



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 13, 2026 – 12:13 PM EDT

PDB ID : 9YAG / pdb_00009yag
Title : TCR-HLA-DQ2.5-glia-w1 complex
Authors : Lim, J.J.; Loh, T.J.; Rossjohn, J.
Deposited on : 2025-09-15
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

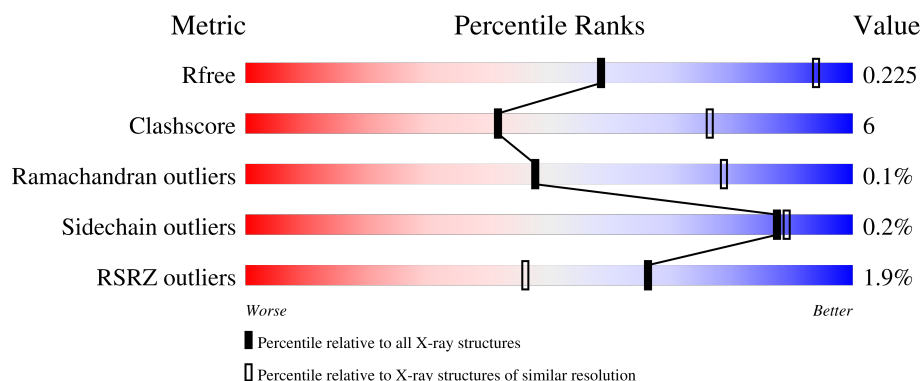
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	183	88% 10% .
1	F	183	89% 10% .
2	B	192	2% 77% 17% 6%
2	G	192	2% 78% 16% 6%
3	C	12	8% 75% 25%

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Mol	Chain	Length	Quality of chain
3	H	12	83%17%
4	D	206	2% 82%16% •
4	I	206	8% 81%16% • •
5	E	244	78%21%
5	J	244	81%18% •

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 13048 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 HLA class II histocompatibility antigen, DQ alpha 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	181	Total	C	N	O	S	0	0	0
			1422	917	231	271	3			
1	A	180	Total	C	N	O	S	0	0	0
			1414	913	230	268	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	46	SER	CYS	conflict	UNP P01909
F	74	CYS	SER	conflict	UNP P01909
A	46	SER	CYS	conflict	UNP P01909
A	74	CYS	SER	conflict	UNP P01909

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DQ 2.5 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	180	Total	C	N	O	S	0	0	0
			1457	923	258	269	7			
2	B	181	Total	C	N	O	S	0	0	0
			1462	926	260	269	7			

- Molecule 3 is a protein called GLIA-W1 PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	12	Total	C	N	O	S	0	0	0
			99	66	15	17	1			
3	C	12	Total	C	N	O	S	0	0	0
			99	66	15	17	1			

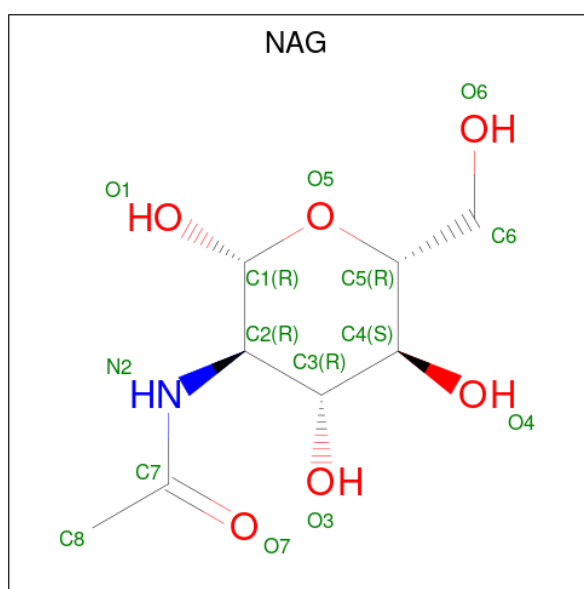
- Molecule 4 is a protein called TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	200	Total	C	N	O	S	0	0	0
			1497	947	243	298	9			
4	D	201	Total	C	N	O	S	0	0	0
			1530	963	249	309	9			

- Molecule 5 is a protein called TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	241	Total	C	N	O	S	0	0	0
			1912	1206	338	362	6			
5	E	243	Total	C	N	O	S	0	0	0
			1926	1213	340	367	6			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



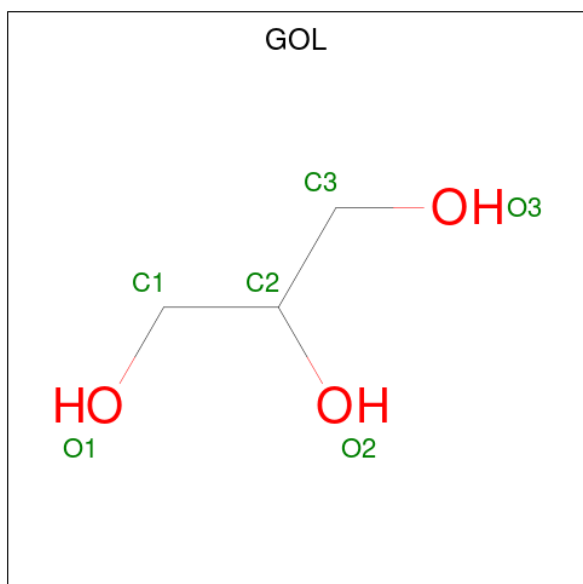
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		
7	I	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	4	Total	O	0	0
			4	4		
8	G	6	Total	O	0	0
			6	6		
8	I	8	Total	O	0	0
			8	8		
8	J	8	Total	O	0	0
			8	8		
8	A	2	Total	O	0	0
			2	2		
8	B	5	Total	O	0	0
			5	5		
8	D	2	Total	O	0	0
			2	2		
8	E	5	Total	O	0	0
			5	5		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

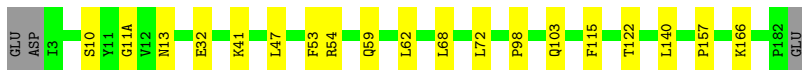
- Molecule 1: HLA class II histocompatibility antigen, DQ alpha 1 chain

Chain F: 



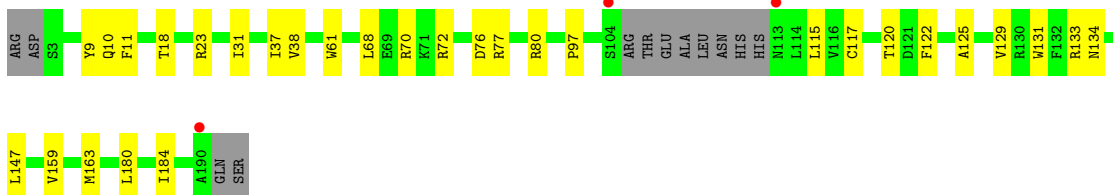
- Molecule 1: HLA class II histocompatibility antigen, DQ alpha 1 chain

Chain A: 



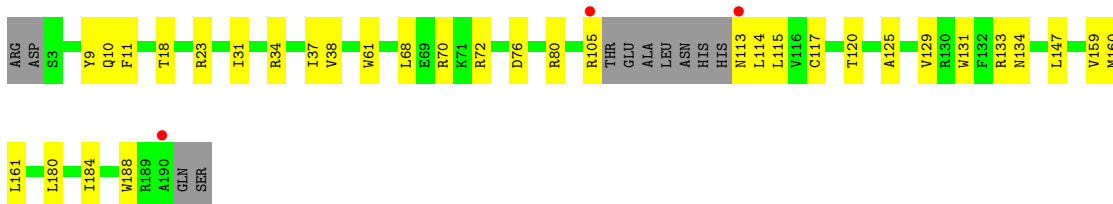
- Molecule 2: HLA class II histocompatibility antigen, DQ 2.5 beta chain

Chain G: 



- Molecule 2: HLA class II histocompatibility antigen, DQ 2.5 beta chain

Chain B: 



- Molecule 3: GLIA-W1 PEPTIDE

Chain H:  83% 17%



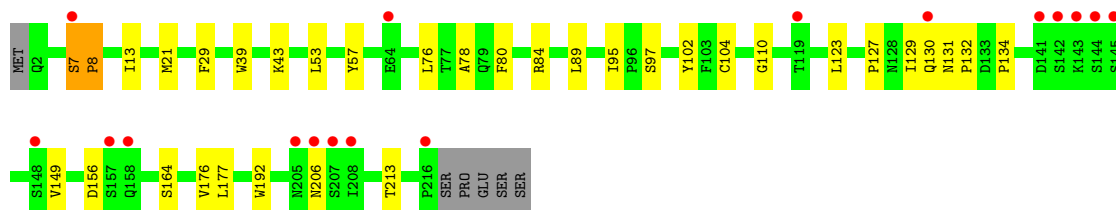
• Molecule 3: GLIA-W1 PEPTIDE

Chain C:  8% 75% 25%



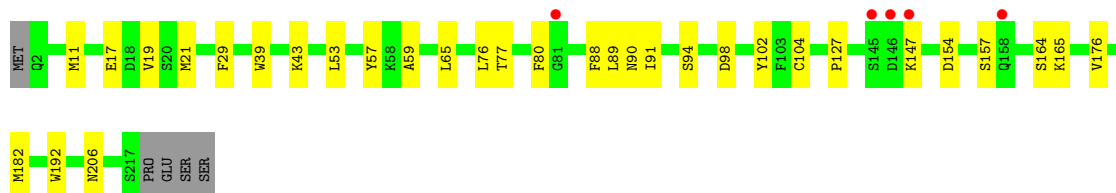
• Molecule 4: TCR alpha chain

Chain I:  8% 81% 16% . .



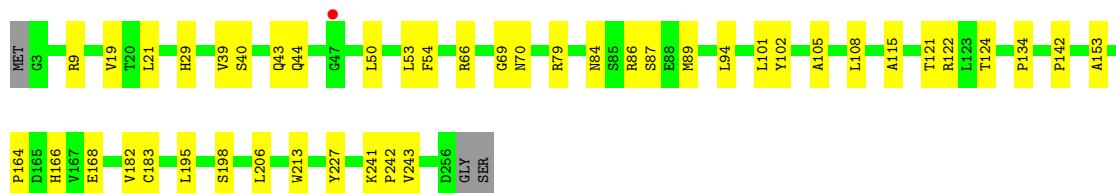
• Molecule 4: TCR alpha chain

Chain D:  2% 82% 16% .



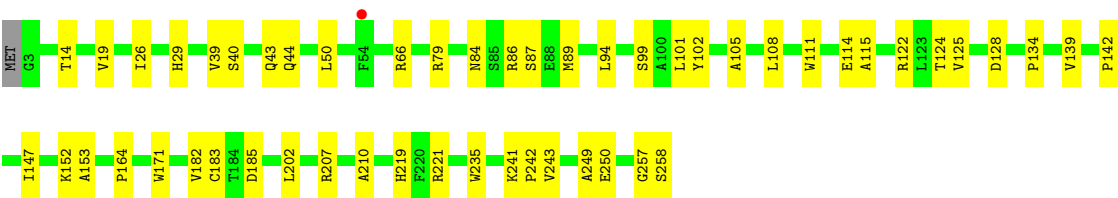
• Molecule 5: TCR beta chain

Chain J:  81% 18% .



• Molecule 5: TCR beta chain

Chain E:  78% 21%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.99Å 122.22Å 249.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 3.20 49.25 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.25-3.20) 99.9 (49.25-3.20)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.185 , 0.226 0.185 , 0.225	Depositor DCC
R_{free} test set	2310 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13048	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.11	0/1456	0.29	0/1994
1	F	0.11	0/1464	0.30	0/2005
2	B	0.12	0/1495	0.32	0/2034
2	G	0.15	0/1490	0.32	0/2027
3	C	0.16	0/105	0.37	0/145
3	H	0.17	0/105	0.42	0/145
4	D	0.11	0/1563	0.31	0/2125
4	I	0.12	0/1530	0.35	0/2086
5	E	0.11	0/1978	0.29	0/2690
5	J	0.10	0/1964	0.28	0/2672
All	All	0.12	0/13150	0.31	0/17923

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
4	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	I	7	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1414	0	1346	15	0
1	F	1422	0	1350	14	0
2	B	1462	0	1417	23	0
2	G	1457	0	1414	20	0
3	C	99	0	89	3	0
3	H	99	0	89	2	0
4	D	1530	0	1433	26	0
4	I	1497	0	1380	22	0
5	E	1926	0	1826	35	0
5	J	1912	0	1814	29	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	D	56	0	52	0	0
6	E	14	0	13	1	0
6	F	14	0	13	0	0
6	I	28	0	26	0	0
6	J	14	0	13	1	0
7	A	12	0	16	0	0
7	F	12	0	16	0	0
7	G	6	0	8	0	0
7	I	6	0	8	0	0
8	A	2	0	0	0	0
8	B	5	0	0	0	0
8	D	2	0	0	0	0
8	E	5	0	0	0	0
8	F	4	0	0	0	0
8	G	6	0	0	0	0
8	I	8	0	0	0	0
8	J	8	0	0	0	0
All	All	13048	0	12349	161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (161) 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:F:54:ARG:H	3:H:0:GLN:HG2	1.50	0.76
5:J:70:ASN:ND2	1:A:53:PHE:O	2.24	0.71
4:D:59:ALA:HA	4:D:80:PHE:HD1	1.56	0.71
4:D:147:LYS:HD2	4:D:192:TRP:HD1	1.58	0.69
2:B:105:ARG:HA	2:B:113:ASN:HB3	1.75	0.67
5:E:19:VAL:HG13	5:E:94:LEU:HD11	1.76	0.67
2:B:125:ALA:HB1	2:B:147:LEU:HD21	1.78	0.66
5:J:19:VAL:HG13	5:J:94:LEU:HD11	1.78	0.66
5:J:43:GLN:HB2	5:J:53:LEU:HD11	1.79	0.65
1:A:13:ASN:HB2	2:B:11:PHE:HB3	1.80	0.64
5:E:39:VAL:HG21	5:E:87:SER:HB2	1.80	0.63
1:F:32:GLU:HB2	1:F:140:LEU:HD21	1.81	0.62
5:J:134:PRO:HD3	5:J:242:PRO:HB3	1.82	0.61
5:J:54:PHE:HZ	5:J:89:MET:HG3	1.65	0.61
5:E:235:TRP:HB2	5:E:241:LYS:HD3	1.83	0.61
4:D:59:ALA:HA	4:D:80:PHE:CD1	2.35	0.60
2:B:37:ILE:HG13	2:B:38:VAL:HG23	1.84	0.59
1:F:60:PHE:CZ	4:I:110:GLY:HA2	2.38	0.59
4:I:43:LYS:HB2	4:I:53:LEU:HD11	1.84	0.59
5:E:134:PRO:HD3	5:E:242:PRO:HB3	1.84	0.58
5:J:79:ARG:HB2	6:J:301:NAG:H83	1.86	0.57
5:E:101:LEU:HB2	5:E:122:ARG:NH2	2.20	0.57
5:J:39:VAL:HG21	5:J:87:SER:HB2	1.86	0.56
4:I:29:PHE:HB2	4:I:39:TRP:NE1	2.19	0.56
5:J:105:ALA:HB1	5:J:115:ALA:HB1	1.88	0.56
1:A:59:GLN:HG2	5:E:66:ARG:CZ	2.35	0.56
2:B:61:TRP:CE2	3:C:7:GLN:HB2	2.41	0.56
1:F:59:GLN:HG2	5:J:66:ARG:CZ	2.36	0.55
5:J:89:MET:HE1	5:J:102:TYR:CD1	2.42	0.55
4:D:127:PRO:O	4:D:157:SER:OG	2.21	0.55
5:J:29:HIS:HA	5:J:108:LEU:HD12	1.89	0.55
1:F:41:LYS:HG2	1:F:62:LEU:HD11	1.89	0.54
5:J:40:SER:HB2	5:J:105:ALA:HB3	1.89	0.54
5:E:105:ALA:HB1	5:E:115:ALA:HB1	1.88	0.54
2:G:37:ILE:HG13	2:G:38:VAL:HG23	1.88	0.54
4:D:164:SER:HA	4:D:206:ASN:HD22	1.72	0.54
4:I:149:VAL:HG12	4:I:192:TRP:HB3	1.89	0.54
4:I:8:PRO:HG3	4:I:21:MET:HA	1.88	0.54
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.43	0.53
2:B:129:VAL:HB	2:B:159:VAL:HG21	1.91	0.53
1:A:32:GLU:HB2	1:A:140:LEU:HD21	1.91	0.53
2:B:10:GLN:HB2	2:B:31:ILE:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:84:ASN:ND2	5:E:86:ARG:HB3	2.24	0.53
4:D:147:LYS:HD2	4:D:192:TRP:CD1	2.42	0.52
5:E:124:THR:HG21	5:E:164:PRO:HB3	1.90	0.52
5:J:142:PRO:HG2	5:J:153:ALA:HB1	1.91	0.52
5:E:79:ARG:HB2	6:E:301:NAG:H83	1.91	0.52
5:J:195:LEU:HB2	5:J:198:SER:HB2	1.90	0.52
4:D:77:THR:HG23	4:D:90:ASN:HB2	1.90	0.52
2:G:77:ARG:NH1	4:I:57:TYR:HB3	2.23	0.52
4:D:127:PRO:HD3	4:D:176:VAL:HG21	1.92	0.52
4:I:95:ILE:HG22	4:I:97:SER:H	1.75	0.51
4:D:39:TRP:HD1	4:D:80:PHE:CE2	2.28	0.51
4:I:164:SER:HA	4:I:206:ASN:HD21	1.76	0.51
1:F:10:SER:C	1:F:11(A):GLY:HA2	2.36	0.51
1:A:59:GLN:HG2	5:E:66:ARG:NE	2.26	0.51
4:I:80:PHE:HE1	4:I:84:ARG:HA	1.77	0.50
4:D:98:ASP:HB2	4:D:102:TYR:OH	2.11	0.50
1:A:10:SER:C	1:A:11(A):GLY:HA2	2.36	0.50
5:E:44:GLN:HE21	5:E:50:LEU:HD11	1.75	0.50
4:I:129:ILE:HG13	4:I:156:ASP:HA	1.93	0.50
5:E:26:ILE:HD12	5:E:29:HIS:CE1	2.47	0.50
2:G:10:GLN:HB2	2:G:31:ILE:HB	1.92	0.50
2:G:61:TRP:CE2	3:H:7:GLN:HB2	2.47	0.50
1:F:13:ASN:HB2	2:G:11:PHE:HB3	1.94	0.49
5:J:124:THR:HG21	5:J:164:PRO:HB3	1.94	0.49
2:G:180:LEU:HD13	2:G:184:ILE:HG13	1.95	0.49
5:E:257:GLY:O	5:E:258:SER:HB2	2.12	0.49
2:G:115:LEU:HG	2:G:163:MET:SD	2.53	0.49
5:E:221:ARG:HG3	5:E:250:GLU:HG2	1.95	0.49
1:A:54:ARG:H	3:C:0:GLN:CD	2.21	0.48
5:E:219:HIS:NE2	5:E:250:GLU:OE1	2.40	0.48
5:J:101:LEU:HB2	5:J:122:ARG:NH2	2.29	0.48
5:J:21:LEU:HG	5:J:121:THR:HG21	1.94	0.47
4:D:43:LYS:HB2	4:D:53:LEU:HD11	1.95	0.47
4:I:80:PHE:CE1	4:I:84:ARG:HA	2.50	0.47
2:G:117:CYS:HB2	2:G:131:TRP:CZ2	2.49	0.47
4:I:134:PRO:HB2	4:I:213:THR:HA	1.97	0.47
2:B:180:LEU:HD13	2:B:184:ILE:HG13	1.97	0.47
4:D:165:LYS:NZ	4:D:206:ASN:HB3	2.30	0.47
2:G:125:ALA:HB1	2:G:147:LEU:HD21	1.97	0.47
4:D:182:MET:HE1	5:E:152:LYS:HE3	1.96	0.47
5:J:241:LYS:HG2	5:J:243:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:PRO:HD3	2:G:120:THR:HG21	1.98	0.46
2:B:114:LEU:HD12	2:B:160:MET:HB3	1.96	0.46
1:A:72:LEU:HD13	2:B:9:TYR:HB2	1.98	0.46
4:I:127:PRO:HD3	4:I:176:VAL:HG21	1.97	0.46
5:E:99:SER:HG	5:E:125:VAL:H	1.63	0.46
5:E:142:PRO:HG2	5:E:153:ALA:HB1	1.97	0.46
5:E:241:LYS:HG2	5:E:243:VAL:HG13	1.97	0.46
5:E:40:SER:HB2	5:E:105:ALA:HB3	1.98	0.46
4:D:29:PHE:HB2	4:D:39:TRP:NE1	2.31	0.46
4:D:21:MET:HE1	4:D:102:TYR:CD1	2.50	0.46
1:F:72:LEU:HD13	2:G:9:TYR:HB2	1.96	0.46
4:I:21:MET:HE1	4:I:102:TYR:CD1	2.51	0.46
1:A:41:LYS:HG2	1:A:62:LEU:HD11	1.98	0.46
2:G:18:THR:HB	2:G:23:ARG:HB2	1.96	0.45
5:E:89:MET:HE1	5:E:102:TYR:CD2	2.51	0.45
2:G:76:ASP:OD1	2:G:80:ARG:HD2	2.16	0.45
2:G:129:VAL:HB	2:G:159:VAL:HG21	1.98	0.45
1:F:59:GLN:HG2	5:J:66:ARG:NE	2.32	0.45
5:E:43:GLN:HG3	5:E:102:TYR:CE2	2.52	0.45
4:D:154:ASP:OD1	5:E:207:ARG:NH1	2.48	0.45
5:J:166:HIS:HB3	5:J:227:TYR:HB2	1.99	0.45
2:G:76:ASP:HA	2:G:80:ARG:HB2	1.98	0.44
2:G:133:ARG:HA	2:G:134:ASN:HA	1.74	0.44
2:B:70:ARG:HG2	4:D:57:TYR:CE1	2.52	0.44
5:E:171:TRP:HD1	5:E:182:VAL:HG13	1.83	0.44
5:J:44:GLN:HE21	5:J:50:LEU:HD11	1.82	0.44
2:B:68:LEU:HD13	2:B:72:ARG:HH21	1.83	0.44
1:A:98:PRO:HD3	2:B:120:THR:HG21	1.99	0.44
4:I:13:ILE:HD13	4:I:123:LEU:HD11	1.99	0.44
5:J:9:ARG:NH2	5:J:168:GLU:OE2	2.47	0.44
2:B:133:ARG:HA	2:B:134:ASN:HA	1.75	0.44
2:B:131:TRP:HB3	2:B:161:LEU:HD22	1.99	0.43
5:J:53:LEU:O	5:J:69:GLY:N	2.35	0.43
2:B:115:LEU:HD23	2:B:115:LEU:HA	1.82	0.43
5:J:43:GLN:HG3	5:J:102:TYR:CE1	2.54	0.43
1:A:122:THR:HG23	1:A:166:LYS:HB3	2.00	0.43
4:D:76:LEU:HD23	4:D:91:ILE:HG12	2.01	0.43
4:I:78:ALA:HB2	4:I:89:LEU:HD13	2.01	0.43
2:B:18:THR:HB	2:B:23:ARG:HB2	2.01	0.43
1:F:156:LEU:HD21	5:E:128:ASP:OD2	2.19	0.43
5:E:29:HIS:HA	5:E:108:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:LEU:HG	2:G:9:TYR:CD1	2.54	0.43
5:J:101:LEU:HB2	5:J:122:ARG:HH21	1.83	0.43
5:E:171:TRP:CD1	5:E:182:VAL:HG13	2.54	0.43
4:I:76:LEU:HD22	4:I:89:LEU:HD11	2.01	0.42
4:I:177:LEU:HB3	5:J:183:CYS:HB2	2.00	0.42
1:A:115:PHE:CE2	2:B:34:ARG:HG3	2.54	0.42
5:J:142:PRO:HD2	5:J:213:TRP:CZ2	2.55	0.42
4:D:21:MET:HE1	4:D:102:TYR:CG	2.54	0.42
1:A:47:LEU:HD12	1:A:47:LEU:HA	1.91	0.42
4:D:76:LEU:HD22	4:D:89:LEU:HD11	2.00	0.42
1:F:124:LEU:HB2	1:F:164:ASP:HB2	2.02	0.42
4:D:57:TYR:OH	5:E:114:GLU:OE2	2.29	0.42
4:D:164:SER:HA	4:D:206:ASN:ND2	2.34	0.42
4:D:65:LEU:HD21	4:D:88:PHE:CZ	2.55	0.42
4:D:17:GLU:O	4:D:94:SER:OG	2.34	0.42
3:C:3:PRO:HG2	5:E:111:TRP:CH2	2.55	0.42
4:I:130:GLN:O	4:I:132:PRO:HD3	2.19	0.41
5:E:101:LEU:HB2	5:E:122:ARG:HH21	1.85	0.41
1:F:116:PRO:O	1:F:118:VAL:N	2.48	0.41
2:G:97:PRO:HB3	2:G:122:PHE:HB3	2.02	0.41
1:A:103:GLN:O	1:A:157:PRO:HD2	2.20	0.41
4:I:29:PHE:HB2	4:I:39:TRP:HE1	1.82	0.41
2:B:115:LEU:HD11	2:B:188:TRP:CE3	2.56	0.41
4:D:165:LYS:HD3	4:D:206:ASN:CG	2.46	0.41
5:E:147:ILE:HG23	5:E:210:ALA:HB1	2.03	0.41
2:G:70:ARG:HG2	4:I:57:TYR:CE1	2.56	0.41
5:J:84:ASN:C	5:J:86:ARG:H	2.27	0.41
5:E:14:THR:HG23	5:E:128:ASP:HA	2.01	0.41
4:D:11:MET:HE1	4:D:19:VAL:HG13	2.03	0.41
4:I:129:ILE:O	4:I:131:ASN:N	2.50	0.41
1:A:68:LEU:HG	2:B:9:TYR:CD1	2.55	0.41
5:J:182:VAL:HG22	5:J:206:LEU:HD13	2.03	0.41
2:B:76:ASP:HA	2:B:80:ARG:HB2	2.03	0.41
5:E:139:VAL:HG23	5:E:249:ALA:HB3	2.03	0.41
2:G:68:LEU:HD13	2:G:72:ARG:HH21	1.85	0.40
5:E:185:ASP:HB2	5:E:202:LEU:HD12	2.02	0.40
2:B:131:TRP:CD1	2:B:161:LEU:HB2	2.55	0.40

There are no symmetry-related clashes.

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	178/183 (97%)	171 (96%)	7 (4%)	0	100	100
1	F	179/183 (98%)	172 (96%)	7 (4%)	0	100	100
2	B	177/192 (92%)	169 (96%)	8 (4%)	0	100	100
2	G	176/192 (92%)	166 (94%)	10 (6%)	0	100	100
3	C	10/12 (83%)	8 (80%)	2 (20%)	0	100	100
3	H	10/12 (83%)	8 (80%)	2 (20%)	0	100	100
4	D	199/206 (97%)	190 (96%)	9 (4%)	0	100	100
4	I	198/206 (96%)	183 (92%)	13 (7%)	2 (1%)	12	45
5	E	241/244 (99%)	232 (96%)	9 (4%)	0	100	100
5	J	239/244 (98%)	232 (97%)	7 (3%)	0	100	100
All	All	1607/1674 (96%)	1531 (95%)	74 (5%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	8	PRO
4	I	7	SER

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	159/167 (95%)	159 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	160/167 (96%)	160 (100%)	0	100	100
2	B	160/176 (91%)	160 (100%)	0	100	100
2	G	160/176 (91%)	160 (100%)	0	100	100
3	C	12/12 (100%)	12 (100%)	0	100	100
3	H	12/12 (100%)	12 (100%)	0	100	100
4	D	170/181 (94%)	169 (99%)	1 (1%)	78	84
4	I	160/181 (88%)	159 (99%)	1 (1%)	78	84
5	E	210/212 (99%)	209 (100%)	1 (0%)	81	85
5	J	208/212 (98%)	208 (100%)	0	100	100
All	All	1411/1496 (94%)	1408 (100%)	3 (0%)	87	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	I	104	CYS
4	D	104	CYS
5	E	183	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	33	GLN
2	G	84	GLN
2	G	150	ASN
4	I	3	GLN
4	I	107	GLN
5	J	18	GLN
5	J	51	GLN
5	J	149	HIS
1	A	126	ASN
2	B	84	GLN
2	B	150	ASN
2	B	156	GLN
4	D	9	GLN
4	D	163	GLN
4	D	206	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

17 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	$\# Z > 2$
6	NAG	I	303	4	14,14,15	0.62	0	17,19,21	0.85	0
7	GOL	G	201	-	5,5,5	0.38	0	5,5,5	0.43	0
6	NAG	F	201	1	14,14,15	0.61	0	17,19,21	0.89	1 (5%)
7	GOL	A	201	-	5,5,5	0.40	0	5,5,5	0.50	0
6	NAG	D	304	4	14,14,15	0.61	0	17,19,21	2.16	3 (17%)
6	NAG	B	201	2	14,14,15	0.67	0	17,19,21	0.83	0
7	GOL	I	301	-	5,5,5	0.38	0	5,5,5	0.50	0
6	NAG	I	302	4	14,14,15	0.72	0	17,19,21	1.01	1 (5%)
7	GOL	A	202	-	5,5,5	0.38	0	5,5,5	0.46	0
6	NAG	A	203	1	14,14,15	0.64	0	17,19,21	0.93	1 (5%)
6	NAG	J	301	5	14,14,15	0.70	0	17,19,21	0.83	0
6	NAG	D	302	4	14,14,15	0.67	0	17,19,21	0.75	0
7	GOL	F	203	-	5,5,5	0.39	0	5,5,5	0.44	0
6	NAG	E	301	5	14,14,15	0.68	0	17,19,21	0.75	0
7	GOL	F	202	-	5,5,5	0.37	0	5,5,5	0.46	0
6	NAG	D	303	4	14,14,15	0.67	0	17,19,21	0.76	0
6	NAG	D	301	4	14,14,15	0.64	0	17,19,21	0.82	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
6	NAG	I	303	4	-	0/6/23/26	0/1/1/1
7	GOL	G	201	-	-	0/4/4/4	-
6	NAG	F	201	1	-	1/6/23/26	0/1/1/1
7	GOL	A	201	-	-	2/4/4/4	-
6	NAG	D	304	4	-	3/6/23/26	0/1/1/1
6	NAG	B	201	2	-	1/6/23/26	0/1/1/1
7	GOL	I	301	-	-	0/4/4/4	-
6	NAG	I	302	4	-	2/6/23/26	0/1/1/1
7	GOL	A	202	-	-	0/4/4/4	-
6	NAG	A	203	1	-	2/6/23/26	0/1/1/1
6	NAG	J	301	5	-	2/6/23/26	0/1/1/1
6	NAG	D	302	4	-	0/6/23/26	0/1/1/1
7	GOL	F	203	-	-	0/4/4/4	-
6	NAG	E	301	5	-	1/6/23/26	0/1/1/1
7	GOL	F	202	-	-	1/4/4/4	-
6	NAG	D	303	4	-	0/6/23/26	0/1/1/1
6	NAG	D	301	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	304	NAG	C1-O5-C5	6.66	121.11	112.19
6	D	304	NAG	C3-C4-C5	3.48	116.54	110.23
6	D	304	NAG	O5-C5-C4	2.78	117.59	110.83
6	I	302	NAG	O5-C1-C2	-2.68	107.15	111.29
6	A	203	NAG	C1-O5-C5	2.60	115.67	112.19
6	F	201	NAG	C1-O5-C5	2.39	115.39	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	201	GOL	O1-C1-C2-C3
6	I	302	NAG	O5-C5-C6-O6
6	D	304	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	D	304	NAG	O5-C5-C6-O6
6	A	203	NAG	O5-C5-C6-O6
6	A	203	NAG	C4-C5-C6-O6
6	I	302	NAG	C4-C5-C6-O6
7	A	201	GOL	O1-C1-C2-O2
6	F	201	NAG	O5-C5-C6-O6
7	F	202	GOL	O1-C1-C2-C3
6	J	301	NAG	C4-C5-C6-O6
6	J	301	NAG	O5-C5-C6-O6
6	E	301	NAG	C1-C2-N2-C7
6	D	304	NAG	C3-C2-N2-C7
6	B	201	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	301	NAG	1	0
6	E	301	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	180/183 (98%)	-0.25	0 100 100	34, 48, 70, 92	0
1	F	181/183 (98%)	-0.29	0 100 100	30, 44, 69, 101	0
2	B	181/192 (94%)	-0.17	3 (1%) 69 49	35, 49, 80, 106	0
2	G	180/192 (93%)	-0.19	3 (1%) 69 49	33, 47, 79, 95	0
3	C	12/12 (100%)	0.31	1 (8%) 17 11	42, 49, 68, 82	0
3	H	12/12 (100%)	0.06	0 100 100	36, 43, 68, 76	0
4	D	201/206 (97%)	0.25	5 (2%) 58 39	32, 59, 89, 120	0
4	I	200/206 (97%)	0.54	17 (8%) 16 11	32, 64, 105, 129	0
5	E	243/244 (99%)	-0.16	1 (0%) 88 79	34, 50, 69, 105	0
5	J	241/244 (98%)	-0.09	1 (0%) 88 79	34, 50, 78, 103	0
All	All	1631/1674 (97%)	-0.04	31 (1%) 66 46	30, 51, 84, 129	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	190	ALA	3.5
4	I	144	SER	3.1
2	B	105	ARG	3.1
4	I	130	GLN	3.1
4	I	142	SER	3.1
4	D	146	ASP	3.0
2	B	190	ALA	2.9
4	I	206	ASN	2.9
4	I	208	ILE	2.9
4	I	148	SER	2.8
4	D	158	GLN	2.7
4	I	157	SER	2.6
2	B	113	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
4	D	147	LYS	2.5
4	I	145	SER	2.5
4	I	158	GLN	2.4
4	I	119	THR	2.3
4	D	81	GLY	2.3
4	I	207	SER	2.3
3	C	11	CYS	2.2
4	I	7	SER	2.2
2	G	104	SER	2.2
4	I	141	ASP	2.2
4	I	64	GLU	2.1
2	G	113	ASN	2.1
5	J	47	GLY	2.1
5	E	54	PHE	2.1
4	D	145	SER	2.1
4	I	143	LYS	2.0
4	I	205	ASN	2.0
4	I	216	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	D	304	14/15	0.41	0.23	107,127,137,143	0
6	NAG	B	201	14/15	0.60	0.15	91,120,129,137	0
7	GOL	F	203	6/6	0.71	0.20	49,69,83,84	0
7	GOL	I	301	6/6	0.71	0.20	67,71,90,92	0
6	NAG	D	303	14/15	0.72	0.15	76,97,104,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	I	302	14/15	0.76	0.16	86,105,116,121	0
6	NAG	D	301	14/15	0.78	0.13	96,108,115,116	0
6	NAG	A	203	14/15	0.81	0.16	58,77,92,94	0
6	NAG	E	301	14/15	0.81	0.12	51,59,66,80	0
7	GOL	A	202	6/6	0.81	0.20	45,72,79,80	0
7	GOL	G	201	6/6	0.82	0.15	63,68,87,96	0
6	NAG	I	303	14/15	0.82	0.14	74,88,104,108	0
6	NAG	D	302	14/15	0.82	0.13	50,75,93,98	0
6	NAG	F	201	14/15	0.84	0.14	54,61,75,76	0
6	NAG	J	301	14/15	0.86	0.12	44,58,64,79	0
7	GOL	F	202	6/6	0.93	0.12	37,55,59,60	0
7	GOL	A	201	6/6	0.94	0.12	38,54,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.