Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:40 PM GMT

PDB ID	:	4MA1
Title	:	Unliganded 3 crystal structure of S25-26 Fab
Authors	:	Haji-Ghassemi, O.; Evans, S.V.
Deposited on	:	2013-08-15
Resolution	:	2.32 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:

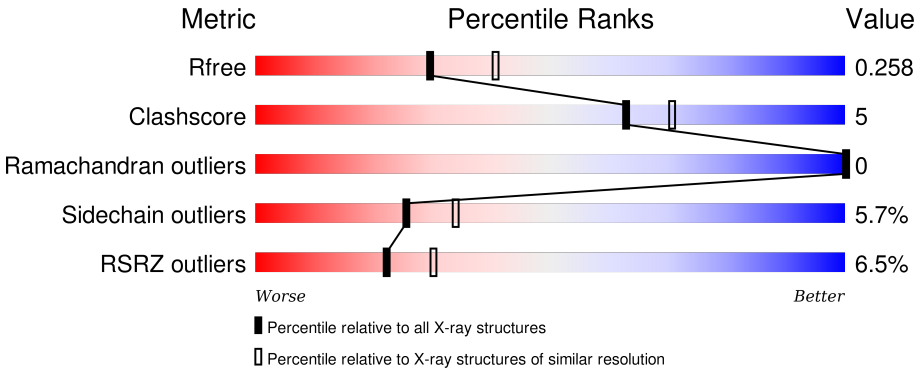
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.32 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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	B	219	3% 87% 11%
1	E	219	26% 79% 16%
1	H	219	3% 87% 11%
2	C	219	2% 90% 9%
2	F	219	4% 89% 10%

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Mol	Chain	Length	Quality of chain
2	L	219	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10552 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 S25-26 Fab (IgG1k) heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	218	Total	C	N	O	S	0	0	0
			1647	1050	273	317	7			
1	E	216	Total	C	N	O	S	0	0	0
			1631	1039	270	315	7			
1	H	218	Total	C	N	O	S	0	1	0
			1653	1053	274	318	8			

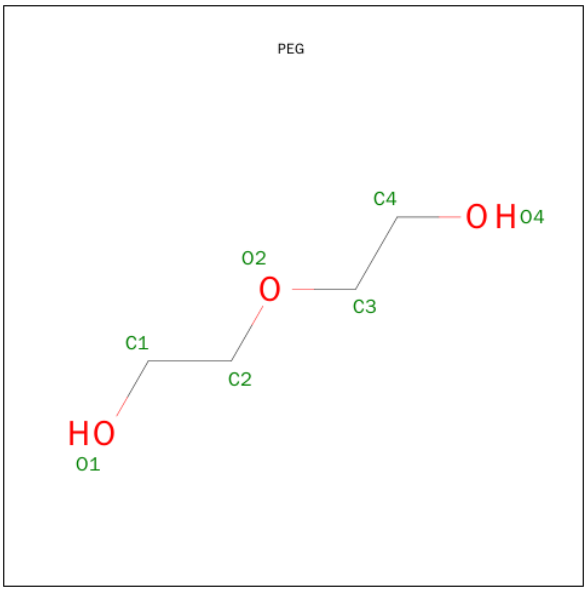
- Molecule 2 is a protein called S25-26 Fab (IgG1k) light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	219	Total	C	N	O	S	0	0	0
			1712	1072	291	342	7			
2	F	219	Total	C	N	O	S	0	0	0
			1712	1072	291	342	7			
2	L	219	Total	C	N	O	S	0	0	0
			1712	1072	291	342	7			

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	5	Total	C	N	O	0	0
			60	34	2	24		
3	E	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 7 4 3	0	0
4	H	1	Total C O 7 4 3	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	2	Total C N O 24 14 1 9	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	7	Total C N O 83 46 2 35	0	0

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total K 1 1	0	0

- Molecule 8 is water.

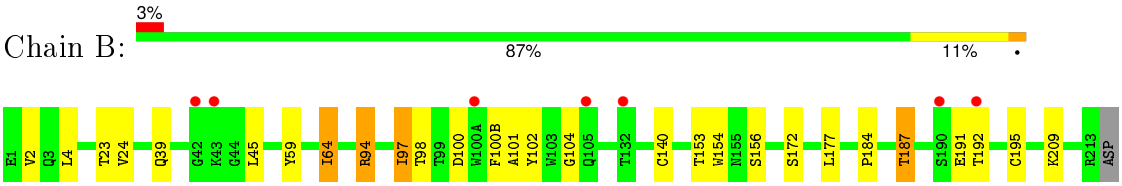
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	38	Total O 38 38	0	0
8	E	16	Total O 16 16	0	0
8	H	62	Total O 62 62	0	0
8	C	34	Total O 34 34	0	0
8	F	47	Total O 47 47	0	0
8	L	46	Total O 46 46	0	0

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.

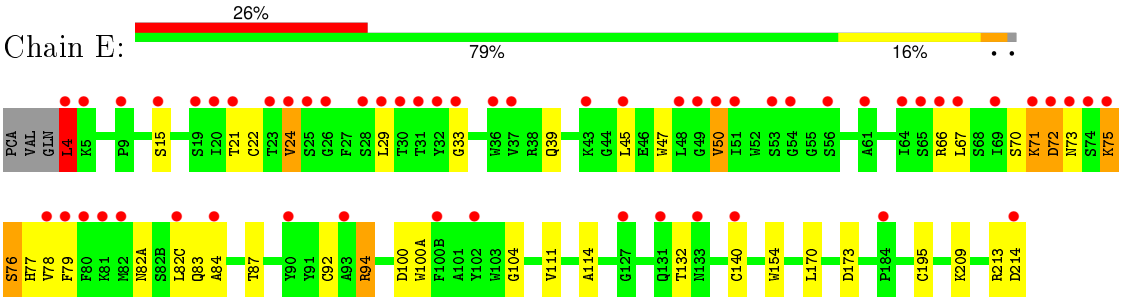
- Molecule 1: S25-26 Fab (IgG1k) heavy chain

Chain B:



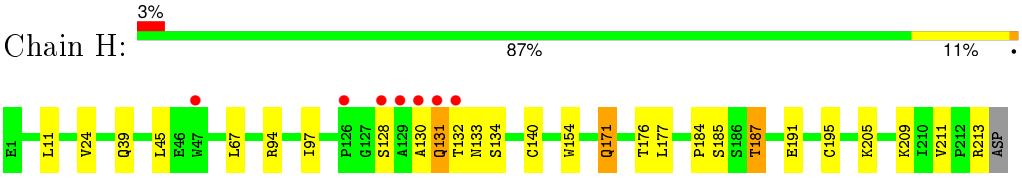
- Molecule 1: S25-26 Fab (IgG1k) heavy chain

Chain E:



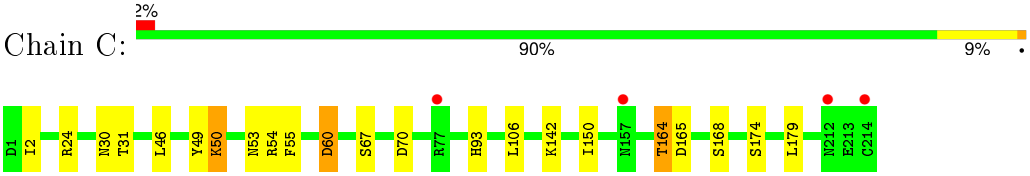
- Molecule 1: S25-26 Fab (IgG1k) heavy chain

Chain H:



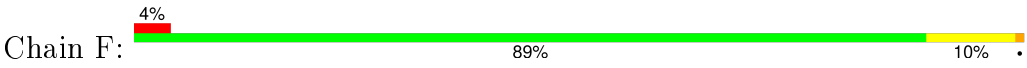
- Molecule 2: S25-26 Fab (IgG1k) light chain

Chain C:



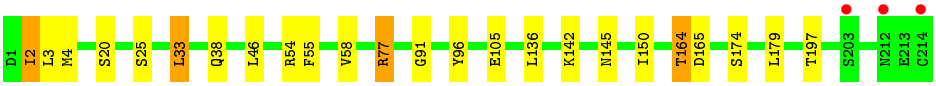
- Molecule 2: S25-26 Fab (IgG1k) light chain

Chain F:



- Molecule 2: S25-26 Fab (IgG1k) light chain

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	196.26Å 66.51Å 122.08Å 90.00° 113.46° 90.00°	Depositor
Resolution (Å)	29.93 – 2.32 29.91 – 2.32	Depositor EDS
% Data completeness (in resolution range)	81.4 (29.93-2.32) 81.4 (29.91-2.32)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.12 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.229 , 0.260 0.230 , 0.258	Depositor DCC
R_{free} test set	2621 reflections (5.38%)	DCC
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 40.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 51319 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10552	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, NAG, GLA, K, GAL, FUC, PEG, PCA, 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	B	0.47	0/1686	0.67	1/2311 (0.0%)
1	E	0.41	0/1677	0.71	4/2297 (0.2%)
1	H	0.49	0/1692	0.71	0/2319
2	C	0.47	0/1752	0.66	0/2376
2	F	0.51	0/1752	0.72	1/2376 (0.0%)
2	L	0.50	0/1752	0.70	1/2376 (0.0%)
All	All	0.47	0/10311	0.70	7/14055 (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
1	B	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	108	ARG	CB-CA-C	-8.07	94.25	110.40
1	E	82(A)	ASN	N-CA-C	5.98	127.14	111.00
1	E	50	VAL	CB-CA-C	-5.69	100.59	111.40
1	B	140	CYS	CA-CB-SG	5.68	124.22	114.00
1	E	4	LEU	CB-CG-CD2	-5.40	101.81	111.00
2	L	33	LEU	CA-CB-CG	-5.22	103.30	115.30
1	E	71	LYS	N-CA-C	5.09	124.75	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	100	ASP	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	B	1647	0	1618	12	0
1	E	1631	0	1598	40	0
1	H	1653	0	1621	12	0
2	C	1712	0	1649	14	0
2	F	1712	0	1649	12	0
2	L	1712	0	1648	15	0
3	B	60	0	52	3	0
3	E	60	0	52	4	0
4	B	7	0	10	0	0
4	H	7	0	10	0	0
5	H	24	0	21	0	0
6	H	83	0	70	0	0
7	L	1	0	0	0	0
8	B	38	0	0	1	0
8	C	34	0	0	2	0
8	E	16	0	0	0	0
8	F	47	0	0	0	0
8	H	62	0	0	0	0
8	L	46	0	0	1	0
All	All	10552	0	9998	107	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 5.

All (107) 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)
3:B:402:FUC:O2	3:B:403:NAG:H82	1.45	1.15
3:E:401:NAG:H62	3:E:402:FUC:H5	1.27	1.08
3:B:402:FUC:HO2	3:B:403:NAG:H82	1.33	0.91
3:E:401:NAG:H62	3:E:402:FUC:C5	2.07	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:LYS:HE3	1:E:73:ASN:OD1	1.82	0.80
1:E:47:TRP:HZ2	1:E:50:VAL:CG2	1.98	0.76
1:E:4:LEU:CD2	1:E:22:CYS:SG	2.77	0.73
1:E:29:LEU:HD13	1:E:72:ASP:HB3	1.71	0.72
1:E:77:HIS:HB3	1:E:79:PHE:HE1	1.54	0.71
1:H:39:GLN:OE1	2:L:38:GLN:NE2	2.20	0.70
1:E:71:LYS:HE3	1:E:73:ASN:ND2	2.06	0.70
1:E:78:VAL:C	1:E:79:PHE:HD1	1.95	0.70
2:C:2:ILE:HD13	2:C:93:HIS:HB2	1.76	0.68
3:B:402:FUC:O2	3:B:403:NAG:C8	2.33	0.67
1:E:4:LEU:HD22	1:E:92:CYS:SG	2.35	0.67
2:F:210:ASN:N	2:F:210:ASN:OD1	2.28	0.67
1:E:71:LYS:HE3	1:E:73:ASN:CG	2.16	0.66
1:E:33:GLY:O	1:E:94:ARG:NH1	2.28	0.66
2:F:2:ILE:HD13	2:F:93:HIS:HB2	1.77	0.65
1:E:77:HIS:HB3	1:E:79:PHE:CE1	2.32	0.65
1:E:71:LYS:CE	1:E:73:ASN:HD21	2.09	0.65
2:C:164:THR:HG23	2:C:165:ASP:O	1.97	0.64
1:E:47:TRP:HZ2	1:E:50:VAL:HG23	1.62	0.64
1:E:71:LYS:HE3	1:E:73:ASN:HD21	1.61	0.64
2:L:164:THR:HG23	2:L:165:ASP:O	2.00	0.62
2:L:2:ILE:HD11	2:L:4:MET:SD	2.40	0.62
1:E:24:VAL:O	1:E:76:SER:HB2	2.00	0.60
2:L:77:ARG:O	2:L:77:ARG:HG2	2.02	0.59
2:C:60:ASP:OD1	2:C:60:ASP:N	2.36	0.59
1:E:71:LYS:NZ	1:E:73:ASN:HD21	2.00	0.58
2:C:30:ASN:OD1	2:C:50:LYS:HE3	2.03	0.58
1:E:4:LEU:HD21	1:E:22:CYS:SG	2.44	0.57
1:E:83:GLN:O	1:E:111:VAL:HG21	2.05	0.57
1:B:154:TRP:CZ3	1:B:195:CYS:HB3	2.40	0.56
1:B:97:ILE:HD11	2:C:49:TYR:CG	2.40	0.56
1:H:131:GLN:HA	1:H:131:GLN:HE21	1.70	0.56
1:E:154:TRP:CZ3	1:E:195:CYS:HB3	2.40	0.56
1:E:82(C):LEU:HB3	1:E:111:VAL:HG11	1.88	0.55
1:B:94:ARG:NH2	1:B:100(B):PHE:O	2.39	0.54
2:C:67:SER:HB3	8:C:308:HOH:O	2.07	0.54
1:E:213:ARG:NH1	2:F:120:PRO:O	2.36	0.54
1:H:128:SER:O	1:H:130:ALA:N	2.41	0.54
2:L:145:ASN:HB3	2:L:197:THR:CG2	2.37	0.54
2:F:164:THR:HG23	2:F:165:ASP:O	2.06	0.54
3:E:401:NAG:C6	3:E:402:FUC:H5	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:24:ARG:HG2	2:C:70:ASP:OD1	2.09	0.52
1:E:47:TRP:CZ2	1:E:50:VAL:HG23	2.42	0.52
1:B:4:LEU:O	1:B:104:GLY:HA2	2.10	0.52
1:H:154:TRP:CZ3	1:H:195:CYS:HB3	2.45	0.52
1:H:171:GLN:NE2	1:H:176:THR:OG1	2.43	0.51
2:L:77:ARG:O	2:L:77:ARG:CG	2.58	0.51
1:B:59:TYR:HB2	1:B:64:ILE:HG13	1.93	0.51
1:E:114:ALA:HB2	1:E:173:ASP:HB3	1.92	0.50
1:E:87:THR:OG1	1:E:111:VAL:HG22	2.11	0.50
2:L:2:ILE:HG23	8:L:401:HOH:O	2.11	0.50
1:H:133:ASN:O	1:H:185:SER:HB2	2.11	0.50
2:L:2:ILE:HD13	2:L:25:SER:HB2	1.94	0.50
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.93	0.50
2:L:150:ILE:HD11	2:L:179:LEU:HD21	1.94	0.49
1:E:75:LYS:HB2	1:E:77:HIS:CE1	2.48	0.49
1:B:39:GLN:HB2	1:B:45:LEU:HD23	1.95	0.48
1:E:84:ALA:HA	1:E:111:VAL:HG23	1.94	0.48
1:E:39:GLN:HB2	1:E:45:LEU:HD23	1.94	0.48
2:C:46:LEU:HD23	2:C:55:PHE:CD1	2.48	0.48
1:E:21:THR:HG23	1:E:79:PHE:CE1	2.49	0.48
2:F:46:LEU:HD23	2:F:55:PHE:CD1	2.49	0.47
1:E:24:VAL:O	1:E:76:SER:CB	2.61	0.47
2:C:49:TYR:O	2:C:53:ASN:HB2	2.15	0.47
2:F:150:ILE:HD11	2:F:179:LEU:HD21	1.96	0.47
1:E:71:LYS:CE	1:E:73:ASN:ND2	2.73	0.47
1:E:100:ASP:HB2	1:E:100(A):TRP:CE3	2.50	0.47
1:H:184:PRO:O	1:H:187:THR:HG22	2.15	0.46
1:E:79:PHE:N	1:E:79:PHE:CD1	2.83	0.46
2:C:150:ILE:HD11	2:C:179:LEU:HD21	1.97	0.46
2:F:16:GLY:HA2	2:F:77:ARG:HG2	1.96	0.45
1:E:47:TRP:HZ2	1:E:50:VAL:HG22	1.78	0.45
3:E:401:NAG:C6	3:E:402:FUC:C5	2.86	0.44
1:H:39:GLN:NE2	2:L:38:GLN:OE1	2.40	0.44
1:B:154:TRP:CH2	1:B:195:CYS:HB3	2.52	0.44
2:F:2:ILE:N	2:F:2:ILE:HD12	2.33	0.44
2:L:54:ARG:HD3	2:L:58:VAL:O	2.17	0.44
1:B:2:VAL:HG21	1:B:100(B):PHE:HA	1.98	0.44
8:B:511:HOH:O	2:F:212:ASN:HB3	2.18	0.44
1:B:177:LEU:C	1:B:177:LEU:HD12	2.38	0.44
2:L:46:LEU:HD23	2:L:55:PHE:CD1	2.52	0.44
1:B:153:THR:HB	1:B:156:SER:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:164:THR:HG22	2:C:174:SER:H	1.83	0.43
2:C:67:SER:CB	8:C:308:HOH:O	2.65	0.43
1:E:29:LEU:CD1	1:E:72:ASP:HB3	2.44	0.42
1:B:184:PRO:O	1:B:187:THR:HG22	2.19	0.42
2:F:170:ASP:C	2:F:170:ASP:OD1	2.58	0.42
2:F:164:THR:HG22	2:F:174:SER:H	1.85	0.42
1:E:154:TRP:CH2	1:E:195:CYS:HB3	2.55	0.42
1:B:101:ALA:HB3	2:C:55:PHE:CE1	2.54	0.42
1:E:4:LEU:HD22	1:E:22:CYS:SG	2.59	0.42
2:L:164:THR:HG22	2:L:174:SER:H	1.85	0.42
2:L:91:GLY:HA2	2:L:96:TYR:CD1	2.55	0.42
1:E:4:LEU:HB3	1:E:104:GLY:HA2	2.02	0.41
1:E:47:TRP:CZ2	1:E:50:VAL:CG2	2.89	0.41
2:C:2:ILE:HD12	2:C:2:ILE:N	2.34	0.41
1:E:79:PHE:N	1:E:79:PHE:HD1	2.17	0.41
1:H:187:THR:OG1	1:H:191:GLU:HG3	2.22	0.40
1:H:133:ASN:CG	1:H:134:SER:N	2.75	0.40
1:E:78:VAL:C	1:E:79:PHE:CD1	2.85	0.40
2:F:27(D):HIS:O	2:F:27(E):ARG:HD2	2.21	0.40
2:L:136:LEU:N	2:L:136:LEU:HD12	2.36	0.40
1:H:177:LEU:C	1:H:177:LEU:HD12	2.41	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	B	216/219 (99%)	212 (98%)	4 (2%)	0	100	100
1	E	214/219 (98%)	205 (96%)	9 (4%)	0	100	100
1	H	217/219 (99%)	213 (98%)	4 (2%)	0	100	100
2	C	217/219 (99%)	214 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	217/219 (99%)	214 (99%)	3 (1%)	0	100	100
2	L	217/219 (99%)	214 (99%)	3 (1%)	0	100	100
All	All	1298/1314 (99%)	1272 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	B	187/188 (100%)	175 (94%)	12 (6%)	22	28
1	E	186/188 (99%)	171 (92%)	15 (8%)	15	18
1	H	188/188 (100%)	173 (92%)	15 (8%)	15	18
2	C	196/196 (100%)	188 (96%)	8 (4%)	37	50
2	F	196/196 (100%)	188 (96%)	8 (4%)	37	50
2	L	196/196 (100%)	188 (96%)	8 (4%)	37	50
All	All	1149/1152 (100%)	1083 (94%)	66 (6%)	25	34

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	23	THR
1	B	24	VAL
1	B	64	ILE
1	B	94	ARG
1	B	97	ILE
1	B	98	THR
1	B	102	TYR
1	B	172	SER
1	B	187	THR
1	B	191	GLU
1	B	192	THR
1	B	209	LYS

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Mol	Chain	Res	Type
1	E	4	LEU
1	E	15	SER
1	E	24	VAL
1	E	66	ARG
1	E	67	LEU
1	E	70	SER
1	E	72	ASP
1	E	75	LYS
1	E	76	SER
1	E	94	ARG
1	E	132	THR
1	E	140	CYS
1	E	170	LEU
1	E	209	LYS
1	E	214	ASP
1	H	11	LEU
1	H	24	VAL
1	H	67	LEU
1	H	94	ARG
1	H	97	ILE
1	H	131	GLN
1	H	132	THR
1	H	140[A]	CYS
1	H	140[B]	CYS
1	H	171	GLN
1	H	187	THR
1	H	205	LYS
1	H	209	LYS
1	H	211	VAL
1	H	213	ARG
2	C	31	THR
2	C	50	LYS
2	C	54	ARG
2	C	60	ASP
2	C	106	LEU
2	C	142	LYS
2	C	164	THR
2	C	168	SER
2	F	18	GLN
2	F	20	SER
2	F	31	THR
2	F	52	SER

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Mol	Chain	Res	Type
2	F	106	LEU
2	F	164	THR
2	F	188	ARG
2	F	210	ASN
2	L	2	ILE
2	L	3	LEU
2	L	20	SER
2	L	33	LEU
2	L	77	ARG
2	L	105	GLU
2	L	142	LYS
2	L	164	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	73	ASN
1	E	77	HIS
1	H	13	GLN
1	H	39	GLN
1	H	131	GLN
1	H	171	GLN
2	F	18	GLN
2	L	38	GLN
2	L	156	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 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	$\#\|Z\|>2$
1	PCA	B	1	1	7,8,9	0.47	0	9,10,12	1.05	0
1	PCA	H	1	1	7,8,9	0.46	0	9,10,12	1.43	2 (22%)

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
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	H	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	1	PCA	CB-CA-C	-3.25	108.31	112.76
1	H	1	PCA	O-C-CA	-2.02	120.11	125.44

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)

19 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	401	1,3	14,14,15	0.67	0	15,19,21	1.28	3 (20%)
3	FUC	B	402	3	10,10,11	0.30	0	14,14,16	0.79	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	403	3	14,14,15	0.61	0	15,19,21	1.61	2 (13%)
3	BMA	B	404	3	11,11,12	0.38	0	14,15,17	0.91	1 (7%)
3	MAN	B	405	3	11,11,12	0.46	0	14,15,17	2.59	1 (7%)
3	NAG	E	401	1,3	14,14,15	0.52	0	15,19,21	1.49	2 (13%)
3	FUC	E	402	3	10,10,11	0.34	0	14,14,16	1.00	1 (7%)
3	NAG	E	403	3	14,14,15	0.46	0	15,19,21	2.31	2 (13%)
3	BMA	E	404	3	11,11,12	0.29	0	14,15,17	2.07	3 (21%)
3	MAN	E	405	3	11,11,12	0.54	0	14,15,17	1.03	1 (7%)
5	NAG	H	401	1,5,6	14,14,15	0.27	0	15,19,21	0.53	0
5	FUC	H	402	5	10,10,11	0.48	0	14,14,16	1.35	2 (14%)
6	NAG	H	403	5,6	14,14,15	1.34	1 (7%)	15,19,21	2.49	4 (26%)
6	BMA	H	404	6	11,11,12	0.44	0	14,15,17	2.39	3 (21%)
6	MAN	H	405	6	11,11,12	0.49	0	14,15,17	1.44	1 (7%)
6	NAG	H	406	6	14,14,15	0.47	0	15,19,21	0.69	0
6	GAL	H	407	6	11,11,12	0.74	0	14,15,17	2.30	4 (28%)
6	GLA	H	408	6	11,11,12	0.41	0	14,15,17	1.05	1 (7%)
6	MAN	H	409	6	11,11,12	0.25	0	14,15,17	0.60	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
3	NAG	B	401	1,3	-	0/6/23/26	0/1/1/1
3	FUC	B	402	3	-	0/0/17/20	0/1/1/1
3	NAG	B	403	3	-	0/6/23/26	0/1/1/1
3	BMA	B	404	3	-	0/2/19/22	0/1/1/1
3	MAN	B	405	3	-	0/2/19/22	0/1/1/1
3	NAG	E	401	1,3	-	0/6/23/26	0/1/1/1
3	FUC	E	402	3	-	0/0/17/20	0/1/1/1
3	NAG	E	403	3	-	0/6/23/26	0/1/1/1
3	BMA	E	404	3	-	0/2/19/22	0/1/1/1
3	MAN	E	405	3	-	0/2/19/22	0/1/1/1
5	NAG	H	401	1,5,6	-	0/6/23/26	0/1/1/1
5	FUC	H	402	5	-	0/0/17/20	0/1/1/1
6	NAG	H	403	5,6	-	0/6/23/26	0/1/1/1
6	BMA	H	404	6	-	0/2/19/22	0/1/1/1
6	MAN	H	405	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	H	406	6	-	0/6/23/26	0/1/1/1
6	GAL	H	407	6	-	0/2/19/22	0/1/1/1
6	GLA	H	408	6	-	0/2/19/22	0/1/1/1
6	MAN	H	409	6	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	403	NAG	O4-C4	-4.39	1.32	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	403	NAG	C4-C3-C2	-6.73	100.77	111.23
6	H	407	GAL	O3-C3-C2	-4.47	101.93	110.00
6	H	404	BMA	C2-C3-C4	-3.56	105.00	111.04
3	B	401	NAG	O6-C6-C5	-3.17	100.86	111.33
6	H	407	GAL	C2-C3-C4	-3.16	105.67	111.04
6	H	408	GLA	O2-C2-C1	-2.52	104.16	109.21
3	B	401	NAG	C3-C4-C5	-2.49	105.86	110.20
5	H	402	FUC	C2-C3-C4	-2.47	106.85	111.04
3	E	401	NAG	O7-C7-C8	-2.42	117.63	122.06
3	E	404	BMA	O3-C3-C2	-2.38	105.69	110.00
6	H	404	BMA	O5-C1-C2	-2.19	107.31	110.86
6	H	407	GAL	C1-C2-C3	-2.12	107.03	109.54
3	B	401	NAG	C2-N2-C7	-2.08	120.37	123.04
3	B	402	FUC	O5-C5-C6	2.03	109.49	106.13
3	B	404	BMA	C3-C4-C5	2.06	113.78	110.20
6	H	403	NAG	O4-C4-C3	2.22	115.34	110.34
3	E	402	FUC	O5-C5-C6	2.33	109.98	106.13
3	E	403	NAG	C3-C4-C5	2.35	114.29	110.20
5	H	402	FUC	O2-C2-C1	2.45	114.11	109.21
3	E	405	MAN	C1-C2-C3	2.49	112.48	109.54
3	E	404	BMA	O5-C1-C2	2.62	115.10	110.86
3	E	401	NAG	C1-O5-C5	3.41	116.58	112.25
3	B	403	NAG	C4-C3-C2	3.84	117.19	111.23
6	H	403	NAG	C3-C2-N2	3.84	119.75	110.56
3	B	403	NAG	C3-C4-C5	4.05	117.25	110.20
6	H	403	NAG	C1-O5-C5	4.73	118.25	112.25
6	H	405	MAN	C1-O5-C5	4.74	118.27	112.25
6	H	407	GAL	C1-O5-C5	5.78	119.59	112.25
3	E	404	BMA	C1-C2-C3	6.13	116.79	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	404	BMA	C1-O5-C5	7.14	121.31	112.25
3	E	403	NAG	C1-O5-C5	8.17	122.61	112.25
3	B	405	MAN	C1-O5-C5	9.15	123.86	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	FUC	3	0
3	B	403	NAG	3	0
3	E	401	NAG	4	0
3	E	402	FUC	4	0

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PEG	B	406	-	6,6,6	0.54	0	5,5,5	0.26	0
4	PEG	H	410	-	6,6,6	0.44	0	5,5,5	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	B	406	-	-	0/4/4/4	0/0/0/0
4	PEG	H	410	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	B	217/219 (99%)	0.22	7 (3%) 51 60	25, 45, 68, 75	0
1	E	216/219 (98%)	1.47	56 (25%) 1 1	36, 70, 134, 182	0
1	H	217/219 (99%)	0.20	7 (3%) 51 60	17, 33, 58, 105	0
2	C	219/219 (100%)	0.28	4 (1%) 71 78	30, 48, 71, 85	0
2	F	219/219 (100%)	0.21	8 (3%) 45 54	26, 39, 60, 79	0
2	L	219/219 (100%)	0.05	3 (1%) 78 83	14, 37, 58, 78	0
All	All	1307/1314 (99%)	0.40	85 (6%) 22 30	14, 43, 89, 182	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	30	THR	11.2
1	E	29	LEU	8.0
1	E	32	TYR	7.4
1	E	71	LYS	6.1
1	E	51	ILE	6.0
1	H	131	GLN	5.7
1	H	129	ALA	5.3
1	E	65	SER	5.3
1	E	73	ASN	5.0
1	E	31	THR	5.0
1	E	61	ALA	4.7
1	E	33	GLY	4.6
1	E	72	ASP	4.5
1	E	28	SER	4.5
2	F	214	CYS	4.3
1	H	128	SER	4.0
1	H	132	THR	4.0
2	C	214	CYS	4.0
1	E	79	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	75	LYS	3.8
1	E	56	SER	3.7
1	E	100(B)	PHE	3.7
1	E	54	GLY	3.7
1	E	36	TRP	3.6
1	E	93	ALA	3.5
1	E	23	THR	3.5
1	E	26	GLY	3.4
1	E	69	ILE	3.3
1	E	37	VAL	3.3
1	E	78	VAL	3.3
2	F	210	ASN	3.3
1	E	131	GLN	3.2
1	E	102	TYR	3.2
1	B	43	LYS	3.1
1	E	24	VAL	3.1
2	C	212	ASN	3.1
1	E	9	PRO	3.0
2	L	203	SER	3.0
2	L	214	CYS	3.0
1	E	20	ILE	3.0
1	E	53	SER	3.0
1	E	15	SER	2.9
1	E	80	PHE	2.9
1	E	19	SER	2.9
1	E	81	LYS	2.8
2	F	169	LYS	2.8
1	E	82	MET	2.8
1	E	84	ALA	2.8
1	E	48	LEU	2.8
2	F	212	ASN	2.7
1	E	64	ILE	2.7
1	E	45	LEU	2.7
1	E	184	PRO	2.7
1	B	100(A)	TRP	2.6
1	E	67	LEU	2.6
1	B	105	GLN	2.6
2	F	42	GLN	2.6
2	C	77	ARG	2.5
1	E	90	TYR	2.5
1	B	190	SER	2.5
1	E	25	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	74	SER	2.4
1	E	49	GLY	2.4
1	E	82(C)	LEU	2.4
1	B	42	GLY	2.4
2	F	2	ILE	2.4
2	F	3	LEU	2.4
1	E	66	ARG	2.4
1	E	214	ASP	2.3
1	H	130	ALA	2.3
2	L	212	ASN	2.3
1	E	21	THR	2.3
1	E	140	CYS	2.3
1	B	192	THR	2.3
1	E	127	GLY	2.2
2	F	163	TRP	2.2
1	E	4	LEU	2.2
1	E	50	VAL	2.1
1	E	43	LYS	2.1
1	B	132	THR	2.1
2	C	157	ASN	2.1
1	E	133	ASN	2.1
1	H	47	TRP	2.1
1	E	5	LYS	2.0
1	H	126	PRO	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
1	PCA	H	1	8/9	0.94	0.18	-	47,50,52,54	0
1	PCA	B	1	8/9	0.75	0.38	-	58,69,74,78	0

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, 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	MAN	H	405	11/12	0.62	0.39	-	97,105,108,111	0
3	BMA	B	404	11/12	0.71	0.37	-	92,99,108,115	0
6	MAN	H	409	11/12	0.79	0.44	-	92,97,99,100	0
5	NAG	H	401	14/15	0.88	0.27	-	41,50,62,74	0
6	GLA	H	408	11/12	0.52	0.51	-	86,92,93,94	0
3	NAG	E	403	14/15	0.63	0.38	-	104,110,114,115	0
3	FUC	E	402	10/11	0.68	0.39	-	95,104,107,109	0
6	BMA	H	404	11/12	0.64	0.33	-	84,93,98,100	0
3	NAG	B	403	14/15	0.49	0.34	-	85,91,98,101	0
3	BMA	E	404	11/12	0.77	0.45	-	97,105,109,109	0
6	NAG	H	406	14/15	0.75	0.37	-	104,107,109,113	0
3	FUC	B	402	10/11	0.76	0.35	-	90,93,96,97	0
3	MAN	E	405	11/12	0.63	0.42	-	77,92,99,101	0
3	NAG	E	401	14/15	0.68	0.30	-	59,71,101,105	0
3	NAG	B	401	14/15	0.85	0.18	-	56,69,80,84	0
6	GAL	H	407	11/12	0.66	0.47	-	89,100,103,105	0
6	NAG	H	403	14/15	0.78	0.23	-	60,64,70,80	0
5	FUC	H	402	10/11	0.54	0.38	-	79,85,91,91	0
3	MAN	B	405	11/12	0.41	0.56	-	108,119,121,122	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	PEG	B	406	7/7	0.84	0.14	1.01	44,46,48,48	0
7	K	L	301	1/1	0.97	0.05	-2.65	39,39,39,39	0
4	PEG	H	410	7/7	0.86	0.14	-	54,56,59,61	0

6.5 Other polymers

There are no such residues in this entry.