Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2017 – 11:24 AM EST

PDB ID	:	5TLK
Title	:	COMPLEX BETWEEN HUMAN CD27 AND FAB FRAGMENTS OF ANTIBODIES M2177 AND H2191
Authors	:	Teplyakov, A.; Obmolova, G.; Malia, T.; Gilliland, G.L.
Deposited on	:	2016-10-11
Resolution	:	2.70 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

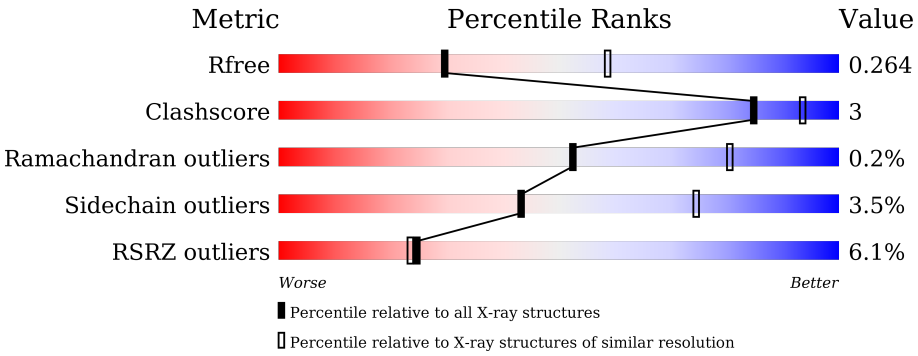
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 <=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	218	90% 8% •
1	E	218	8% 88% 10% ••
2	B	229	3% 85% 8% 7%
2	F	229	24% 86% 6% • 7%
3	C	218	% 90% 8% ••
3	G	218	2% 86% 12% •

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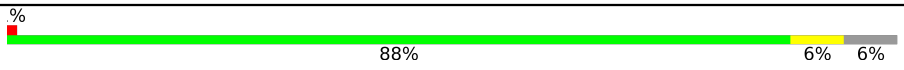
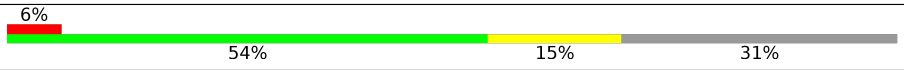
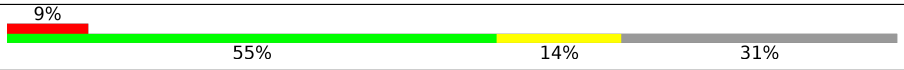
Mol	Chain	Length	Quality of chain
4	D	226	
4	H	226	
5	X	109	
5	Y	109	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14287 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 M2177 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1647	1029	274	339	5			
1	E	215	Total	C	N	O	S	0	0	0
			1647	1029	274	339	5			

- Molecule 2 is a protein called M2177 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1598	1017	261	314	6			
2	F	212	Total	C	N	O	S	0	0	0
			1592	1014	260	312	6			

- Molecule 3 is a protein called H2191 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	215	Total	C	N	O	S	0	0	0
			1672	1048	286	332	6			
3	G	215	Total	C	N	O	S	0	0	0
			1672	1048	286	332	6			

- Molecule 4 is a protein called H2191 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	212	Total	C	N	O	S	0	0	0
			1584	1001	268	309	6			
4	H	211	Total	C	N	O	S	0	0	0
			1578	998	267	307	6			

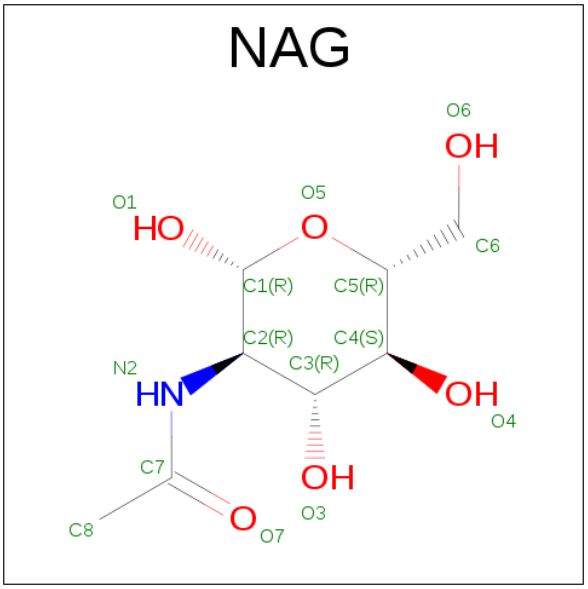
- Molecule 5 is a protein called CD27 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	75	Total	C	N	O	S	0	0	0
			583	351	113	106	13			
5	Y	75	Total	C	N	O	S	0	0	0
			583	351	113	106	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	102	GLY	-	expression tag	UNP P26842
X	103	GLY	-	expression tag	UNP P26842
X	104	HIS	-	expression tag	UNP P26842
X	105	HIS	-	expression tag	UNP P26842
X	106	HIS	-	expression tag	UNP P26842
X	107	HIS	-	expression tag	UNP P26842
X	108	HIS	-	expression tag	UNP P26842
X	109	HIS	-	expression tag	UNP P26842
Y	102	GLY	-	expression tag	UNP P26842
Y	103	GLY	-	expression tag	UNP P26842
Y	104	HIS	-	expression tag	UNP P26842
Y	105	HIS	-	expression tag	UNP P26842
Y	106	HIS	-	expression tag	UNP P26842
Y	107	HIS	-	expression tag	UNP P26842
Y	108	HIS	-	expression tag	UNP P26842
Y	109	HIS	-	expression tag	UNP P26842

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	X	1	Total C N O 14 8 1 5	0	0
6	X	1	Total C N O 14 8 1 5	0	0
6	Y	1	Total C N O 14 8 1 5	0	0
6	Y	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is water.

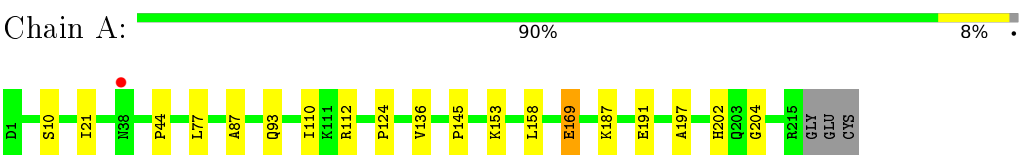
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	14	Total O 14 14	0	0
7	B	17	Total O 17 17	0	0
7	C	12	Total O 12 12	0	0
7	D	15	Total O 15 15	0	0
7	E	1	Total O 1 1	0	0
7	G	3	Total O 3 3	0	0
7	H	8	Total O 8 8	0	0
7	X	4	Total O 4 4	0	0
7	Y	1	Total O 1 1	0	0

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.

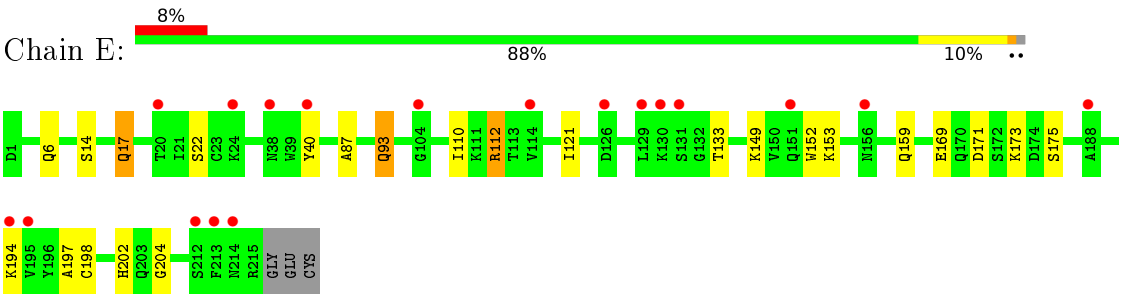
- Molecule 1: M2177 LIGHT CHAIN

Chain A:



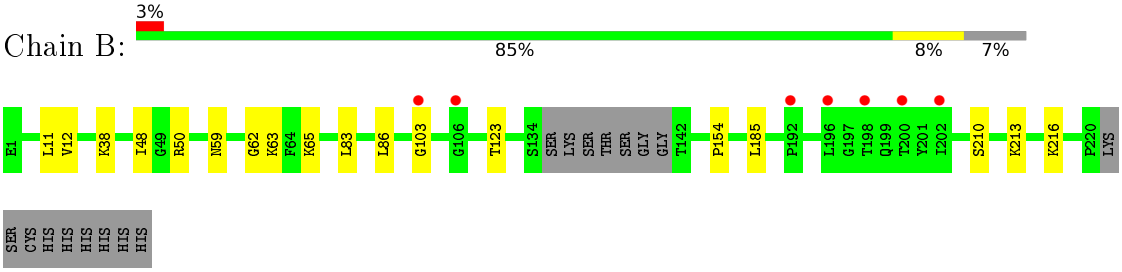
- Molecule 1: M2177 LIGHT CHAIN

Chain E:



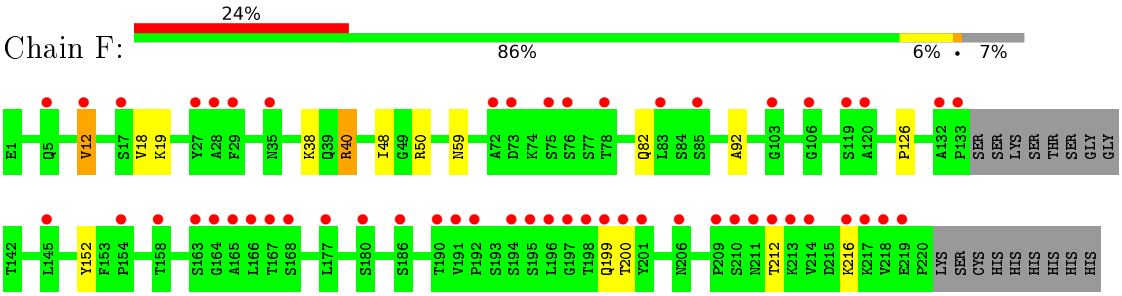
- Molecule 2: M2177 HEAVY CHAIN

Chain B:



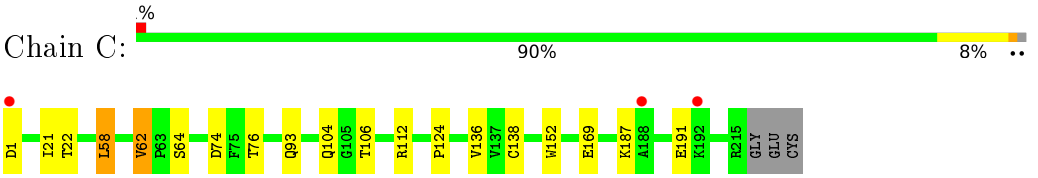
- Molecule 2: M2177 HEAVY CHAIN

Chain F:



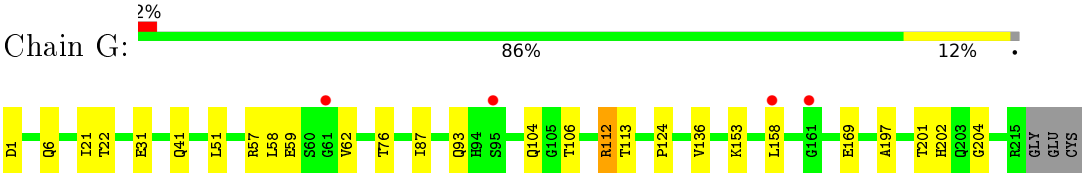
- Molecule 3: H2191 LIGHT CHAIN

Chain C:



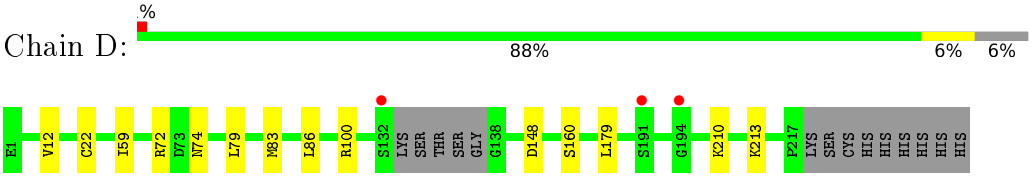
• Molecule 3: H2191 LIGHT CHAIN

Chain G:



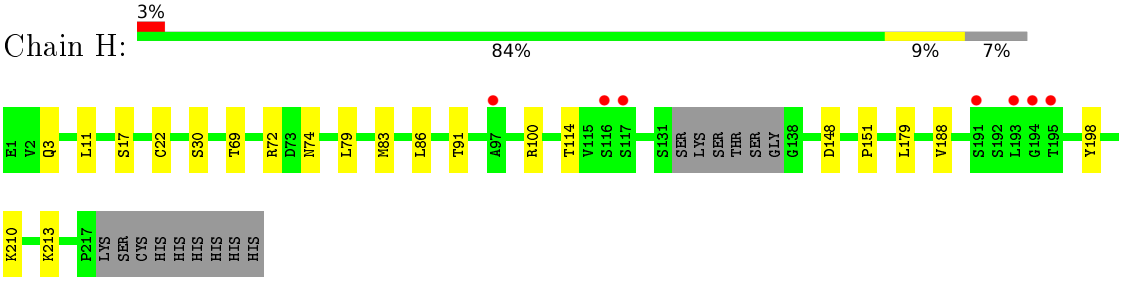
• Molecule 4: H2191 HEAVY CHAIN

Chain D:



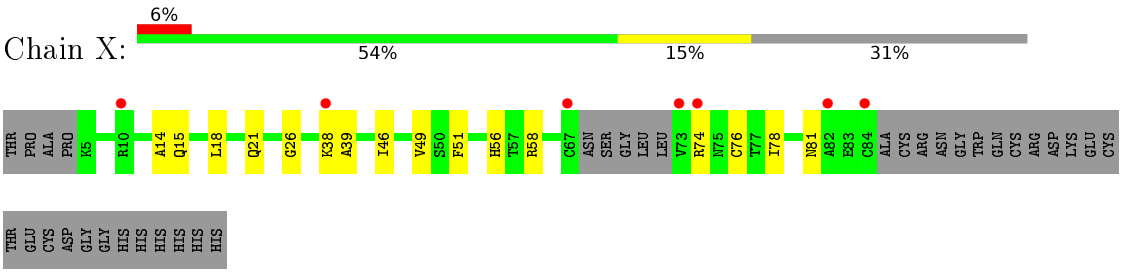
• Molecule 4: H2191 HEAVY CHAIN

Chain H:



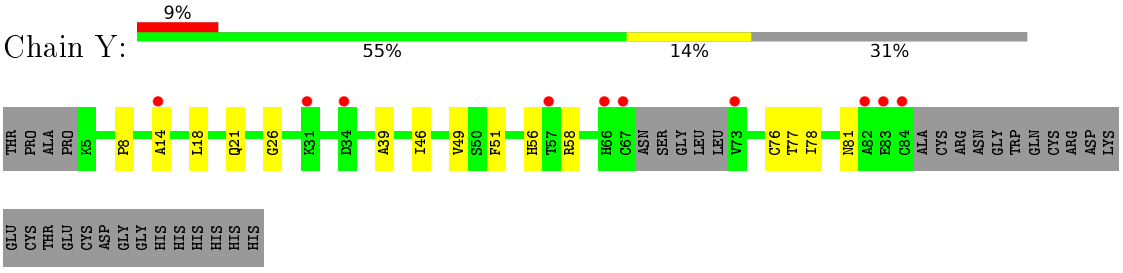
• Molecule 5: CD27 antigen

Chain X:



• Molecule 5: CD27 antigen

Chain Y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	139.71Å 52.96Å 140.60Å 90.00° 109.52° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 29.21 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.70) 98.6 (29.21-2.69)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.213 , 0.263 0.213 , 0.264	Depositor DCC
R_{free} test set	1105 reflections (2.10%)	DCC
Wilson B-factor (Å^2)	56.4	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14287	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.52 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2904e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PCA, 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	0.39	0/1683	0.61	1/2288 (0.0%)
1	E	0.40	0/1683	0.59	0/2288
2	B	0.40	0/1633	0.59	1/2225 (0.0%)
2	F	0.44	0/1627	0.60	0/2217
3	C	0.39	0/1711	0.61	0/2320
3	G	0.40	0/1711	0.61	0/2320
4	D	0.39	0/1616	0.62	0/2201
4	H	0.40	0/1610	0.60	0/2193
5	X	0.39	0/598	0.59	0/807
5	Y	0.38	0/598	0.59	0/807
All	All	0.40	0/14470	0.60	2/19666 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	185	LEU	CA-CB-CG	5.08	126.98	115.30
1	A	158	LEU	CA-CB-CG	5.02	126.84	115.30

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	1647	0	1583	10	0
1	E	1647	0	1583	10	0
2	B	1598	0	1554	7	0
2	F	1592	0	1549	7	0
3	C	1672	0	1629	8	0
3	G	1672	0	1629	10	0
4	D	1584	0	1544	5	0
4	H	1578	0	1539	8	0
5	X	583	0	529	10	0
5	Y	583	0	529	7	0
6	X	28	0	25	0	0
6	Y	28	0	25	0	0
7	A	14	0	0	0	0
7	B	17	0	0	0	0
7	C	12	0	0	0	0
7	D	15	0	0	0	0
7	E	1	0	0	0	0
7	G	3	0	0	0	0
7	H	8	0	0	0	0
7	X	4	0	0	0	0
7	Y	1	0	0	0	0
All	All	14287	0	13718	81	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 3.

All (81) 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:D:72:ARG:HE	4:D:74:ASN:HD21	1.26	0.80
1:A:44:PRO:HG3	1:A:169:GLU:HG2	1.67	0.76
2:B:50:ARG:HH11	2:B:59:ASN:HD22	1.37	0.73
2:F:50:ARG:HH11	2:F:59:ASN:HD22	1.46	0.63
1:E:153:LYS:HB2	1:E:197:ALA:HB3	1.83	0.61
4:H:72:ARG:HE	4:H:74:ASN:HD21	1.47	0.59
1:A:187:LYS:O	1:A:191:GLU:HG2	2.04	0.58
1:E:14:SER:HB2	1:E:17:GLN:HG3	1.85	0.58
5:Y:76:CYS:SG	5:Y:81:ASN:HA	2.45	0.57
5:X:21:GLN:HB2	5:X:39:ALA:HA	1.87	0.57
5:X:76:CYS:SG	5:X:81:ASN:HA	2.45	0.56
1:A:202:HIS:CD2	1:A:204:GLY:H	2.22	0.56
3:G:22:THR:HG22	3:G:76:THR:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:56:HIS:HD2	5:Y:58:ARG:HB2	1.71	0.55
3:G:21:ILE:HD12	3:G:106:THR:HG21	1.90	0.54
4:D:160:SER:HB2	4:H:30:SER:HB2	1.89	0.54
3:C:22:THR:HG22	3:C:76:THR:HG22	1.90	0.53
5:X:56:HIS:HD2	5:X:58:ARG:HB2	1.74	0.53
5:Y:46:ILE:HB	5:Y:49:VAL:HB	1.91	0.53
1:E:112:ARG:HG2	1:E:175:SER:HB2	1.90	0.52
4:H:22:CYS:HB3	4:H:79:LEU:HB3	1.91	0.52
5:X:51:PHE:CE1	5:X:81:ASN:HB3	2.44	0.52
2:B:12:VAL:HG11	2:B:86:LEU:HD12	1.92	0.51
4:D:22:CYS:HB3	4:D:79:LEU:HB3	1.92	0.51
5:X:56:HIS:CD2	5:X:58:ARG:HB2	2.46	0.51
1:E:40:TYR:HE2	1:E:93:GLN:HE21	1.60	0.49
3:C:58:LEU:CD2	3:C:62:VAL:HG22	2.43	0.48
4:H:83:MET:HB3	4:H:86:LEU:HD21	1.94	0.48
3:C:58:LEU:HD21	3:C:62:VAL:HG22	1.96	0.47
1:E:202:HIS:CD2	1:E:204:GLY:H	2.32	0.47
1:E:87:ALA:HB2	1:E:110:ILE:HG12	1.96	0.47
3:G:59:GLU:O	3:G:62:VAL:HG22	2.15	0.47
3:G:124:PRO:HD3	3:G:136:VAL:HG22	1.97	0.47
2:F:19:LYS:HE3	2:F:82:GLN:HB2	1.96	0.46
5:Y:56:HIS:CD2	5:Y:58:ARG:HB2	2.50	0.46
1:E:202:HIS:HD2	1:E:204:GLY:H	1.64	0.45
2:B:62:GLY:HA2	2:B:65:LYS:HE2	1.97	0.45
3:C:187:LYS:O	3:C:191:GLU:HG2	2.16	0.45
2:F:126:PRO:HB3	2:F:152:TYR:HB3	1.98	0.45
2:F:38:LYS:HE2	2:F:40:ARG:HD3	1.98	0.45
1:A:153:LYS:HB2	1:A:197:ALA:HB3	1.98	0.45
2:B:123:THR:HG22	2:B:210:SER:HB3	1.99	0.45
2:F:40:ARG:HD2	2:F:92:ALA:HB2	1.99	0.45
3:C:21:ILE:HD12	3:C:106:THR:HG21	1.99	0.44
4:D:83:MET:HB3	4:D:86:LEU:HD21	1.99	0.44
4:H:91:THR:HG23	4:H:114:THR:HA	1.98	0.44
5:X:26:GLY:HA2	5:X:78:ILE:O	2.17	0.44
2:B:83:LEU:HB3	2:B:86:LEU:HD21	1.98	0.44
4:D:148:ASP:HB3	4:D:179:LEU:HD13	1.99	0.44
2:F:38:LYS:HB2	2:F:48:ILE:HD11	2.00	0.44
4:H:188:VAL:HG11	4:H:198:TYR:CE1	2.53	0.44
2:F:12:VAL:HG21	2:F:18:VAL:HB	2.00	0.43
3:G:202:HIS:CD2	3:G:204:GLY:H	2.35	0.43
1:A:44:PRO:HG3	1:A:169:GLU:CG	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:21:GLN:HB2	5:Y:39:ALA:HA	2.00	0.43
5:X:56:HIS:CD2	5:X:58:ARG:H	2.37	0.43
2:B:11:LEU:HD22	2:B:154:PRO:HD3	2.01	0.43
1:A:124:PRO:HD3	1:A:136:VAL:HG22	2.00	0.42
3:C:58:LEU:HD11	3:C:64:SER:HA	2.01	0.42
1:A:202:HIS:HD2	1:A:204:GLY:H	1.64	0.42
4:H:148:ASP:HB3	4:H:179:LEU:HD13	2.01	0.42
5:X:46:ILE:HB	5:X:49:VAL:HB	2.01	0.42
4:H:11:LEU:HB2	4:H:151:PRO:HG3	2.01	0.41
3:C:138:CYS:HB2	3:C:152:TRP:CH2	2.55	0.41
3:G:58:LEU:HD22	3:G:62:VAL:HG23	2.03	0.41
5:Y:26:GLY:HA2	5:Y:78:ILE:O	2.20	0.41
1:A:145:PRO:O	1:A:202:HIS:HE1	2.04	0.41
1:A:21:ILE:HD12	1:A:77:LEU:HD23	2.01	0.41
2:B:38:LYS:HB2	2:B:48:ILE:HD11	2.03	0.41
1:E:121:ILE:HD12	1:E:198:CYS:HB2	2.03	0.41
1:E:6:GLN:HA	1:E:22:SER:O	2.21	0.41
5:X:51:PHE:CD1	5:X:81:ASN:HB3	2.55	0.41
5:Y:51:PHE:CE1	5:Y:81:ASN:HB3	2.56	0.41
3:C:124:PRO:HD3	3:C:136:VAL:HG22	2.02	0.41
3:G:112:ARG:HD3	3:G:113:THR:O	2.21	0.40
3:G:41:GLN:HB2	3:G:51:LEU:HD11	2.03	0.40
5:X:56:HIS:HD2	5:X:58:ARG:H	1.69	0.40
1:A:87:ALA:HB2	1:A:110:ILE:HG12	2.04	0.40
3:G:153:LYS:HB2	3:G:197:ALA:HB3	2.03	0.40
1:E:152:TRP:HB2	1:E:159:GLN:HB2	2.03	0.40
3:G:6:GLN:HB2	3:G:104:GLN:HE21	1.87	0.40

There are no symmetry-related clashes.

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	213/218 (98%)	206 (97%)	7 (3%)	0	100 100
1	E	213/218 (98%)	203 (95%)	10 (5%)	0	100 100
2	B	209/229 (91%)	201 (96%)	7 (3%)	1 (0%)	34 63
2	F	208/229 (91%)	193 (93%)	15 (7%)	0	100 100
3	C	213/218 (98%)	208 (98%)	5 (2%)	0	100 100
3	G	213/218 (98%)	202 (95%)	11 (5%)	0	100 100
4	D	208/226 (92%)	205 (99%)	3 (1%)	0	100 100
4	H	207/226 (92%)	200 (97%)	7 (3%)	0	100 100
5	X	71/109 (65%)	67 (94%)	3 (4%)	1 (1%)	14 35
5	Y	71/109 (65%)	66 (93%)	3 (4%)	2 (3%)	6 15
All	All	1826/2000 (91%)	1751 (96%)	71 (4%)	4 (0%)	52 80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	Y	14	ALA
5	X	14	ALA
5	Y	8	PRO
2	B	103	GLY

5.3.2 Protein sidechains (i)

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	185/187 (99%)	181 (98%)	4 (2%)	60 86
1	E	185/187 (99%)	176 (95%)	9 (5%)	31 61
2	B	176/190 (93%)	173 (98%)	3 (2%)	68 90
2	F	175/190 (92%)	169 (97%)	6 (3%)	44 75
3	C	191/193 (99%)	183 (96%)	8 (4%)	36 68
3	G	191/193 (99%)	182 (95%)	9 (5%)	32 63
4	D	175/188 (93%)	170 (97%)	5 (3%)	50 80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	H	174/188 (93%)	168 (97%)	6 (3%)	44 75
5	X	67/95 (70%)	63 (94%)	4 (6%)	24 50
5	Y	67/95 (70%)	65 (97%)	2 (3%)	48 79
All	All	1586/1706 (93%)	1530 (96%)	56 (4%)	43 74

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	93	GLN
1	A	112	ARG
1	A	169	GLU
2	B	63	LYS
2	B	213	LYS
2	B	216	LYS
3	C	1	ASP
3	C	58	LEU
3	C	62	VAL
3	C	74	ASP
3	C	93	GLN
3	C	104	GLN
3	C	112	ARG
3	C	169	GLU
4	D	12	VAL
4	D	59	ILE
4	D	100	ARG
4	D	210	LYS
4	D	213	LYS
1	E	17	GLN
1	E	93	GLN
1	E	112	ARG
1	E	133	THR
1	E	149	LYS
1	E	169	GLU
1	E	171	ASP
1	E	173	LYS
1	E	194	LYS
2	F	12	VAL
2	F	40	ARG
2	F	199	GLN
2	F	200	THR

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Mol	Chain	Res	Type
2	F	212	THR
2	F	216	LYS
3	G	1	ASP
3	G	31	GLU
3	G	57	ARG
3	G	87	ILE
3	G	93	GLN
3	G	112	ARG
3	G	158	LEU
3	G	169	GLU
3	G	201	THR
4	H	3	GLN
4	H	17	SER
4	H	69	THR
4	H	100	ARG
4	H	210	LYS
4	H	213	LYS
5	X	15	GLN
5	X	18	LEU
5	X	38	LYS
5	X	74	ARG
5	Y	18	LEU
5	Y	77	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	57	ASN
1	A	78	ASN
1	A	93	GLN
1	A	164	GLN
1	A	202	HIS
2	B	59	ASN
3	C	93	GLN
3	C	164	GLN
4	D	74	ASN
4	D	77	ASN
4	D	82	GLN
4	D	208	ASN
1	E	57	ASN
1	E	93	GLN

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Mol	Chain	Res	Type
1	E	202	HIS
2	F	59	ASN
2	F	82	GLN
3	G	93	GLN
3	G	104	GLN
3	G	151	GLN
3	G	202	HIS
4	H	74	ASN
4	H	77	ASN
5	X	15	GLN
5	X	56	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

4 non-standard protein/DNA/RNA residues 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	PCA	B	1	2	7,8,9	0.51	0	9,10,12	1.14	1 (11%)
4	PCA	D	1	4	7,8,9	0.43	0	9,10,12	1.24	2 (22%)
2	PCA	F	1	2	7,8,9	0.51	0	9,10,12	0.95	0
4	PCA	H	1	4	7,8,9	0.46	0	9,10,12	1.25	1 (11%)

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	PCA	B	1	2	-	0/0/11/13	0/1/1/1
4	PCA	D	1	4	-	0/0/11/13	0/1/1/1
2	PCA	F	1	2	-	0/0/11/13	0/1/1/1
4	PCA	H	1	4	-	0/0/11/13	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(^{o})	Ideal(^{o})
4	H	1	PCA	OE-CD-CG	-2.22	122.46	126.85
4	D	1	PCA	O-C-CA	-2.04	120.10	125.69
4	D	1	PCA	OE-CD-CG	-2.03	122.84	126.85
2	B	1	PCA	O-C-CA	-2.01	120.18	125.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	X	301	5,6	14,14,15	0.54	0	15,19,21	1.07	2 (13%)
6	NAG	X	302	6	14,14,15	0.50	0	15,19,21	1.04	1 (6%)
6	NAG	Y	301	5,6	14,14,15	0.62	0	15,19,21	0.82	0
6	NAG	Y	302	6	14,14,15	0.52	0	15,19,21	1.23	2 (13%)

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	X	301	5,6	-	0/6/23/26	0/1/1/1
6	NAG	X	302	6	-	0/6/23/26	0/1/1/1
6	NAG	Y	301	5,6	-	0/6/23/26	0/1/1/1
6	NAG	Y	302	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	X	301	NAG	C4-C3-C2	2.08	114.57	111.34
6	X	301	NAG	C2-N2-C7	2.12	125.87	123.11
6	Y	302	NAG	C4-C3-C2	2.38	115.04	111.34
6	Y	302	NAG	C1-O5-C5	2.65	116.04	112.14
6	X	302	NAG	C1-O5-C5	2.90	116.41	112.14

There are no chirality outliers.

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, 95^{th} 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	215/218 (98%)	0.09	1 (0%) 91 93	29, 45, 63, 78	0
1	E	215/218 (98%)	0.62	18 (8%) 14 11	53, 72, 106, 117	0
2	B	212/229 (92%)	0.15	7 (3%) 50 50	25, 47, 77, 92	0
2	F	211/229 (92%)	1.29	54 (25%) 1 1	57, 89, 120, 133	0
3	C	215/218 (98%)	0.05	3 (1%) 78 77	29, 48, 74, 84	0
3	G	215/218 (98%)	0.28	4 (1%) 70 70	40, 65, 87, 102	0
4	D	211/226 (93%)	0.06	3 (1%) 78 77	31, 50, 77, 98	0
4	H	210/226 (92%)	0.25	7 (3%) 50 50	38, 58, 78, 94	0
5	X	75/109 (68%)	0.39	7 (9%) 11 8	33, 51, 74, 83	0
5	Y	75/109 (68%)	0.91	10 (13%) 4 3	50, 75, 90, 95	0
All	All	1854/2000 (92%)	0.37	114 (6%) 25 23	25, 58, 99, 133	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	200	THR	6.9
2	F	196	LEU	6.5
4	H	194	GLY	5.3
2	F	217	LYS	5.3
2	F	192	PRO	5.3
2	F	209	PRO	4.9
2	F	214	VAL	4.5
2	F	191	VAL	4.4
2	F	198	THR	4.2
2	F	85	SER	4.1
2	F	197	GLY	4.0
2	F	195	SER	4.0
5	Y	66	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
2	F	165	ALA	3.9
5	X	82	ALA	3.6
5	Y	67	CYS	3.6
2	F	103	GLY	3.6
5	Y	31	LYS	3.5
2	B	202	ILE	3.5
2	F	201	TYR	3.4
1	E	130	LYS	3.4
2	F	168	SER	3.4
2	F	119	SER	3.3
2	F	213	LYS	3.3
5	Y	14	ALA	3.3
2	F	145	LEU	3.3
2	B	200	THR	3.3
4	D	191	SER	3.2
2	F	132	ALA	3.2
5	X	67	CYS	3.2
4	H	195	THR	3.1
1	E	131	SER	3.1
2	F	164	GLY	3.0
2	F	194	SER	3.0
1	E	194	LYS	2.9
2	F	76	SER	2.9
4	H	191	SER	2.9
4	H	117	SER	2.9
2	F	12	VAL	2.9
5	Y	82	ALA	2.9
2	F	163	SER	2.9
5	Y	57	THR	2.9
5	Y	84	CYS	2.8
2	F	78	THR	2.8
2	F	5	GLN	2.8
2	F	190	THR	2.8
5	X	73	VAL	2.7
2	F	177	LEU	2.7
2	B	106	GLY	2.7
5	X	74	ARG	2.7
1	E	126	ASP	2.7
5	Y	83	GLU	2.6
1	E	24	LYS	2.6
2	F	27	TYR	2.6
1	E	214	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	212	SER	2.6
2	F	75	SER	2.6
2	F	166	LEU	2.5
3	C	188	ALA	2.5
2	F	17	SER	2.5
2	F	210	SER	2.4
3	C	1	ASP	2.4
2	B	198	THR	2.4
2	F	28	ALA	2.4
2	F	218	VAL	2.4
4	D	194	GLY	2.4
1	E	20	THR	2.4
1	E	38	ASN	2.4
2	F	212	THR	2.4
1	A	38	ASN	2.4
2	F	29	PHE	2.4
2	F	199	GLN	2.4
2	F	158	THR	2.4
1	E	195	VAL	2.4
5	X	10	ARG	2.4
3	G	158	LEU	2.3
5	Y	73	VAL	2.3
2	F	206	ASN	2.3
2	F	180	SER	2.3
2	F	186	SER	2.3
2	F	73	ASP	2.2
5	Y	34	ASP	2.2
2	F	120	ALA	2.2
2	F	219	GLU	2.2
2	F	216	LYS	2.2
5	X	84	CYS	2.2
2	F	154	PRO	2.2
3	C	192	LYS	2.2
3	G	161	GLY	2.2
2	F	211	ASN	2.2
2	F	133	PRO	2.2
2	F	106	GLY	2.2
2	B	196	LEU	2.2
2	B	103	GLY	2.2
3	G	61	GLY	2.1
4	H	97	ALA	2.1
2	F	35	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	167	THR	2.1
4	D	132	SER	2.1
2	F	83	LEU	2.1
5	X	38	LYS	2.1
1	E	129	LEU	2.1
1	E	188	ALA	2.1
1	E	156	ASN	2.1
3	G	95	SER	2.1
1	E	114	VAL	2.1
4	H	193	LEU	2.0
1	E	40	TYR	2.0
1	E	151	GLN	2.0
2	B	192	PRO	2.0
2	F	72	ALA	2.0
4	H	116	SER	2.0
1	E	104	GLY	2.0
1	E	213	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	PCA	H	1	8/9	0.83	0.32	-	72,75,78,80	0
2	PCA	F	1	8/9	0.83	0.43	-	76,87,91,94	0
4	PCA	D	1	8/9	0.92	0.15	-	55,67,70,71	0
2	PCA	B	1	8/9	0.83	0.41	-	67,78,88,95	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. 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, 95^{th} 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	NAG	Y	301	14/15	0.74	0.39	-	103,110,123,124	0
6	NAG	X	302	14/15	0.65	0.43	-	116,131,139,144	0
6	NAG	X	301	14/15	0.80	0.27	-	79,90,100,114	0
6	NAG	Y	302	14/15	0.61	0.46	-	120,131,134,140	0

6.5 Other polymers (i)

There are no such residues in this entry.