



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:13 AM GMT

PDB ID : 2WBJ
Title : TCR complex
Authors : Harkiolaki, M.; Holmes, S.L.; Svendsen, P.; Gregersen, J.W.; Jensen, L.T.;
McMahon, R.; Friese, M.A.; Van Boxel, G.; Etzensperger, R.; Tzartos, J.S.;
Kranc, K.; Sainsbury, S.; Harlos, K.; Mellins, E.D.; Palace, J.; Esiri, M.M.;
Van Der Merwe, P.A.; Jones, E.Y.; Fugger, L.
Deposited on : 2009-03-02
Resolution : 3.00 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

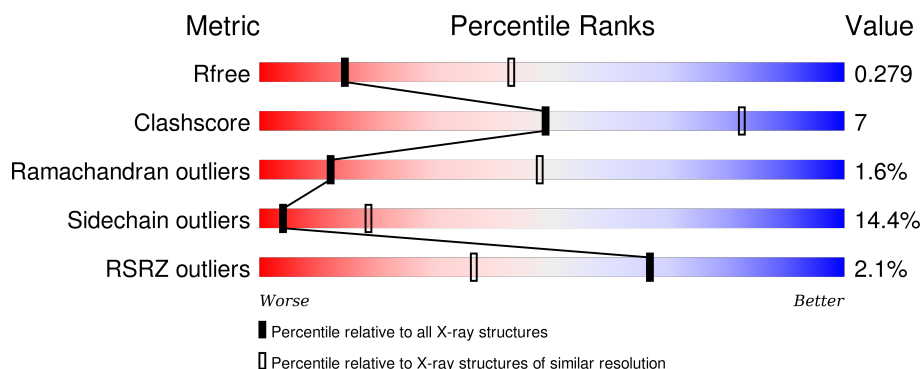
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	194	<div> <div>2%</div> <div>74% 15% • 8%</div> </div>
1	E	194	<div> <div>71% 18% • 9%</div> </div>
2	B	200	<div> <div>2%</div> <div>77% 11% • 11%</div> </div>
2	F	200	<div> <div>2%</div> <div>74% 19% • 6%</div> </div>
3	C	219	<div> <div>4%</div> <div>65% 18% • • 12%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	219	
4	D	279	
4	H	279	

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
5	NAG	A	1181	X	-	-	-
5	NAG	E	1186	X	-	-	-
5	NAG	F	1191	X	-	-	-
7	NAG	E	1181	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13235 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, DR ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1465	950	238	272	5			
1	E	177	Total	C	N	O	S	0	0	0
			1456	945	237	269	5			

- Molecule 2 is a protein called HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DRB1-15 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	179	Total	C	N	O	S	0	0	0
			1478	939	259	274	6			
2	F	188	Total	C	N	O	S	0	0	0
			1548	980	275	287	6			

- Molecule 3 is a protein called OB TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	193	Total	C	N	O	S	0	0	0
			1511	934	263	307	7			
3	G	190	Total	C	N	O	S	0	0	0
			1484	919	258	300	7			

- Molecule 4 is a protein called OB TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	270	Total	C	N	O	S	0	0	0
			2105	1323	366	408	8			
4	H	260	Total	C	N	O	S	0	0	0
			2056	1297	356	396	7			

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

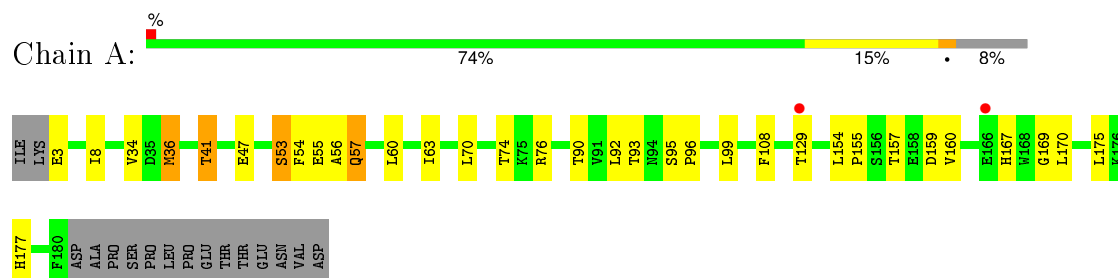
- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	5	Total	C	N	O	0	0
			61	34	2	25		

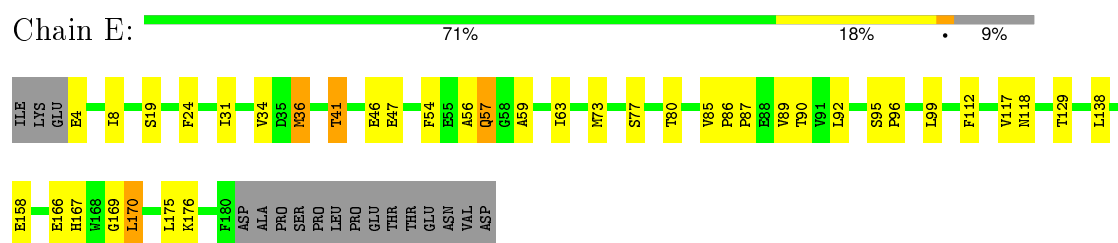
3 Residue-property plots [i](#)

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.

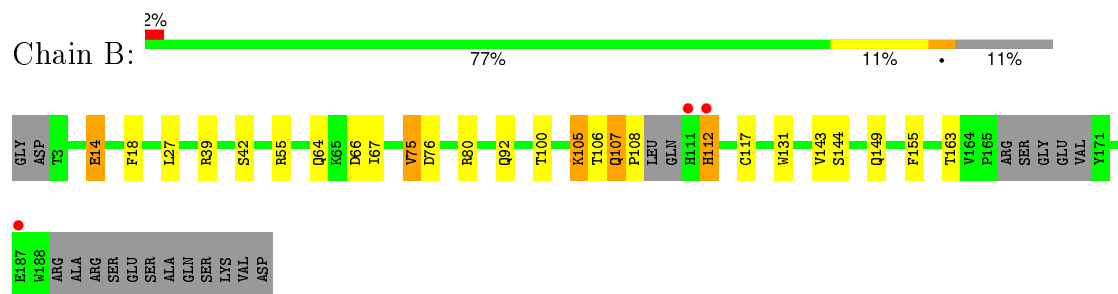
- Molecule 1: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR ALPHA CHAIN



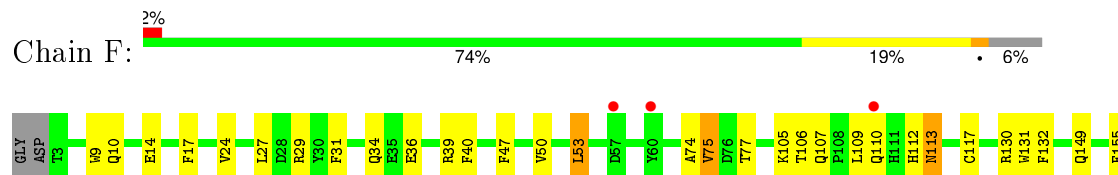
- Molecule 1: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR ALPHA CHAIN

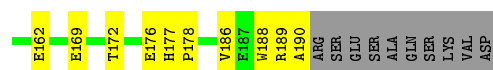


- Molecule 2: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DRB1-15 BETA CHAIN

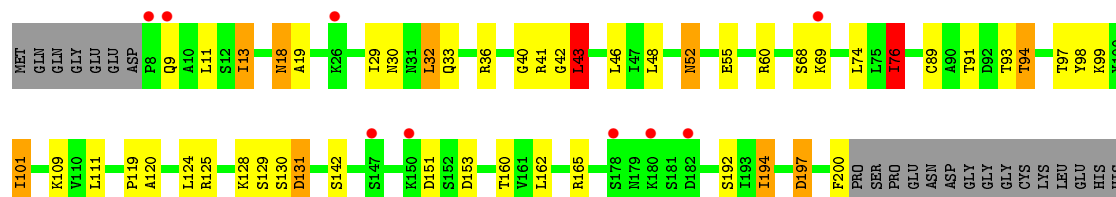


- Molecule 2: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DRB1-15 BETA CHAIN

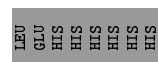
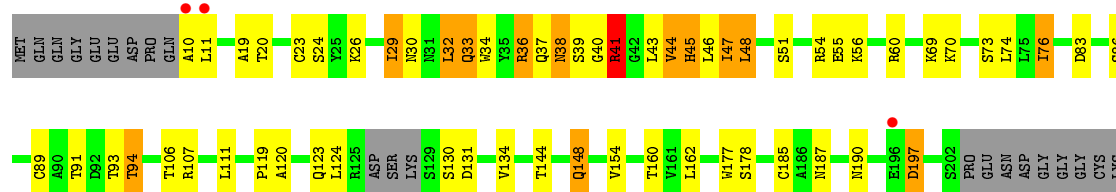




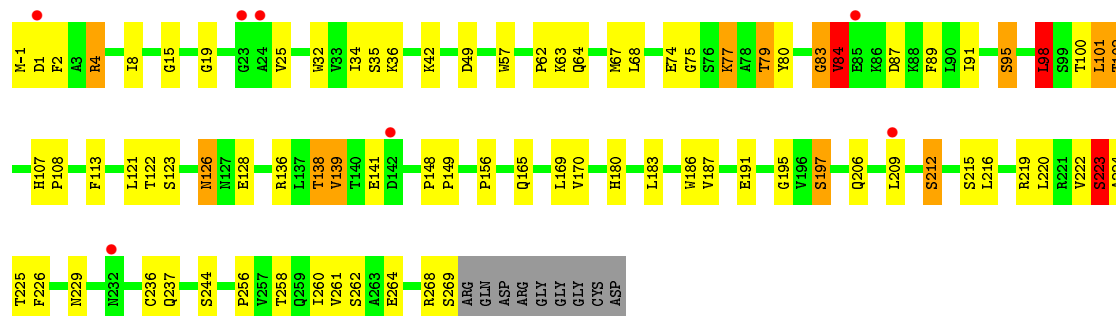
• Molecule 3: OB TCR



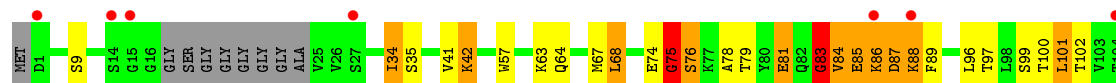
• Molecule 3: OB TCR

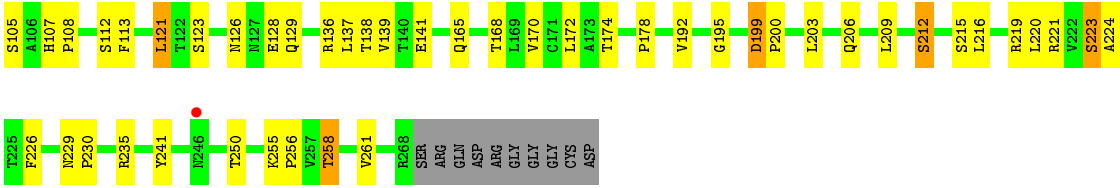


• Molecule 4: OB TCR



• Molecule 4: OB TCR





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.71Å 130.27Å 180.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.41 – 3.00 29.62 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (105.41-3.00) 99.6 (29.62-3.00)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.247 , 0.288 0.240 , 0.279	Depositor DCC
R_{free} test set	2659 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 52144 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13235	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: SO4, BMA, NAG, MAN

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	0.38	0/1510	0.50	0/2059
1	E	0.37	0/1501	0.53	0/2047
2	B	0.37	0/1519	0.49	0/2064
2	F	0.36	0/1591	0.48	0/2163
3	C	0.36	0/1537	0.53	0/2077
3	G	0.37	0/1509	0.58	1/2041 (0.0%)
4	D	0.37	0/2161	0.54	2/2936 (0.1%)
4	H	0.37	0/2111	0.54	1/2870 (0.0%)
All	All	0.37	0/13439	0.53	4/18257 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	C	0	1
3	G	0	1
4	D	0	5
4	H	0	5
7	E	1	0
All	All	1	13

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	32	LEU	CA-CB-CG	5.83	128.71	115.30
4	H	121	LEU	CA-CB-CG	5.45	127.82	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	223	SER	N-CA-C	5.17	124.97	111.00
4	D	98	LEU	CA-CB-CG	5.11	127.05	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	E	1181	NAG	C1

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	112	HIS	Peptide
3	C	76	ILE	Peptide
4	D	15	GLY	Peptide
4	D	222	VAL	Peptide
4	D	83	GLY	Peptide
4	D	84	VAL	Peptide
4	D	87	ASP	Peptide
3	G	56	LYS	Peptide
4	H	223	SER	Peptide
4	H	75	GLY	Peptide
4	H	78	ALA	Peptide
4	H	83	GLY	Peptide
4	H	86	LYS	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	1465	0	1401	18	0
1	E	1456	0	1394	22	0
2	B	1478	0	1398	14	0
2	F	1548	0	1473	20	0
3	C	1511	0	1465	25	0
3	G	1484	0	1438	28	0
4	D	2105	0	2005	36	0
4	H	2056	0	1962	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	F	5	0	0	0	0
7	E	61	0	52	2	0
All	All	13235	0	12640	185	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 7.

All (185) 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)
4:H:223:SER:CB	4:H:226:PHE:HB3	1.57	1.32
4:H:223:SER:HB2	4:H:226:PHE:HB3	1.21	1.15
4:D:83:GLY:HA2	4:D:84:VAL:HB	1.27	1.15
4:H:223:SER:HB3	4:H:226:PHE:HB3	1.33	1.10
4:H:223:SER:HB2	4:H:226:PHE:CB	1.94	0.96
1:A:8:ILE:HG12	2:B:14:GLU:HB3	1.47	0.94
1:E:57:GLN:H	1:E:57:GLN:HE21	1.16	0.93
3:G:40:GLY:HA3	3:G:41:ARG:HB2	1.52	0.91
3:C:130:SER:N	3:C:131:ASP:HA	1.88	0.88
4:H:86:LYS:HB3	4:H:87:ASP:HB2	1.57	0.87
3:G:47:ILE:HG13	3:G:48:LEU:H	1.41	0.84
4:H:86:LYS:HB3	4:H:87:ASP:CB	2.11	0.81
1:E:118:ASN:HB2	1:E:166:GLU:HG3	1.62	0.81
1:A:167:HIS:CD2	1:A:169:GLY:H	1.99	0.79
1:A:167:HIS:HD2	1:A:169:GLY:H	1.31	0.77
3:G:148:GLN:HA	3:G:148:GLN:HE21	1.52	0.74
3:C:162:LEU:HG	4:D:197:SER:HB3	1.69	0.73
1:A:41:THR:HG21	1:A:54:PHE:O	1.87	0.73
3:G:124:LEU:HB2	3:G:134:VAL:HG23	1.70	0.73
3:C:32:LEU:HB2	3:C:91:THR:HG22	1.71	0.73
2:F:14:GLU:HG3	2:F:27:LEU:HB2	1.70	0.72
1:E:41:THR:HG21	1:E:54:PHE:O	1.89	0.71
3:C:130:SER:H	3:C:131:ASP:HA	1.54	0.71
1:E:167:HIS:HA	7:E:1181:NAG:H81	1.70	0.70
4:D:83:GLY:CA	4:D:84:VAL:HB	2.16	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:75:GLY:N	4:H:76:SER:HB3	2.09	0.68
3:C:120:ALA:HA	3:C:197:ASP:HB3	1.76	0.68
1:A:57:GLN:HE21	1:A:57:GLN:H	1.41	0.67
3:G:39:SER:HB2	3:G:40:GLY:HA2	1.76	0.67
2:F:149:GLN:HG2	2:F:155:PHE:CE2	2.29	0.67
4:H:123:SER:OG	4:H:128:GLU:HB2	1.95	0.66
3:G:40:GLY:HA3	3:G:41:ARG:CB	2.25	0.66
4:H:86:LYS:CB	4:H:87:ASP:HB2	2.26	0.66
1:E:41:THR:HG22	1:E:56:ALA:HB2	1.77	0.66
4:D:223:SER:HB2	4:D:226:PHE:HB2	1.78	0.65
4:H:86:LYS:HB2	4:H:88:LYS:H	1.60	0.65
3:G:124:LEU:HD22	4:H:170:VAL:HG12	1.78	0.65
4:D:83:GLY:HA2	4:D:84:VAL:CB	2.17	0.65
3:G:36:ARG:HH11	3:G:38:ASN:HD21	1.43	0.64
1:A:41:THR:HG22	1:A:56:ALA:HB2	1.79	0.63
3:C:30:ASN:ND2	3:C:94:THR:HB	2.12	0.63
3:G:120:ALA:HA	3:G:197:ASP:HB3	1.81	0.63
2:B:14:GLU:HG3	2:B:27:LEU:HB2	1.80	0.62
4:H:241:TYR:HA	4:H:258:THR:HB	1.82	0.62
4:H:107:HIS:HB3	4:H:108:PRO:HD2	1.82	0.61
3:C:52:ASN:H	3:C:52:ASN:HD22	1.49	0.60
3:G:39:SER:CB	3:G:40:GLY:HA2	2.31	0.60
3:G:47:ILE:HG13	3:G:48:LEU:N	2.13	0.60
3:C:124:LEU:HD22	4:D:170:VAL:HG12	1.82	0.60
4:H:86:LYS:HB2	4:H:88:LYS:N	2.16	0.60
3:G:10:ALA:HB3	3:G:106:THR:HG22	1.83	0.60
3:C:119:PRO:HG2	3:C:194:ILE:HG21	1.84	0.59
4:D:223:SER:HB2	4:D:226:PHE:CB	2.32	0.59
1:E:36:MET:CE	1:E:63:ILE:HG13	2.32	0.59
4:H:68:LEU:HD13	4:H:81:GLU:HG3	1.84	0.59
3:C:129:SER:HB3	3:C:130:SER:HA	1.83	0.58
4:H:223:SER:CB	4:H:226:PHE:CB	2.51	0.58
4:D:268:ARG:O	4:D:269:SER:CB	2.52	0.58
1:E:8:ILE:HG12	2:F:14:GLU:HB3	1.86	0.58
3:G:19:ALA:HB3	3:G:76:ILE:HG23	1.85	0.57
4:D:165:GLN:O	4:D:224:ALA:HB2	2.03	0.57
3:G:37:GLN:O	3:G:38:ASN:HB2	2.05	0.57
3:G:44:VAL:O	3:G:45:HIS:HB3	2.04	0.56
3:C:19:ALA:HB3	3:C:76:ILE:HG23	1.86	0.56
1:E:57:GLN:NE2	1:E:57:GLN:H	1.97	0.56
2:F:74:ALA:HA	2:F:77:THR:HG22	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:206:GLN:HB2	4:D:212:SER:HB2	1.87	0.56
4:H:86:LYS:HB3	4:H:87:ASP:CA	2.38	0.54
3:G:47:ILE:CG1	3:G:48:LEU:H	2.15	0.54
1:E:36:MET:HE1	1:E:63:ILE:HG13	1.90	0.54
2:B:105:LYS:HB2	2:B:108:PRO:HD3	1.90	0.53
4:D:268:ARG:O	4:D:269:SER:HB3	2.08	0.53
3:G:30:ASN:ND2	3:G:94:THR:HB	2.24	0.53
4:D:183:LEU:HD21	4:D:236:CYS:SG	2.47	0.53
4:H:41:VAL:HG11	4:H:137:LEU:HD13	1.90	0.53
4:H:165:GLN:O	4:H:224:ALA:HB2	2.09	0.53
4:H:85:GLU:HG3	4:H:88:LYS:HG2	1.89	0.52
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.45	0.52
4:D:123:SER:OG	4:D:128:GLU:HB2	2.08	0.52
1:A:3:GLU:HB2	2:B:18:PHE:CD2	2.44	0.52
4:D:156:PRO:HD3	4:D:169:LEU:HG	1.91	0.52
4:H:42:LYS:HE3	4:H:100:THR:HG21	1.92	0.52
4:H:86:LYS:CA	4:H:87:ASP:HB2	2.40	0.52
4:D:149:PRO:O	4:D:261:VAL:HG21	2.11	0.51
1:E:95:SER:HB2	1:E:96:PRO:HD2	1.93	0.50
3:C:13:ILE:HG23	3:C:109:LYS:HB2	1.93	0.50
1:A:95:SER:HB2	1:A:96:PRO:HD2	1.94	0.50
1:A:55:GLU:OE2	4:D:4:ARG:NH1	2.45	0.50
4:D:148:PRO:HD3	4:D:256:PRO:HB3	1.94	0.50
4:D:268:ARG:HG3	4:D:269:SER:H	1.77	0.50
3:C:18:ASN:HD22	3:C:18:ASN:N	2.09	0.50
2:B:105:LYS:HG2	2:B:106:THR:N	2.27	0.49
2:F:29:ARG:HD2	2:F:36:GLU:OE2	2.12	0.49
4:H:34:ILE:HG12	4:H:178:PRO:HG3	1.94	0.49
1:E:4:GLU:HB2	2:F:17:PHE:O	2.13	0.48
3:G:47:ILE:CG1	3:G:48:LEU:N	2.74	0.48
1:E:89:VAL:HG12	1:E:176:LYS:HG3	1.95	0.48
2:B:64:GLN:HE21	2:B:67:ILE:HD12	1.79	0.48
3:G:33:GLN:HG3	3:G:48:LEU:HD23	1.96	0.48
4:D:42:LYS:HG3	4:D:102:THR:HB	1.96	0.48
3:C:30:ASN:HD21	3:C:94:THR:HB	1.79	0.48
3:C:129:SER:CB	3:C:130:SER:HA	2.43	0.47
2:F:117:CYS:HB2	2:F:131:TRP:CZ2	2.49	0.47
1:E:87:PRO:HD3	1:E:167:HIS:CD2	2.49	0.47
1:A:70:LEU:O	1:A:74:THR:HG23	2.13	0.47
4:D:223:SER:HB3	4:D:224:ALA:H	1.46	0.47
2:B:75:VAL:HG13	2:B:80:ARG:HH12	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:VAL:HB	1:A:177:HIS:HE1	1.80	0.47
2:F:105:LYS:HE2	2:F:112:HIS:CD2	2.49	0.47
1:E:167:HIS:CD2	1:E:169:GLY:H	2.32	0.47
3:C:101:ILE:H	3:C:101:ILE:HG13	1.65	0.47
4:D:77:LYS:H	4:D:77:LYS:HD2	1.80	0.46
4:H:223:SER:HB3	4:H:226:PHE:CB	2.25	0.46
4:H:206:GLN:HB2	4:H:212:SER:HB2	1.97	0.46
3:C:42:GLY:O	3:C:43:LEU:HB2	2.15	0.46
4:H:223:SER:HB2	4:H:226:PHE:CA	2.46	0.46
3:C:119:PRO:O	3:C:197:ASP:HA	2.15	0.46
3:G:60:ARG:NH1	3:G:83:ASP:OD2	2.36	0.46
3:C:98:TYR:CE2	4:D:4:ARG:HD2	2.51	0.46
2:F:10:GLN:HB2	2:F:31:PHE:HB2	1.98	0.45
2:B:105:LYS:HG2	2:B:107:GLN:H	1.81	0.45
1:A:167:HIS:HD2	1:A:169:GLY:N	2.08	0.45
1:A:36:MET:HE1	1:A:63:ILE:HG13	1.99	0.45
2:F:105:LYS:HB3	2:F:107:GLN:O	2.17	0.45
4:H:86:LYS:CB	4:H:88:LYS:N	2.79	0.45
3:C:60:ARG:NH1	3:C:76:ILE:HD11	2.32	0.45
2:F:24:VAL:HB	2:F:75:VAL:HG22	1.99	0.44
4:D:149:PRO:HG2	4:D:261:VAL:CG2	2.48	0.44
2:B:76:ASP:OD1	2:B:80:ARG:NH1	2.50	0.44
1:E:24:PHE:HB3	1:E:31:ILE:HD12	2.00	0.44
1:E:34:VAL:HG12	1:E:41:THR:HB	1.99	0.44
1:E:87:PRO:HA	1:E:112:PHE:HB3	2.00	0.44
3:G:119:PRO:O	3:G:197:ASP:HA	2.18	0.44
2:F:149:GLN:HG2	2:F:155:PHE:HE2	1.81	0.44
3:G:60:ARG:NH1	3:G:76:ILE:HD11	2.33	0.44
2:B:105:LYS:HA	2:B:112:HIS:HB2	2.00	0.44
4:H:75:GLY:CA	4:H:76:SER:HB3	2.48	0.43
7:E:1181:NAG:H61	7:E:1182:NAG:H82	2.00	0.43
1:E:87:PRO:HD2	1:E:170:LEU:HD22	2.00	0.43
2:B:143:VAL:HG22	2:B:144:SER:N	2.33	0.43
2:F:40:PHE:HB2	2:F:47:PHE:CE2	2.52	0.43
4:D:95:SER:HB2	4:D:98:LEU:H	1.84	0.43
3:G:197:ASP:OD2	3:G:197:ASP:N	2.51	0.43
4:D:186:TRP:CE2	4:D:191:GLU:HB3	2.54	0.43
4:H:229:ASN:HA	4:H:230:PRO:HD3	1.79	0.43
2:F:177:HIS:CG	2:F:178:PRO:HD2	2.53	0.43
4:H:168:THR:HG23	4:H:221:ARG:HB2	2.00	0.43
2:F:113:ASN:HD22	2:F:113:ASN:C	2.22	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:MET:HG3	2:F:9:TRP:CZ3	2.54	0.43
4:H:57:TRP:CE2	4:H:101:LEU:HB2	2.54	0.42
1:A:154:LEU:HA	1:A:155:PRO:HD3	1.90	0.42
3:C:32:LEU:HD12	3:C:33:GLN:N	2.35	0.42
1:E:34:VAL:HG21	1:E:59:ALA:HB3	2.00	0.42
2:F:132:PHE:HB2	2:F:172:THR:HB	2.01	0.42
3:G:23:CYS:HB2	3:G:34:TRP:CH2	2.54	0.42
3:G:154:VAL:HG13	3:G:178:SER:HB2	2.02	0.42
2:B:149:GLN:HG2	2:B:155:PHE:CE2	2.54	0.42
3:C:32:LEU:HD11	3:C:89:CYS:HB2	2.02	0.41
1:A:53:SER:HA	4:D:-1:MET:HA	2.01	0.41
4:H:255:LYS:HA	4:H:256:PRO:HD3	1.90	0.41
1:A:57:GLN:HA	1:A:60:LEU:HD12	2.02	0.41
4:D:123:SER:HB3	4:D:126:ASN:O	2.21	0.41
2:F:31:PHE:CE2	2:F:36:GLU:HB2	2.55	0.41
3:C:41:ARG:HA	4:D:113:PHE:CZ	2.55	0.41
2:B:64:GLN:NE2	2:B:67:ILE:HD12	2.36	0.41
4:D:107:HIS:O	4:D:139:VAL:HG21	2.20	0.41
4:D:57:TRP:CE2	4:D:101:LEU:HB2	2.55	0.41
4:D:107:HIS:HB3	4:D:108:PRO:HD2	2.03	0.41
4:H:113:PHE:HD1	4:H:136:ARG:HG3	1.86	0.41
2:F:188:TRP:CH2	2:F:190:ALA:HB2	2.56	0.41
4:D:32:TRP:HB3	4:D:180:HIS:CD2	2.56	0.41
3:C:124:LEU:HD22	4:D:170:VAL:CG1	2.49	0.41
3:G:29:ILE:CG1	3:G:91:THR:HB	2.51	0.41
4:H:83:GLY:HA3	4:H:84:VAL:HA	1.85	0.41
3:C:97:THR:OG1	3:C:99:LYS:HG2	2.21	0.41
4:D:138:THR:CG2	4:D:180:HIS:CE1	3.04	0.40
1:A:57:GLN:H	1:A:57:GLN:NE2	2.11	0.40
3:G:134:VAL:HG12	3:G:177:TRP:HB3	2.03	0.40
1:A:36:MET:HE3	1:A:60:LEU:HD23	2.03	0.40
1:E:77:SER:HB3	2:F:53:LEU:HD11	2.04	0.40
3:G:29:ILE:HG23	3:G:30:ASN:N	2.36	0.40
4:D:138:THR:HG22	4:D:180:HIS:CE1	2.57	0.40
4:H:199:ASP:HA	4:H:200:PRO:HD3	1.96	0.40
4:D:1:ASP:HB3	4:D:2:PHE:H	1.67	0.40
1:E:85:VAL:HA	1:E:86:PRO:HD2	1.95	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	176/194 (91%)	170 (97%)	6 (3%)	0	100	100
1	E	175/194 (90%)	170 (97%)	5 (3%)	0	100	100
2	B	173/200 (86%)	165 (95%)	7 (4%)	1 (1%)	30	72
2	F	186/200 (93%)	175 (94%)	10 (5%)	1 (0%)	34	76
3	C	191/219 (87%)	166 (87%)	22 (12%)	3 (2%)	12	48
3	G	186/219 (85%)	160 (86%)	21 (11%)	5 (3%)	6	32
4	D	268/279 (96%)	237 (88%)	22 (8%)	9 (3%)	5	25
4	H	256/279 (92%)	234 (91%)	16 (6%)	6 (2%)	8	36
All	All	1611/1784 (90%)	1477 (92%)	109 (7%)	25 (2%)	12	48

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	84	VAL
4	D	223	SER
3	G	38	ASN
3	G	47	ILE
4	H	76	SER
4	H	83	GLY
3	C	40	GLY
2	F	169	GLU
3	G	41	ARG
4	H	87	ASP
3	C	9	GLN
3	C	43	LEU
4	D	79	THR
3	G	131	ASP
2	B	107	GLN
4	D	74	GLU
4	D	80	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	45	HIS
4	D	62	PRO
4	H	75	GLY
4	D	75	GLY
4	H	84	VAL
4	H	195	GLY
4	D	19	GLY
4	D	195	GLY

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	163/178 (92%)	146 (90%)	17 (10%)	9	32
1	E	162/178 (91%)	146 (90%)	16 (10%)	10	35
2	B	163/180 (91%)	153 (94%)	10 (6%)	23	61
2	F	170/180 (94%)	156 (92%)	14 (8%)	14	46
3	C	173/195 (89%)	142 (82%)	31 (18%)	2	11
3	G	170/195 (87%)	133 (78%)	37 (22%)	1	6
4	D	231/237 (98%)	188 (81%)	43 (19%)	2	10
4	H	228/237 (96%)	186 (82%)	42 (18%)	2	10
All	All	1460/1580 (92%)	1250 (86%)	210 (14%)	4	18

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL
1	A	36	MET
1	A	41	THR
1	A	47	GLU
1	A	53	SER
1	A	57	GLN
1	A	76	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	90	THR
1	A	92	LEU
1	A	93	THR
1	A	99	LEU
1	A	108	PHE
1	A	129	THR
1	A	157	THR
1	A	159	ASP
1	A	170	LEU
1	A	175	LEU
2	B	14	GLU
2	B	39	ARG
2	B	42	SER
2	B	55	ARG
2	B	66	ASP
2	B	75	VAL
2	B	92	GLN
2	B	100	THR
2	B	105	LYS
2	B	163	THR
3	C	11	LEU
3	C	13	ILE
3	C	18	ASN
3	C	29	ILE
3	C	32	LEU
3	C	36	ARG
3	C	43	LEU
3	C	46	LEU
3	C	48	LEU
3	C	52	ASN
3	C	55	GLU
3	C	68	SER
3	C	69	LYS
3	C	74	LEU
3	C	76	ILE
3	C	93	THR
3	C	94	THR
3	C	101	ILE
3	C	111	LEU
3	C	125	ARG
3	C	128	LYS
3	C	131	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	142	SER
3	C	151	ASP
3	C	153	ASP
3	C	160	THR
3	C	165	ARG
3	C	192	SER
3	C	194	ILE
3	C	197	ASP
3	C	200	PHE
4	D	4	ARG
4	D	8	ILE
4	D	25	VAL
4	D	34	ILE
4	D	35	SER
4	D	36	LYS
4	D	49	ASP
4	D	63	LYS
4	D	64	GLN
4	D	67	MET
4	D	68	LEU
4	D	77	LYS
4	D	79	THR
4	D	89	PHE
4	D	91	ILE
4	D	95	SER
4	D	98	LEU
4	D	100	THR
4	D	101	LEU
4	D	102	THR
4	D	121	LEU
4	D	122	THR
4	D	126	ASN
4	D	136	ARG
4	D	138	THR
4	D	139	VAL
4	D	141	GLU
4	D	187	VAL
4	D	197	SER
4	D	209	LEU
4	D	212	SER
4	D	215	SER
4	D	216	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	219	ARG
4	D	220	LEU
4	D	225	THR
4	D	229	ASN
4	D	237	GLN
4	D	244	SER
4	D	258	THR
4	D	260	ILE
4	D	262	SER
4	D	264	GLU
1	E	19	SER
1	E	36	MET
1	E	41	THR
1	E	46	GLU
1	E	47	GLU
1	E	57	GLN
1	E	80	THR
1	E	90	THR
1	E	92	LEU
1	E	99	LEU
1	E	117	VAL
1	E	129	THR
1	E	138	LEU
1	E	158	GLU
1	E	170	LEU
1	E	175	LEU
2	F	34	GLN
2	F	39	ARG
2	F	50	VAL
2	F	53	LEU
2	F	75	VAL
2	F	106	THR
2	F	109	LEU
2	F	110	GLN
2	F	113	ASN
2	F	130	ARG
2	F	162	GLU
2	F	176	GLU
2	F	186	VAL
2	F	189	ARG
3	G	11	LEU
3	G	20	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	24	SER
3	G	26	LYS
3	G	29	ILE
3	G	32	LEU
3	G	33	GLN
3	G	36	ARG
3	G	41	ARG
3	G	43	LEU
3	G	44	VAL
3	G	46	LEU
3	G	48	LEU
3	G	51	SER
3	G	54	ARG
3	G	55	GLU
3	G	69	LYS
3	G	70	LYS
3	G	73	SER
3	G	74	LEU
3	G	76	ILE
3	G	86	SER
3	G	89	CYS
3	G	93	THR
3	G	94	THR
3	G	107	ARG
3	G	111	LEU
3	G	123	GLN
3	G	130	SER
3	G	144	THR
3	G	148	GLN
3	G	160	THR
3	G	162	LEU
3	G	185	CYS
3	G	187	ASN
3	G	190	ASN
3	G	197	ASP
4	H	9	SER
4	H	34	ILE
4	H	35	SER
4	H	42	LYS
4	H	63	LYS
4	H	64	GLN
4	H	67	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	68	LEU
4	H	74	GLU
4	H	79	THR
4	H	81	GLU
4	H	85	GLU
4	H	88	LYS
4	H	89	PHE
4	H	96	LEU
4	H	97	THR
4	H	99	SER
4	H	101	LEU
4	H	102	THR
4	H	105	SER
4	H	112	SER
4	H	121	LEU
4	H	126	ASN
4	H	129	GLN
4	H	138	THR
4	H	139	VAL
4	H	141	GLU
4	H	172	LEU
4	H	174	THR
4	H	192	VAL
4	H	199	ASP
4	H	203	LEU
4	H	209	LEU
4	H	212	SER
4	H	215	SER
4	H	216	LEU
4	H	219	ARG
4	H	220	LEU
4	H	235	ARG
4	H	250	THR
4	H	258	THR
4	H	261	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	143	HIS
1	A	167	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	177	HIS
2	B	64	GLN
2	B	113	ASN
3	C	18	ASN
3	C	22	ASN
3	C	30	ASN
3	C	37	GLN
3	C	52	ASN
4	D	60	GLN
4	D	73	ASN
4	D	82	GLN
4	D	180	HIS
4	D	237	GLN
4	D	239	GLN
1	E	57	GLN
1	E	149	HIS
2	F	70	GLN
2	F	96	GLN
2	F	110	GLN
2	F	112	HIS
2	F	113	ASN
2	F	149	GLN
3	G	30	ASN
3	G	31	ASN
3	G	33	GLN
3	G	38	ASN
3	G	148	GLN
3	G	187	ASN
4	H	73	ASN
4	H	188	ASN
4	H	229	ASN
4	H	232	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

5 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	$\# Z > 2$
7	NAG	E	1181	1,7	14,14,15	0.46	0	15,19,21	1.11	1 (6%)
7	NAG	E	1182	7	14,14,15	0.50	0	15,19,21	1.05	2 (13%)
7	BMA	E	1183	7	11,11,12	0.43	0	14,15,17	0.99	1 (7%)
7	MAN	E	1184	7	11,11,12	0.55	0	14,15,17	0.63	0
7	MAN	E	1185	7	11,11,12	0.69	0	14,15,17	1.19	2 (14%)

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
7	NAG	E	1181	1,7	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	E	1182	7	-	0/6/23/26	0/1/1/1
7	BMA	E	1183	7	-	0/2/19/22	0/1/1/1
7	MAN	E	1184	7	-	0/2/19/22	0/1/1/1
7	MAN	E	1185	7	-	0/2/19/22	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(°)
7	E	1182	NAG	C4-C3-C2	2.08	114.47	111.23
7	E	1182	NAG	C1-O5-C5	2.15	114.98	112.25
7	E	1185	MAN	C2-C3-C4	2.18	114.75	111.04
7	E	1185	MAN	C3-C4-C5	2.85	115.16	110.20
7	E	1183	BMA	C1-C2-C3	2.86	112.93	109.54
7	E	1181	NAG	C1-O5-C5	3.46	116.64	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	E	1181	NAG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	1181	NAG	2	0
7	E	1182	NAG	1	0

5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
5	NAG	A	1181	1	14,14,15	0.46	0	15,19,21	0.93	1 (6%)
5	NAG	B	1189	2	14,14,15	0.53	0	15,19,21	1.02	0
6	SO4	B	1190	-	4,4,4	0.28	0	6,6,6	0.18	0
6	SO4	C	1201	-	4,4,4	0.20	0	6,6,6	0.13	0
5	NAG	E	1186	1	14,14,15	0.55	0	15,19,21	0.89	0
5	NAG	F	1191	2	14,14,15	0.48	0	15,19,21	0.64	0
6	SO4	F	1192	-	4,4,4	0.21	0	6,6,6	0.16	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
5	NAG	A	1181	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	B	1189	2	-	0/6/23/26	0/1/1/1
6	SO4	B	1190	-	-	0/0/0/0	0/0/0/0
6	SO4	C	1201	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1186	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	F	1191	2	1/1/5/7	0/6/23/26	0/1/1/1
6	SO4	F	1192	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1181	NAG	C1-O5-C5	2.51	115.43	112.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	F	1191	NAG	C1
5	E	1186	NAG	C1
5	A	1181	NAG	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	178/194 (91%)	-0.16	2 (1%) 82 58	55, 61, 69, 78	0
1	E	177/194 (91%)	-0.27	0 100 100	55, 61, 69, 71	0
2	B	179/200 (89%)	-0.01	3 (1%) 73 45	49, 62, 71, 96	0
2	F	188/200 (94%)	-0.05	3 (1%) 74 47	49, 63, 71, 86	0
3	C	193/219 (88%)	0.13	9 (4%) 35 14	53, 66, 78, 88	0
3	G	190/219 (86%)	0.04	3 (1%) 74 47	53, 66, 74, 89	0
4	D	270/279 (96%)	0.04	7 (2%) 59 29	50, 64, 76, 95	0
4	H	260/279 (93%)	0.10	8 (3%) 52 24	51, 63, 73, 83	0
All	All	1635/1784 (91%)	-0.01	35 (2%) 67 36	49, 63, 73, 96	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	112	HIS	4.8
4	H	1	ASP	4.3
2	B	111	HIS	3.8
3	C	26	LYS	3.6
3	C	69	LYS	3.5
4	D	142	ASP	3.3
4	H	104	THR	3.2
4	H	14	SER	3.1
4	D	1	ASP	3.1
1	A	129	THR	2.9
3	C	150	LYS	2.9
4	H	246	ASN	2.8
4	H	86	LYS	2.8
3	C	8	PRO	2.7
2	B	187	GLU	2.6
4	D	23	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	H	27	SER	2.6
2	F	57	ASP	2.5
2	F	110	GLN	2.5
2	F	60	TYR	2.5
3	G	196	GLU	2.4
3	C	180	LYS	2.3
4	H	88	LYS	2.3
3	C	9	GLN	2.3
3	C	147	SER	2.3
4	H	15	GLY	2.3
4	D	24	ALA	2.2
1	A	166	GLU	2.1
4	D	232	ASN	2.1
4	D	85	GLU	2.1
3	C	182	ASP	2.1
3	C	178	SER	2.1
3	G	10	ALA	2.1
4	D	209	LEU	2.0
3	G	11	LEU	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(\AA^2)	Q<0.9
7	NAG	E	1181	14/15	0.91	0.27	1.52	51,60,65,66	0
7	BMA	E	1183	11/12	0.90	0.39	-	83,86,89,98	0
7	MAN	E	1185	11/12	0.55	0.49	-	105,109,111,112	0
7	MAN	E	1184	11/12	0.86	0.42	-	87,91,92,93	0
7	NAG	E	1182	14/15	0.92	0.44	-	72,76,77,79	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
6	SO4	C	1201	5/5	0.92	0.18	0.08	91,91,92,93	0
6	SO4	F	1192	5/5	0.93	0.23	-0.42	56,58,59,61	0
6	SO4	B	1190	5/5	0.97	0.26	-0.66	51,52,54,54	0
5	NAG	E	1186	14/15	0.77	0.42	-	94,99,103,104	0
5	NAG	A	1181	14/15	0.83	0.34	-	86,92,95,96	0
5	NAG	F	1191	14/15	0.77	0.42	-	95,101,104,106	0
5	NAG	B	1189	14/15	0.86	0.36	-	74,82,87,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.