Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:06 PM GMT

PDB ID	:	5AFM
Title	:	alpha7-AChBP in complex with lobeline and fragment 4
Authors	:	Spurny, R.; Debaveye, S.; Farinha, A.; Veys, K.; Gossas, T.; Atack, J.; Bertrand, D.; Kemp, J.; Vos, A.; Danielson, U.H.; Tresadern, G.; Ulens, C.
Deposited on	:	2015-01-22
Resolution	:	2.85 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 ①) were used in the production of this report:

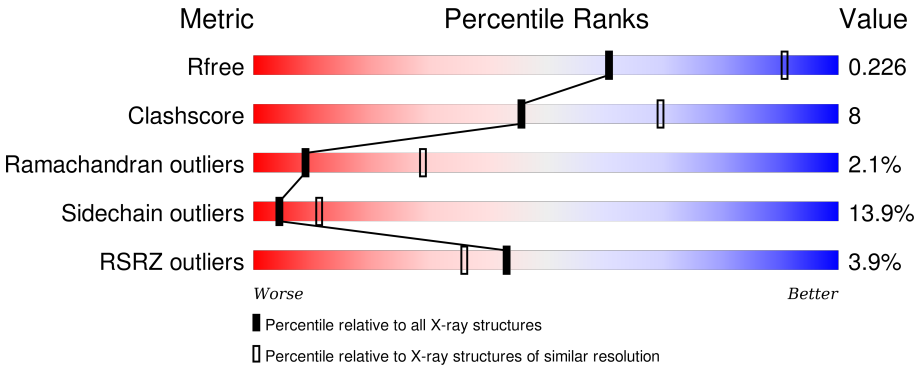
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	205	4% 74% 20% 5%
1	C	205	4% 74% 20% 6%
1	D	205	% 72% 22% 5%
1	E	205	% 75% 21% .
2	B	207	9% 73% 22% .

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
4	L0B	D	1205	-	-	-	X
5	GOL	A	1206	-	-	-	X
5	GOL	C	1206	-	-	X	X
5	GOL	D	1206	-	-	-	X
5	GOL	E	1206	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9054 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.

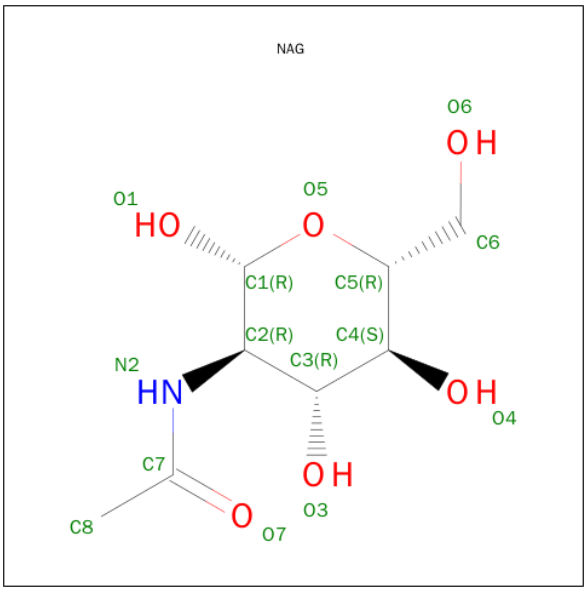
- Molecule 1 is a protein called ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1670	1071	279	313	7			
1	C	205	Total	C	N	O	S	0	0	0
			1670	1071	279	313	7			
1	D	205	Total	C	N	O	S	0	0	0
			1670	1071	279	313	7			
1	E	205	Total	C	N	O	S	0	0	0
			1670	1071	279	313	7			

- Molecule 2 is a protein called ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7.

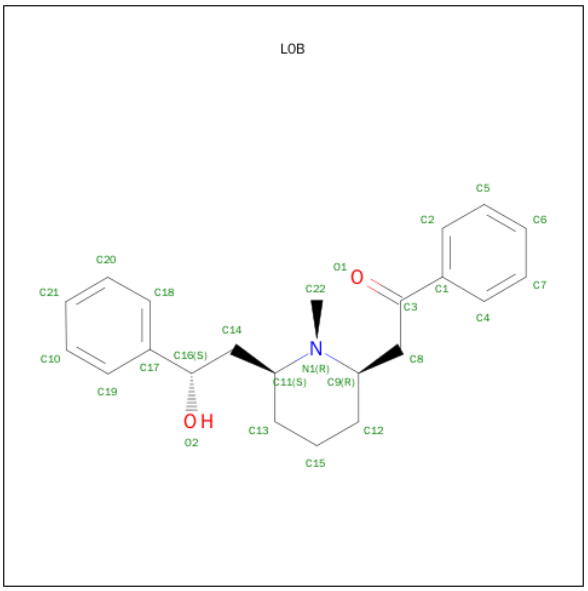
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	S	0	0	0
			1687	1080	284	316	7			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



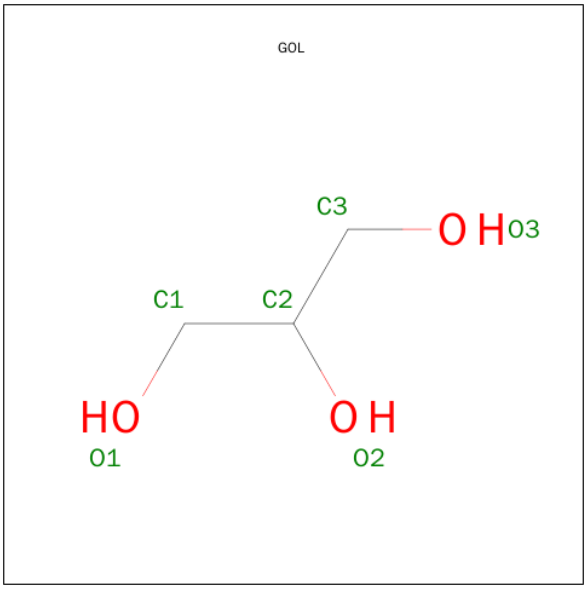
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	E	1	Total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

- Molecule 4 is ALPHA-LOBELINE (three-letter code: L0B) (formula: $C_{22}H_{27}NO_2$).



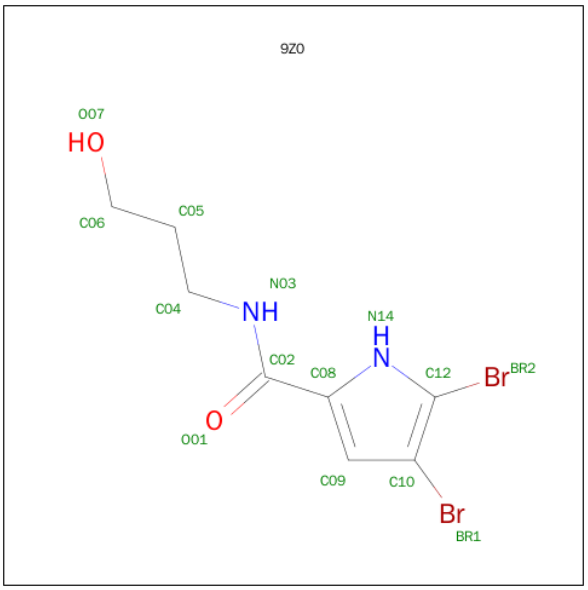
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			25	22	1	2		
4	B	1	Total	C	N	O	0	0
			25	22	1	2		
4	C	1	Total	C	N	O	0	0
			25	22	1	2		
4	D	1	Total	C	N	O	0	0
			25	22	1	2		
4	E	1	Total	C	N	O	0	0
			25	22	1	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0

- Molecule 6 is 4,5-DIBROMO-N-(3-HYDROXYPROPYL)-1H-PYRROLE-2-CARBOXAMIDE (three-letter code: 9Z0) (formula: $C_8H_{10}Br_2N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Br C N O 14 2 8 2 2	0	0
6	B	1	Total Br C N O 14 2 8 2 2	0	0
6	C	1	Total Br C N O 14 2 8 2 2	0	0
6	D	1	Total Br C N O 14 2 8 2 2	0	0
6	E	1	Total Br C N O 14 2 8 2 2	0	0

- Molecule 7 is water.

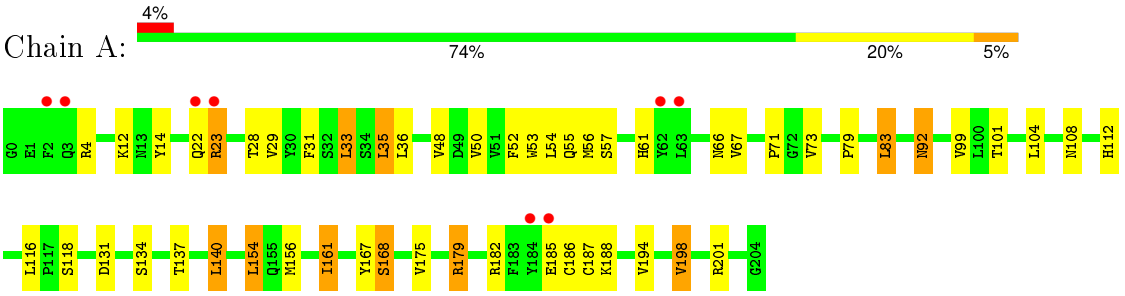
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	73	Total O 73 73	0	0
7	B	40	Total O 40 40	0	0
7	C	73	Total O 73 73	0	0
7	D	75	Total O 75 75	0	0
7	E	67	Total O 67 67	0	0

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.

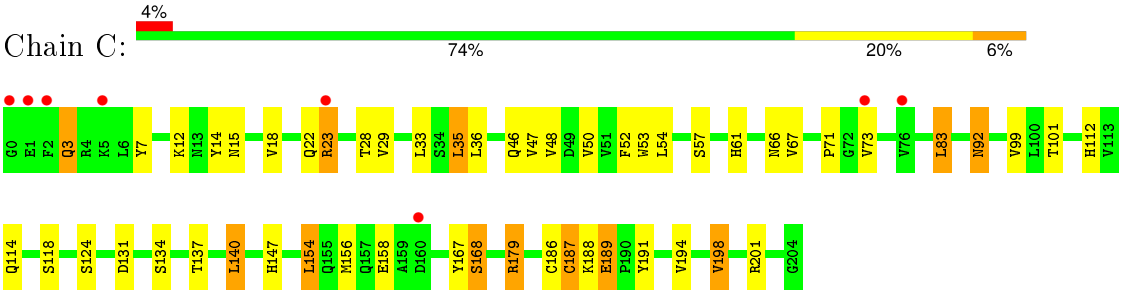
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

Chain A:



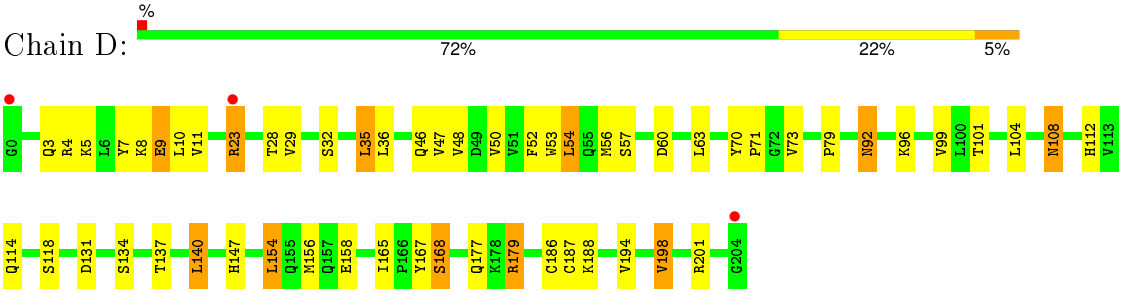
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

Chain C:



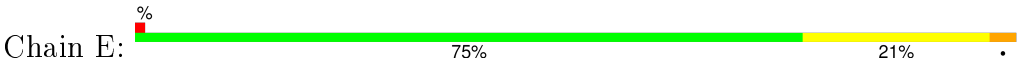
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

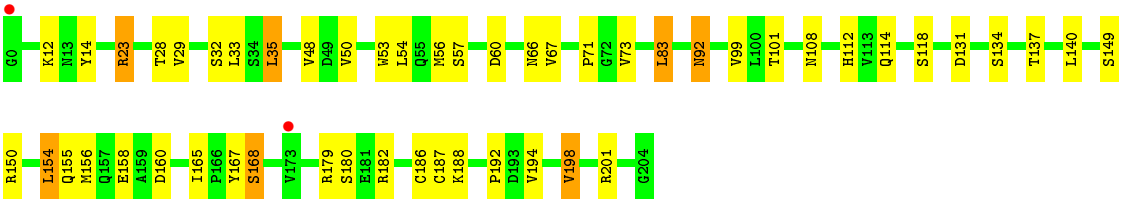
Chain D:



• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

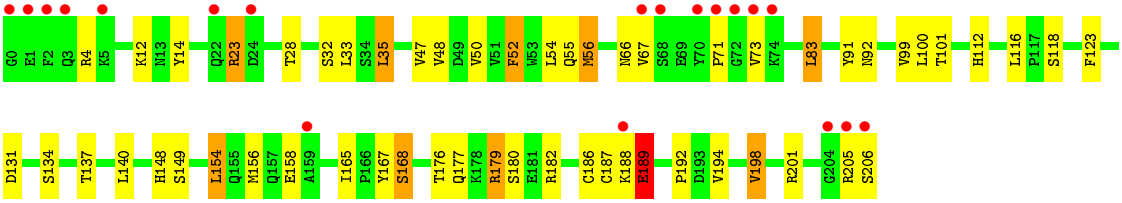
Chain E:





• Molecule 2: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.70Å 119.60Å 143.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.72 – 2.85 47.72 – 2.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.72-2.85) 99.7 (47.72-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.161 , 0.217 0.168 , 0.226	Depositor DCC
R_{free} test set	1552 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	67.5	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 83.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 31080 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9054	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: 9Z0, GOL, NAG, L0B

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	0.51	1/1715 (0.1%)	0.78	0/2333
1	C	0.51	0/1715	0.78	1/2333 (0.0%)
1	D	0.55	0/1715	0.82	1/2333 (0.0%)
1	E	0.52	0/1715	0.77	0/2333
2	B	0.47	0/1732	0.77	0/2355
All	All	0.51	1/8592 (0.0%)	0.78	2/11687 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	ILE	CG1-CD1	5.45	1.88	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	187	CYS	N-CA-C	5.88	126.87	111.00
1	D	10	LEU	C-N-CA	5.10	134.46	121.70

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	1670	0	1633	19	0
1	C	1670	0	1633	25	0
1	D	1670	0	1633	32	0
1	E	1670	0	1633	24	0
2	B	1687	0	1651	24	0
3	A	28	0	26	4	0
3	B	28	0	26	3	0
3	C	28	0	26	1	0
3	D	28	0	26	5	0
3	E	28	0	26	6	0
4	A	25	0	27	0	0
4	B	25	0	27	1	0
4	C	25	0	27	4	0
4	D	25	0	27	4	0
4	E	25	0	27	0	0
5	A	6	0	8	2	0
5	C	6	0	7	4	0
5	D	6	0	8	3	0
5	E	6	0	8	1	0
6	A	14	0	10	1	0
6	B	14	0	10	2	0
6	C	14	0	10	0	0
6	D	14	0	10	1	0
6	E	14	0	10	0	0
7	A	73	0	0	0	0
7	B	40	0	0	1	0
7	C	73	0	0	2	0
7	D	75	0	0	5	0
7	E	67	0	0	2	0
All	All	9054	0	8529	132	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 8.

All (132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:CD1	1:A:161:ILE:CG1	1.88	1.47
2:B:52:PHE:CE1	6:B:1208:9Z0:BR2	2.73	0.97
1:E:160:ASP:HB2	7:E:2019:HOH:O	1.67	0.94
2:B:52:PHE:CZ	6:B:1208:9Z0:BR2	2.77	0.93
2:B:33:LEU:HD21	2:B:52:PHE:CD2	2.10	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:301:NAG:H61	3:C:302:NAG:H82	1.66	0.77
1:D:147:HIS:HE1	7:D:2035:HOH:O	1.67	0.77
3:A:301:NAG:H61	3:A:302:NAG:H82	1.68	0.74
4:C:1205:L0B:H10	1:D:53:TRP:CD2	2.23	0.73
3:B:301:NAG:H61	3:B:302:NAG:H82	1.71	0.72
3:E:301:NAG:H61	3:E:302:NAG:H82	1.69	0.71
2:B:156:MET:SD	2:B:177:GLN:HG2	2.31	0.71
3:D:301:NAG:H61	3:D:302:NAG:H82	1.74	0.70
2:B:55:GLN:HA	2:B:116:LEU:HD12	1.73	0.70
1:C:101:THR:HG23	1:C:118:SER:HB2	1.78	0.65
2:B:33:LEU:HD21	2:B:52:PHE:HD2	1.62	0.65
1:C:92:ASN:HA	5:C:1206:GOL:H12	1.79	0.64
5:C:1206:GOL:H32	1:D:165:ILE:HD13	1.78	0.64
1:D:4:ARG:HH11	1:D:4:ARG:HG2	1.63	0.64
1:E:101:THR:HG23	1:E:118:SER:HB2	1.81	0.63
1:A:92:ASN:HA	5:A:1206:GOL:H31	1.81	0.63
1:D:101:THR:HG23	1:D:118:SER:HB2	1.80	0.63
2:B:101:THR:HG23	2:B:118:SER:HB2	1.81	0.62
1:D:46:GLN:HE21	1:E:167:TYR:HB2	1.65	0.61
1:D:154:LEU:HD13	1:D:194:VAL:HG23	1.84	0.60
2:B:154:LEU:HD13	2:B:194:VAL:HG23	1.84	0.58
1:A:101:THR:HG23	1:A:118:SER:HB2	1.84	0.58
5:C:1206:GOL:H32	1:D:165:ILE:CD1	2.34	0.58
1:A:186:CYS:SG	1:A:187:CYS:N	2.77	0.57
1:C:57:SER:HB2	1:C:112:HIS:CE1	2.39	0.57
1:A:154:LEU:HD13	1:A:194:VAL:HG23	1.86	0.57
5:D:1206:GOL:H11	1:E:165:ILE:HD11	1.87	0.57
1:E:154:LEU:HD13	1:E:194:VAL:HG23	1.87	0.56
5:D:1206:GOL:H11	1:E:165:ILE:CD1	2.37	0.55
5:A:1206:GOL:H12	2:B:165:ILE:HD11	1.89	0.54
1:D:92:ASN:HA	5:D:1206:GOL:H32	1.90	0.54
1:C:156:MET:HG3	1:C:179:ARG:HB3	1.90	0.54
1:E:156:MET:HB2	7:E:2053:HOH:O	2.06	0.54
1:D:11:VAL:N	7:D:2003:HOH:O	2.40	0.53
4:D:1205:L0B:H5	1:E:114:GLN:NE2	2.24	0.53
1:A:112:HIS:CD2	3:A:301:NAG:H62	2.44	0.52
1:C:14:TYR:HE2	1:C:83:LEU:HA	1.74	0.52
1:D:112:HIS:CD2	3:D:301:NAG:H62	2.44	0.52
1:C:191:TYR:CE2	4:C:1205:L0B:H121	2.45	0.52
1:A:22:GLN:HB3	1:A:61:HIS:CE1	2.44	0.52
6:D:1207:9Z0:H041	7:D:2039:HOH:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:MET:HG3	1:D:179:ARG:HB3	1.93	0.51
1:A:156:MET:HG3	1:A:179:ARG:HB3	1.93	0.50
1:C:154:LEU:HD13	1:C:194:VAL:HG23	1.92	0.50
1:E:14:TYR:HE2	1:E:83:LEU:HA	1.77	0.50
2:B:32:SER:HB3	2:B:55:GLN:HB2	1.93	0.50
1:A:14:TYR:HE2	1:A:83:LEU:HA	1.76	0.50
2:B:156:MET:HG3	2:B:179:ARG:HB3	1.94	0.49
2:B:52:PHE:HZ	2:B:123:PHE:HZ	1.59	0.49
1:E:108:ASN:ND2	3:E:301:NAG:O5	2.46	0.49
1:C:35:LEU:HD21	1:C:50:VAL:HG22	1.95	0.49
1:C:114:GLN:HG2	7:C:2022:HOH:O	2.12	0.49
2:B:176:THR:HA	7:B:2029:HOH:O	2.11	0.49
1:C:46:GLN:HE21	1:D:167:TYR:HB2	1.78	0.49
4:D:1205:L0B:H10	1:E:53:TRP:CG	2.47	0.48
1:A:31:PHE:CZ	1:A:33:LEU:HD22	2.48	0.48
1:E:108:ASN:HD22	1:E:112:HIS:HB3	1.78	0.48
4:C:1205:L0B:H5	1:D:114:GLN:NE2	2.29	0.48
2:B:14:TYR:HE2	2:B:83:LEU:HA	1.76	0.48
6:A:1207:9Z0:H062	2:B:100:LEU:O	2.13	0.48
1:E:112:HIS:CD2	3:E:301:NAG:H62	2.48	0.48
4:C:1205:L0B:H10	1:D:53:TRP:CE3	2.48	0.47
1:C:186:CYS:SG	1:C:187:CYS:N	2.88	0.47
1:D:108:ASN:ND2	3:D:301:NAG:O5	2.48	0.47
1:E:186:CYS:SG	1:E:187:CYS:N	2.88	0.47
1:D:35:LEU:HD21	1:D:50:VAL:HG22	1.97	0.47
1:C:187:CYS:C	1:C:189:GLU:H	2.18	0.46
1:A:52:PHE:HZ	1:A:140:LEU:HD23	1.81	0.46
1:D:96:LYS:NZ	7:D:2041:HOH:O	2.48	0.46
2:B:52:PHE:HZ	2:B:123:PHE:CZ	2.33	0.46
2:B:112:HIS:CD2	3:B:301:NAG:H62	2.51	0.46
1:D:186:CYS:SG	1:D:187:CYS:N	2.88	0.46
2:B:35:LEU:HD21	2:B:50:VAL:HG22	1.98	0.46
3:A:301:NAG:HO4	3:A:302:NAG:C1	2.28	0.46
1:E:35:LEU:HD21	1:E:50:VAL:HG22	1.98	0.46
1:C:57:SER:HB2	1:C:112:HIS:HE1	1.79	0.45
1:E:92:ASN:HA	5:E:1206:GOL:H32	1.98	0.45
1:A:55:GLN:HG2	1:A:116:LEU:HD22	1.98	0.45
1:D:177:GLN:HB2	7:D:2065:HOH:O	2.16	0.45
1:C:147:HIS:HE1	7:C:2029:HOH:O	1.99	0.45
1:E:108:ASN:CG	3:E:301:NAG:C1	2.85	0.45
2:B:148:HIS:ND1	2:B:189:GLU:HG2	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:SER:HB2	1:E:112:HIS:NE2	2.32	0.45
1:A:35:LEU:HD21	1:A:50:VAL:HG22	1.98	0.45
1:D:9:GLU:HG3	1:D:70:TYR:OH	2.17	0.44
1:D:60:ASP:HB3	1:D:63:LEU:HD12	2.00	0.44
1:C:3:GLN:HE21	1:C:7:TYR:HE1	1.64	0.44
1:D:52:PHE:HZ	1:D:140:LEU:HD23	1.82	0.44
1:E:155:GLN:HA	1:E:155:GLN:NE2	2.33	0.44
3:D:301:NAG:O4	3:D:302:NAG:O5	2.31	0.44
4:D:1205:L0B:H10	1:E:53:TRP:CD1	2.53	0.44
1:A:137:THR:HA	1:A:198:VAL:O	2.18	0.44
3:E:301:NAG:O4	3:E:302:NAG:O5	2.29	0.43
1:D:54:LEU:HD13	1:D:56:MET:HE2	2.01	0.43
1:A:167:TYR:O	1:A:168:SER:CB	2.66	0.43
1:A:36:LEU:HD11	1:A:53:TRP:HB2	2.01	0.43
1:A:108:ASN:CG	3:A:301:NAG:C1	2.87	0.43
1:D:167:TYR:O	1:D:168:SER:CB	2.66	0.43
1:C:22:GLN:HG3	1:C:61:HIS:CE1	2.53	0.43
1:C:15:ASN:H	1:D:4:ARG:HH12	1.66	0.42
2:B:137:THR:HA	2:B:198:VAL:O	2.19	0.42
1:E:167:TYR:O	1:E:168:SER:CB	2.68	0.42
2:B:91:TYR:CD2	4:B:1207:L0B:H18	2.54	0.42
1:C:18:VAL:HG22	1:D:7:TYR:CD2	2.54	0.42
1:D:137:THR:HA	1:D:198:VAL:O	2.19	0.42
3:E:301:NAG:HO4	3:E:302:NAG:C5	2.33	0.42
2:B:167:TYR:O	2:B:168:SER:CB	2.67	0.42
3:D:301:NAG:HO4	3:D:302:NAG:C5	2.33	0.41
1:C:137:THR:HA	1:C:198:VAL:O	2.20	0.41
2:B:180:SER:O	2:B:192:PRO:HA	2.20	0.41
3:B:301:NAG:O4	3:B:302:NAG:O5	2.31	0.41
1:D:5:LYS:O	1:D:9:GLU:HG2	2.19	0.41
1:E:180:SER:O	1:E:192:PRO:HA	2.20	0.41
1:C:167:TYR:O	1:C:168:SER:CB	2.68	0.41
4:D:1205:L0B:H132	4:D:1205:L0B:H222	1.79	0.41
1:D:79:PRO:HA	1:D:104:LEU:HD23	2.02	0.41
1:E:137:THR:HA	1:E:198:VAL:O	2.20	0.41
1:C:187:CYS:O	1:C:188:LYS:HB2	2.20	0.41
1:A:79:PRO:HA	1:A:104:LEU:HD23	2.02	0.41
1:E:14:TYR:OH	1:E:60:ASP:OD2	2.32	0.41
1:C:52:PHE:HZ	1:C:140:LEU:HD23	1.85	0.41
2:B:56:MET:HB2	2:B:56:MET:HE2	1.97	0.40
1:D:36:LEU:HD11	1:D:53:TRP:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:SER:CB	5:C:1206:GOL:H31	2.51	0.40
1:C:36:LEU:HD11	1:C:53:TRP:HB2	2.03	0.40
1:C:15:ASN:H	1:D:4:ARG:NH1	2.20	0.40
1:A:175:VAL:HG22	1:A:198:VAL:HG13	2.04	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	203/205 (99%)	193 (95%)	6 (3%)	4 (2%)	9 30
1	C	203/205 (99%)	193 (95%)	6 (3%)	4 (2%)	9 30
1	D	203/205 (99%)	193 (95%)	7 (3%)	3 (2%)	13 38
1	E	203/205 (99%)	193 (95%)	6 (3%)	4 (2%)	9 30
2	B	205/207 (99%)	193 (94%)	6 (3%)	6 (3%)	6 20
All	All	1017/1027 (99%)	965 (95%)	31 (3%)	21 (2%)	9 29

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	23	ARG
1	D	23	ARG
1	A	23	ARG
2	B	23	ARG
2	B	149	SER
1	D	73	VAL
1	E	12	LYS
1	E	23	ARG
2	B	12	LYS
2	B	71	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	12	LYS
1	C	71	PRO
1	D	71	PRO
1	A	12	LYS
1	A	71	PRO
2	B	189	GLU
1	E	71	PRO
1	A	73	VAL
2	B	73	VAL
1	E	73	VAL
1	C	73	VAL

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	190/190 (100%)	164 (86%)	26 (14%)	4 12
1	C	190/190 (100%)	166 (87%)	24 (13%)	5 14
1	D	190/190 (100%)	165 (87%)	25 (13%)	5 13
1	E	190/190 (100%)	163 (86%)	27 (14%)	4 11
2	B	192/192 (100%)	162 (84%)	30 (16%)	3 8
All	All	952/952 (100%)	820 (86%)	132 (14%)	4 11

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	23	ARG
1	A	28	THR
1	A	29	VAL
1	A	33	LEU
1	A	35	LEU
1	A	48	VAL
1	A	54	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	56	MET
1	A	57	SER
1	A	66	ASN
1	A	67	VAL
1	A	83	LEU
1	A	92	ASN
1	A	99	VAL
1	A	131	ASP
1	A	134	SER
1	A	140	LEU
1	A	154	LEU
1	A	168	SER
1	A	179	ARG
1	A	182	ARG
1	A	185	GLU
1	A	188	LYS
1	A	198	VAL
1	A	201	ARG
2	B	4	ARG
2	B	23	ARG
2	B	28	THR
2	B	35	LEU
2	B	47	VAL
2	B	48	VAL
2	B	52	PHE
2	B	54	LEU
2	B	56	MET
2	B	66	ASN
2	B	67	VAL
2	B	83	LEU
2	B	92	ASN
2	B	99	VAL
2	B	131	ASP
2	B	134	SER
2	B	140	LEU
2	B	154	LEU
2	B	158	GLU
2	B	168	SER
2	B	179	ARG
2	B	182	ARG
2	B	186	CYS
2	B	187	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	188	LYS
2	B	189	GLU
2	B	198	VAL
2	B	201	ARG
2	B	205	ARG
2	B	206	SER
1	C	3	GLN
1	C	23	ARG
1	C	28	THR
1	C	29	VAL
1	C	33	LEU
1	C	35	LEU
1	C	47	VAL
1	C	48	VAL
1	C	54	LEU
1	C	66	ASN
1	C	67	VAL
1	C	83	LEU
1	C	92	ASN
1	C	99	VAL
1	C	131	ASP
1	C	134	SER
1	C	140	LEU
1	C	154	LEU
1	C	158	GLU
1	C	168	SER
1	C	179	ARG
1	C	189	GLU
1	C	198	VAL
1	C	201	ARG
1	D	3	GLN
1	D	8	LYS
1	D	9	GLU
1	D	23	ARG
1	D	28	THR
1	D	29	VAL
1	D	32	SER
1	D	35	LEU
1	D	47	VAL
1	D	48	VAL
1	D	54	LEU
1	D	57	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	92	ASN
1	D	99	VAL
1	D	108	ASN
1	D	131	ASP
1	D	134	SER
1	D	140	LEU
1	D	154	LEU
1	D	158	GLU
1	D	168	SER
1	D	179	ARG
1	D	188	LYS
1	D	198	VAL
1	D	201	ARG
1	E	23	ARG
1	E	28	THR
1	E	29	VAL
1	E	32	SER
1	E	33	LEU
1	E	35	LEU
1	E	48	VAL
1	E	54	LEU
1	E	56	MET
1	E	66	ASN
1	E	67	VAL
1	E	83	LEU
1	E	92	ASN
1	E	99	VAL
1	E	131	ASP
1	E	134	SER
1	E	140	LEU
1	E	149	SER
1	E	150	ARG
1	E	154	LEU
1	E	158	GLU
1	E	168	SER
1	E	179	ARG
1	E	182	ARG
1	E	188	LYS
1	E	198	VAL
1	E	201	ARG

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

Mol	Chain	Res	Type
1	A	61	HIS
1	A	112	HIS
2	B	22	GLN
2	B	55	GLN
2	B	147	HIS
1	C	3	GLN
1	C	46	GLN
1	C	112	HIS
1	C	147	HIS
1	D	46	GLN
1	E	22	GLN
1	E	108	ASN
1	E	112	HIS
1	E	114	GLN
1	E	155	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

24 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	$\#\|Z\|>2$
4	L0B	A	1205	-	27,27,27	0.90	1 (3%)	30,36,36	1.00	2 (6%)
5	GOL	A	1206	-	5,5,5	0.97	0	5,5,5	1.23	1 (20%)
6	9Z0	A	1207	-	12,14,14	1.88	2 (16%)	10,18,18	1.87	2 (20%)
3	NAG	A	301	-	14,14,15	1.28	3 (21%)	15,19,21	1.87	5 (33%)
3	NAG	A	302	-	14,14,15	1.50	4 (28%)	15,19,21	1.94	4 (26%)
4	L0B	B	1207	-	27,27,27	0.75	0	30,36,36	1.13	4 (13%)
6	9Z0	B	1208	-	12,14,14	1.76	2 (16%)	10,18,18	2.57	6 (60%)
3	NAG	B	301	-	14,14,15	1.24	3 (21%)	15,19,21	1.70	5 (33%)
3	NAG	B	302	-	14,14,15	1.66	6 (42%)	15,19,21	2.15	4 (26%)
4	L0B	C	1205	-	27,27,27	0.80	1 (3%)	30,36,36	1.32	2 (6%)
5	GOL	C	1206	-	5,5,5	1.57	1 (20%)	5,5,5	2.49	3 (60%)
6	9Z0	C	1207	-	12,14,14	1.84	2 (16%)	10,18,18	2.11	4 (40%)
3	NAG	C	301	-	14,14,15	1.35	3 (21%)	15,19,21	1.49	4 (26%)
3	NAG	C	302	-	14,14,15	1.55	4 (28%)	15,19,21	1.94	3 (20%)
4	L0B	D	1205	-	27,27,27	0.74	0	30,36,36	1.33	7 (23%)
5	GOL	D	1206	-	5,5,5	1.08	0	5,5,5	2.07	1 (20%)
6	9Z0	D	1207	-	12,14,14	1.98	3 (25%)	10,18,18	1.89	4 (40%)
3	NAG	D	301	-	14,14,15	1.26	2 (14%)	15,19,21	2.31	4 (26%)
3	NAG	D	302	-	14,14,15	1.49	2 (14%)	15,19,21	1.93	3 (20%)
4	L0B	E	1205	-	27,27,27	0.65	0	30,36,36	0.99	4 (13%)
5	GOL	E	1206	-	5,5,5	1.20	1 (20%)	5,5,5	2.61	2 (40%)
6	9Z0	E	1207	-	12,14,14	1.70	2 (16%)	10,18,18	2.13	5 (50%)
3	NAG	E	301	-	14,14,15	1.22	3 (21%)	15,19,21	1.64	3 (20%)
3	NAG	E	302	-	14,14,15	1.55	3 (21%)	15,19,21	1.98	3 (20%)

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	L0B	A	1205	-	-	0/16/30/30	0/3/3/3
5	GOL	A	1206	-	-	0/4/4/4	0/0/0/0
6	9Z0	A	1207	-	-	0/6/9/9	0/1/1/1
3	NAG	A	301	-	-	0/6/23/26	0/1/1/1
3	NAG	A	302	-	-	0/6/23/26	0/1/1/1
4	L0B	B	1207	-	-	0/16/30/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	9Z0	B	1208	-	-	0/6/9/9	0/1/1/1
3	NAG	B	301	-	-	0/6/23/26	0/1/1/1
3	NAG	B	302	-	-	0/6/23/26	0/1/1/1
4	L0B	C	1205	-	-	0/16/30/30	0/3/3/3
5	GOL	C	1206	-	-	0/4/4/4	0/0/0/0
6	9Z0	C	1207	-	-	0/6/9/9	0/1/1/1
3	NAG	C	301	-	-	0/6/23/26	0/1/1/1
3	NAG	C	302	-	-	0/6/23/26	0/1/1/1
4	L0B	D	1205	-	-	0/16/30/30	0/3/3/3
5	GOL	D	1206	-	-	0/4/4/4	0/0/0/0
6	9Z0	D	1207	-	-	0/6/9/9	0/1/1/1
3	NAG	D	301	-	-	0/6/23/26	0/1/1/1
3	NAG	D	302	-	-	0/6/23/26	0/1/1/1
4	L0B	E	1205	-	-	0/16/30/30	0/3/3/3
5	GOL	E	1206	-	-	0/4/4/4	0/0/0/0
6	9Z0	E	1207	-	-	0/6/9/9	0/1/1/1
3	NAG	E	301	-	-	0/6/23/26	0/1/1/1
3	NAG	E	302	-	-	0/6/23/26	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1206	GOL	O2-C2	-2.54	1.35	1.43
4	C	1205	L0B	C17-C16	-2.29	1.48	1.52
3	C	301	NAG	O5-C1	-2.22	1.40	1.43
5	E	1206	GOL	C1-C2	-2.17	1.44	1.52
4	A	1205	L0B	C17-C16	-2.03	1.48	1.52
3	A	301	NAG	C4-C3	2.00	1.57	1.52
3	B	301	NAG	O3-C3	2.02	1.47	1.43
3	C	302	NAG	C4-C3	2.05	1.57	1.52
3	A	302	NAG	C4-C5	2.05	1.57	1.53
3	B	302	NAG	C4-C5	2.08	1.57	1.53
3	B	302	NAG	C3-C2	2.10	1.57	1.52
3	C	302	NAG	C4-C5	2.12	1.57	1.53
3	B	302	NAG	O5-C5	2.13	1.48	1.43
3	A	302	NAG	C4-C3	2.14	1.58	1.52
3	E	302	NAG	C4-C3	2.15	1.58	1.52
3	E	301	NAG	C3-C2	2.20	1.57	1.52
3	D	301	NAG	C4-C5	2.21	1.57	1.53
3	E	301	NAG	C4-C3	2.22	1.58	1.52
3	B	302	NAG	O3-C3	2.22	1.48	1.43
3	A	301	NAG	C3-C2	2.29	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1207	9Z0	BR1-C10	2.33	1.95	1.89
3	D	301	NAG	C4-C3	2.35	1.58	1.52
3	B	301	NAG	C3-C2	2.35	1.57	1.52
3	D	302	NAG	C3-C2	2.36	1.57	1.52
3	A	301	NAG	C4-C5	2.38	1.58	1.53
3	A	302	NAG	C3-C2	2.39	1.58	1.52
3	C	302	NAG	C3-C2	2.40	1.58	1.52
3	C	301	NAG	C3-C2	2.40	1.58	1.52
3	E	301	NAG	C1-C2	2.51	1.55	1.52
3	B	301	NAG	C4-C3	2.51	1.59	1.52
3	E	302	NAG	C4-C5	2.54	1.58	1.53
3	C	301	NAG	C4-C3	2.56	1.59	1.52
6	B	1208	9Z0	BR2-C12	2.59	1.94	1.90
3	A	302	NAG	C1-C2	2.60	1.56	1.52
3	B	302	NAG	C4-C3	2.60	1.59	1.52
3	D	302	NAG	C1-C2	2.64	1.56	1.52
3	B	302	NAG	C1-C2	2.69	1.56	1.52
3	E	302	NAG	C1-C2	2.77	1.56	1.52
6	E	1207	9Z0	BR2-C12	2.85	1.94	1.90
3	C	302	NAG	C1-C2	2.85	1.56	1.52
6	A	1207	9Z0	BR2-C12	3.64	1.95	1.90
6	C	1207	9Z0	BR2-C12	3.88	1.96	1.90
6	D	1207	9Z0	BR2-C12	4.19	1.96	1.90
6	D	1207	9Z0	C02-N03	4.57	1.43	1.33
6	C	1207	9Z0	C02-N03	4.62	1.43	1.33
6	E	1207	9Z0	C02-N03	4.63	1.43	1.33
6	A	1207	9Z0	C02-N03	4.84	1.44	1.33
6	B	1208	9Z0	C02-N03	4.95	1.44	1.33

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1206	GOL	C3-C2-C1	-5.14	90.95	111.12
4	C	1205	L0B	C22-N1-C9	-5.08	108.80	113.20
3	D	301	NAG	C1-O5-C5	-4.90	106.03	112.25
5	D	1206	GOL	C3-C2-C1	-4.12	94.97	111.12
5	C	1206	GOL	O1-C1-C2	-3.97	90.91	110.18
3	A	301	NAG	C1-O5-C5	-3.83	107.39	112.25
4	A	1205	L0B	C22-N1-C11	-3.61	110.08	113.20
3	D	301	NAG	C8-C7-N2	-3.58	109.26	116.11
6	B	1208	9Z0	BR1-C10-C12	-3.49	123.83	127.63
4	B	1207	L0B	C22-N1-C11	-3.43	110.24	113.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	301	NAG	C1-O5-C5	-3.29	108.08	112.25
4	D	1205	L0B	C22-N1-C11	-2.99	110.61	113.20
5	C	1206	GOL	O2-C2-C1	-2.95	95.13	108.65
6	C	1207	9Z0	BR1-C10-C12	-2.92	124.45	127.63
3	E	301	NAG	C1-O5-C5	-2.81	108.68	112.25
6	E	1207	9Z0	BR1-C10-C12	-2.81	124.57	127.63
4	C	1205	L0B	C14-C16-C17	-2.55	106.64	111.36
5	C	1206	GOL	C3-C2-C1	-2.54	101.15	111.12
3	A	301	NAG	C4-C3-C2	-2.54	107.28	111.23
4	B	1207	L0B	C22-N1-C9	-2.53	111.01	113.20
4	E	1205	L0B	C22-N1-C9	-2.47	111.06	113.20
4	E	1205	L0B	C14-C11-C13	-2.46	108.34	113.10
5	E	1206	GOL	O1-C1-C2	-2.43	98.40	110.18
3	D	301	NAG	C4-C3-C2	-2.43	107.45	111.23
4	B	1207	L0B	C14-C11-C13	-2.42	108.42	113.10
3	C	301	NAG	C4-C3-C2	-2.40	107.50	111.23
3	C	301	NAG	C1-O5-C5	-2.39	109.21	112.25
4	D	1205	L0B	C8-C3-C1	-2.32	116.24	118.72
3	C	302	NAG	C8-C7-N2	-2.25	111.81	116.11
4	D	1205	L0B	C14-C16-C17	-2.25	107.20	111.36
3	B	301	NAG	C4-C3-C2	-2.18	107.84	111.23
4	B	1207	L0B	C8-C3-C1	-2.15	116.42	118.72
5	A	1206	GOL	C3-C2-C1	-2.11	102.84	111.12
4	E	1205	L0B	C14-C16-C17	-2.11	107.45	111.36
6	B	1208	9Z0	BR2-C12-C10	-2.10	123.56	126.70
4	D	1205	L0B	C13-C11-N1	-2.06	107.26	111.42
3	A	302	NAG	C8-C7-N2	-2.06	112.17	116.11
4	A	1205	L0B	C14-C11-C13	-2.05	109.14	113.10
3	E	302	NAG	O7-C7-N2	2.01	125.95	121.86
6	E	1207	9Z0	BR1-C10-C09	2.03	127.59	124.40
3	B	301	NAG	C3-C2-N2	2.03	115.43	110.56
6	C	1207	9Z0	BR1-C10-C09	2.05	127.63	124.40
3	C	301	NAG	O4-C4-C3	2.09	115.05	110.34
6	D	1207	9Z0	BR1-C10-C12	2.10	129.92	127.63
3	A	302	NAG	C3-C2-N2	2.11	115.62	110.56
3	D	302	NAG	C2-N2-C7	2.13	125.77	123.04
4	E	1205	L0B	O1-C3-C8	2.15	123.16	120.75
3	A	301	NAG	C2-N2-C7	2.15	125.81	123.04
3	B	301	NAG	O4-C4-C3	2.16	115.20	110.34
6	E	1207	9Z0	C05-C04-N03	2.17	118.54	112.19
3	A	302	NAG	C4-C3-C2	2.18	114.62	111.23
3	E	301	NAG	O3-C3-C4	2.21	115.31	110.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	302	NAG	C4-C3-C2	2.22	114.69	111.23
3	E	302	NAG	O4-C4-C5	2.24	115.17	109.24
4	D	1205	L0B	C15-C12-C9	2.25	114.98	110.86
3	B	302	NAG	C3-C2-N2	2.29	116.04	110.56
3	B	302	NAG	C4-C3-C2	2.31	114.83	111.23
4	D	1205	L0B	O1-C3-C8	2.35	123.38	120.75
3	B	301	NAG	O3-C3-C4	2.36	115.66	110.34
3	C	302	NAG	C4-C3-C2	2.48	115.08	111.23
6	B	1208	9Z0	C05-C04-N03	2.50	119.52	112.19
3	A	301	NAG	O4-C4-C3	2.56	116.10	110.34
4	D	1205	L0B	O2-C16-C14	2.60	114.08	108.94
3	B	302	NAG	O4-C4-C5	2.64	116.23	109.24
6	D	1207	9Z0	C08-C02-N03	2.68	119.03	115.42
3	C	301	NAG	O3-C3-C4	2.75	116.53	110.34
6	B	1208	9Z0	BR1-C10-C09	2.95	129.04	124.40
6	C	1207	9Z0	C05-C04-N03	2.96	120.85	112.19
6	D	1207	9Z0	C04-C05-C06	3.06	118.32	112.94
6	A	1207	9Z0	C04-C05-C06	3.06	118.33	112.94
3	A	301	NAG	C3-C2-N2	3.09	117.96	110.56
6	B	1208	9Z0	C04-C05-C06	3.10	118.40	112.94
6	E	1207	9Z0	C04-C05-C06	3.14	118.47	112.94
6	D	1207	9Z0	C05-C04-N03	3.34	121.97	112.19
6	E	1207	9Z0	C08-C02-N03	3.63	120.31	115.42
3	E	301	NAG	C3-C2-N2	3.65	119.31	110.56
6	A	1207	9Z0	C05-C04-N03	3.69	123.00	112.19
3	D	301	NAG	C3-C2-N2	3.90	119.89	110.56
6	C	1207	9Z0	C08-C02-N03	3.92	120.70	115.42
6	B	1208	9Z0	C08-C02-N03	4.43	121.38	115.42
3	C	302	NAG	C1-O5-C5	5.81	119.62	112.25
3	A	302	NAG	C1-O5-C5	5.94	119.78	112.25
3	E	302	NAG	C1-O5-C5	6.06	119.94	112.25
3	D	302	NAG	C1-O5-C5	6.19	120.10	112.25
3	B	302	NAG	C1-O5-C5	6.62	120.65	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1206	GOL	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1207	9Z0	1	0
3	A	301	NAG	4	0
3	A	302	NAG	2	0
4	B	1207	L0B	1	0
6	B	1208	9Z0	2	0
3	B	301	NAG	3	0
3	B	302	NAG	2	0
4	C	1205	L0B	4	0
5	C	1206	GOL	4	0
3	C	301	NAG	1	0
3	C	302	NAG	1	0
4	D	1205	L0B	4	0
5	D	1206	GOL	3	0
6	D	1207	9Z0	1	0
3	D	301	NAG	5	0
3	D	302	NAG	3	0
5	E	1206	GOL	1	0
3	E	301	NAG	6	0
3	E	302	NAG	3	0

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	A	205/205 (100%)	0.17	8 (3%) 43 36	47, 78, 136, 155	0
1	C	205/205 (100%)	0.09	8 (3%) 43 36	51, 79, 138, 160	0
1	D	205/205 (100%)	-0.04	3 (1%) 76 73	45, 70, 110, 158	0
1	E	205/205 (100%)	-0.02	2 (0%) 84 81	45, 72, 120, 137	0
2	B	207/207 (100%)	0.48	19 (9%) 11 7	56, 96, 142, 187	0
All	All	1027/1027 (100%)	0.14	40 (3%) 43 36	45, 79, 136, 187	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	0	GLY	8.8
2	B	206	SER	7.3
2	B	205	ARG	5.7
2	B	0	GLY	5.3
2	B	2	PHE	4.6
1	A	23	ARG	4.5
2	B	73	VAL	4.5
1	C	73	VAL	4.2
2	B	5	LYS	3.8
1	D	204	GLY	3.6
2	B	68	SER	3.5
1	E	173	VAL	3.4
1	C	1	GLU	3.3
1	A	62	TYR	3.2
1	A	3	GLN	3.2
2	B	204	GLY	3.1
1	D	0	GLY	2.8
1	A	22	GLN	2.8
1	E	0	GLY	2.7
1	C	2	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	23	ARG	2.6
1	A	2	PHE	2.6
2	B	72	GLY	2.6
1	A	184	TYR	2.6
2	B	74	LYS	2.6
2	B	24	ASP	2.5
1	A	63	LEU	2.5
2	B	67	VAL	2.5
1	C	160	ASP	2.4
2	B	1	GLU	2.2
1	C	76	VAL	2.2
1	C	23	ARG	2.2
1	C	5	LYS	2.2
2	B	188	LYS	2.2
2	B	159	ALA	2.2
2	B	71	PRO	2.1
1	A	185	GLU	2.1
2	B	3	GLN	2.1
2	B	22	GLN	2.0
2	B	70	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no 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
5	GOL	A	1206	6/6	0.90	0.45	9.51	99,100,101,101	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	GOL	D	1206	6/6	0.91	0.39	9.03	72,73,74,77	0
5	GOL	C	1206	6/6	0.92	0.38	5.73	66,67,68,70	0
5	GOL	E	1206	6/6	0.90	0.32	3.67	65,67,69,73	0
4	L0B	D	1205	25/25	0.95	0.24	2.93	27,60,97,136	0
4	L0B	B	1207	25/25	0.91	0.31	1.73	45,86,171,300	0
4	L0B	A	1205	25/25	0.95	0.30	1.21	57,74,295,300	0
4	L0B	E	1205	25/25	0.93	0.22	0.60	36,75,167,260	0
4	L0B	C	1205	25/25	0.93	0.19	0.40	40,78,115,189	0
6	9Z0	D	1207	14/14	0.94	0.19	-0.30	27,67,202,297	2
6	9Z0	A	1207	14/14	0.96	0.19	-0.47	34,65,190,236	2
6	9Z0	C	1207	14/14	0.96	0.20	-0.56	47,61,104,126	2
6	9Z0	E	1207	14/14	0.97	0.18	-0.61	23,46,148,205	2
6	9Z0	B	1208	14/14	0.93	0.19	-0.67	25,86,240,251	2
3	NAG	E	301	14/15	0.94	0.15	-	84,91,97,98	0
3	NAG	A	302	14/15	0.83	0.22	-	141,149,156,159	0
3	NAG	E	302	14/15	0.86	0.17	-	116,124,135,136	0
3	NAG	C	302	14/15	0.64	0.33	-	157,168,177,181	0
3	NAG	B	301	14/15	0.85	0.18	-	117,126,132,134	0
3	NAG	B	302	14/15	0.70	0.30	-	123,132,143,144	0
3	NAG	D	301	14/15	0.93	0.14	-	86,92,96,98	0
3	NAG	C	301	14/15	0.93	0.11	-	100,106,117,117	0
3	NAG	A	301	14/15	0.84	0.20	-	91,97,106,107	0
3	NAG	D	302	14/15	0.75	0.29	-	154,158,167,168	0

6.5 Other polymers (i)

There are no such residues in this entry.