Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:38 PM GMT

PDB ID	:	4M7Z
Title	:	Unliganded 1 crystal structure of S25-26 Fab
Authors	:	Haji-Ghassemi, O.; Evans, S.V.; Muller-Loennies, S.; Saldova, R.; Muniyappa, M.; Brade, L.; Rudd, P.M.; Harvey, D.J.; Kosma, P.; Brade, H.
Deposited on	:	2013-08-12
Resolution	:	2.75 Å(reported)

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

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

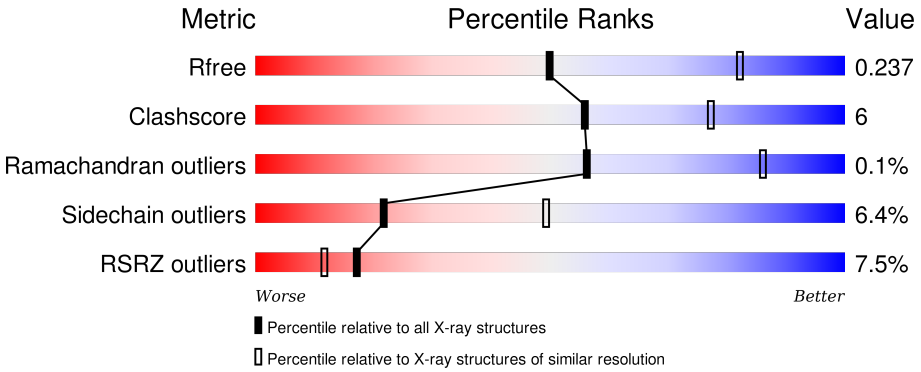
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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

Mol	Chain	Length	Quality of chain
1	B	219	7%, 85%, 11%
1	H	219	7%, 88%, 9%
2	C	219	2%, 87%, 12%
2	L	219	13%, 84%, 15%

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	PG4	B	404	-	-	-	X
4	PG4	B	405	-	-	-	X
4	PG4	H	402	-	-	-	X
4	PG4	L	301	-	-	-	X
5	PEG	B	407	-	-	-	X
5	PEG	B	408	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6973 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

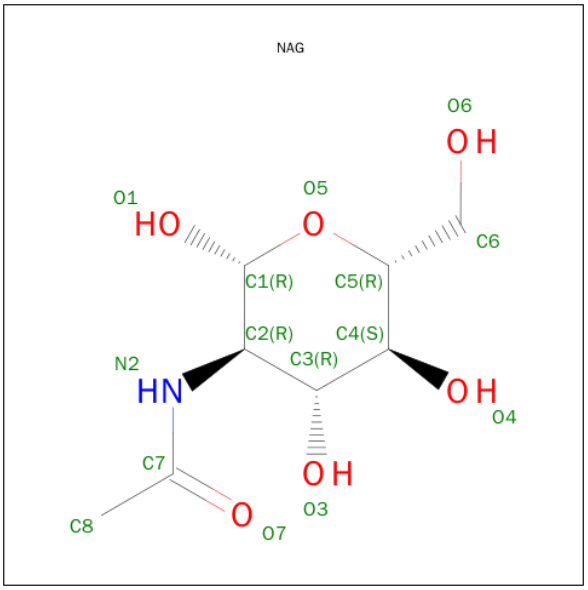
- Molecule 1 is a protein called S25-26 Fab (Igg1k) Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	216	Total	C	N	O	S	0	0	0
			1631	1039	270	315	7			
1	H	215	Total	C	N	O	S	0	0	0
			1623	1035	269	312	7			

- Molecule 2 is a protein called S25-26 Fab (Igg1k) Light Chain.

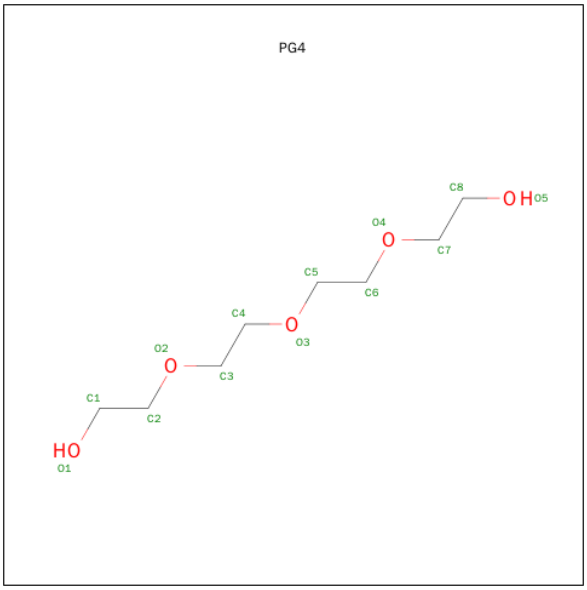
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	219	Total	C	N	O	S	0	0	0
			1712	1072	291	342	7			
2	L	218	Total	C	N	O	S	0	0	0
			1706	1069	290	341	6			

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



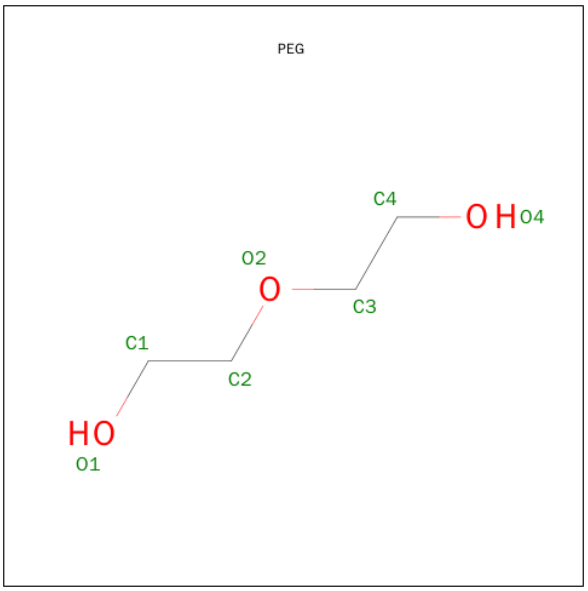
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 14 8 1 5	0	0
3	H	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 13 8 5	0	0
4	B	1	Total C O 13 8 5	0	0
4	B	1	Total C O 13 8 5	0	0
4	B	1	Total C O 13 8 5	0	0
4	H	1	Total C O 13 8 5	0	0
4	C	1	Total C O 13 8 5	0	0
4	L	1	Total C O 13 8 5	0	0
4	L	1	Total C O 13 8 5	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total Ca 1 1	0	0
6	B	1	Total Ca 1 1	0	0
6	L	1	Total Ca 1 1	0	0

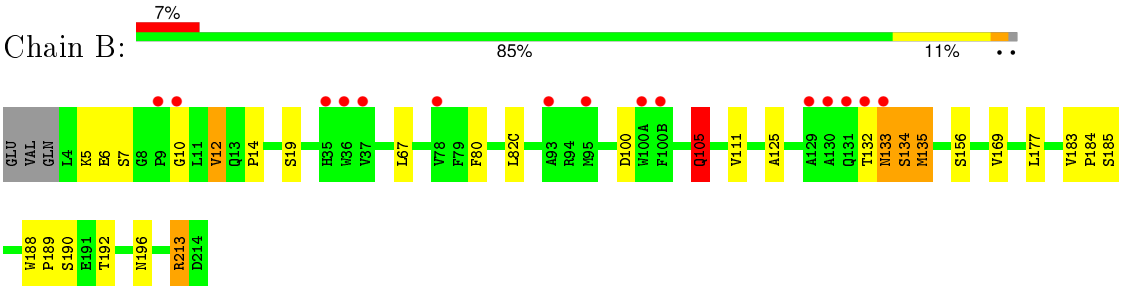
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	44	Total O 44 44	0	0
7	H	22	Total O 22 22	0	0
7	C	38	Total O 38 38	0	0
7	L	20	Total O 20 20	0	0

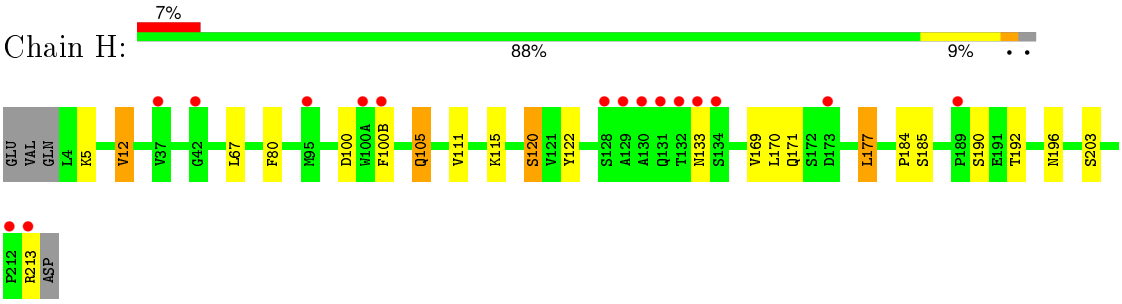
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

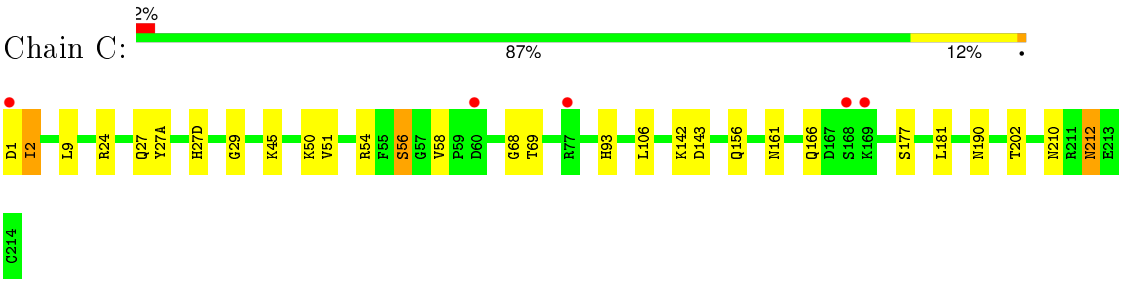
- Molecule 1: S25-26 Fab (Igg1k) Heavy Chain



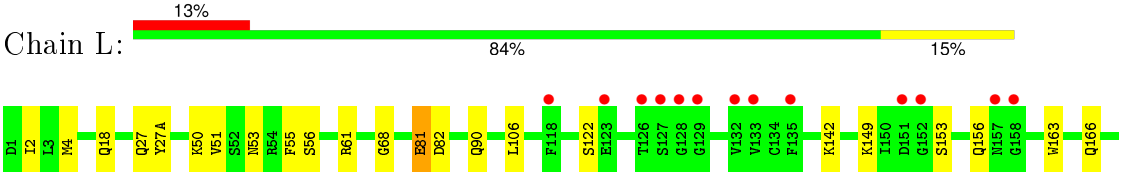
- Molecule 1: S25-26 Fab (Igg1k) Heavy Chain

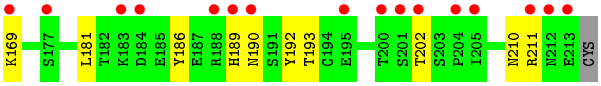


- Molecule 2: S25-26 Fab (Igg1k) Light Chain



- Molecule 2: S25-26 Fab (Igg1k) Light Chain




K169
S177
L181
T182
K183
D184
E185
Y186
E187
R188
H189
N190
S191
Y192
T193
C194
E195
T200
S201
T202
S203
P204
I205
N210
R211
N212
E213
CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.30Å 111.99Å 156.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.76 – 2.75 24.75 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.76-2.75) 100.0 (24.75-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.28 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.216 , 0.238 0.215 , 0.237	Depositor DCC
R_{free} test set	1992 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	66.4	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 26.7	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 39858 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6973	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: PG4, PEG, CA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	B	0.54	0/1677	0.70	1/2297 (0.0%)
1	H	0.51	0/1669	0.71	0/2286
2	C	0.55	0/1752	0.72	0/2376
2	L	0.51	0/1746	0.72	0/2368
All	All	0.53	0/6844	0.71	1/9327 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	105	GLN	CB-CA-C	-5.22	99.96	110.40

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	B	1631	0	1598	35	0
1	H	1623	0	1593	9	0
2	C	1712	0	1649	15	0
2	L	1706	0	1644	26	0
3	B	14	0	13	0	0
3	H	14	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	52	0	71	0	0
4	C	13	0	18	0	0
4	H	13	0	17	0	0
4	L	26	0	36	0	0
5	B	21	0	30	3	0
5	C	7	0	10	0	0
5	H	7	0	10	0	0
5	L	7	0	10	0	0
6	B	1	0	0	0	0
6	H	1	0	0	0	0
6	L	1	0	0	1	0
7	B	44	0	0	0	0
7	C	38	0	0	2	0
7	H	22	0	0	1	0
7	L	20	0	0	0	0
All	All	6973	0	6712	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 6.

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)
2:L:192:TYR:CE2	2:L:211:ARG:CZ	2.36	1.08
1:B:135:MET:HE3	1:B:184:PRO:HA	1.37	1.07
2:L:189:HIS:HB2	2:L:211:ARG:NH1	1.78	0.99
1:B:135:MET:CE	1:B:183:VAL:C	2.37	0.93
1:B:135:MET:HE1	1:B:184:PRO:N	1.82	0.93
2:L:189:HIS:HB2	2:L:211:ARG:HH11	1.40	0.87
1:B:135:MET:HE2	1:B:183:VAL:C	1.98	0.83
1:B:135:MET:CE	1:B:184:PRO:HA	2.08	0.83
2:L:192:TYR:CZ	2:L:211:ARG:NH1	2.46	0.82
1:B:135:MET:CE	1:B:184:PRO:N	2.41	0.82
2:L:192:TYR:CE2	2:L:211:ARG:NH1	2.48	0.82
1:B:135:MET:CE	1:B:184:PRO:CA	2.59	0.80
1:B:135:MET:HE2	1:B:183:VAL:O	1.82	0.80
1:B:135:MET:HA	1:B:135:MET:HE3	1.65	0.78
3:H:401:NAG:O7	3:H:401:NAG:O3	2.05	0.75
1:B:135:MET:HE3	1:B:184:PRO:CA	2.15	0.75
2:C:2:ILE:HD13	2:C:27:GLN:HB2	1.70	0.73
2:L:189:HIS:CB	2:L:211:ARG:NH1	2.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:SER:HA	5:B:406:PEG:H41	1.73	0.69
1:H:100:ASP:O	2:L:55:PHE:CE1	2.47	0.68
1:B:135:MET:CE	1:B:183:VAL:O	2.41	0.67
1:B:6:GLU:H	1:B:105:GLN:HE22	1.41	0.67
2:L:2:ILE:HD12	2:L:27:GLN:HB2	1.77	0.66
2:L:192:TYR:CD2	2:L:211:ARG:NH2	2.63	0.66
1:B:135:MET:HE1	1:B:184:PRO:CA	2.27	0.65
1:B:125:ALA:O	1:B:213:ARG:NH1	2.30	0.64
2:L:81:GLU:OE2	6:L:304:CA:CA	1.74	0.64
1:B:135:MET:CE	1:B:135:MET:HA	2.28	0.63
1:H:105:GLN:HE21	1:H:105:GLN:H	1.46	0.62
2:L:50:LYS:HB2	2:L:53:ASN:HD22	1.64	0.61
2:C:54:ARG:NH1	2:C:58:VAL:O	2.34	0.61
1:B:105:GLN:HE21	1:B:105:GLN:H	1.49	0.61
1:B:14:PRO:O	1:B:82(C):LEU:O	2.18	0.61
2:L:190:ASN:C	2:L:211:ARG:NH2	2.55	0.60
2:L:61:ARG:NH2	2:L:82:ASP:OD2	2.34	0.60
1:B:134:SER:O	1:B:185:SER:N	2.26	0.59
2:L:192:TYR:CD2	2:L:211:ARG:CZ	2.85	0.59
1:B:135:MET:HE1	1:B:183:VAL:C	2.18	0.57
2:C:54:ARG:HD3	7:C:404:HOH:O	2.05	0.56
3:H:401:NAG:C7	3:H:401:NAG:HO3	2.13	0.56
1:B:6:GLU:N	1:B:105:GLN:HE22	2.04	0.55
1:B:7:SER:HA	5:B:406:PEG:C4	2.38	0.54
1:B:105:GLN:NE2	1:B:105:GLN:H	2.08	0.52
1:H:5:LYS:HE3	7:H:522:HOH:O	2.10	0.52
2:L:192:TYR:CE2	2:L:211:ARG:NE	2.79	0.50
2:C:27(D):HIS:CD2	2:C:29:GLY:H	2.29	0.50
1:H:120:SER:HB3	1:H:122:TYR:CZ	2.46	0.50
1:B:67:LEU:HD11	1:B:80:PHE:CE2	2.47	0.50
2:L:189:HIS:O	2:L:211:ARG:NE	2.44	0.50
1:B:135:MET:HE1	1:B:184:PRO:CD	2.42	0.49
1:H:67:LEU:HD11	1:H:80:PHE:CE2	2.48	0.49
1:H:105:GLN:NE2	1:H:105:GLN:H	2.11	0.49
2:C:27(A):TYR:CE2	2:C:68:GLY:HA2	2.46	0.49
2:C:27(D):HIS:HD2	2:C:29:GLY:H	1.59	0.49
2:L:106:LEU:H	2:L:166:GLN:HE22	1.59	0.48
2:C:50:LYS:O	2:C:51:VAL:HB	2.12	0.48
2:C:161:ASN:ND2	2:C:177:SER:OG	2.46	0.48
2:L:50:LYS:O	2:L:51:VAL:HB	2.14	0.48
2:L:27(A):TYR:CE2	2:L:68:GLY:HA2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:177:LEU:C	1:H:177:LEU:HD12	2.35	0.47
2:C:106:LEU:H	2:C:166:GLN:HE22	1.62	0.47
2:C:24:ARG:HA	2:C:69:THR:O	2.16	0.46
1:B:156:SER:HB2	1:H:184:PRO:HG2	1.96	0.46
2:L:142:LYS:HB3	2:L:142:LYS:HE2	1.67	0.46
1:B:12:VAL:O	1:B:111:VAL:HA	2.16	0.46
1:H:12:VAL:O	1:H:111:VAL:HA	2.16	0.46
2:L:190:ASN:HA	2:L:211:ARG:HD3	1.99	0.45
1:B:100:ASP:HB3	2:C:56:SER:HB2	1.98	0.44
2:L:190:ASN:O	2:L:210:ASN:HA	2.18	0.44
2:C:2:ILE:HD11	2:C:93:HIS:CD2	2.52	0.43
2:C:54:ARG:CD	7:C:404:HOH:O	2.65	0.43
1:B:177:LEU:C	1:B:177:LEU:HD12	2.39	0.43
2:L:192:TYR:HE2	2:L:211:ARG:NE	2.17	0.43
1:B:6:GLU:H	1:B:105:GLN:NE2	2.14	0.42
2:L:149:LYS:HB2	2:L:193:THR:HB	2.02	0.42
1:B:133:ASN:OD1	1:B:133:ASN:N	2.52	0.42
2:C:190:ASN:O	2:C:210:ASN:HA	2.20	0.42
2:L:186:TYR:CE1	2:L:192:TYR:CE2	3.08	0.41
2:C:161:ASN:HD22	2:C:177:SER:HA	1.85	0.41
1:B:188:TRP:CG	1:B:189:PRO:HA	2.56	0.41
1:B:19:SER:HA	1:B:80:PHE:O	2.21	0.41
1:B:134:SER:O	1:B:184:PRO:HA	2.21	0.40
1:B:10:GLY:N	5:B:406:PEG:H12	2.36	0.40
2:L:4:MET:HE2	2:L:90:GLN:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	214/219 (98%)	210 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	213/219 (97%)	208 (98%)	5 (2%)	0	100 100
2	C	217/219 (99%)	210 (97%)	6 (3%)	1 (0%)	34 67
2	L	216/219 (99%)	211 (98%)	5 (2%)	0	100 100
All	All	860/876 (98%)	839 (98%)	20 (2%)	1 (0%)	56 86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	212	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	186/189 (98%)	174 (94%)	12 (6%)	21 48
1	H	185/189 (98%)	169 (91%)	16 (9%)	13 33
2	C	196/196 (100%)	185 (94%)	11 (6%)	26 56
2	L	195/196 (100%)	185 (95%)	10 (5%)	29 61
All	All	762/770 (99%)	713 (94%)	49 (6%)	22 49

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	5	LYS
1	B	12	VAL
1	B	105	GLN
1	B	132	THR
1	B	133	ASN
1	B	134	SER
1	B	135	MET
1	B	169	VAL
1	B	190	SER
1	B	192	THR

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Mol	Chain	Res	Type
1	B	196	ASN
1	B	213	ARG
1	H	12	VAL
1	H	100(B)	PHE
1	H	105	GLN
1	H	115	LYS
1	H	120	SER
1	H	133	ASN
1	H	169	VAL
1	H	170	LEU
1	H	171	GLN
1	H	177	LEU
1	H	185	SER
1	H	190	SER
1	H	192	THR
1	H	196	ASN
1	H	203	SER
1	H	213	ARG
2	C	1	ASP
2	C	2	ILE
2	C	9	LEU
2	C	45	LYS
2	C	56	SER
2	C	142	LYS
2	C	143	ASP
2	C	156	GLN
2	C	181	LEU
2	C	202	THR
2	C	212	ASN
2	L	18	GLN
2	L	56	SER
2	L	81	GLU
2	L	122	SER
2	L	153	SER
2	L	156	GLN
2	L	163	TRP
2	L	169	LYS
2	L	181	LEU
2	L	202	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	77	HIS
1	B	105	GLN
1	B	131	GLN
1	B	164	HIS
1	B	171	GLN
1	H	77	HIS
1	H	105	GLN
1	H	164	HIS
2	C	27(D)	HIS
2	C	53	ASN
2	C	138	ASN
2	C	161	ASN
2	C	166	GLN
2	C	210	ASN
2	C	212	ASN
2	L	18	GLN
2	L	30	ASN
2	L	53	ASN
2	L	138	ASN
2	L	156	GLN
2	L	166	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

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
3	NAG	B	401	1	14,14,15	0.42	0	15,19,21	1.06	0
4	PG4	B	402	-	12,12,12	0.69	0	11,11,11	0.50	0
4	PG4	B	403	-	12,12,12	0.49	0	11,11,11	0.53	0
4	PG4	B	404	6	12,12,12	0.59	0	11,11,11	0.36	0
4	PG4	B	405	-	12,12,12	0.64	0	11,11,11	0.42	0
5	PEG	B	406	-	6,6,6	0.59	0	5,5,5	0.53	0
5	PEG	B	407	-	6,6,6	0.51	0	5,5,5	0.17	0
5	PEG	B	408	-	6,6,6	0.56	0	5,5,5	0.39	0
4	PG4	C	301	-	12,12,12	0.69	0	11,11,11	0.37	0
5	PEG	C	302	-	6,6,6	0.47	0	5,5,5	0.28	0
3	NAG	H	401	1	14,14,15	0.28	0	15,19,21	0.53	0
4	PG4	H	402	6	12,12,12	0.74	0	11,11,11	0.45	0
5	PEG	H	403	-	6,6,6	0.46	0	5,5,5	0.33	0
4	PG4	L	301	-	12,12,12	0.55	0	11,11,11	0.18	0
4	PG4	L	302	-	12,12,12	0.62	0	11,11,11	0.35	0
5	PEG	L	303	-	6,6,6	0.57	0	5,5,5	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	401	1	-	0/6/23/26	0/1/1/1
4	PG4	B	402	-	-	0/10/10/10	0/0/0/0
4	PG4	B	403	-	-	0/10/10/10	0/0/0/0
4	PG4	B	404	6	-	0/10/10/10	0/0/0/0
4	PG4	B	405	-	-	0/10/10/10	0/0/0/0
5	PEG	B	406	-	-	0/4/4/4	0/0/0/0
5	PEG	B	407	-	-	0/4/4/4	0/0/0/0
5	PEG	B	408	-	-	0/4/4/4	0/0/0/0
4	PG4	C	301	-	-	0/10/10/10	0/0/0/0
5	PEG	C	302	-	-	0/4/4/4	0/0/0/0
3	NAG	H	401	1	-	0/6/23/26	0/1/1/1
4	PG4	H	402	6	-	0/10/10/10	0/0/0/0
5	PEG	H	403	-	-	0/4/4/4	0/0/0/0
4	PG4	L	301	-	-	0/10/10/10	0/0/0/0
4	PG4	L	302	-	-	0/10/10/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	L	303	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	406	PEG	3	0
3	H	401	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	B	216/219 (98%)	0.25	15 (6%) 20 14	29, 41, 61, 70	0
1	H	215/219 (98%)	0.52	16 (7%) 17 12	27, 60, 96, 120	0
2	C	219/219 (100%)	0.11	5 (2%) 64 57	26, 40, 55, 71	0
2	L	218/219 (99%)	0.55	29 (13%) 4 3	27, 62, 128, 149	0
All	All	868/876 (99%)	0.36	65 (7%) 17 12	26, 45, 104, 149	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	129	ALA	6.5
1	B	100(A)	TRP	5.6
2	C	168	SER	5.3
1	H	132	THR	5.3
1	H	130	ALA	5.1
1	H	100(A)	TRP	4.5
1	B	100(B)	PHE	4.5
1	H	131	GLN	4.4
2	L	157	ASN	4.4
2	L	158	GLY	4.1
2	L	190	ASN	3.9
2	L	202	THR	3.9
2	L	212	ASN	3.9
1	H	133	ASN	3.9
2	C	169	LYS	3.7
1	B	9	PRO	3.7
1	B	131	GLN	3.6
2	L	126	THR	3.5
1	H	128	SER	3.5
2	L	132	VAL	3.5
1	B	93	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
2	L	128	GLY	3.2
1	B	132	THR	3.2
2	L	188	ARG	3.2
1	H	100(B)	PHE	3.1
2	L	205	ILE	3.1
2	L	183	LYS	3.0
1	H	213	ARG	3.0
1	B	10	GLY	3.0
2	L	127	SER	2.9
2	L	213	GLU	2.9
2	L	184	ASP	2.9
2	L	189	HIS	2.8
2	L	195	GLU	2.8
2	L	201	SER	2.8
1	B	35	HIS	2.8
2	L	177	SER	2.7
2	L	151	ASP	2.7
2	L	211	ARG	2.7
1	H	173	ASP	2.6
2	L	123	GLU	2.6
1	B	133	ASN	2.5
2	L	169	LYS	2.5
1	B	130	ALA	2.4
2	L	129	GLY	2.4
1	H	212	PRO	2.3
2	L	152	GLY	2.3
2	C	1	ASP	2.3
1	H	134	SER	2.3
1	B	36	TRP	2.3
2	L	135	PHE	2.3
2	L	204	PRO	2.3
1	B	78	VAL	2.3
2	L	133	VAL	2.3
1	B	129	ALA	2.3
2	C	60	ASP	2.2
1	H	95	MET	2.2
1	H	37	VAL	2.2
2	L	200	THR	2.2
1	H	42	GLY	2.1
1	B	95	MET	2.1
2	C	77	ARG	2.1
1	B	37	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	189	PRO	2.0
2	L	118	PHE	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
4	PG4	H	402	13/13	0.90	0.22	12.53	37,37,37,37	0
5	PEG	B	407	7/7	0.84	0.40	9.73	37,37,37,37	0
4	PG4	B	404	13/13	0.88	0.28	5.09	37,37,37,37	0
4	PG4	B	405	13/13	0.87	0.31	3.64	37,37,37,37	0
5	PEG	B	408	7/7	0.81	0.32	2.56	37,37,37,37	0
4	PG4	L	301	13/13	0.83	0.33	2.08	37,37,37,37	0
4	PG4	B	402	13/13	0.85	0.28	1.61	37,37,37,37	0
4	PG4	B	403	13/13	0.81	0.23	1.40	37,37,37,37	0
5	PEG	B	406	7/7	0.81	0.34	1.05	37,37,37,37	0
5	PEG	L	303	7/7	0.87	0.22	0.42	37,37,37,37	0
5	PEG	C	302	7/7	0.94	0.14	-1.41	37,37,37,37	0
6	CA	L	304	1/1	0.91	0.10	-	37,37,37,37	1
3	NAG	B	401	14/15	0.90	0.31	-	37,37,37,37	0
4	PG4	C	301	13/13	0.88	0.35	-	37,37,37,37	0
5	PEG	H	403	7/7	0.86	0.38	-	37,37,37,37	0
6	CA	B	409	1/1	0.98	0.06	-	37,37,37,37	0
4	PG4	L	302	13/13	0.89	0.40	-	37,37,37,37	0
3	NAG	H	401	14/15	0.79	0.40	-	37,37,37,37	0
6	CA	H	404	1/1	0.97	0.05	-	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.