



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2024 – 09:04 AM EST

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

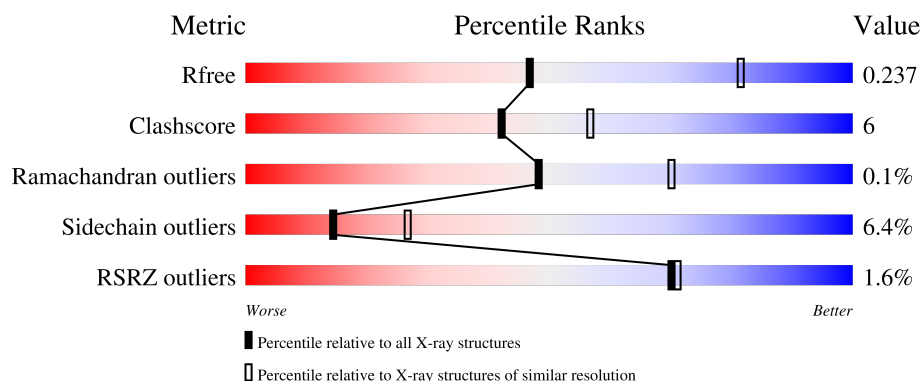
1 Overall quality at a glance

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}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	B	219	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	H	219	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>..</div> </div> </div>
2	C	219	<div> <div></div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
2	L	219	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>15%</div> </div> </div>

2 Entry composition [i](#)

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.

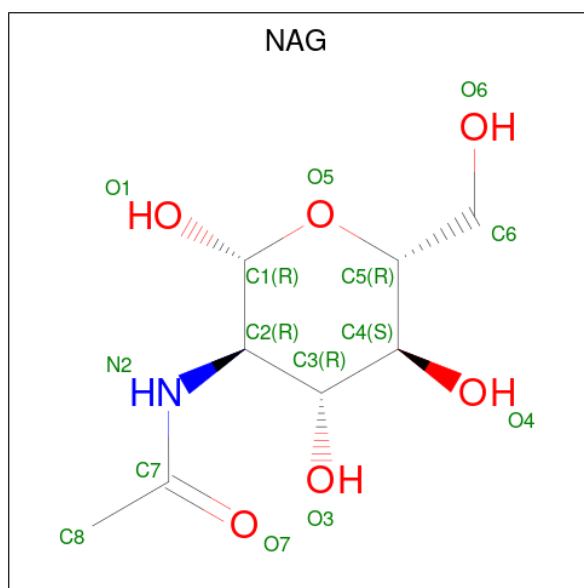
- Molecule 1 is a protein called S25-26 Fab (Igglk) Heavy Chain.

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 (Igglk) Light Chain.

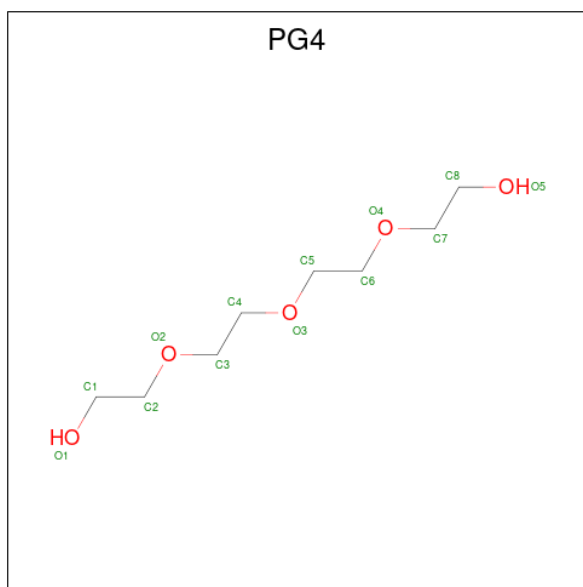
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	219	Total	C	N	O	S	0	0	0
			1712	1072	291	342	7			
2	L	218	Total	C	N	O	S	0	0	0
			1706	1069	290	341	6			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

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

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

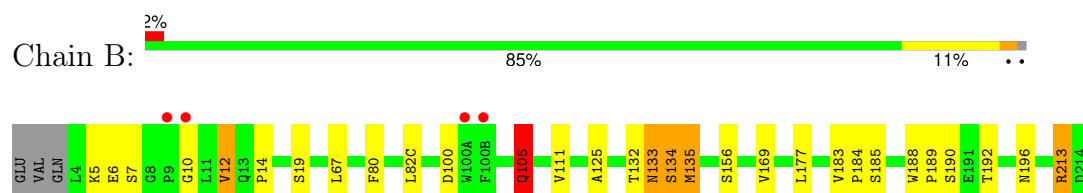
- Molecule 7 is water.

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

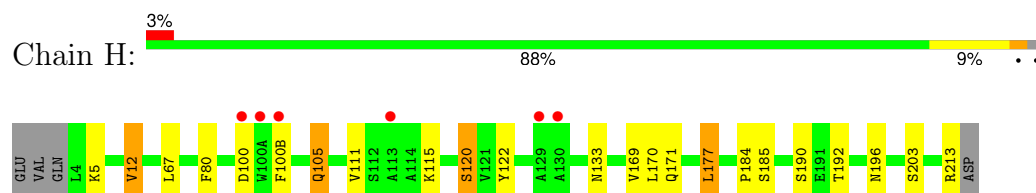
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

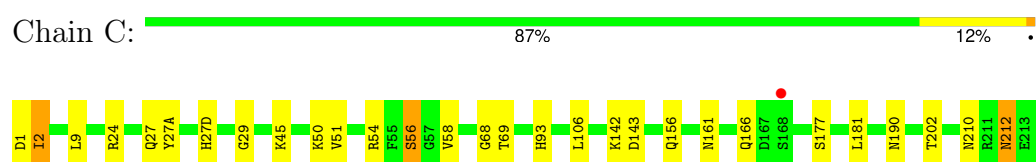
- Molecule 1: S25-26 Fab (IgG1k) Heavy Chain



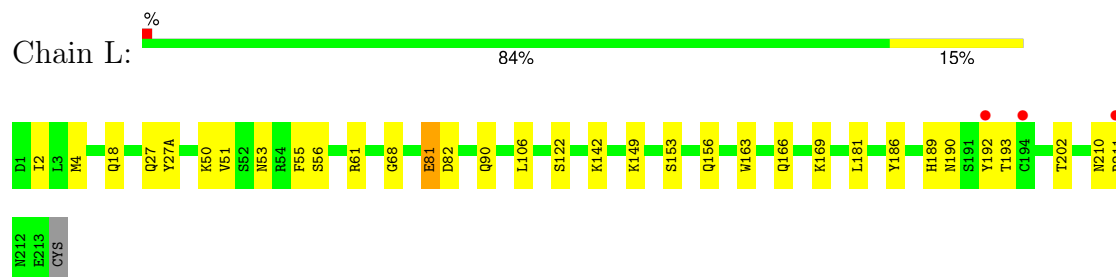
- Molecule 1: S25-26 Fab (IgG1k) Heavy Chain



- Molecule 2: S25-26 Fab (IgG1k) Light Chain



- Molecule 2: S25-26 Fab (IgG1k) Light Chain



4 Data and refinement statistics

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 24.76 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.76-2.75) 99.8 (24.76-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.76Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.238 0.215 , 0.237	Depositor DCC
R_{free} test set	1992 reflections (5.01%)	wwPDB-VP
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 , 24.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: PG4, NAG, PEG, CA

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(°)	Ideal(°)
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 [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	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:HE3	1:B:135:MET:HA	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:6:GLU:H	1:B:105:GLN:HE22	1.41	0.67
1:B:135:MET:CE	1:B:183:VAL:O	2.41	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:HO3	3:H:401:NAG:C7	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:H	1:B:105:GLN:NE2	2.08	0.52
1:H:5:LYS:HE3	7:H:522:HOH:O	2.10	0.52
1:H:120:SER:HB3	1:H:122:TYR:CZ	2.46	0.50
2:C:27(D):HIS:CD2	2:C:29:GLY:H	2.29	0.50
2:L:192:TYR:CE2	2:L:211:ARG:NE	2.79	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:H	1:H:105:GLN:NE2	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:C:50:LYS:O	2:C:51:VAL:HB	2.12	0.48
2:L:106:LEU:H	2:L:166:GLN:HE22	1.59	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
1:H:177:LEU:C	1:H:177:LEU:HD12	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:LEU:H	2:C:166:GLN:HE22	1.62	0.47
2:L:27(A):TYR:CE2	2:L:68:GLY:HA2	2.50	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:HE2	2:L:142:LYS:HB3	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
1:B:133:ASN:N	1:B:133:ASN:OD1	2.52	0.42
2:L:149:LYS:HB2	2:L:193:THR:HB	2.02	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

5.3.1 Protein backbone

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%)	25	41
2	L	216/219 (99%)	211 (98%)	5 (2%)	0	100	100
All	All	860/876 (98%)	839 (98%)	20 (2%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	212	ASN

5.3.2 Protein sidechains ⓘ

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%)	14	26
1	H	185/189 (98%)	169 (91%)	16 (9%)	8	15
2	C	196/196 (100%)	185 (94%)	11 (6%)	17	32
2	L	195/196 (100%)	185 (95%)	10 (5%)	20	36
All	All	762/770 (99%)	713 (94%)	49 (6%)	14	27

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

Sometimes 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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
4	PG4	B	402	-	12,12,12	0.69	0	11,11,11	0.50	0
4	PG4	L	302	-	12,12,12	0.62	0	11,11,11	0.35	0
4	PG4	L	301	-	12,12,12	0.55	0	11,11,11	0.20	0
5	PEG	L	303	-	6,6,6	0.58	0	5,5,5	0.57	0
4	PG4	B	404	6	12,12,12	0.59	0	11,11,11	0.38	0
5	PEG	B	408	-	6,6,6	0.56	0	5,5,5	0.40	0
4	PG4	B	405	-	12,12,12	0.64	0	11,11,11	0.44	0
4	PG4	C	301	-	12,12,12	0.68	0	11,11,11	0.39	0
5	PEG	B	407	-	6,6,6	0.52	0	5,5,5	0.19	0
4	PG4	H	402	6	12,12,12	0.74	0	11,11,11	0.47	0
5	PEG	H	403	-	6,6,6	0.46	0	5,5,5	0.30	0
5	PEG	B	406	-	6,6,6	0.60	0	5,5,5	0.52	0
3	NAG	H	401	1	14,14,15	0.29	0	17,19,21	0.56	0
4	PG4	B	403	-	12,12,12	0.49	0	11,11,11	0.53	0
5	PEG	C	302	-	6,6,6	0.48	0	5,5,5	0.25	0
3	NAG	B	401	1	14,14,15	0.44	0	17,19,21	1.14	1 (5%)

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	PG4	B	402	-	-	5/10/10/10	-
4	PG4	L	302	-	-	2/10/10/10	-
4	PG4	L	301	-	-	6/10/10/10	-
5	PEG	L	303	-	-	3/4/4/4	-
4	PG4	B	404	6	-	5/10/10/10	-
5	PEG	B	408	-	-	4/4/4/4	-
4	PG4	B	405	-	-	6/10/10/10	-
4	PG4	C	301	-	-	5/10/10/10	-
5	PEG	B	407	-	-	3/4/4/4	-
4	PG4	H	402	6	-	4/10/10/10	-
5	PEG	H	403	-	-	1/4/4/4	-
5	PEG	B	406	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	H	401	1	-	3/6/23/26	0/1/1/1
4	PG4	B	403	-	-	9/10/10/10	-
5	PEG	C	302	-	-	1/4/4/4	-
3	NAG	B	401	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(°)	Ideal(°)
3	B	401	NAG	O5-C1-C2	-2.14	107.98	111.29

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	301	PG4	O1-C1-C2-O2
5	B	408	PEG	O1-C1-C2-O2
4	B	403	PG4	O3-C5-C6-O4
4	C	301	PG4	O2-C3-C4-O3
4	B	405	PG4	O2-C3-C4-O3
4	B	403	PG4	O1-C1-C2-O2
4	B	403	PG4	O4-C7-C8-O5
5	B	406	PEG	O1-C1-C2-O2
4	B	402	PG4	O1-C1-C2-O2
5	B	408	PEG	O2-C3-C4-O4
5	C	302	PEG	O2-C3-C4-O4
4	B	404	PG4	O3-C5-C6-O4
4	B	402	PG4	O4-C7-C8-O5
4	L	301	PG4	O2-C3-C4-O3
3	H	401	NAG	C3-C2-N2-C7
3	H	401	NAG	C4-C5-C6-O6
4	H	402	PG4	O3-C5-C6-O4
4	L	301	PG4	C1-C2-O2-C3
5	L	303	PEG	C1-C2-O2-C3
4	B	403	PG4	O2-C3-C4-O3
4	B	405	PG4	C8-C7-O4-C6
4	B	403	PG4	C4-C3-O2-C2
4	B	402	PG4	C8-C7-O4-C6
4	B	405	PG4	C6-C5-O3-C4
4	B	403	PG4	C3-C4-O3-C5
4	B	403	PG4	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
4	B	404	PG4	C8-C7-O4-C6
4	B	405	PG4	C5-C6-O4-C7
4	L	301	PG4	C5-C6-O4-C7
4	B	403	PG4	C8-C7-O4-C6
4	B	404	PG4	O4-C7-C8-O5
4	H	402	PG4	O4-C7-C8-O5
4	B	402	PG4	C4-C3-O2-C2
4	L	302	PG4	C5-C6-O4-C7
4	B	403	PG4	C1-C2-O2-C3
4	H	402	PG4	C4-C3-O2-C2
5	B	407	PEG	O1-C1-C2-O2
4	B	402	PG4	C3-C4-O3-C5
3	H	401	NAG	O5-C5-C6-O6
5	L	303	PEG	C4-C3-O2-C2
5	B	407	PEG	O2-C3-C4-O4
5	L	303	PEG	O1-C1-C2-O2
4	B	404	PG4	C4-C3-O2-C2
4	L	301	PG4	O1-C1-C2-O2
5	B	406	PEG	C4-C3-O2-C2
4	C	301	PG4	C4-C3-O2-C2
5	H	403	PEG	C4-C3-O2-C2
4	C	301	PG4	C8-C7-O4-C6
4	B	405	PG4	O3-C5-C6-O4
4	B	405	PG4	O4-C7-C8-O5
4	L	301	PG4	C3-C4-O3-C5
4	C	301	PG4	O3-C5-C6-O4
4	B	404	PG4	C1-C2-O2-C3
5	B	407	PEG	C1-C2-O2-C3
4	L	301	PG4	C6-C5-O3-C4
5	B	408	PEG	C1-C2-O2-C3
4	L	302	PG4	O1-C1-C2-O2
5	B	408	PEG	C4-C3-O2-C2
4	H	402	PG4	C6-C5-O3-C4

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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	B	216/219 (98%)	-0.38	4 (1%) 66 67	29, 41, 61, 70	0
1	H	215/219 (98%)	-0.08	6 (2%) 55 56	27, 60, 96, 120	0
2	C	219/219 (100%)	-0.48	1 (0%) 87 89	26, 40, 55, 71	0
2	L	218/219 (99%)	-0.13	3 (1%) 73 75	27, 62, 128, 149	0
All	All	868/876 (99%)	-0.27	14 (1%) 70 71	26, 45, 104, 149	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	100(B)	PHE	3.9
1	H	129	ALA	3.4
2	C	168	SER	3.4
1	B	100(A)	TRP	3.2
1	B	9	PRO	3.1
1	B	100(B)	PHE	2.8
1	H	100(A)	TRP	2.6
2	L	211	ARG	2.5
1	H	130	ALA	2.5
1	B	10	GLY	2.5
2	L	194	CYS	2.3
1	H	113	ALA	2.3
1	H	100	ASP	2.2
2	L	192	TYR	2.2

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 monosaccharides 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. 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	B-factors(\AA^2)	Q<0.9
5	PEG	B	408	7/7	0.62	0.18	37,37,37,37	0
5	PEG	B	406	7/7	0.68	0.15	37,37,37,37	0
5	PEG	L	303	7/7	0.71	0.14	37,37,37,37	0
3	NAG	H	401	14/15	0.72	0.20	37,37,37,37	0
4	PG4	L	301	13/13	0.81	0.16	37,37,37,37	0
3	NAG	B	401	14/15	0.83	0.14	37,37,37,37	0
5	PEG	B	407	7/7	0.83	0.15	37,37,37,37	0
4	PG4	B	403	13/13	0.84	0.12	37,37,37,37	0
5	PEG	H	403	7/7	0.85	0.13	37,37,37,37	0
4	PG4	C	301	13/13	0.85	0.11	37,37,37,37	0
4	PG4	L	302	13/13	0.87	0.12	37,37,37,37	0
4	PG4	H	402	13/13	0.87	0.11	37,37,37,37	0
4	PG4	B	405	13/13	0.88	0.15	37,37,37,37	0
4	PG4	B	402	13/13	0.88	0.12	37,37,37,37	0
4	PG4	B	404	13/13	0.92	0.10	37,37,37,37	0
5	PEG	C	302	7/7	0.93	0.10	37,37,37,37	0
6	CA	L	304	1/1	0.94	0.06	37,37,37,37	1
6	CA	B	409	1/1	0.97	0.04	37,37,37,37	0
6	CA	H	404	1/1	0.98	0.04	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.