



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:19 PM UTC

PDB ID : 4M93 / pdb_00004m93
Title : Unliganded 2 crystal structure of S25-26 Fab
Authors : Haji-Ghassemi, O.; Evans, S.V.
Deposited on : 2013-08-14
Resolution : 2.09 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

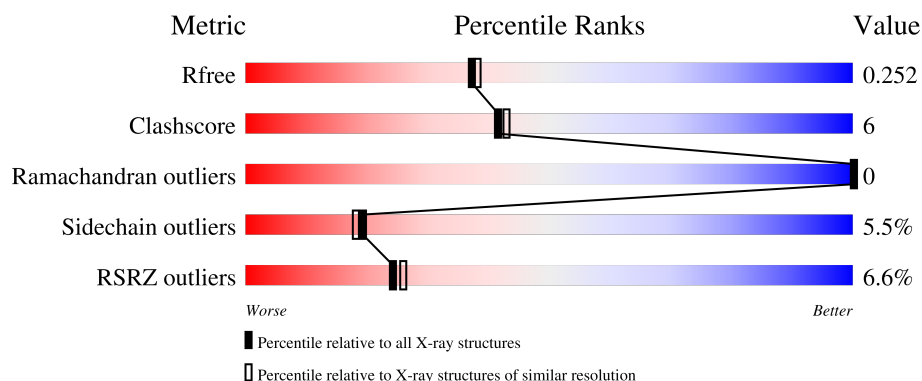
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	C	219	3% 84% 15% .
1	L	219	10% 84% 13% .
2	B	218	5% 83% 15% .
2	H	218	9% 90% 8% .

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
5	ACT	B	303	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7037 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.

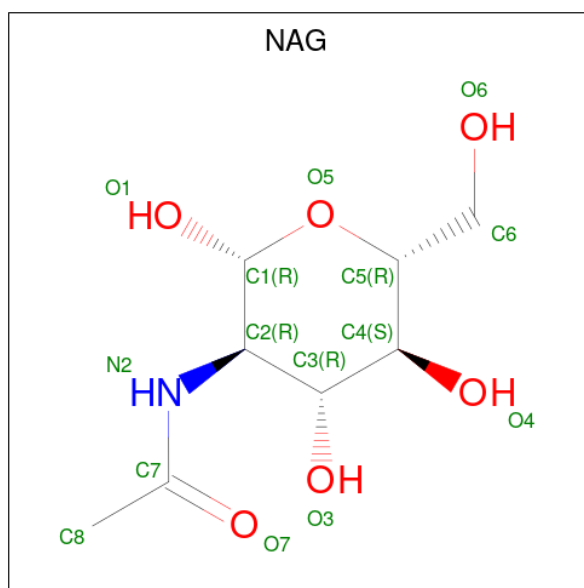
- Molecule 1 is a protein called S25-26 Fab (IgG1k) light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	218	Total	C	N	O	S	0	0	0
			1706	1069	290	341	6			
1	C	218	Total	C	N	O	S	0	1	0
			1712	1072	291	342	7			

- Molecule 2 is a protein called S25-26 Fab (IgG1k) heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1647	1050	273	317	7			
2	B	218	Total	C	N	O	S	0	2	0
			1659	1056	275	319	9			

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

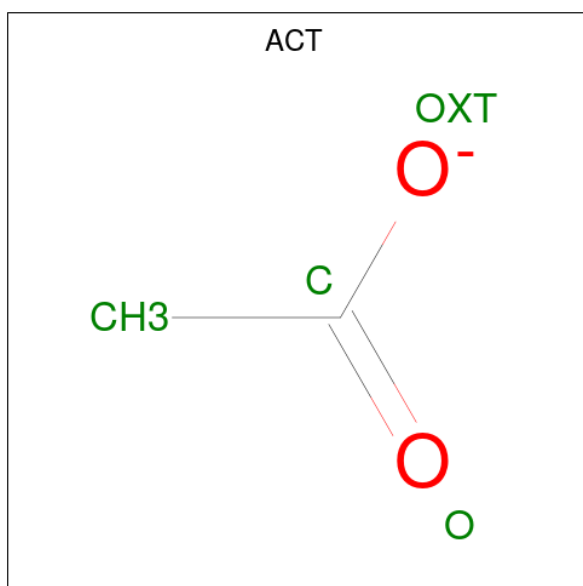


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	46	Total	O	0	0
			46	46		

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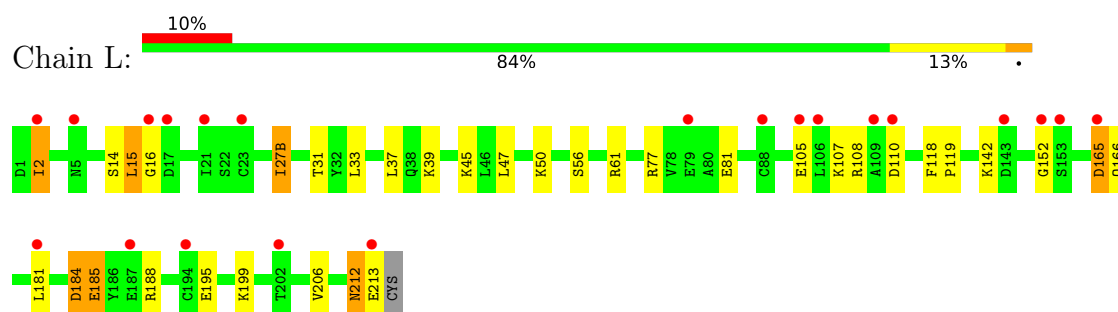
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	70	Total 70	O 70	0	0
6	C	79	Total 79	O 79	0	0
6	B	77	Total 77	O 77	0	0

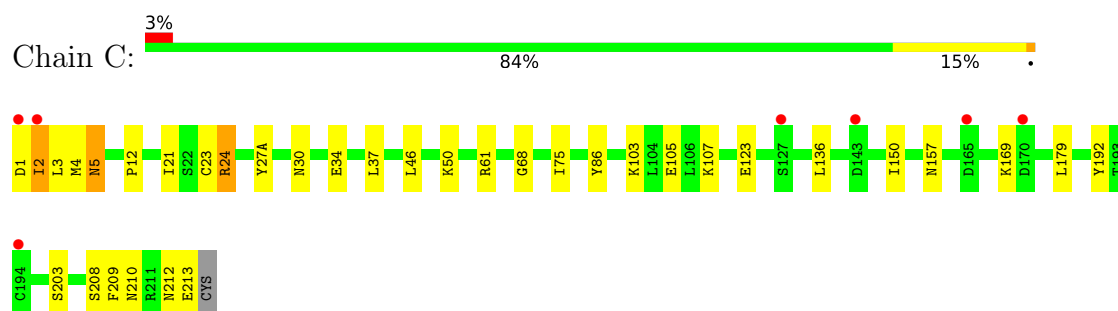
3 Residue-property plots [i](#)

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.

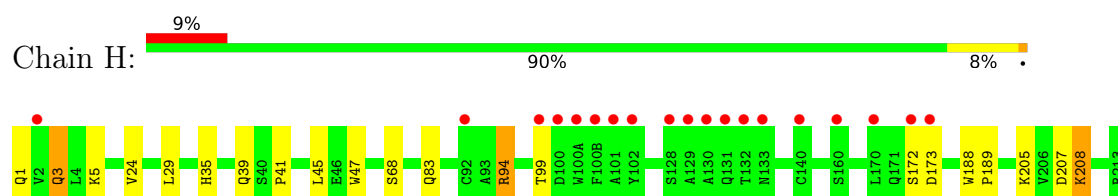
- Molecule 1: S25-26 Fab (IgG1k) light chain



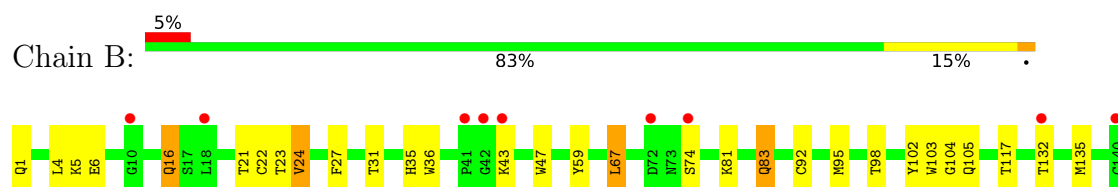
- Molecule 1: S25-26 Fab (IgG1k) light chain



- Molecule 2: S25-26 Fab (IgG1k) heavy chain



- Molecule 2: S25-26 Fab (IgG1k) heavy chain





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.89Å 88.81Å 101.89Å 90.00° 102.06° 90.00°	Depositor
Resolution (Å)	24.87 – 2.09 24.87 – 2.09	Depositor EDS
% Data completeness (in resolution range)	96.7 (24.87-2.09) 98.0 (24.87-2.09)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.06Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.218 , 0.251 0.215 , 0.252	Depositor DCC
R_{free} test set	3113 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.2	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	7037	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, PCA, 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	C	0.70	0/1752	0.85	0/2376
1	L	0.78	8/1746 (0.5%)	0.88	3/2368 (0.1%)
2	B	0.64	0/1698	0.89	2/2327 (0.1%)
2	H	0.67	0/1686	0.87	0/2311
All	All	0.70	8/6882 (0.1%)	0.87	5/9382 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	108	ARG	CA-C	7.87	1.62	1.52
1	L	16	GLY	N-CA	-7.60	1.33	1.45
1	L	110	ASP	C-N	5.98	1.41	1.33
1	L	15	LEU	CA-C	5.92	1.60	1.52
1	L	152	GLY	N-CA	5.58	1.53	1.45
1	L	16	GLY	C-N	-5.44	1.26	1.33
1	L	16	GLY	C-O	-5.25	1.16	1.24
1	L	152	GLY	C-N	5.03	1.40	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	108	ARG	O-C-N	6.13	129.70	123.26
1	L	108	ARG	CA-C-O	-6.13	114.88	121.38
1	L	27(B)	ILE	CB-CA-C	5.30	117.42	111.80
2	B	117	THR	CA-C-N	5.26	123.45	119.66
2	B	117	THR	C-N-CA	5.26	123.45	119.66

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	C	1712	0	1647	23	0
1	L	1706	0	1644	16	0
2	B	1659	0	1624	27	0
2	H	1647	0	1618	18	0
3	B	14	0	13	0	0
3	H	14	0	13	0	0
4	B	1	0	0	0	0
5	B	12	0	9	5	0
6	B	77	0	0	3	0
6	C	79	0	0	5	0
6	H	70	0	0	3	0
6	L	46	0	0	0	0
All	All	7037	0	6568	85	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 (85) 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:H:94:ARG:HH11	2:H:94:ARG:HG2	1.06	1.19
2:B:4:LEU:HD11	2:B:102:TYR:HB2	1.48	0.96
2:B:21:THR:OG1	5:B:305:ACT:H3	1.70	0.92
2:H:94:ARG:HG2	2:H:94:ARG:NH1	1.85	0.89
2:B:35:HIS:HD2	2:B:47:TRP:HE1	1.17	0.89
1:C:24:ARG:HH11	1:C:24:ARG:HG3	1.42	0.84
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.24	0.83
1:C:103:LYS:HE3	6:C:371:HOH:O	1.78	0.82
2:B:4:LEU:HD11	2:B:102:TYR:CB	2.09	0.82
5:B:303:ACT:OXT	5:B:304:ACT:H1	1.83	0.78
2:H:41:PRO:HD2	6:H:436:HOH:O	1.87	0.73
2:B:16:GLN:HE21	2:B:16:GLN:HA	1.53	0.72
2:H:35:HIS:CD2	2:H:47:TRP:HE1	2.12	0.65
2:B:35:HIS:CD2	2:B:47:TRP:HE1	2.08	0.65
2:B:4:LEU:CD1	2:B:102:TYR:CB	2.75	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:MET:HE3	1:C:23:CYS:SG	2.39	0.63
2:B:4:LEU:CD1	2:B:102:TYR:HB3	2.28	0.63
1:C:209:PHE:HA	5:B:303:ACT:H3	1.82	0.61
2:B:172:SER:OG	2:B:173:ASP:N	2.32	0.61
2:B:6:GLU:H	2:B:105:GLN:HE21	1.47	0.61
1:L:39:LYS:HE2	1:L:81:GLU:O	2.01	0.61
2:B:22[B]:CYS:SG	2:B:36:TRP:CH2	2.94	0.60
1:L:105:GLU:HB2	1:L:166:GLN:HE22	1.66	0.60
1:L:37:LEU:HB2	1:L:47:LEU:HD11	1.82	0.59
2:B:4:LEU:N	2:B:4:LEU:HD12	2.18	0.57
2:B:135:MET:HE3	2:B:182:THR:HG22	1.86	0.57
1:L:185:GLU:HA	1:L:188:ARG:HD3	1.87	0.56
1:L:212:ASN:H	1:L:212:ASN:HD22	1.52	0.56
2:H:172:SER:OG	2:H:173:ASP:N	2.39	0.56
2:H:41:PRO:HA	6:H:449:HOH:O	2.04	0.56
1:C:123:GLU:HB2	6:C:352:HOH:O	2.07	0.54
1:C:2:ILE:HD12	1:C:2:ILE:N	2.23	0.54
1:C:210:ASN:H	5:B:303:ACT:H3	1.73	0.53
2:H:94:ARG:HH11	2:H:94:ARG:CG	1.97	0.53
2:B:83:GLN:HG3	6:B:434:HOH:O	2.11	0.51
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.91	0.51
1:C:2:ILE:N	1:C:2:ILE:CD1	2.74	0.51
2:H:35:HIS:HE1	6:H:432:HOH:O	1.93	0.50
2:B:5:LYS:HG3	2:B:23:THR:HB	1.93	0.50
2:B:36:TRP:CZ2	2:B:92[B]:CYS:SG	3.05	0.49
1:L:27(B):ILE:O	1:L:27(B):ILE:HG13	2.12	0.49
1:C:24:ARG:HG3	1:C:24:ARG:NH1	2.18	0.49
2:B:59:TYR:CD1	2:B:67:LEU:HD23	2.46	0.49
2:B:213:ARG:C	6:B:448:HOH:O	2.55	0.49
1:L:195:GLU:HG2	1:L:206:VAL:HG22	1.95	0.48
1:C:34:GLU:HG2	1:C:46:LEU:HD11	1.96	0.48
2:H:35:HIS:HD2	2:H:47:TRP:NE1	2.03	0.48
1:L:2:ILE:CD1	1:L:2:ILE:N	2.77	0.47
1:C:24:ARG:HH11	1:C:24:ARG:CG	2.20	0.47
2:H:3:GLN:HG2	2:H:5:LYS:HE3	1.98	0.46
1:C:212:ASN:ND2	6:C:366:HOH:O	2.49	0.45
2:B:16:GLN:HA	2:B:16:GLN:NE2	2.29	0.45
1:L:31:THR:O	1:L:50:LYS:HA	2.17	0.45
1:L:61:ARG:HD2	1:L:77:ARG:O	2.17	0.45
1:C:150:ILE:HD11	1:C:179:LEU:HD21	1.98	0.45
2:B:192:THR:OG1	2:B:209:LYS:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:27(B):ILE:HD11	1:L:33:LEU:HB2	1.98	0.44
2:B:4:LEU:HD12	2:B:102:TYR:HB3	1.98	0.44
2:B:24:VAL:HG22	2:B:27:PHE:CZ	2.53	0.44
2:H:207:ASP:O	2:H:208:LYS:HD2	2.17	0.44
1:C:61:ARG:O	1:C:75:ILE:HA	2.18	0.44
1:L:212:ASN:O	1:L:213:GLU:HB2	2.18	0.43
1:C:12:PRO:HB2	1:C:107:LYS:HE3	2.00	0.43
1:C:210:ASN:H	5:B:303:ACT:CH3	2.31	0.43
1:C:3:LEU:HG	1:C:5:ASN:ND2	2.34	0.43
1:C:21:ILE:HB	6:C:355:HOH:O	2.18	0.43
1:C:37:LEU:HD13	1:C:86:TYR:CZ	2.54	0.43
1:L:105:GLU:HB2	1:L:166:GLN:NE2	2.32	0.42
2:B:4:LEU:HD13	2:B:103:TRP:C	2.44	0.42
1:C:192:TYR:O	1:C:208:SER:HB2	2.19	0.42
2:B:172:SER:HG	2:B:173:ASP:H	1.63	0.42
1:L:184:ASP:OD1	1:L:184:ASP:N	2.48	0.42
2:H:205:LYS:HE3	2:H:205:LYS:HB2	1.81	0.42
1:C:5:ASN:ND2	6:C:324:HOH:O	2.51	0.42
2:B:35:HIS:HE1	6:B:446:HOH:O	2.02	0.41
2:H:83:GLN:NE2	2:H:83:GLN:HA	2.35	0.41
2:H:83:GLN:HA	2:H:83:GLN:HE21	1.85	0.41
1:C:30:ASN:ND2	1:C:50:LYS:NZ	2.68	0.41
2:H:24:VAL:HG21	2:H:29:LEU:HD21	2.02	0.41
2:H:188:TRP:CD1	2:H:189:PRO:HA	2.56	0.41
2:B:6:GLU:OE2	2:B:104:GLY:HA3	2.19	0.41
1:L:118:PHE:HA	1:L:119:PRO:HD2	1.90	0.41
1:L:165:ASP:OD1	1:L:165:ASP:N	2.44	0.40
1:C:27(A):TYR:CE2	1:C:68:GLY:HA2	2.57	0.40
2:B:6:GLU:HG2	2:B:22[B]:CYS:SG	2.61	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	C	217/219 (99%)	214 (99%)	3 (1%)	0	100	100
1	L	216/219 (99%)	210 (97%)	6 (3%)	0	100	100
2	B	218/218 (100%)	212 (97%)	6 (3%)	0	100	100
2	H	216/218 (99%)	214 (99%)	2 (1%)	0	100	100
All	All	867/874 (99%)	850 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	C	196/196 (100%)	186 (95%)	10 (5%)	21	21
1	L	195/196 (100%)	182 (93%)	13 (7%)	15	12
2	B	189/187 (101%)	175 (93%)	14 (7%)	13	10
2	H	187/187 (100%)	182 (97%)	5 (3%)	39	45
All	All	767/766 (100%)	725 (94%)	42 (6%)	19	18

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	ILE
1	L	14	SER
1	L	15	LEU
1	L	45	LYS
1	L	56	SER
1	L	107	LYS
1	L	142	LYS
1	L	165	ASP
1	L	181	LEU
1	L	184	ASP
1	L	185	GLU
1	L	199	LYS
1	L	212	ASN

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Mol	Chain	Res	Type
2	H	3	GLN
2	H	68	SER
2	H	94	ARG
2	H	99	THR
2	H	208	LYS
1	C	1	ASP
1	C	2	ILE
1	C	5	ASN
1	C	24	ARG
1	C	105	GLU
1	C	136	LEU
1	C	157	ASN
1	C	169	LYS
1	C	203	SER
1	C	213	GLU
2	B	16	GLN
2	B	24	VAL
2	B	31	THR
2	B	43	LYS
2	B	67	LEU
2	B	74	SER
2	B	81	LYS
2	B	83	GLN
2	B	95	MET
2	B	98	THR
2	B	132	THR
2	B	160	SER
2	B	185	SER
2	B	209	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	18	GLN
1	L	27	GLN
1	L	28	ASN
1	L	38	GLN
1	L	166	GLN
1	L	210	ASN
1	L	212	ASN
2	H	3	GLN
2	H	35	HIS

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Mol	Chain	Res	Type
2	H	39	GLN
2	H	77	HIS
2	H	83	GLN
1	C	5	ASN
1	C	28	ASN
1	C	30	ASN
1	C	38	GLN
1	C	166	GLN
1	C	212	ASN
2	B	3	GLN
2	B	16	GLN
2	B	35	HIS
2	B	39	GLN
2	B	105	GLN
2	B	133	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	PCA	B	1	2	7,8,9	0.64	0	9,10,12	1.16	1 (11%)
2	PCA	H	1	2	7,8,9	1.22	1 (14%)	9,10,12	1.06	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
2	PCA	B	1	2	-	0/0/11/13	0/1/1/1
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	PCA	CB-CG	2.12	1.58	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	PCA	CB-CA-C	-2.29	109.51	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
5	ACT	B	304	-	3,3,3	0.85	0	3,3,3	0.76	0
5	ACT	B	303	-	3,3,3	1.09	0	3,3,3	0.86	0
3	NAG	H	301	2	14,14,15	0.64	0	17,19,21	1.84	4 (23%)
3	NAG	B	301	2	14,14,15	0.49	0	17,19,21	2.18	4 (23%)
5	ACT	B	305	-	3,3,3	0.84	0	3,3,3	0.80	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	H	301	2	-	0/6/23/26	0/1/1/1
3	NAG	B	301	2	-	4/6/23/26	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(°)	Ideal(°)
3	B	301	NAG	C1-O5-C5	6.81	121.31	112.19
3	H	301	NAG	C3-C4-C5	-3.91	103.15	110.23
3	H	301	NAG	C1-O5-C5	3.61	117.02	112.19
3	H	301	NAG	O5-C5-C6	3.39	114.27	107.66
3	B	301	NAG	O5-C5-C4	2.87	117.81	110.83
3	B	301	NAG	C1-C2-N2	2.34	114.13	110.43
3	B	301	NAG	C2-N2-C7	2.33	126.03	122.90
3	H	301	NAG	C4-C3-C2	-2.06	108.00	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	NAG	C8-C7-N2-C2
3	B	301	NAG	O7-C7-N2-C2
3	B	301	NAG	C4-C5-C6-O6
3	B	301	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	304	ACT	1	0
5	B	303	ACT	4	0
5	B	305	ACT	1	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, 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	C	218/219 (99%)	0.34	7 (3%) 50 53	15, 31, 51, 70	1 (0%)
1	L	218/219 (99%)	0.71	21 (9%) 13 14	22, 41, 69, 83	0
2	B	217/218 (99%)	0.57	10 (4%) 37 39	13, 36, 56, 74	2 (0%)
2	H	217/218 (99%)	0.63	19 (8%) 15 16	12, 35, 65, 90	1 (0%)
All	All	870/874 (99%)	0.56	57 (6%) 24 26	12, 35, 64, 90	4 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	92	CYS	10.3
2	H	100(A)	TRP	4.7
2	H	129	ALA	4.3
1	L	109	ALA	4.1
1	L	152	GLY	3.7
1	L	153	SER	3.4
2	H	2	VAL	3.4
1	C	170	ASP	3.2
2	H	102	TYR	3.0
2	B	195	CYS	2.9
2	H	100(B)	PHE	2.9
2	B	74	SER	2.9
1	C	1	ASP	2.8
2	H	140	CYS	2.8
1	L	2	ILE	2.8
2	H	128	SER	2.8
1	L	23	CYS	2.8
2	B	10	GLY	2.7
2	H	133	ASN	2.7
1	L	17	ASP	2.7
2	H	173	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	165	ASP	2.6
1	C	143	ASP	2.6
1	C	2	ILE	2.6
2	B	42	GLY	2.6
2	B	140	CYS	2.5
1	L	143	ASP	2.5
1	L	187	GLU	2.5
1	C	127	SER	2.4
2	H	99	THR	2.4
2	H	170	LEU	2.3
1	L	106	LEU	2.3
2	B	72	ASP	2.3
1	L	105	GLU	2.3
2	H	172	SER	2.3
1	L	110	ASP	2.3
1	L	88	CYS	2.2
1	L	181	LEU	2.2
1	L	5	ASN	2.2
2	B	41	PRO	2.2
2	H	101	ALA	2.2
2	H	160	SER	2.2
1	L	21	ILE	2.2
1	L	79	GLU	2.2
1	L	194	CYS	2.2
2	B	43	LYS	2.2
1	L	16	GLY	2.1
2	H	130	ALA	2.1
1	L	213	GLU	2.1
1	C	194[A]	CYS	2.1
1	C	165	ASP	2.1
2	H	100	ASP	2.1
2	H	131	GLN	2.1
2	H	132	THR	2.1
2	B	132	THR	2.1
1	L	202	THR	2.0
2	B	18	LEU	2.0

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

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($\text{\AA}^2$)	Q<0.9
2	PCA	H	1	8/9	0.43	0.20	92,106,111,115	0
2	PCA	B	1	8/9	0.84	0.13	41,44,47,48	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	NAG	B	301	14/15	0.50	0.17	52,61,65,65	0
5	ACT	B	305	4/4	0.67	0.22	48,53,55,56	0
3	NAG	H	301	14/15	0.73	0.14	44,52,58,58	0
5	ACT	B	303	4/4	0.84	0.25	33,34,35,41	0
5	ACT	B	304	4/4	0.88	0.11	35,37,38,41	0
4	CA	B	302	1/1	0.94	0.12	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.