.6
1	B	191	ARG	3.6
1	B	202	SER	3.6
1	B	361	SER	3.6
1	C	207	THR	3.6
1	A	346	MET	3.6
1	C	190	GLN	3.6
1	A	123	ARG	3.6
1	B	313	ARG	3.6
1	C	114	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	98	SER	3.5
1	A	131	THR	3.5
1	C	150	MET	3.5
1	A	335	ILE	3.5
1	A	296	ASN	3.5
1	C	200	TYR	3.5
1	B	244	PHE	3.5
1	A	223	ASN	3.5
1	A	295	HIS	3.5
1	A	309	VAL	3.5
1	A	354	HIS	3.5
1	B	241	VAL	3.5
1	A	344	GLN	3.5
1	A	71	CYS	3.5
1	B	138	CYS	3.5
1	C	71	CYS	3.5
1	B	324	PRO	3.5
1	C	195	GLN	3.5
1	C	348	ASP	3.5
1	C	179	TRP	3.5
1	A	319	GLY	3.5
1	B	451	VAL	3.5
1	A	212	SER	3.5
1	A	127	THR	3.5
1	A	483	ASN	3.5
1	A	20	VAL	3.5
1	A	121	LEU	3.5
1	A	201	VAL	3.5
1	A	300	LEU	3.5
1	B	38	GLU	3.4
1	C	363	TYR	3.4
1	C	229	MET	3.4
1	B	137	ALA	3.4
1	A	399	PHE	3.4
1	C	353	TYR	3.4
1	A	182	HIS	3.4
1	A	137	ALA	3.4
1	B	26	ARG	3.4
1	A	479	ASN	3.4
1	C	465	GLY	3.4
1	B	40	THR	3.4
1	A	474	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	221	LYS	3.4
1	A	368	GLU	3.4
1	A	183	HIS	3.4
1	A	331	LEU	3.4
1	A	436	THR	3.4
1	A	485	THR	3.4
1	C	469	PHE	3.4
1	C	492	GLU	3.4
1	C	32	HIS	3.4
1	A	315	VAL	3.4
1	C	369	SER	3.4
1	A	267	ILE	3.4
1	A	81	SER	3.3
1	A	11	TYR	3.3
1	A	83	ILE	3.3
1	A	255	TYR	3.3
1	A	425	ALA	3.3
1	B	189	GLU	3.3
1	C	393	GLU	3.3
1	B	462	LEU	3.3
1	C	45	LEU	3.3
1	B	253	PRO	3.3
1	C	148	ARG	3.3
1	C	157	GLY	3.3
1	A	473	CYS	3.3
1	B	126	TRP	3.3
1	A	434	GLU	3.3
1	B	326	ILE	3.3
1	C	54	LEU	3.3
1	C	204	GLY	3.3
1	C	420	VAL	3.3
1	A	218	THR	3.3
1	A	435	ARG	3.3
1	A	382	ASN	3.3
1	C	169	ASN	3.3
1	C	236	LEU	3.3
1	A	394	ALA	3.3
1	A	67	GLY	3.2
1	C	275	GLU	3.2
1	A	414	GLU	3.2
1	B	475	ASP	3.2
1	C	438	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	259	ILE	3.2
1	A	132	THR	3.2
1	C	273	THR	3.2
1	A	194	TYR	3.2
1	A	268	MET	3.2
1	A	193	LEU	3.2
1	C	48	LEU	3.2
1	A	110	THR	3.2
1	C	203	VAL	3.2
1	C	413	MET	3.2
1	C	216	ILE	3.2
1	B	163	ALA	3.2
1	A	305	CYS	3.2
1	A	126	TRP	3.2
1	A	406	LEU	3.1
1	B	430	LEU	3.1
1	B	216	ILE	3.1
1	A	57	GLY	3.1
1	A	185	ASN	3.1
1	B	121	LEU	3.1
1	B	279	THR	3.1
1	A	150	MET	3.1
1	A	359	GLN	3.1
1	C	57	GLY	3.1
1	B	288	ILE	3.1
1	B	115	PHE	3.1
1	C	233	TRP	3.1
1	C	487	ASP	3.1
1	C	281	CYS	3.1
1	A	256	GLY	3.1
1	C	75	LEU	3.1
1	A	64	TRP	3.1
1	B	169	ASN	3.1
1	C	90	VAL	3.1
1	C	384	VAL	3.1
1	B	367	LYS	3.1
1	C	100	ASN	3.1
1	C	209	ASN	3.1
1	A	248	GLY	3.1
1	A	48	LEU	3.0
1	A	244	PHE	3.0
1	A	338	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	271	GLU	3.0
1	A	476	GLU	3.0
1	B	242	ILE	3.0
1	C	373	ALA	3.0
1	C	323	VAL	3.0
1	A	21	ASP	3.0
1	C	483	ASN	3.0
1	A	46	CYS	3.0
1	A	47	ARG	3.0
1	A	272	LYS	3.0
1	A	106	LYS	3.0
1	A	38	GLU	3.0
1	A	113	THR	3.0
1	B	226	GLY	3.0
1	B	264	SER	3.0
1	C	255	TYR	3.0
1	B	181	ILE	3.0
1	A	144	PRO	3.0
1	A	173	GLU	3.0
1	A	462	LEU	2.9
1	C	81	SER	2.9
1	B	80	TRP	2.9
1	B	254	GLU	2.9
1	A	284	PRO	2.9
1	C	119	LYS	2.9
1	A	227	GLY	2.9
1	A	264	SER	2.9
1	B	204	GLY	2.9
1	C	476	GLU	2.9
1	C	96	PRO	2.9
1	A	311	SER	2.9
1	A	159	ASN	2.9
1	A	72	ASP	2.9
1	C	268	MET	2.9
1	A	310	LYS	2.9
1	C	149	ASN	2.9
1	C	53	PRO	2.9
1	B	84	VAL	2.9
1	C	105	LEU	2.9
1	B	467	PHE	2.9
1	C	132	THR	2.9
1	A	482	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	228	ARG	2.9
1	A	257	PHE	2.9
1	C	217	ALA	2.9
1	A	372	LYS	2.9
1	A	490	LYS	2.9
1	A	360	GLY	2.9
1	C	211	ARG	2.8
1	A	285	LEU	2.8
1	B	401	ASN	2.8
1	B	5	ASP	2.8
1	C	317	ALA	2.8
1	A	180	GLY	2.8
1	A	398	GLU	2.8
1	C	349	GLY	2.8
1	C	435	ARG	2.8
1	A	442	SER	2.8
1	A	308	TYR	2.8
1	A	28	VAL	2.8
1	B	272	LYS	2.8
1	A	461	GLU	2.8
1	C	55	GLU	2.8
1	A	139	ALA	2.8
1	C	133	GLY	2.8
1	C	416	GLY	2.8
1	C	174	GLN	2.8
1	A	16	SER	2.8
1	C	297	ILE	2.8
1	A	102	TYR	2.8
1	C	102	TYR	2.8
1	A	25	GLU	2.8
1	B	122	PRO	2.8
1	A	213	ILE	2.8
1	B	211	ARG	2.8
1	C	409	LEU	2.8
1	C	247	THR	2.8
1	C	139	ALA	2.8
1	A	468	GLU	2.8
1	C	46	CYS	2.8
1	C	167	TYR	2.8
1	C	395	VAL	2.8
1	C	289	ASN	2.8
1	A	453	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	40	THR	2.8
1	A	68	ASN	2.8
1	A	357	ASN	2.8
1	B	305	CYS	2.8
1	B	258	LYS	2.8
1	C	18	GLU	2.7
1	C	110	THR	2.7
1	C	482	LYS	2.7
1	C	277	CYS	2.7
1	A	162	ILE	2.7
1	A	313	ARG	2.7
1	A	423	TYR	2.7
1	B	72	ASP	2.7
1	A	178	ILE	2.7
1	B	465	GLY	2.7
1	C	213	ILE	2.7
1	B	343	TRP	2.7
1	B	437	LEU	2.7
1	A	290	THR	2.7
1	A	444	VAL	2.7
1	A	317	ALA	2.7
1	C	199	THR	2.7
1	A	400	SER	2.7
1	B	99	PHE	2.7
1	C	338	PHE	2.7
1	B	255	TYR	2.7
1	C	101	ASP	2.7
1	A	299	PRO	2.7
1	B	473	CYS	2.7
1	B	239	TRP	2.7
1	C	202	SER	2.7
1	C	197	VAL	2.7
1	A	142	ASP	2.7
1	A	108	LEU	2.7
1	A	111	SER	2.7
1	C	220	PRO	2.7
1	C	260	SER	2.7
1	A	222	VAL	2.7
1	C	343	TRP	2.7
1	C	371	GLN	2.7
1	C	356	SER	2.6
1	A	294	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	231	PHE	2.6
1	C	396	GLY	2.6
1	A	429	VAL	2.6
1	B	151	VAL	2.6
1	B	359	GLN	2.6
1	C	351	TYR	2.6
1	A	37	LEU	2.6
1	C	437	LEU	2.6
1	C	69	PRO	2.6
1	C	354	HIS	2.6
1	A	120	ILE	2.6
1	A	437	LEU	2.6
1	C	16	SER	2.6
1	B	453	MET	2.6
1	C	431	MET	2.6
1	A	249	ASN	2.6
1	A	86	LYS	2.6
1	C	86	LYS	2.6
1	C	332	PHE	2.6
1	C	454	GLN	2.6
1	B	179	TRP	2.6
1	C	278	GLU	2.6
1	A	44	LYS	2.5
1	A	395	VAL	2.5
1	B	474	ASP	2.5
1	B	133	GLY	2.5
1	B	284	PRO	2.5
1	C	410	ASN	2.5
1	A	87	GLU	2.5
1	A	22	THR	2.5
1	A	343	TRP	2.5
1	A	148	ARG	2.5
1	A	420	VAL	2.5
1	A	438	ASP	2.5
1	B	98	SER	2.5
1	C	205	THR	2.5
1	C	165	ARG	2.5
1	A	99	PHE	2.5
1	C	99	PHE	2.5
1	B	427	LEU	2.5
1	B	267	ILE	2.5
1	A	440	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	495	SER	2.5
1	C	459	VAL	2.5
1	A	404	ARG	2.5
1	C	61	ILE	2.5
1	C	391	GLN	2.5
1	C	485	THR	2.5
1	C	486	TYR	2.5
1	B	209	ASN	2.5
1	C	400	SER	2.5
1	B	390	THR	2.5
1	A	339	ILE	2.5
1	B	246	SER	2.5
1	C	261	LYS	2.4
1	A	65	LEU	2.4
1	A	217	ALA	2.4
1	A	41	HIS	2.4
1	A	191	ARG	2.4
1	A	432	GLU	2.4
1	A	471	HIS	2.4
1	B	466	CYS	2.4
1	B	208	LEU	2.4
1	B	223	ASN	2.4
1	A	130	THR	2.4
1	B	83	ILE	2.4
1	B	215	GLU	2.4
1	A	197	VAL	2.4
1	B	59	CYS	2.4
1	B	65	LEU	2.4
1	B	256	GLY	2.4
1	C	290	THR	2.4
1	A	238	THR	2.4
1	B	273	THR	2.4
1	A	421	TRP	2.4
1	C	335	ILE	2.4
1	A	460	LYS	2.4
1	C	210	LYS	2.4
1	B	53	PRO	2.4
1	C	306	PRO	2.4
1	C	392	PHE	2.4
1	A	424	ASN	2.4
1	C	254	GLU	2.4
1	B	331	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	258	LYS	2.4
1	A	273	THR	2.4
1	C	125	GLN	2.4
1	B	259	ILE	2.4
1	A	220	PRO	2.4
1	A	448	TYR	2.4
1	B	27	ASN	2.4
1	C	230	GLU	2.4
1	B	164	LYS	2.4
1	A	312	ASP	2.4
1	A	320	LEU	2.4
1	B	429	VAL	2.4
1	A	356	SER	2.4
1	A	168	ASN	2.3
1	C	324	PRO	2.3
1	A	281	CYS	2.3
1	B	472	LYS	2.3
1	C	106	LYS	2.3
1	C	477	CYS	2.3
1	B	56	LEU	2.3
1	B	250	LEU	2.3
1	B	212	SER	2.3
1	A	155	LYS	2.3
1	B	42	ASN	2.3
1	B	346	MET	2.3
1	B	364	ALA	2.3
1	A	439	PHE	2.3
1	A	151	VAL	2.3
1	A	154	THR	2.3
1	C	263	GLY	2.3
1	A	304	GLU	2.3
1	A	179	TRP	2.3
1	A	76	SER	2.3
1	C	145	SER	2.3
1	C	355	HIS	2.3
1	B	362	GLY	2.3
1	A	275	GLU	2.3
1	A	492	GLU	2.3
1	C	383	SER	2.3
1	C	6	GLN	2.3
1	C	382	ASN	2.3
1	A	378	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	381	VAL	2.3
1	A	481	VAL	2.3
1	B	177	ILE	2.3
1	B	297	ILE	2.3
1	A	279	THR	2.3
1	C	11	TYR	2.3
1	A	112	VAL	2.3
1	A	466	CYS	2.2
1	A	24	LEU	2.2
1	A	465	GLY	2.2
1	B	187	ASP	2.2
1	B	459	VAL	2.2
1	C	84	VAL	2.2
1	C	245	GLU	2.2
1	C	380	LYS	2.2
1	C	36	ILE	2.2
1	A	266	GLY	2.2
1	A	160	TYR	2.2
1	B	315	VAL	2.2
1	B	145	SER	2.2
1	B	224	GLY	2.2
1	B	424	ASN	2.2
1	A	452	ARG	2.2
1	B	421	TRP	2.2
1	A	291	THR	2.2
1	C	20	VAL	2.2
1	A	33	ALA	2.2
1	C	453	MET	2.2
1	A	303	GLY	2.2
1	A	54	LEU	2.2
1	B	35	ASP	2.2
1	C	419	ASP	2.2
1	C	440	HIS	2.2
1	B	414	GLU	2.2
1	B	338	PHE	2.2
1	C	439	PHE	2.2
1	A	235	LEU	2.2
1	A	158	SER	2.1
1	B	87	GLU	2.1
1	A	314	LEU	2.1
1	B	358	ASP	2.1
1	C	331	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	390	THR	2.1
1	B	135	SER	2.1
1	B	481	VAL	2.1
1	B	397	LYS	2.1
1	C	491	TYR	2.1
1	B	93	LEU	2.1
1	B	257	PHE	2.1
1	C	389	ASN	2.1
1	C	462	LEU	2.1
1	A	170	THR	2.1
1	B	161	PRO	2.1
1	C	107	HIS	2.1
1	A	204	GLY	2.1
1	A	188	ALA	2.1
1	B	252	ALA	2.1
1	B	58	ASP	2.1
1	A	464	ASN	2.1
1	C	280	LYS	2.1
1	C	112	VAL	2.1
1	A	410	ASN	2.1
1	A	66	LEU	2.1
1	B	236	LEU	2.1
1	B	41	HIS	2.1
1	B	180	GLY	2.1
1	B	489	PRO	2.1
1	C	182	HIS	2.1
1	C	299	PRO	2.1
1	C	342	GLY	2.1
1	B	476	GLU	2.1
1	C	94	CYS	2.1
1	B	464	ASN	2.1
1	B	45	LEU	2.1
1	C	214	PRO	2.1
1	B	312	ASP	2.1
1	B	375	ASP	2.1
1	C	35	ASP	2.1
1	C	358	ASP	2.1
1	A	347	VAL	2.1
1	C	344	GLN	2.1
1	C	73	ARG	2.1
1	C	377	ILE	2.1
1	A	426	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	370	THR	2.1
1	A	133	GLY	2.0
1	C	164	LYS	2.0
1	C	411	LYS	2.0
1	A	246	SER	2.0
1	C	480	SER	2.0
1	C	47	ARG	2.0
1	C	137	ALA	2.0
1	C	472	LYS	2.0
1	C	303	GLY	2.0
1	A	340	GLU	2.0
1	B	149	ASN	2.0
1	A	365	ALA	2.0
1	C	163	ALA	2.0
1	B	178	ILE	2.0
1	B	22	THR	2.0
1	B	448	TYR	2.0
1	C	460	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

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
3	SIA	C	1497	20/21	0.57	0.37	0.14	54,58,60,61	0
3	GAL	B	1500	11/12	0.76	0.25	-0.17	82,84,85,85	0
3	SIA	B	1499	20/21	0.83	0.19	-0.65	77,79,81,81	0
3	GAL	C	1498	11/12	0.73	0.36	-	63,66,67,68	0
3	NAG	C	1499	15/15	0.76	0.28	-	70,74,74,75	0
3	NAG	B	1501	15/15	0.56	0.49	-	86,89,89,90	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	C	1500	14/15	0.48	0.44	0.89	78,79,80,80	0
2	NAG	A	1500	13/15	0.68	0.19	-	69,70,71,72	0
2	NAG	A	1499	14/15	0.58	0.36	-	111,114,114,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.