



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:07 PM GMT

PDB ID : 5AFL
Title : alpha7-AChBP in complex with lobeline and fragment 3
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 : 2.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

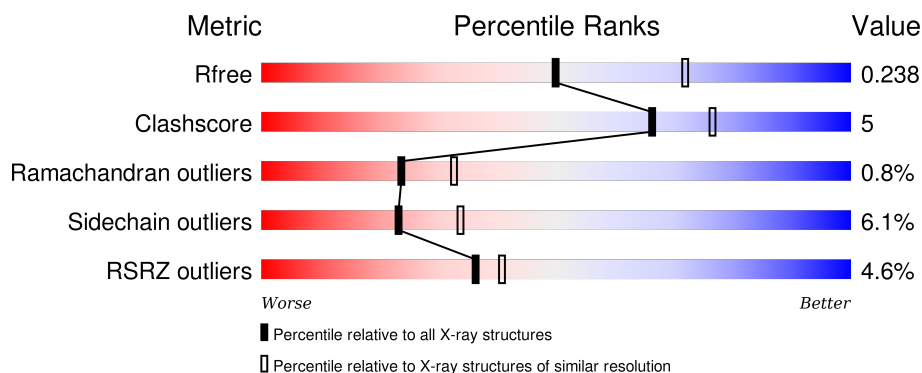
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	205	<div> <div>5%</div> <div>86%</div> <div>12%</div> <div>•</div> </div>
1	B	205	<div> <div>5%</div> <div>85%</div> <div>14%</div> <div></div> </div>
1	C	205	<div> <div>6%</div> <div>85%</div> <div>13%</div> <div>•</div> </div>
1	D	205	<div> <div>5%</div> <div>81%</div> <div>18%</div> <div>•</div> </div>
1	E	205	<div> <div>%</div> <div>88%</div> <div>10%</div> <div>•</div> </div>

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
2	BMA	A	303	X	-	-	-
3	L0B	A	1205	-	-	-	X
3	L0B	C	1205	-	-	-	X
4	GOL	A	1207	-	-	-	X
4	GOL	B	1206	-	-	-	X
4	GOL	D	1206	-	-	-	X
4	GOL	E	1206	-	-	-	X
6	TLA	B	1205	-	-	-	X
8	FHV	E	1207	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8945 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.

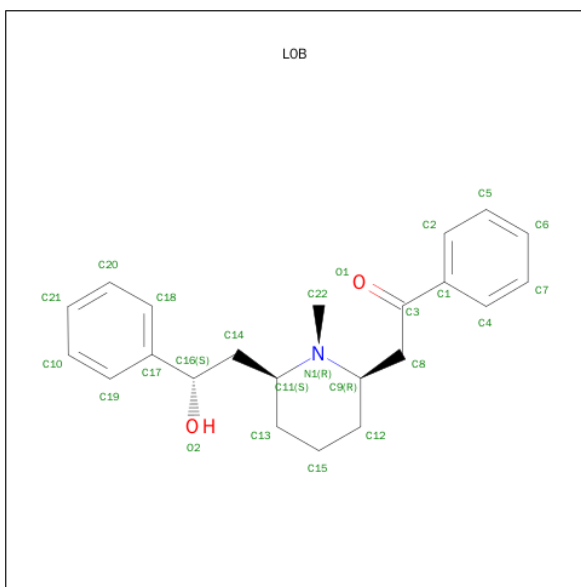
- Molecule 1 is a protein called ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	1	0
			1680	1076	281	316	7			
1	B	205	Total	C	N	O	S	0	0	0
			1671	1071	279	314	7			
1	C	205	Total	C	N	O	S	0	0	0
			1671	1071	279	314	7			
1	D	205	Total	C	N	O	S	0	0	0
			1671	1071	279	314	7			
1	E	205	Total	C	N	O	S	0	1	0
			1679	1076	280	315	8			

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

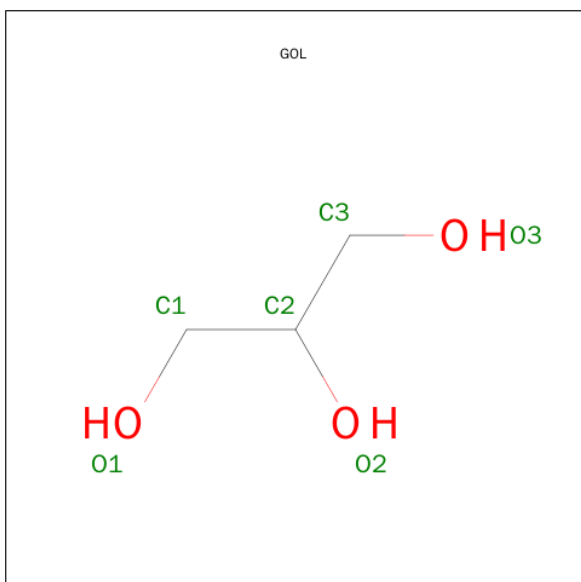
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 3 is ALPHA-LOBELINE (three-letter code: L0B) (formula: C₂₂H₂₇NO₂).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).

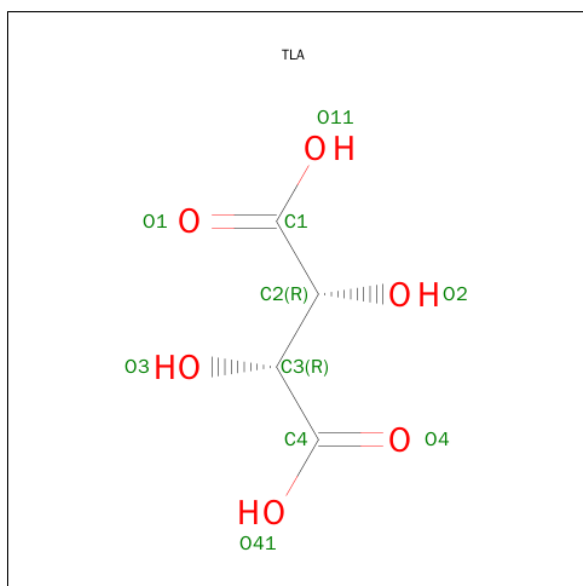


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total C N O 28 16 2 10	0	0
5	C	2	Total C N O 28 16 2 10	0	0
5	D	2	Total C N O 28 16 2 10	0	0

- Molecule 6 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).

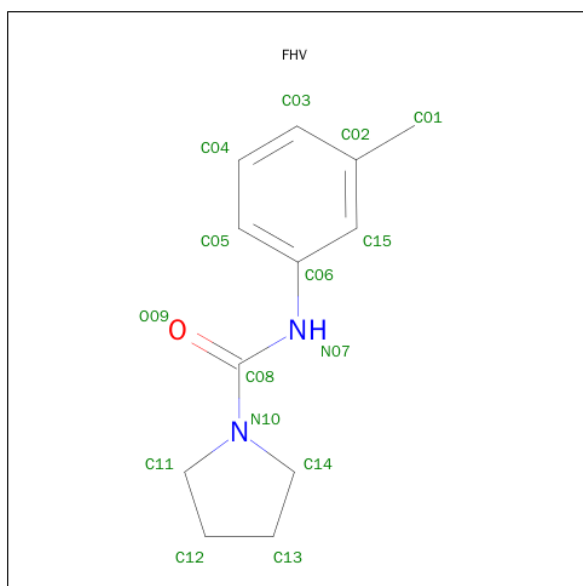


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 10 4 6	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is N-(3-METHYLPHENYL)PYRROLIDINE-1-CARBOXAMIDE (three-letter code: FHV) (formula: C₁₂H₁₆N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	1	Total	C	N	O	0	0
			15	12	2	1		

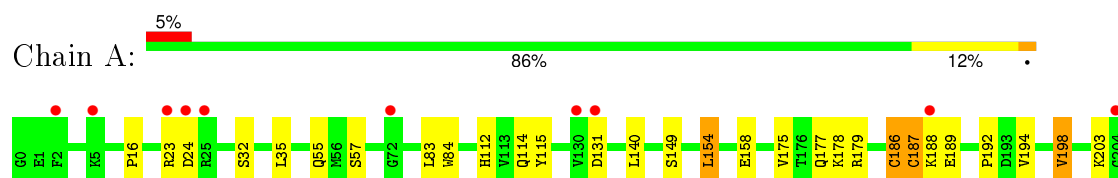
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	58	Total	O	0	0
			58	58		
9	B	48	Total	O	0	0
			48	48		
9	C	35	Total	O	0	0
			35	35		
9	D	37	Total	O	0	0
			37	37		
9	E	53	Total	O	0	0
			53	53		

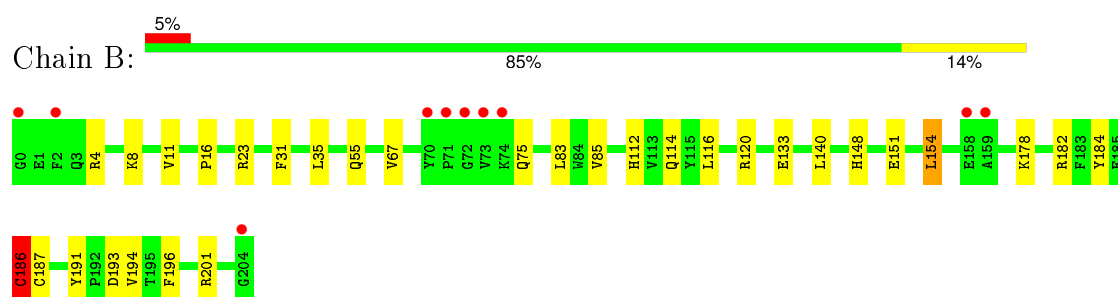
3 Residue-property plots [i](#)

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.

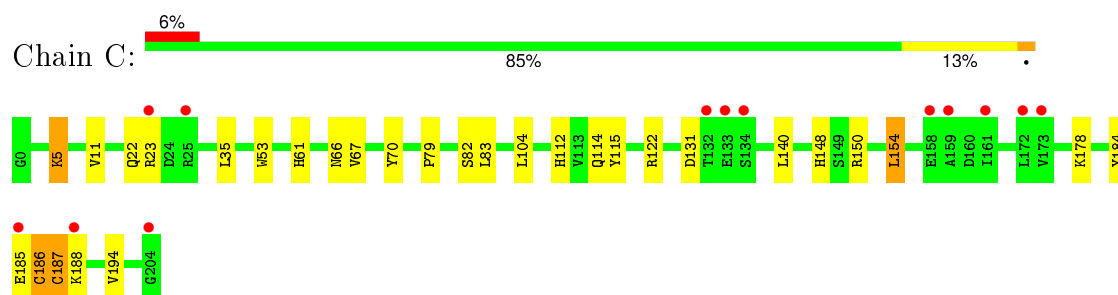
- Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7



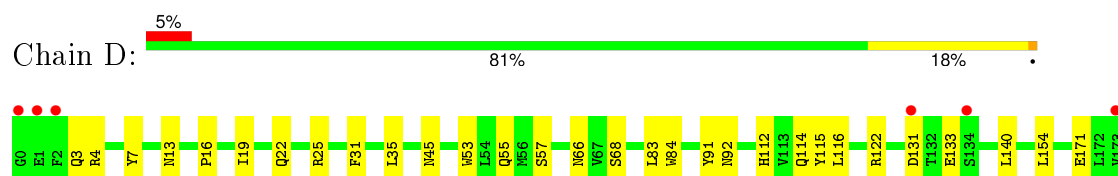
- Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

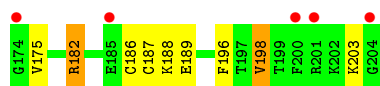


- Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7

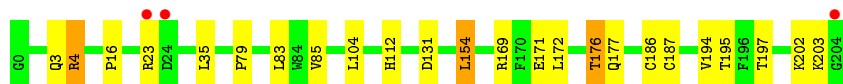
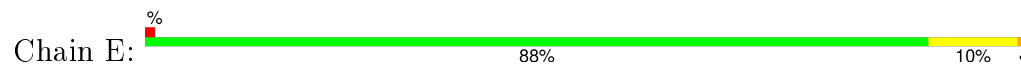


- Molecule 1: ACETYLCHOLINE-BINDING PROTEIN, NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-7





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.81Å 112.30Å 143.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.83 – 2.38 46.98 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.3 (41.83-2.38) 91.0 (46.98-2.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.171 , 0.231 0.184 , 0.238	Depositor DCC
R_{free} test set	2582 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 55695 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8945	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, NDG, TLA, FHV, 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	0.40	0/1725	0.55	0/2345
1	B	0.39	0/1716	0.56	0/2333
1	C	0.33	0/1716	0.51	0/2333
1	D	0.37	0/1716	0.53	0/2333
1	E	0.43	0/1724	0.60	1/2343 (0.0%)
All	All	0.38	0/8597	0.55	1/11687 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	1	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	83	LEU	CA-CB-CG	5.42	127.76	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	303	BMA	C1

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	1680	0	1639	15	0
1	B	1671	0	1632	17	0
1	C	1671	0	1631	13	0
1	D	1671	0	1632	22	0
1	E	1679	0	1640	15	0
2	A	50	0	43	1	0
3	A	25	0	27	0	0
3	C	50	0	54	4	0
3	D	25	0	27	2	0
3	E	25	0	27	3	0
4	A	12	0	16	4	0
4	B	6	0	8	3	0
4	D	6	0	8	1	0
4	E	6	0	8	3	0
5	B	28	0	25	1	0
5	C	28	0	25	1	0
5	D	28	0	25	1	0
6	B	10	0	4	1	0
7	E	28	0	25	1	0
8	E	15	0	16	1	0
9	A	58	0	0	5	0
9	B	48	0	0	1	0
9	C	35	0	0	3	0
9	D	37	0	0	3	0
9	E	53	0	0	1	0
All	All	8945	0	8512	84	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 (84) 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:C:186:CYS:SG	1:C:187:CYS:N	2.53	0.81
1:E:177:GLN:OE1	9:E:2014:HOH:O	2.02	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:OH	9:A:2035:HOH:O	2.09	0.70
1:B:16:PRO:HB2	4:B:1206:GOL:H31	1.74	0.69
1:B:154:LEU:HD13	1:B:194:VAL:HG23	1.75	0.69
1:A:16:PRO:HB2	4:A:1207:GOL:H31	1.75	0.66
1:A:175:VAL:HG22	1:A:198:VAL:HB	1.78	0.66
1:B:186:CYS:SG	1:B:187:CYS:N	2.69	0.65
1:C:154:LEU:HD13	1:C:194:VAL:HG23	1.78	0.65
1:E:112:HIS:CD2	7:E:301:NAG:H62	2.34	0.61
1:A:57:SER:HB3	1:A:114:GLN:HG3	1.83	0.61
4:A:1206:GOL:H12	1:B:120:ARG:HH12	1.66	0.60
1:B:186:CYS:N	9:B:2043:HOH:O	2.34	0.60
1:E:85:VAL:HG22	4:E:1206:GOL:H12	1.84	0.59
1:C:53:TRP:CG	3:C:1205:L0B:H10	2.38	0.58
1:E:16:PRO:HB2	4:E:1206:GOL:H31	1.85	0.58
1:C:115:TYR:OH	9:C:2026:HOH:O	2.16	0.58
1:D:13:ASN:O	1:E:4:ARG:NH2	2.37	0.58
9:A:2044:HOH:O	1:B:75:GLN:NE2	2.36	0.58
1:A:186:CYS:N	9:A:2054:HOH:O	2.37	0.57
1:D:55:GLN:HG2	1:D:116:LEU:HD22	1.87	0.56
1:D:31:PHE:HE2	1:D:196:PHE:HE2	1.54	0.56
1:B:85:VAL:HG22	4:B:1206:GOL:H12	1.88	0.55
1:D:115:TYR:OH	9:D:2028:HOH:O	2.18	0.53
1:C:186:CYS:N	9:C:2035:HOH:O	2.42	0.52
1:D:112:HIS:CD2	5:D:301:NAG:H62	2.44	0.52
4:A:1206:GOL:C1	1:B:120:ARG:HH12	2.22	0.51
1:A:186:CYS:SG	1:A:187:CYS:N	2.84	0.51
1:D:171:GLU:HB2	1:D:203:LYS:HG2	1.92	0.51
1:D:3:GLN:NE2	9:D:2001:HOH:O	2.43	0.51
1:D:57:SER:HB3	1:D:114:GLN:HG3	1.93	0.50
1:D:122:ARG:NH1	9:D:2011:HOH:O	2.32	0.50
1:C:22:GLN:HE21	1:C:61:HIS:CD2	2.30	0.50
1:E:154:LEU:HD13	1:E:194:VAL:HG23	1.94	0.50
1:B:31:PHE:HE2	1:B:196:PHE:HE1	1.60	0.49
1:E:85:VAL:H	4:E:1206:GOL:H12	1.77	0.49
1:D:22:GLN:HB2	1:D:25:ARG:HB2	1.95	0.49
1:B:112:HIS:CG	5:B:301:NAG:H62	2.47	0.49
1:E:176:THR:HG23	1:E:197:THR:HB	1.94	0.48
3:E:1205:L0B:H141	3:E:1205:L0B:H223	1.68	0.48
1:C:112:HIS:CD2	5:C:301:NAG:H62	2.48	0.48
1:D:57:SER:HB2	1:D:112:HIS:NE2	2.28	0.48
1:C:79:PRO:HA	1:C:104:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HD13	1:A:194:VAL:HG23	1.96	0.47
1:C:5:LYS:HD2	1:C:70:TYR:HE2	1.80	0.47
1:D:3:GLN:O	1:D:7:TYR:HD1	1.98	0.47
1:D:19:ILE:HG13	1:D:84:TRP:CZ2	2.51	0.46
1:A:149:SER:OG	1:A:192:PRO:HD3	2.15	0.45
1:A:32:SER:HB3	1:A:55:GLN:HB2	1.98	0.45
1:E:177:GLN:HA	1:E:195:THR:O	2.16	0.45
3:C:1206:L0B:H10	1:D:53:TRP:CG	2.52	0.45
1:B:31:PHE:CE2	1:B:196:PHE:HE1	2.35	0.45
1:D:175:VAL:HG22	1:D:198:VAL:HB	1.99	0.45
1:B:85:VAL:H	4:B:1206:GOL:H12	1.81	0.45
1:A:84:TRP:HA	4:A:1207:GOL:H12	1.99	0.45
1:E:186:CYS:SG	1:E:187:CYS:N	2.90	0.45
1:A:178:LYS:HB2	1:A:178:LYS:HE3	1.80	0.45
1:D:186:CYS:SG	1:D:187:CYS:N	2.90	0.45
1:D:182:ARG:CZ	1:D:182:ARG:HB3	2.46	0.44
1:B:133:GLU:O	1:B:201:ARG:NH1	2.48	0.44
3:C:1205:L0B:H81C	3:C:1205:L0B:H221	1.75	0.44
1:C:22:GLN:HE21	1:C:61:HIS:CG	2.36	0.44
1:A:203:LYS:NZ	9:A:2049:HOH:O	2.48	0.44
1:B:8:LYS:O	1:B:11:VAL:HG12	2.18	0.43
1:A:112:HIS:CD2	2:A:301:NAG:H62	2.54	0.43
1:E:79:PRO:HA	1:E:104:LEU:HD23	1.99	0.43
1:D:45:ASN:OD1	1:E:169:ARG:NH1	2.50	0.43
3:C:1206:L0B:H19	1:D:53:TRP:CE2	2.53	0.43
1:B:11:VAL:HG23	6:B:1205:TLA:O3	2.19	0.43
1:A:114:GLN:OE1	3:E:1205:L0B:H6	2.20	0.42
1:E:202:LYS:HE3	1:E:202:LYS:HB2	1.79	0.42
1:D:92:ASN:OD1	1:D:92:ASN:N	2.51	0.42
1:C:122:ARG:NH1	9:C:2013:HOH:O	2.36	0.42
1:B:148:HIS:CE1	1:B:151:GLU:HG3	2.55	0.41
3:E:1205:L0B:H221	3:E:1205:L0B:H81C	1.76	0.41
1:D:91:TYR:OH	3:D:1205:L0B:H131	2.20	0.41
1:A:179:ARG:HD2	9:A:2047:HOH:O	2.20	0.41
1:E:3:GLN:HB3	8:E:1207:FHV:H013	2.01	0.41
1:C:148:HIS:CE1	1:C:150:ARG:HB2	2.56	0.41
1:D:16:PRO:HB2	4:D:1206:GOL:H31	2.03	0.41
1:B:184:TYR:HE1	1:B:191:TYR:HB2	1.84	0.41
3:D:1205:L0B:H141	3:D:1205:L0B:H223	1.81	0.41
1:C:184:TYR:O	1:C:186:CYS:N	2.54	0.41
1:E:171:GLU:HB2	1:E:203:LYS:HG2	2.02	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	204/205 (100%)	199 (98%)	3 (2%)	2 (1%)	19	26
1	B	203/205 (99%)	197 (97%)	4 (2%)	2 (1%)	19	26
1	C	203/205 (99%)	198 (98%)	2 (1%)	3 (2%)	13	15
1	D	203/205 (99%)	200 (98%)	3 (2%)	0	100	100
1	E	204/205 (100%)	198 (97%)	5 (2%)	1 (0%)	34	46
All	All	1017/1025 (99%)	992 (98%)	17 (2%)	8 (1%)	24	33

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	E	23	ARG
1	B	23	ARG
1	B	186	CYS
1	C	23	ARG
1	A	186	CYS
1	C	185	GLU
1	C	186	CYS

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	191/190 (100%)	179 (94%)	12 (6%)	22	32
1	B	190/190 (100%)	177 (93%)	13 (7%)	20	28
1	C	190/190 (100%)	176 (93%)	14 (7%)	17	24
1	D	190/190 (100%)	177 (93%)	13 (7%)	20	28
1	E	191/190 (100%)	185 (97%)	6 (3%)	47	67
All	All	952/950 (100%)	894 (94%)	58 (6%)	23	34

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	A	35	LEU
1	A	83	LEU
1	A	131	ASP
1	A	140	LEU
1	A	154	LEU
1	A	158	GLU
1	A	177	GLN
1	A	187	CYS
1	A	188	LYS
1	A	189	GLU
1	A	198	VAL
1	B	4	ARG
1	B	35	LEU
1	B	55	GLN
1	B	67	VAL
1	B	83	LEU
1	B	114	GLN
1	B	116	LEU
1	B	140	LEU
1	B	154	LEU
1	B	178	LYS
1	B	182	ARG
1	B	186	CYS
1	B	193	ASP
1	C	5	LYS
1	C	11	VAL
1	C	35	LEU
1	C	66	ASN
1	C	67	VAL
1	C	82	SER

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Mol	Chain	Res	Type
1	C	83	LEU
1	C	114	GLN
1	C	131	ASP
1	C	140	LEU
1	C	154	LEU
1	C	178	LYS
1	C	187	CYS
1	C	188	LYS
1	D	4	ARG
1	D	35	LEU
1	D	66	ASN
1	D	68	SER
1	D	83	LEU
1	D	131	ASP
1	D	133	GLU
1	D	140	LEU
1	D	154	LEU
1	D	182	ARG
1	D	188	LYS
1	D	189	GLU
1	D	198	VAL
1	E	4	ARG
1	E	35	LEU
1	E	131	ASP
1	E	154	LEU
1	E	172	LEU
1	E	176	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	22	GLN
1	C	61	HIS

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 ⓘ

12 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$
2	NAG	A	301	1,2	14,14,15	0.53	0	15,19,21	1.11	1 (6%)
2	NAG	A	302	2	14,14,15	0.62	0	15,19,21	1.31	2 (13%)
2	BMA	A	303	2	11,11,12	0.29	0	14,15,17	0.91	0
2	BMA	A	304	2	11,11,12	0.58	0	14,15,17	1.28	1 (7%)
5	NAG	B	301	1,5	14,14,15	0.56	0	15,19,21	0.79	0
5	NAG	B	302	5	14,14,15	0.51	0	15,19,21	0.79	0
5	NAG	C	301	1,5	14,14,15	0.49	0	15,19,21	0.92	1 (6%)
5	NAG	C	302	5	14,14,15	0.40	0	15,19,21	1.15	2 (13%)
5	NAG	D	301	1,5	14,14,15	0.53	0	15,19,21	0.74	0
5	NAG	D	302	5	14,14,15	0.52	0	15,19,21	0.57	0
7	NAG	E	301	1,7	14,14,15	0.56	0	15,19,21	1.42	3 (20%)
7	NDG	E	302	7	14,14,15	0.38	0	15,19,21	1.45	1 (6%)

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	NAG	A	301	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	302	2	-	0/6/23/26	0/1/1/1
2	BMA	A	303	2	1/1/4/5	0/2/19/22	0/1/1/1
2	BMA	A	304	2	-	0/2/19/22	1/1/1/1
5	NAG	B	301	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	302	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	301	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	302	5	-	0/6/23/26	0/1/1/1
5	NAG	D	301	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	302	5	-	0/6/23/26	0/1/1/1
7	NAG	E	301	1,7	-	0/6/23/26	0/1/1/1
7	NDG	E	302	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	301	NAG	C2-N2-C7	-3.95	117.97	123.04
2	A	302	NAG	C1-O5-C5	-3.34	108.01	112.25
2	A	304	BMA	C3-C4-C5	-2.83	105.27	110.20
2	A	302	NAG	C2-N2-C7	-2.49	119.85	123.04
7	E	301	NAG	C6-C5-C4	-2.29	107.37	113.02
5	C	302	NAG	C2-N2-C7	-2.27	120.12	123.04
7	E	301	NAG	C1-O5-C5	2.30	115.17	112.25
5	C	301	NAG	C1-O5-C5	2.59	115.54	112.25
2	A	301	NAG	O5-C5-C6	2.63	113.03	107.35
5	C	302	NAG	C1-O5-C5	2.68	115.65	112.25
7	E	302	NDG	C1-O-C5	4.47	117.92	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	303	BMA	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	304	BMA	C1-C2-C3-C4-C5-O5

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAG	1	0
5	B	301	NAG	1	0
5	C	301	NAG	1	0
5	D	301	NAG	1	0

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

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
3	L0B	A	1205	-	27,27,27	0.62	0	30,36,36	1.22	3 (10%)
4	GOL	A	1206	-	5,5,5	0.30	0	5,5,5	0.38	0
4	GOL	A	1207	-	5,5,5	0.40	0	5,5,5	0.47	0
6	TLA	B	1205	-	3,9,9	1.71	1 (33%)	6,12,12	1.15	1 (16%)
4	GOL	B	1206	-	5,5,5	0.33	0	5,5,5	0.58	0
3	L0B	C	1205	-	27,27,27	0.52	0	30,36,36	1.24	3 (10%)
3	L0B	C	1206	-	27,27,27	0.54	0	30,36,36	1.07	3 (10%)
3	L0B	D	1205	-	27,27,27	0.53	0	30,36,36	1.11	2 (6%)
4	GOL	D	1206	-	5,5,5	0.31	0	5,5,5	0.57	0
3	L0B	E	1205	-	27,27,27	0.60	1 (3%)	30,36,36	1.57	4 (13%)
4	GOL	E	1206	-	5,5,5	0.34	0	5,5,5	0.46	0
8	FHV	E	1207	-	16,16,16	3.01	7 (43%)	19,21,21	1.98	3 (15%)

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	L0B	A	1205	-	-	0/16/30/30	0/3/3/3
4	GOL	A	1206	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1207	-	-	0/4/4/4	0/0/0/0
6	TLA	B	1205	-	-	0/4/12/12	0/0/0/0
4	GOL	B	1206	-	-	0/4/4/4	0/0/0/0
3	L0B	C	1205	-	-	0/16/30/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	L0B	C	1206	-	-	0/16/30/30	0/3/3/3
3	L0B	D	1205	-	-	0/16/30/30	0/3/3/3
4	GOL	D	1206	-	-	0/4/4/4	0/0/0/0
3	L0B	E	1205	-	-	0/16/30/30	0/3/3/3
4	GOL	E	1206	-	-	0/4/4/4	0/0/0/0
8	FHV	E	1207	-	-	0/8/15/15	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	1207	FHV	C11-N10	-2.43	1.41	1.47
3	E	1205	L0B	C17-C16	-2.20	1.48	1.52
6	B	1205	TLA	O2-C2	-2.01	1.38	1.42
8	E	1207	FHV	O09-C08	2.04	1.27	1.23
8	E	1207	FHV	C15-C02	2.05	1.42	1.38
8	E	1207	FHV	C04-C05	3.66	1.46	1.38
8	E	1207	FHV	C06-N07	4.01	1.49	1.41
8	E	1207	FHV	C08-N07	5.82	1.45	1.36
8	E	1207	FHV	C08-N10	7.71	1.51	1.36

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1205	L0B	C22-N1-C11	-4.81	109.04	113.20
3	A	1205	L0B	C22-N1-C9	-4.72	109.12	113.20
3	C	1205	L0B	C22-N1-C9	-4.58	109.24	113.20
3	E	1205	L0B	C22-N1-C9	-4.48	109.32	113.20
3	D	1205	L0B	C22-N1-C11	-3.92	109.81	113.20
8	E	1207	FHV	O09-C08-N10	-3.78	115.99	121.77
3	C	1205	L0B	C22-N1-C11	-3.34	110.31	113.20
3	E	1205	L0B	C14-C11-C13	-3.31	106.71	113.10
3	C	1206	L0B	C22-N1-C9	-3.21	110.42	113.20
3	E	1205	L0B	C14-C16-C17	-3.10	105.62	111.36
3	A	1205	L0B	C14-C11-C13	-3.03	107.25	113.10
3	C	1206	L0B	C22-N1-C11	-2.85	110.74	113.20
3	C	1205	L0B	C14-C11-C13	-2.63	108.02	113.10
3	D	1205	L0B	C22-N1-C9	-2.61	110.94	113.20
3	C	1206	L0B	C14-C11-C13	-2.29	108.67	113.10
6	B	1205	TLA	C4-C3-C2	-2.11	109.02	113.35
3	A	1205	L0B	C22-N1-C11	-2.05	111.43	113.20
8	E	1207	FHV	C03-C02-C15	2.89	122.71	117.95
8	E	1207	FHV	N07-C08-N10	5.42	122.09	116.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1206	GOL	2	0
4	A	1207	GOL	2	0
6	B	1205	TLA	1	0
4	B	1206	GOL	3	0
3	C	1205	L0B	2	0
3	C	1206	L0B	2	0
3	D	1205	L0B	2	0
4	D	1206	GOL	1	0
3	E	1205	L0B	3	0
4	E	1206	GOL	3	0
8	E	1207	FHV	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	205/205 (100%)	0.41	10 (4%) 33 38	25, 43, 81, 122	0
1	B	205/205 (100%)	0.29	10 (4%) 33 38	25, 47, 91, 119	0
1	C	205/205 (100%)	0.39	13 (6%) 23 27	35, 61, 99, 135	0
1	D	205/205 (100%)	0.41	11 (5%) 29 34	32, 53, 88, 111	0
1	E	205/205 (100%)	0.17	3 (1%) 76 78	27, 42, 72, 108	0
All	All	1025/1025 (100%)	0.33	47 (4%) 36 41	25, 49, 91, 135	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	159	ALA	6.6
1	B	204	GLY	6.2
1	D	204	GLY	5.3
1	C	204	GLY	4.6
1	A	23	ARG	3.9
1	A	204	GLY	3.9
1	C	134	SER	3.8
1	D	131	ASP	3.8
1	E	24	ASP	3.7
1	B	159	ALA	3.6
1	B	158	GLU	3.6
1	D	134	SER	3.6
1	D	173	VAL	3.5
1	A	24	ASP	3.2
1	D	2	PHE	3.2
1	B	0	GLY	3.0
1	A	2	PHE	2.9
1	B	2	PHE	2.7
1	B	74	LYS	2.7
1	C	173	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	158	GLU	2.6
1	A	130	VAL	2.6
1	C	188	LYS	2.6
1	B	72	GLY	2.5
1	A	25	ARG	2.5
1	E	204	GLY	2.5
1	B	70	TYR	2.5
1	D	174	GLY	2.5
1	C	133	GLU	2.4
1	A	188	LYS	2.4
1	E	23	ARG	2.4
1	A	72	GLY	2.4
1	C	185	GLU	2.3
1	C	132	THR	2.3
1	A	131	ASP	2.3
1	C	172	LEU	2.3
1	C	25	ARG	2.2
1	C	23	ARG	2.2
1	D	201	ARG	2.2
1	D	0	GLY	2.2
1	C	161	ILE	2.2
1	D	1	GLU	2.1
1	D	200	PHE	2.1
1	D	185	GLU	2.1
1	B	73	VAL	2.1
1	A	5	LYS	2.0
1	B	71	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	B	301	14/15	0.91	0.24	-	59,71,80,95	0
5	NAG	D	302	14/15	0.75	0.29	-	97,118,131,139	0
2	BMA	A	304	11/12	0.84	0.18	-	65,69,78,88	0
7	NDG	E	302	14/15	0.92	0.21	-	72,86,101,108	0
5	NAG	C	302	14/15	0.75	0.33	-	98,106,119,124	0
2	NAG	A	301	14/15	0.96	0.10	-	36,47,52,53	0
7	NAG	E	301	14/15	0.94	0.11	-	45,56,62,74	0
5	NAG	C	301	14/15	0.97	0.10	-	60,73,78,79	0
2	BMA	A	303	11/12	0.88	0.15	-	59,64,78,79	0
2	NAG	A	302	14/15	0.96	0.10	-	42,48,58,60	0
5	NAG	D	301	14/15	0.95	0.11	-	68,77,89,97	0
5	NAG	B	302	14/15	0.88	0.30	-	74,107,116,120	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	TLA	B	1205	10/10	0.86	0.60	17.16	108,127,138,139	0
4	GOL	A	1207	6/6	0.64	0.34	11.34	54,64,70,71	0
3	L0B	A	1205	25/25	0.92	0.25	6.90	45,60,71,75	0
8	FHV	E	1207	15/15	0.85	0.33	6.31	57,64,77,80	0
3	L0B	C	1205	25/25	0.81	0.28	5.05	64,76,84,92	0
4	GOL	E	1206	6/6	0.69	0.25	3.90	50,72,75,77	0
4	GOL	D	1206	6/6	0.74	0.25	3.11	57,64,68,69	0
4	GOL	B	1206	6/6	0.69	0.20	2.50	41,51,58,59	0
3	L0B	C	1206	25/25	0.85	0.27	2.00	61,88,102,105	0
4	GOL	A	1206	6/6	0.81	0.18	1.88	64,80,83,84	0
3	L0B	E	1205	25/25	0.94	0.19	1.38	39,56,80,83	0
3	L0B	D	1205	25/25	0.93	0.16	0.40	43,58,66,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.