



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:16 PM UTC

PDB ID : 8B7H / pdb_00008b7h
Title : Crystal structure of human Gremlin-1 in complex with Fab
Authors : Schulze, M.-S.; Martinez-Fleites, C.
Deposited on : 2022-09-30
Resolution : 1.95 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
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

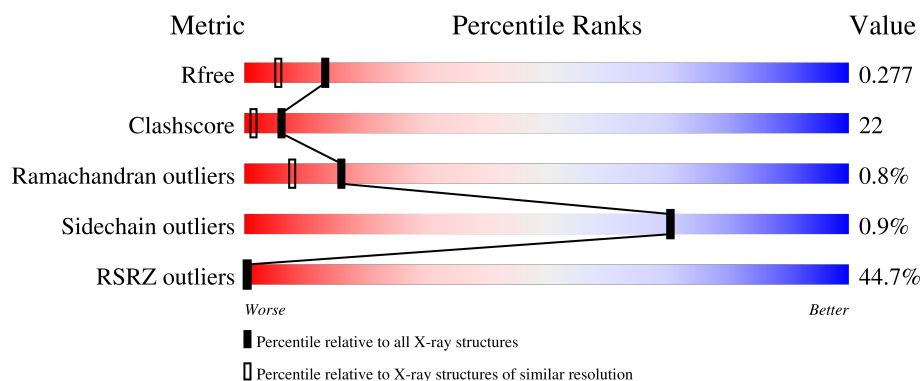
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	L	219	36% 74% 23% .
2	H	227	34% 65% 30% ..
3	A	139	53% 20% 29% .. 47%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4039 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 Fab antibody fragment (light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	219	Total	C	N	O	S	0	0	0
			1701	1064	285	346	6			

- Molecule 2 is a protein called Fab antibody fragment (heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1668	1055	268	337	8			

- Molecule 3 is a protein called Gremlin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	74	Total	C	N	O	S	0	0	0
			608	383	111	104	10			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	initiating methionine	UNP O60565
A	26	GLY	-	expression tag	UNP O60565
A	27	SER	-	expression tag	UNP O60565
A	28	SER	-	expression tag	UNP O60565
A	29	HIS	-	expression tag	UNP O60565
A	30	HIS	-	expression tag	UNP O60565
A	31	HIS	-	expression tag	UNP O60565
A	32	HIS	-	expression tag	UNP O60565
A	33	HIS	-	expression tag	UNP O60565
A	34	HIS	-	expression tag	UNP O60565
A	35	SER	-	expression tag	UNP O60565
A	36	SER	-	expression tag	UNP O60565
A	37	GLY	-	expression tag	UNP O60565
A	38	GLU	-	expression tag	UNP O60565

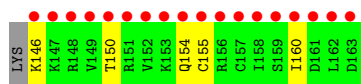
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Chain	Residue	Modelled	Actual	Comment	Reference
A	39	ASN	-	expression tag	UNP O60565
A	40	LEU	-	expression tag	UNP O60565
A	41	TYR	-	expression tag	UNP O60565
A	42	PHE	-	expression tag	UNP O60565
A	43	GLN	-	expression tag	UNP O60565
A	44	GLY	-	expression tag	UNP O60565
A	45	SER	-	expression tag	UNP O60565

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	27	Total	O	0	0
			27	27		
4	H	35	Total	O	0	0
			35	35		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	65.74Å 80.65Å 252.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.96 – 1.95 50.96 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.96-1.95) 99.1 (50.96-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.265 , 0.275 0.269 , 0.277	Depositor DCC
R_{free} test set	2472 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4039	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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

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	L	0.80	0/1738	1.05	4/2362 (0.2%)
2	H	0.83	1/1710 (0.1%)	1.12	5/2332 (0.2%)
3	A	0.65	0/617	1.00	2/821 (0.2%)
All	All	0.80	1/4065 (0.0%)	1.08	11/5515 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	196	PRO	C-O	-5.06	1.18	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	30	THR	N-CA-C	-7.20	104.23	112.87
2	H	171	THR	N-CA-C	-6.07	106.52	114.04
1	L	27	GLN	CB-CA-C	-5.78	109.90	116.54
1	L	98	TYR	N-CA-C	-5.43	105.44	111.36
1	L	26	SER	N-CA-C	-5.41	102.00	110.17
2	H	226	SER	CA-C-O	-5.38	115.69	122.63
3	A	115	GLY	N-CA-C	5.33	118.25	111.37
3	A	126	LYS	N-CA-C	-5.30	106.94	113.41
2	H	130	PRO	CB-CA-C	-5.24	103.47	110.85
2	H	176	THR	CB-CA-C	5.17	119.06	110.78
1	L	156	ASP	CB-CA-C	5.04	118.88	111.73

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	L	1701	0	1641	47	0
2	H	1668	0	1607	90	0
3	A	608	0	613	64	0
4	H	35	0	0	0	0
4	L	27	0	0	0	0
All	All	4039	0	3861	176	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 22.

All (176) 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:33:TYR:CE1	3:A:127:LYS:HD3	1.84	1.11
2:H:33:TYR:HE1	3:A:127:LYS:HD3	1.22	1.01
2:H:2:VAL:HG11	2:H:113:TYR:CD2	1.99	0.98
3:A:107:PRO:HA	3:A:116:SER:HA	1.44	0.97
2:H:161:VAL:HG23	2:H:189:LEU:HD21	1.46	0.97
2:H:161:VAL:CG2	2:H:189:LEU:HD21	1.96	0.94
2:H:27:TYR:HD1	2:H:28:THR:H	1.18	0.89
2:H:67:ARG:HD3	2:H:87:ARG:HH11	1.35	0.89
3:A:81:THR:OG1	3:A:90:ARG:O	1.92	0.88
1:L:31:TYR:HB2	1:L:98:TYR:HE1	1.41	0.85
2:H:50:LEU:HD11	2:H:59:ILE:HG13	1.60	0.84
2:H:105:SER:HB2	3:A:127:LYS:HG2	1.59	0.83
3:A:106:ILE:HB	3:A:117:PHE:HB2	1.59	0.82
2:H:52:ASP:HB3	2:H:56:GLY:H	1.43	0.82
3:A:75:THR:HG23	3:A:96:PHE:O	1.83	0.79
3:A:110:ILE:HD12	3:A:110:ILE:O	1.83	0.79
2:H:32:TYR:C	3:A:127:LYS:HZ1	1.89	0.79
2:H:33:TYR:CD1	3:A:127:LYS:HD3	2.18	0.78
2:H:161:VAL:CG2	2:H:189:LEU:CD2	2.62	0.78
2:H:33:TYR:N	3:A:127:LYS:NZ	2.35	0.74
2:H:32:TYR:CA	3:A:127:LYS:NZ	2.51	0.74
3:A:134:THR:HG22	3:A:146:LYS:HG2	1.70	0.74
3:A:122:PHE:CE2	3:A:124:LYS:HD3	2.23	0.73
2:H:32:TYR:HA	2:H:105:SER:OG	1.91	0.71
2:H:32:TYR:CA	3:A:127:LYS:HZ1	2.03	0.70
2:H:33:TYR:H	3:A:127:LYS:HZ2	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:101:ARG:HG3	2:H:101:ARG:O	1.94	0.68
2:H:22:CYS:HB3	2:H:79:ALA:HB3	1.77	0.67
2:H:211:HIS:ND1	2:H:214:SER:HB2	2.11	0.66
1:L:99:ASP:CG	1:L:100:THR:H	2.03	0.66
1:L:31:TYR:HB2	1:L:98:TYR:CE1	2.29	0.66
1:L:24:LYS:HB3	1:L:24:LYS:NZ	2.11	0.65
2:H:31:ASP:C	3:A:127:LYS:HZ3	2.05	0.63
1:L:99:ASP:OD1	1:L:100:THR:N	2.32	0.63
2:H:32:TYR:HA	3:A:127:LYS:NZ	2.14	0.61
2:H:130:PRO:HB3	2:H:156:TYR:HB3	1.82	0.61
2:H:11:VAL:HG21	2:H:158:PRO:HG3	1.82	0.61
2:H:29:PHE:C	2:H:31:ASP:H	2.09	0.61
2:H:29:PHE:C	2:H:31:ASP:N	2.54	0.61
1:L:84:LEU:HD11	1:L:109:LEU:HD21	1.83	0.60
2:H:2:VAL:HG11	2:H:113:TYR:HD2	1.60	0.60
1:L:188:LYS:O	1:L:192:GLU:HG3	2.02	0.60
2:H:28:THR:O	2:H:31:ASP:HB3	2.02	0.60
3:A:154:GLN:HG2	3:A:155:CYS:H	1.67	0.60
2:H:131:SER:HB3	2:H:133:PHE:CZ	2.37	0.60
1:L:25:SER:O	1:L:75:THR:HG23	2.02	0.59
2:H:207:CYS:SG	2:H:220:LYS:HB3	2.43	0.59
2:H:76:THR:O	2:H:78:THR:CG2	2.51	0.58
2:H:33:TYR:H	3:A:127:LYS:NZ	1.97	0.58
1:L:66:ASP:C	1:L:68:PHE:H	2.11	0.58
1:L:26:SER:O	1:L:27:GLN:C	2.45	0.57
3:A:122:PHE:HE2	3:A:124:LYS:HD3	1.66	0.57
2:H:2:VAL:CG1	2:H:113:TYR:CD2	2.83	0.57
2:H:31:ASP:C	3:A:127:LYS:NZ	2.63	0.57
2:H:166:ASN:ND2	2:H:206:ILE:H	2.02	0.56
2:H:76:THR:O	2:H:78:THR:HG23	2.04	0.56
1:L:4:MET:HE1	1:L:25:SER:HB3	1.86	0.56
3:A:80:GLN:HG3	3:A:81:THR:H	1.71	0.56
3:A:80:GLN:HG3	3:A:81:THR:N	2.20	0.56
2:H:33:TYR:N	3:A:127:LYS:HZ1	2.00	0.56
3:A:76:GLN:HB3	3:A:96:PHE:CZ	2.40	0.56
1:L:29:VAL:HG11	1:L:96:GLN:HB2	1.88	0.55
2:H:112:ASP:HB2	2:H:113:TYR:HD1	1.70	0.55
2:H:78:THR:OG1	2:H:80:TYR:CE2	2.59	0.55
3:A:130:THR:C	3:A:131:MET:HG3	2.31	0.55
2:H:131:SER:N	2:H:154:LYS:O	2.39	0.55
1:L:219:CYS:SG	2:H:227:CYS:SG	3.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:226:SER:O	2:H:227:CYS:C	2.50	0.55
3:A:94:ASN:C	3:A:95:ARG:HD2	2.32	0.55
1:L:24:LYS:HB3	1:L:24:LYS:HZ2	1.71	0.55
2:H:33:TYR:HE1	3:A:127:LYS:CD	2.08	0.54
3:A:73:CYS:O	3:A:74:LYS:HG2	2.07	0.54
2:H:31:ASP:OD1	3:A:126:LYS:HG2	2.08	0.54
2:H:156:TYR:OH	2:H:189:LEU:HD23	2.07	0.53
3:A:78:LEU:HG	3:A:96:PHE:HD2	1.73	0.53
3:A:94:ASN:O	3:A:95:ARG:HD2	2.08	0.53
2:H:51:VAL:HG23	2:H:58:THR:HG22	1.90	0.53
3:A:122:PHE:HB2	3:A:160:ILE:HD11	1.91	0.53
2:H:164:SER:OG	2:H:208:ASN:HB2	2.09	0.53
1:L:66:ASP:C	1:L:68:PHE:N	2.66	0.53
3:A:106:ILE:N	3:A:117:PHE:O	2.42	0.53
2:H:32:TYR:N	3:A:127:LYS:NZ	2.57	0.52
2:H:71:THR:OG1	2:H:80:TYR:HB2	2.09	0.52
2:H:33:TYR:N	3:A:127:LYS:HZ2	1.98	0.52
2:H:163:VAL:HG22	2:H:209:VAL:HG22	1.91	0.52
2:H:166:ASN:HD21	2:H:206:ILE:H	1.57	0.52
3:A:106:ILE:HB	3:A:117:PHE:CB	2.37	0.52
3:A:109:HIS:HB2	3:A:115:GLY:HA3	1.92	0.52
2:H:50:LEU:C	2:H:50:LEU:HD12	2.34	0.52
1:L:15:LEU:C	1:L:17:GLU:H	2.18	0.51
3:A:110:ILE:O	3:A:114:GLU:HB2	2.11	0.51
1:L:34:ASN:O	1:L:35:ASN:C	2.54	0.51
1:L:18:ARG:HG3	1:L:82:ASN:HA	1.93	0.51
1:L:37:ASN:O	1:L:56:TRP:HA	2.11	0.51
2:H:33:TYR:HD1	3:A:127:LYS:HZ2	1.59	0.50
2:H:32:TYR:N	3:A:127:LYS:HZ1	2.09	0.50
1:L:55:TYR:CE2	1:L:61:GLU:OE1	2.65	0.50
2:H:101:ARG:O	2:H:101:ARG:CG	2.58	0.50
2:H:112:ASP:HB2	2:H:113:TYR:CD1	2.47	0.50
1:L:20:THR:OG1	1:L:80:THR:HG22	2.12	0.50
2:H:34:MET:HG2	2:H:79:ALA:HB2	1.94	0.50
2:H:32:TYR:C	3:A:127:LYS:NZ	2.59	0.49
3:A:104:PHE:CZ	3:A:119:SER:HB3	2.47	0.49
1:L:21:ILE:HD12	1:L:79:LEU:HD23	1.94	0.48
1:L:31:TYR:O	1:L:32:SER:C	2.57	0.48
2:H:2:VAL:CG1	2:H:113:TYR:HD2	2.23	0.48
3:A:122:PHE:CD2	3:A:124:LYS:HD3	2.48	0.48
2:H:31:ASP:OD1	3:A:126:LYS:CG	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:32:SER:O	1:L:33:SER:C	2.54	0.48
1:L:67:ARG:O	1:L:81:ILE:HA	2.13	0.48
1:L:75:THR:HG22	1:L:75:THR:O	2.14	0.48
2:H:32:TYR:HA	3:A:127:LYS:HZ3	1.77	0.47
1:L:56:TRP:CD1	1:L:97:TYR:HH	2.32	0.47
1:L:31:TYR:CE1	1:L:33:SER:HB2	2.49	0.47
1:L:189:ALA:O	1:L:193:LYS:HG3	2.15	0.47
3:A:77:PRO:HA	3:A:95:ARG:HA	1.97	0.47
1:L:99:ASP:CG	1:L:100:THR:N	2.69	0.46
1:L:34:ASN:O	1:L:36:LYS:HD3	2.15	0.46
1:L:167:SER:OG	2:H:177:PHE:HB3	2.16	0.46
2:H:2:VAL:HG11	2:H:113:TYR:CE2	2.48	0.46
2:H:30:THR:HA	2:H:53:PRO:HB2	1.98	0.46
1:L:99:ASP:O	1:L:100:THR:C	2.57	0.46
3:A:101:CYS:SG	3:A:123:CYS:SG	3.14	0.45
3:A:76:GLN:HB3	3:A:96:PHE:CE2	2.51	0.45
1:L:38:TYR:HB3	1:L:97:TYR:CD2	2.52	0.45
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.52	0.45
1:L:168:VAL:HG22	1:L:180:LEU:HD12	1.99	0.45
2:H:76:THR:C	2:H:78:THR:HG23	2.42	0.44
2:H:130:PRO:CB	2:H:156:TYR:HB3	2.46	0.44
2:H:1:GLN:O	2:H:26:GLY:HA3	2.17	0.44
3:A:124:LYS:HB2	3:A:125:PRO:HD2	1.99	0.44
1:L:55:TYR:CD1	1:L:59:THR:OG1	2.67	0.44
3:A:110:ILE:O	3:A:110:ILE:CD1	2.60	0.44
1:L:152:GLN:CD	1:L:159:LEU:HD23	2.42	0.44
3:A:120:CYS:SG	3:A:121:SER:N	2.91	0.44
2:H:131:SER:HB3	2:H:133:PHE:CE2	2.53	0.43
2:H:157:PHE:HA	2:H:158:PRO:HA	1.78	0.43
2:H:4:LEU:HD11	2:H:29:PHE:CZ	2.53	0.43
2:H:60:TYR:CE1	2:H:70:ILE:HD12	2.53	0.43
3:A:106:ILE:O	3:A:116:SER:HA	2.17	0.43
1:L:68:PHE:CE2	1:L:81:ILE:HD13	2.54	0.43
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.99	0.43
2:H:24:VAL:HG21	2:H:29:PHE:CG	2.54	0.43
3:A:101:CYS:HB3	3:A:121:SER:HB2	2.01	0.43
2:H:51:VAL:CG1	2:H:70:ILE:HG22	2.48	0.42
3:A:94:ASN:OD1	3:A:95:ARG:N	2.37	0.42
1:L:32:SER:C	1:L:35:ASN:H	2.27	0.42
2:H:27:TYR:HD1	2:H:28:THR:N	2.00	0.42
2:H:76:THR:O	2:H:78:THR:HG22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:161:VAL:CG2	2:H:189:LEU:HD23	2.48	0.42
3:A:134:THR:HG22	3:A:146:LYS:CG	2.45	0.42
1:L:129:GLN:HG2	1:L:134:THR:O	2.19	0.42
2:H:6:GLU:HA	2:H:21:SER:O	2.19	0.42
2:H:162:THR:OG1	2:H:210:ASN:HB3	2.19	0.42
3:A:136:ASN:O	3:A:137:CYS:C	2.62	0.42
1:L:55:TYR:HE1	1:L:56:TRP:CZ3	2.38	0.42
2:H:161:VAL:HG21	2:H:189:LEU:CD2	2.48	0.42
2:H:211:HIS:CE1	2:H:214:SER:HB2	2.54	0.42
3:A:105:TYR:O	3:A:106:ILE:HG13	2.20	0.42
2:H:107:TYR:CD1	2:H:108:PRO:HA	2.55	0.41
3:A:128:PHE:HB3	3:A:150:THR:HG22	2.01	0.41
2:H:36:TRP:CD2	2:H:81:MET:HB2	2.55	0.41
3:A:134:THR:HA	3:A:146:LYS:HA	2.02	0.41
3:A:104:PHE:CD1	3:A:104:PHE:C	2.99	0.41
1:L:15:LEU:C	1:L:17:GLU:N	2.78	0.41
1:L:67:ARG:HG2	1:L:83:SER:HB2	2.02	0.41
1:L:145:TYR:CG	1:L:146:PRO:HA	2.56	0.41
3:A:107:PRO:HB2	3:A:108:ARG:H	1.66	0.41
3:A:71:ASP:N	3:A:102:ASN:HD21	2.18	0.41
2:H:6:GLU:OE2	2:H:95:TYR:HA	2.21	0.41
2:H:27:TYR:CE2	2:H:100:ALA:HB1	2.56	0.41
1:L:34:ASN:C	1:L:36:LYS:N	2.78	0.40
1:L:180:LEU:C	1:L:180:LEU:HD23	2.46	0.40
2:H:27:TYR:CE1	2:H:32:TYR:HE2	2.39	0.40
1:L:112:LYS:HE3	1:L:112:LYS:HB3	1.85	0.40
2:H:76:THR:O	2:H:77:ASP:C	2.64	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	L	217/219 (99%)	197 (91%)	19 (9%)	1 (0%)	24	16
2	H	217/227 (96%)	208 (96%)	9 (4%)	0	100	100
3	A	66/139 (48%)	49 (74%)	14 (21%)	3 (4%)	2	0
All	All	500/585 (86%)	454 (91%)	42 (8%)	4 (1%)	16	8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	107	PRO
3	A	109	HIS
1	L	32	SER
3	A	108	ARG

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	L	194/194 (100%)	192 (99%)	2 (1%)	68	67
2	H	187/192 (97%)	186 (100%)	1 (0%)	81	82
3	A	72/130 (55%)	71 (99%)	1 (1%)	59	56
All	All	453/516 (88%)	449 (99%)	4 (1%)	70	70

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	30	LEU
1	L	33	SER
2	H	131	SER
3	A	109	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	152	GLN
1	L	165	GLN
1	L	204	GLN
2	H	38	GLN
2	H	166	ASN
3	A	118	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	219/219 (100%)	1.77	79 (36%) 1 0	23, 50, 81, 107	0
2	H	221/227 (97%)	1.78	77 (34%) 1 0	22, 39, 81, 87	0
3	A	74/139 (53%)	5.30	74 (100%) 0 0	86, 122, 144, 149	0
All	All	514/585 (87%)	2.28	230 (44%) 0 0	22, 51, 131, 149	0

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	98	TYR	12.9
3	A	149	VAL	9.8
3	A	106	ILE	9.2
2	H	29	PHE	9.2
3	A	96	PHE	8.2
3	A	72	TRP	7.9
3	A	104	PHE	7.6
3	A	78	LEU	7.5
3	A	110	ILE	7.5
1	L	98	TYR	7.4
3	A	105	TYR	7.4
3	A	92	ILE	7.0
3	A	117	PHE	6.9
2	H	27	TYR	6.9
3	A	158	ILE	6.8
3	A	128	PHE	6.8
3	A	152	VAL	6.7
3	A	93	ILE	6.7
2	H	51	VAL	6.6
2	H	130	PRO	6.5
3	A	79	LYS	6.4
3	A	153	LYS	6.4
3	A	125	PRO	6.3

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Mol	Chain	Res	Type	RSRZ
2	H	131	SER	6.2
1	L	31	TYR	6.2
3	A	103	SER	6.1
2	H	100	ALA	6.1
3	A	75	THR	6.1
3	A	100	GLN	6.1
3	A	101	CYS	6.0
3	A	122	PHE	6.0
1	L	53	LEU	6.0
3	A	77	PRO	6.0
1	L	30	LEU	6.0
3	A	131	MET	5.8
3	A	135	LEU	5.8
3	A	102	ASN	5.8
3	A	123	CYS	5.8
3	A	119	SER	5.6
3	A	99	GLY	5.6
2	H	79	ALA	5.6
2	H	106	TYR	5.5
3	A	133	VAL	5.4
3	A	118	GLN	5.4
3	A	124	LYS	5.4
3	A	74	LYS	5.3
1	L	56	TRP	5.3
3	A	107	PRO	5.3
3	A	162	LEU	5.2
1	L	57	ALA	5.2
1	L	68	PHE	5.2
3	A	127	LYS	5.1
1	L	59	THR	5.1
3	A	115	GLY	5.1
2	H	30	THR	5.1
1	L	199	CYS	5.0
2	H	78	THR	5.0
3	A	150	THR	5.0
3	A	160	ILE	5.0
3	A	130	THR	5.0
2	H	132	VAL	4.9
1	L	219	CYS	4.9
3	A	97	CYS	4.9
3	A	157	CYS	4.9
3	A	156	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
3	A	81	THR	4.8
3	A	126	LYS	4.8
2	H	101	ARG	4.8
2	H	59	ILE	4.8
3	A	71	ASP	4.7
2	H	31	ASP	4.7
3	A	76	GLN	4.7
2	H	104	GLY	4.6
2	H	98	THR	4.6
3	A	154	GLN	4.6
3	A	137	CYS	4.6
1	L	33	SER	4.5
3	A	120	CYS	4.5
2	H	74	THR	4.5
1	L	58	SER	4.5
2	H	145	GLY	4.5
3	A	121	SER	4.4
2	H	226	SER	4.4
2	H	28	THR	4.4
3	A	114	GLU	4.3
1	L	72	GLY	4.3
2	H	32	TYR	4.3
2	H	50	LEU	4.2
2	H	33	TYR	4.2
3	A	155	CYS	4.2
2	H	107	TYR	4.2
3	A	134	THR	4.1
2	H	72	ALA	4.1
3	A	129	THR	4.0
3	A	159	SER	4.0
1	L	217	GLY	4.0
2	H	71	THR	4.0
2	H	2	VAL	4.0
3	A	147	LYS	4.0
2	H	70	ILE	4.0
2	H	52	ASP	3.9
1	L	37	ASN	3.9
2	H	4	LEU	3.9
1	L	18	ARG	3.9
3	A	95	ARG	3.8
2	H	129	GLY	3.8
2	H	34	MET	3.8

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Mol	Chain	Res	Type	RSRZ
2	H	227	CYS	3.8
3	A	148	ARG	3.8
3	A	109	HIS	3.7
2	H	80	TYR	3.7
1	L	39	LEU	3.7
2	H	113	TYR	3.7
1	L	99	ASP	3.7
3	A	146	LYS	3.7
2	H	108	PRO	3.7
1	L	19	ALA	3.6
1	L	38	TYR	3.6
1	L	111	ILE	3.6
2	H	53	PRO	3.6
2	H	111	PHE	3.6
2	H	56	GLY	3.6
1	L	29	VAL	3.6
1	L	60	ARG	3.6
2	H	26	GLY	3.6
3	A	136	ASN	3.5
2	H	102	GLY	3.5
1	L	5	THR	3.5
1	L	15	LEU	3.5
1	L	75	THR	3.5
2	H	110	HIS	3.5
1	L	66	ASP	3.5
2	H	55	ASP	3.5
2	H	77	ASP	3.5
1	L	97	TYR	3.5
1	L	36	LYS	3.4
2	H	109	ASN	3.4
1	L	2	ILE	3.4
3	A	132	MET	3.4
1	L	3	VAL	3.3
3	A	80	GLN	3.3
1	L	1	ASP	3.3
1	L	74	GLY	3.3
3	A	73	CYS	3.3
1	L	78	THR	3.2
1	L	73	SER	3.2
1	L	21	ILE	3.2
2	H	24	VAL	3.2
1	L	16	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	L	77	PHE	3.2
2	H	73	ASP	3.1
1	L	26	SER	3.1
2	H	42	GLY	3.1
1	L	84	LEU	3.1
1	L	32	SER	3.1
2	H	64	PHE	3.0
3	A	116	SER	3.0
2	H	58	THR	3.0
3	A	91	THR	3.0
1	L	65	PRO	3.0
1	L	54	ILE	3.0
1	L	81	ILE	3.0
1	L	67	ARG	3.0
1	L	11	LEU	3.0
2	H	75	SER	3.0
1	L	52	LEU	2.9
1	L	79	LEU	2.9
3	A	151	ARG	2.9
1	L	100	THR	2.9
1	L	103	PHE	2.9
1	L	13	VAL	2.9
2	H	201	GLY	2.9
2	H	5	VAL	2.8
1	L	55	TYR	2.8
2	H	68	VAL	2.8
1	L	76	ASP	2.8
3	A	163	ASP	2.8
2	H	87	ARG	2.8
1	L	206	LEU	2.8
1	L	14	SER	2.7
2	H	138	SER	2.7
2	H	25	SER	2.7
1	L	86	ALA	2.7
3	A	94	ASN	2.7
1	L	64	VAL	2.7
2	H	161	VAL	2.7
1	L	41	TRP	2.7
2	H	112	ASP	2.7
1	L	62	SER	2.7
2	H	103	SER	2.7
3	A	90	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	105	SER	2.6
1	L	27	GLN	2.6
1	L	23	CYS	2.6
2	H	35	HIS	2.6
2	H	99	ASP	2.6
3	A	108	ARG	2.6
2	H	3	GLN	2.6
1	L	195	LYS	2.6
2	H	60	TYR	2.5
1	L	4	MET	2.4
2	H	65	GLN	2.4
1	L	70	GLY	2.4
2	H	66	GLY	2.4
1	L	28	SER	2.4
2	H	76	THR	2.4
2	H	202	THR	2.4
1	L	90	ALA	2.4
3	A	161	ASP	2.3
1	L	35	ASN	2.3
2	H	47	TRP	2.3
2	H	114	TRP	2.3
2	H	97	ALA	2.3
1	L	34	ASN	2.3
1	L	47	GLY	2.2
1	L	63	GLY	2.2
1	L	71	SER	2.2
1	L	20	THR	2.2
2	H	23	LYS	2.2
1	L	209	PRO	2.2
2	H	200	LEU	2.2
2	H	43	LYS	2.2
1	L	131	LYS	2.1
1	L	96	GLN	2.1
2	H	57	GLU	2.1
2	H	215	ASN	2.1
1	L	93	PHE	2.0
1	L	83	SER	2.0
1	L	102	THR	2.0
1	L	94	CYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.