Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:17 AM GMT

PDB ID	:	3LIZ
Title	:	crystal structure of bla g 2 complexed with Fab 4C3
Authors	:	Li, M.; Gustchina, A.; Glesner, J.; Wunschmann, S.; Pomes, A.; Wlodawer, A.
Deposited on	:	2010-01-25
Resolution	:	1.80 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:

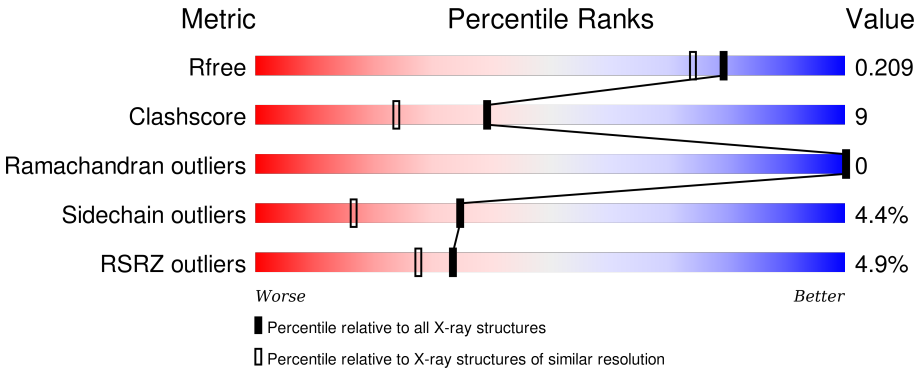
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	334	4% 83% 15%
2	L	211	% 81% 18%
3	H	253	9% 72% 9% 16%

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	NAG	A	502	-	-	-	X
5	NAG	A	601	-	-	-	X
8	EDO	A	339	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6859 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 Aspartic protease Bla g 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	8	0
			2573	1645	421	493	14			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLU	-	expression tag	UNP P54958
A	-9	ALA	-	expression tag	UNP P54958
A	-8	GLU	-	expression tag	UNP P54958
A	-7	ALA	-	expression tag	UNP P54958
A	-6	SER	-	expression tag	UNP P54958
A	-5	ILE	-	expression tag	UNP P54958
A	93	GLN	ASN	engineered	UNP P54958

- Molecule 2 is a protein called 4C3 monoclonal antibody Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	10	0
			1710	1075	282	347	6			

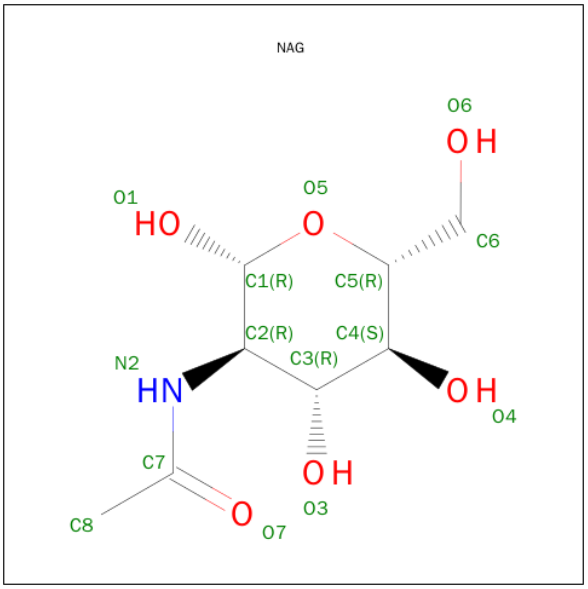
- Molecule 3 is a protein called 4C3 monoclonal antibody Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	213	Total	C	N	O	S	0	2	0
			1608	1020	266	314	8			

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

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

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



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

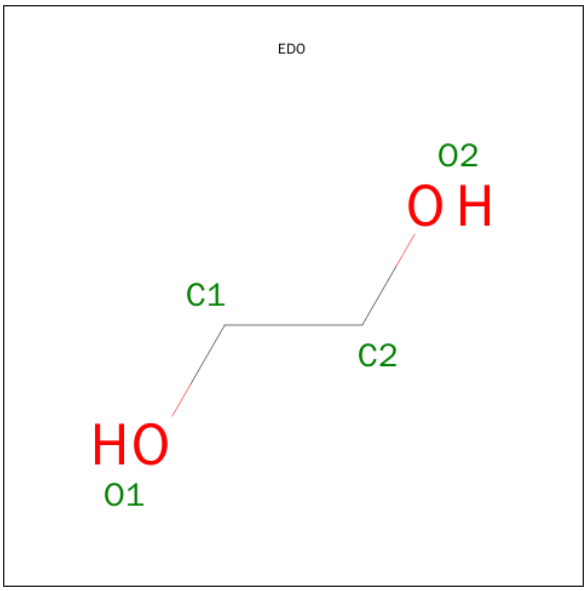
- Molecule 6 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Cd	0	0
			3	3		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total	Zn	0	0
			5	5		
7	L	2	Total	Zn	0	0
			2	2		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0

- Molecule 9 is water.

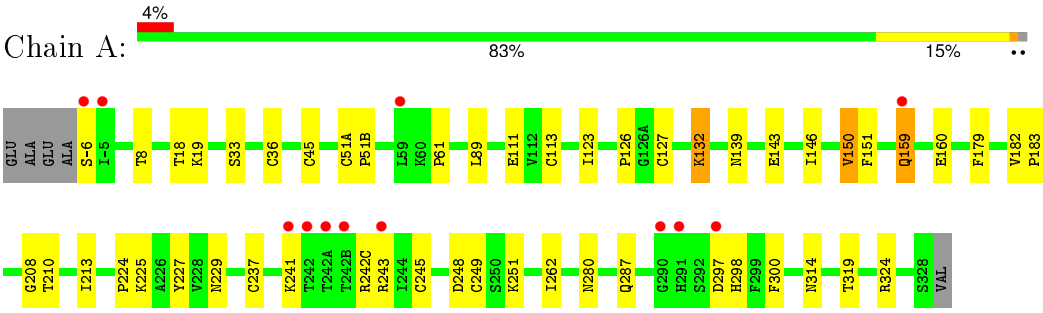
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	412	Total O 412 412	0	0
9	L	269	Total O 269 269	0	0
9	H	189	Total O 189 189	0	0

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.

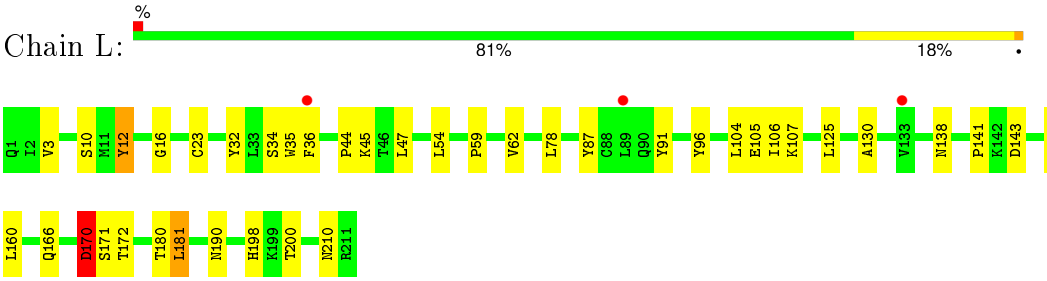
- Molecule 1: Aspartic protease Bla g 2

Chain A:



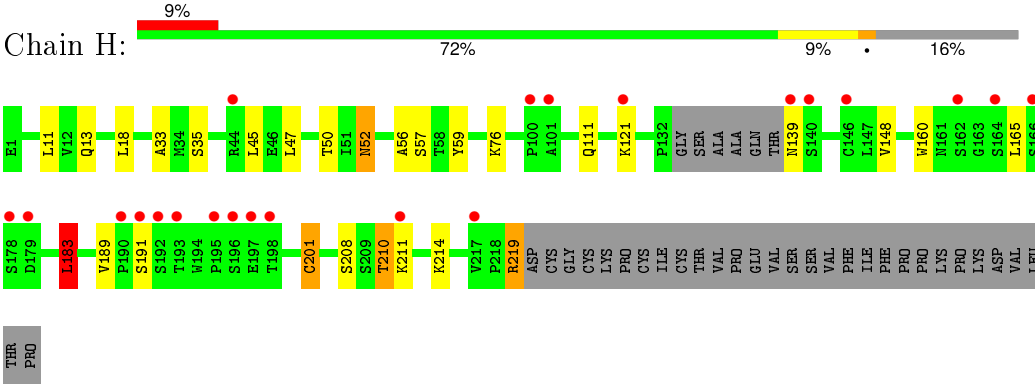
- Molecule 2: 4C3 monoclonal antibody Light Chain

Chain L:



- Molecule 3: 4C3 monoclonal antibody Heavy Chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	155.21Å 105.28Å 109.15Å 90.00° 132.58° 90.00°	Depositor
Resolution (Å)	29.49 – 1.80 29.49 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.49-1.80) 99.3 (29.49-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.4.0057	Depositor
R, R_{free}	0.177 , 0.202 0.183 , 0.209	Depositor DCC
R_{free} test set	3593 reflections (3.13%)	DCC
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.7	EDS
Estimated twinning fraction	0.012 for -h+k-l,-l,-k 0.000 for -h-k-l,l,k 0.015 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 118367 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6859	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: ZN, BMA, NAG, EDO, CD, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.72	4/2659 (0.2%)	0.71	3/3611 (0.1%)
2	L	0.54	0/1772	0.73	2/2402 (0.1%)
3	H	0.47	0/1655	0.63	1/2261 (0.0%)
All	All	0.61	4/6086 (0.1%)	0.69	6/8274 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	GLY	C-N	10.70	1.58	1.34
1	A	8	THR	C-N	10.22	1.57	1.34
1	A	146	ILE	C-N	7.95	1.52	1.34
1	A	61	PRO	C-N	5.51	1.46	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	183	LEU	CA-CB-CG	7.59	132.75	115.30
1	A	208	GLY	O-C-N	-6.20	112.78	122.70
2	L	170	ASP	CB-CG-OD1	-5.87	113.02	118.30
2	L	170	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	150[A]	VAL	CB-CA-C	-5.51	100.93	111.40
1	A	150[B]	VAL	CB-CA-C	-5.51	100.93	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2573	0	2507	48	0
2	L	1710	0	1669	37	0
3	H	1608	0	1587	24	0
4	A	50	0	43	2	0
5	A	14	0	13	2	0
6	A	3	0	0	0	0
7	A	5	0	0	0	0
7	L	2	0	0	0	0
8	A	24	0	36	1	0
9	A	412	0	0	28	0
9	H	189	0	0	7	0
9	L	269	0	0	21	0
All	All	6859	0	5855	106	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 9.

All (106) 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:213:ILE:HD12	9:A:725:HOH:O	1.38	1.22
1:A:127:CYS:HB2	9:A:784:HOH:O	1.43	1.17
1:A:319:THR:HG22	9:A:739:HOH:O	1.53	1.06
1:A:249:CYS:HB3	9:A:624:HOH:O	1.62	1.00
3:H:35[A]:SER:OG	3:H:50[A]:THR:HG22	1.69	0.92
2:L:180:THR:HG23	9:L:263:HOH:O	1.78	0.84
2:L:105:GLU:HG2	9:L:600:HOH:O	1.78	0.81
1:A:36:CYS:HB2	9:A:784:HOH:O	1.85	0.76
1:A:224:PRO:HG2	9:A:777:HOH:O	1.87	0.75
1:A:324:ARG:NH1	9:A:813:HOH:O	2.12	0.74
1:A:150[B]:VAL:HG12	1:A:314:ASN:HA	1.70	0.74
2:L:62:VAL:O	9:L:771:HOH:O	2.07	0.71
9:L:214:HOH:O	3:H:170:HIS:CE1	2.42	0.71
1:A:89:LEU:HG	9:A:610:HOH:O	1.91	0.71
1:A:183:PRO:HA	9:A:739:HOH:O	1.88	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:59:PRO:O	9:L:771:HOH:O	2.09	0.70
4:A:502:NAG:H61	3:H:56:ALA:HB2	1.74	0.69
1:A:45:CYS:SG	9:A:840:HOH:O	2.51	0.68
2:L:180:THR:HG22	9:L:484:HOH:O	1.96	0.66
1:A:151:PHE:HZ	9:A:632:HOH:O	1.81	0.63
1:A:18:THR:HB	9:A:610:HOH:O	1.98	0.63
2:L:198:HIS:HD2	2:L:200:THR:OG1	1.81	0.62
1:A:297:ASP:O	9:A:777:HOH:O	2.16	0.61
1:A:150[A]:VAL:CG2	5:A:601:NAG:H81	2.30	0.61
1:A:248[B]:ASP:OD2	9:A:108:HOH:O	2.17	0.60
2:L:45[B]:LYS:HE2	9:L:655:HOH:O	2.02	0.60
2:L:107:LYS:HE3	9:L:850:HOH:O	2.03	0.58
2:L:106:ILE:H	2:L:166:GLN:HE22	1.52	0.57
1:A:237[B]:CYS:HB3	1:A:245[B]:CYS:HB3	1.85	0.57
1:A:113:CYS:HB3	9:A:582:HOH:O	2.04	0.57
2:L:170:ASP:O	2:L:171:SER:HB2	2.04	0.57
3:H:33:ALA:HB1	9:H:540:HOH:O	2.05	0.57
2:L:36[A]:PHE:CD2	2:L:44:PRO:HB3	2.39	0.56
4:A:501:NAG:H5	9:A:813:HOH:O	2.05	0.56
2:L:155:ARG:HB3	2:L:157[B]:ASN:OD1	2.05	0.56
1:A:132:LYS:N	1:A:132:LYS:HD2	2.21	0.55
2:L:12[A]:TYR:CE2	9:L:783:HOH:O	2.54	0.54
2:L:143:ASP:HB3	9:L:796:HOH:O	2.07	0.54
1:A:227:TYR:HE2	9:A:777:HOH:O	1.92	0.53
2:L:54:LEU:CD1	9:L:771:HOH:O	2.57	0.53
1:A:241:LYS:HD2	1:A:243:ARG:HH12	1.73	0.52
9:L:214:HOH:O	3:H:170:HIS:HE1	1.82	0.52
2:L:45[B]:LYS:HE2	9:L:365:HOH:O	2.10	0.51
1:A:297:ASP:HB3	9:A:549:HOH:O	2.09	0.51
2:L:12[A]:TYR:HE2	9:L:783:HOH:O	1.93	0.51
1:A:298:HIS:NE2	1:A:300:PHE:CZ	2.79	0.51
1:A:182:VAL:HG11	1:A:262:ILE:HG23	1.91	0.51
3:H:211:LYS:HG3	9:H:732:HOH:O	2.11	0.50
1:A:297:ASP:N	1:A:297:ASP:OD1	2.43	0.50
2:L:190[B]:ASN:ND2	2:L:210:ASN:HD22	2.09	0.50
2:L:138:ASN:ND2	9:L:214:HOH:O	2.33	0.50
2:L:170:ASP:HB3	2:L:172:THR:H	1.78	0.49
1:A:111:GLU:HG2	9:A:781:HOH:O	2.12	0.49
1:A:19[A]:LYS:NZ	9:A:638:HOH:O	2.46	0.49
1:A:51(A):CYS:HA	1:A:51(B):PRO:HD3	1.77	0.48
2:L:190[B]:ASN:ND2	2:L:210:ASN:ND2	2.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:SER:HA	1:A:123:ILE:HG13	1.94	0.48
3:H:76:LYS:HE2	9:H:815:HOH:O	2.13	0.48
1:A:189:SER:HB2	9:A:725:HOH:O	2.14	0.48
3:H:50[B]:THR:CG2	9:H:540:HOH:O	2.61	0.48
3:H:52:ASN:ND2	3:H:57:SER:H	2.12	0.48
3:H:219:ARG:NH1	9:H:696:HOH:O	2.28	0.47
1:A:298:HIS:CE1	1:A:300:PHE:CZ	3.03	0.47
1:A:251:LYS:HE3	9:L:301:HOH:O	2.14	0.47
1:A:182:VAL:HB	9:A:792:HOH:O	2.15	0.47
3:H:177:GLN:HB2	9:H:461:HOH:O	2.14	0.46
3:H:47:LEU:HD11	3:H:50[A]:THR:HG23	1.96	0.46
2:L:141:PRO:O	2:L:198:HIS:HE1	1.99	0.46
2:L:3:VAL:HG22	9:L:490:HOH:O	2.15	0.46
1:A:160:GLU:HG3	8:A:343:EDO:O2	2.15	0.46
3:H:208:SER:OG	3:H:210:THR:OG1	2.31	0.46
1:A:191:LYS:HE2	1:A:298:HIS:CE1	2.51	0.46
3:H:52:ASN:HD22	3:H:52:ASN:N	2.14	0.46
2:L:54:LEU:HD11	9:L:771:HOH:O	2.16	0.45
1:A:139:ASN:O	1:A:143:GLU:HG2	2.16	0.45
2:L:36[A]:PHE:HZ	3:H:45:LEU:HD13	1.81	0.45
9:A:829:HOH:O	3:H:52:ASN:HA	2.17	0.45
1:A:251:LYS:HE2	2:L:32:TYR:CZ	2.51	0.45
3:H:50[A]:THR:OG1	3:H:59:TYR:HB3	2.17	0.44
1:A:150[A]:VAL:HG21	5:A:601:NAG:H81	1.98	0.44
1:A:241:LYS:HB3	1:A:243:ARG:NH1	2.33	0.44
2:L:36[A]:PHE:CZ	3:H:45:LEU:HD13	2.52	0.44
2:L:91:TYR:HA	2:L:96:TYR:CD2	2.53	0.44
1:A:225:LYS:HG3	1:A:229:ASN:ND2	2.33	0.44
1:A:251:LYS:HE2	2:L:32:TYR:CE1	2.54	0.43
1:A:191:LYS:HG3	9:A:725:HOH:O	2.18	0.43
2:L:47:LEU:CD2	9:L:655:HOH:O	2.66	0.43
1:A:225:LYS:HB3	1:A:225:LYS:HE3	1.82	0.43
2:L:130:ALA:O	2:L:181:LEU:HD12	2.17	0.43
2:L:16:GLY:HA2	9:L:232:HOH:O	2.19	0.42
3:H:160:TRP:CZ3	3:H:201:CYS:HB3	2.54	0.42
9:A:829:HOH:O	3:H:33:ALA:HB1	2.19	0.42
3:H:52:ASN:HD21	3:H:56:ALA:N	2.18	0.42
3:H:52:ASN:HD22	3:H:52:ASN:H	1.66	0.42
2:L:45[B]:LYS:CE	9:L:655:HOH:O	2.66	0.42
2:L:78:LEU:HD11	2:L:104:LEU:HD21	2.02	0.42
1:A:280:ASN:HB3	9:A:511:HOH:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:SER:CB	9:A:725:HOH:O	2.68	0.41
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.55	0.41
3:H:13:GLN:NE2	9:H:833:HOH:O	2.54	0.41
2:L:36[A]:PHE:CZ	2:L:87:TYR:HB2	2.56	0.40
1:A:210:THR:HG23	9:A:777:HOH:O	2.21	0.40
1:A:182:VAL:HG11	1:A:262:ILE:CG2	2.51	0.40
3:H:148:VAL:HB	3:H:183:LEU:HD22	2.04	0.40
1:A:159:GLN:CD	1:A:159:GLN:H	2.24	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	335/334 (100%)	329 (98%)	6 (2%)	0	100	100
2	L	219/211 (104%)	215 (98%)	4 (2%)	0	100	100
3	H	211/253 (83%)	209 (99%)	2 (1%)	0	100	100
All	All	765/798 (96%)	753 (98%)	12 (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	A	291/286 (102%)	284 (98%)	7 (2%)	57 41
2	L	199/189 (105%)	191 (96%)	8 (4%)	38 20
3	H	183/217 (84%)	168 (92%)	15 (8%)	14 4
All	All	673/692 (97%)	643 (96%)	30 (4%)	35 16

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-6	SER
1	A	126	PRO
1	A	132	LYS
1	A	159	GLN
1	A	179	PHE
1	A	242(C)	ARG
1	A	287	GLN
2	L	10	SER
2	L	12[A]	TYR
2	L	12[B]	TYR
2	L	34	SER
2	L	125	LEU
2	L	160	LEU
2	L	170	ASP
2	L	181	LEU
3	H	11	LEU
3	H	18	LEU
3	H	52	ASN
3	H	111	GLN
3	H	121	LYS
3	H	139	ASN
3	H	165	LEU
3	H	177	GLN
3	H	183	LEU
3	H	189	VAL
3	H	191	SER
3	H	201	CYS
3	H	210	THR
3	H	214	LYS
3	H	219	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	211	GLN
2	L	145	ASN
2	L	156	GLN
2	L	166	GLN
2	L	198	HIS
2	L	210	ASN
3	H	3	GLN
3	H	52	ASN
3	H	77	ASN
3	H	139	ASN
3	H	170	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

4 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	$\#\|Z\| > 2$
4	NAG	A	501	1,4	14,14,15	0.48	0	15,19,21	1.16	1 (6%)
4	NAG	A	502	4	14,14,15	0.50	0	15,19,21	1.05	1 (6%)
4	BMA	A	503	4	11,11,12	0.77	0	14,15,17	1.24	2 (14%)
4	MAN	A	504	4	11,11,12	0.66	0	14,15,17	2.06	4 (28%)

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	NAG	A	501	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	502	4	-	0/6/23/26	0/1/1/1
4	BMA	A	503	4	-	0/2/19/22	0/1/1/1
4	MAN	A	504	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503	BMA	O3-C3-C2	2.11	113.82	110.00
4	A	502	NAG	C1-O5-C5	2.32	115.19	112.25
4	A	504	MAN	C1-O5-C5	2.92	115.95	112.25
4	A	503	BMA	C1-O5-C5	2.99	116.04	112.25
4	A	501	NAG	C1-O5-C5	3.15	116.25	112.25
4	A	504	MAN	C3-C4-C5	3.52	116.33	110.20
4	A	504	MAN	C2-C3-C4	3.59	117.14	111.04
4	A	504	MAN	C1-C2-C3	4.36	114.69	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	NAG	1	0
4	A	502	NAG	1	0

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 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	$\#\|Z\|>2$
8	EDO	A	338	-	3,3,3	0.40	0	2,2,2	0.66	0
8	EDO	A	339	-	3,3,3	0.45	0	2,2,2	0.52	0
8	EDO	A	340	-	3,3,3	0.33	0	2,2,2	0.69	0
8	EDO	A	341	-	3,3,3	0.48	0	2,2,2	0.39	0
8	EDO	A	342	-	3,3,3	0.47	0	2,2,2	0.53	0
8	EDO	A	343	-	3,3,3	0.42	0	2,2,2	0.53	0
5	NAG	A	601	1	14,14,15	0.43	0	15,19,21	1.06	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
8	EDO	A	338	-	-	0/1/1/1	0/0/0/0
8	EDO	A	339	-	-	0/1/1/1	0/0/0/0
8	EDO	A	340	-	-	0/1/1/1	0/0/0/0
8	EDO	A	341	-	-	0/1/1/1	0/0/0/0
8	EDO	A	342	-	-	0/1/1/1	0/0/0/0
8	EDO	A	343	-	-	0/1/1/1	0/0/0/0
5	NAG	A	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	601	NAG	C3-C2-N2	-2.56	104.43	110.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	343	EDO	1	0
5	A	601	NAG	2	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	329/334 (98%)	-0.15	12 (3%) 46 40	20, 28, 43, 67	1 (0%)
2	L	211/211 (100%)	0.08	3 (1%) 78 74	26, 32, 39, 45	1 (0%)
3	H	213/253 (84%)	0.57	22 (10%) 9 6	27, 36, 67, 73	0
All	All	753/798 (94%)	0.12	37 (4%) 33 27	20, 31, 56, 73	2 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242(B)	THR	7.4
1	A	-6	SER	7.2
1	A	242(A)	THR	6.9
1	A	-5	ILE	5.3
1	A	241	LYS	4.8
3	H	139	ASN	3.7
3	H	192	SER	3.6
1	A	59	LEU	3.6
1	A	291	HIS	3.6
3	H	217	VAL	3.6
3	H	196	SER	3.6
3	H	164	SER	3.4
1	A	242	THR	3.4
3	H	198	THR	3.4
3	H	178	SER	3.4
2	L	89	LEU	3.3
2	L	36[A]	PHE	3.1
3	H	146	CYS	3.1
1	A	159	GLN	3.0
3	H	197	GLU	2.9
3	H	211	LYS	2.8
3	H	121	LYS	2.8
3	H	100	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	290	GLY	2.7
3	H	162	SER	2.7
3	H	193	THR	2.6
1	A	243	ARG	2.6
2	L	133	VAL	2.4
3	H	101	ALA	2.3
3	H	140	SER	2.3
3	H	44	ARG	2.2
3	H	179	ASP	2.1
1	A	297	ASP	2.1
3	H	190	PRO	2.1
3	H	195	PRO	2.1
3	H	191	SER	2.1
3	H	166	SER	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, 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	NAG	A	502	14/15	0.93	0.16	3.42	40,47,49,54	0
4	NAG	A	501	14/15	0.95	0.09	-0.80	26,29,36,37	0
4	BMA	A	503	11/12	0.75	0.26	-	59,62,68,73	0
4	MAN	A	504	11/12	0.71	0.37	-	76,77,78,78	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, 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
8	EDO	A	339	4/4	0.84	0.22	6.20	56,58,58,59	0
5	NAG	A	601	14/15	0.84	0.20	3.43	45,49,55,56	0
7	ZN	A	334	1/1	0.99	0.07	-1.28	32,32,32,32	1
7	ZN	A	333	1/1	1.00	0.05	-2.02	22,22,22,22	0
6	CD	A	332	1/1	1.00	0.04	-3.38	28,28,28,28	0
7	ZN	L	212	1/1	0.98	0.04	-3.92	53,53,53,53	1
6	CD	A	331	1/1	0.99	0.07	-	21,21,21,21	1
7	ZN	L	213	1/1	0.98	0.04	-	58,58,58,58	0
7	ZN	A	336	1/1	0.62	0.09	-	95,95,95,95	0
6	CD	A	330	1/1	0.99	0.07	-	24,24,24,24	0
7	ZN	A	337	1/1	0.95	0.04	-	69,69,69,69	0
8	EDO	A	341	4/4	0.78	0.30	-	76,76,76,77	0
8	EDO	A	338	4/4	0.88	0.19	-	64,64,65,67	0
8	EDO	A	342	4/4	0.80	0.26	-	54,57,58,58	0
8	EDO	A	343	4/4	0.79	0.31	-	66,67,68,69	0
7	ZN	A	335	1/1	0.99	0.12	-	35,35,35,35	1
8	EDO	A	340	4/4	0.91	0.23	-	62,62,62,62	0

6.5 Other polymers

There are no such residues in this entry.