



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:04 AM UTC

PDB ID : 7LCV / pdb_00007lcv
Title : Factor H enhancing human antibody fragment (Fab) to meningococcal Factor H binding protein
Authors : Beernink, P.T.; Sands, N.
Deposited on : 2021-01-11
Resolution : 1.70 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

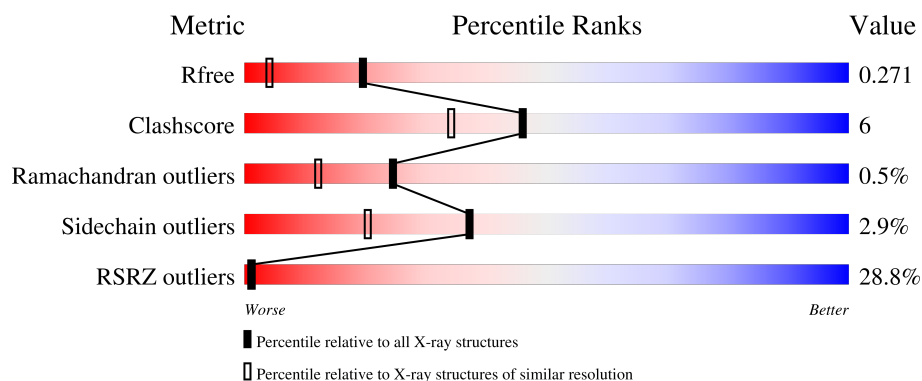
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	A	227	35% 60% 19% .. 18%
2	B	217	29% 82% 16% ..
3	C	263	14% 76% 10% . 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9631 atoms, of which 4599 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 Immunoglobulin heavy chain Fd fragment.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	186	Total	C	H	N	O	S	0	0	0
			2707	871	1327	228	275	6			

- Molecule 2 is a protein called Immunoglobulin kappa light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	215	Total	C	H	N	O	S	0	2	0
			3216	1022	1576	275	335	8			

- Molecule 3 is a protein called Factor H binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	227	Total	C	H	N	O	S	0	0	0
			3405	1062	1696	307	339	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	256	LEU	-	expression tag	UNP Q6VRZ6
C	257	GLU	-	expression tag	UNP Q6VRZ6
C	258	HIS	-	expression tag	UNP Q6VRZ6
C	259	HIS	-	expression tag	UNP Q6VRZ6
C	260	HIS	-	expression tag	UNP Q6VRZ6
C	261	HIS	-	expression tag	UNP Q6VRZ6
C	262	HIS	-	expression tag	UNP Q6VRZ6
C	263	HIS	-	expression tag	UNP Q6VRZ6

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Cl 1	0	0

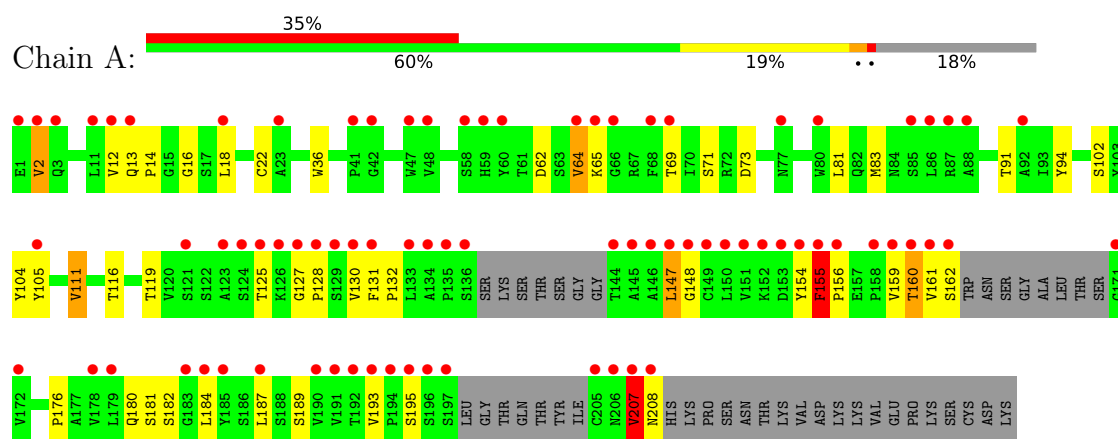
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total 65	O 65	0	0
5	B	109	Total 109	O 109	0	0
5	C	127	Total 127	O 127	0	0

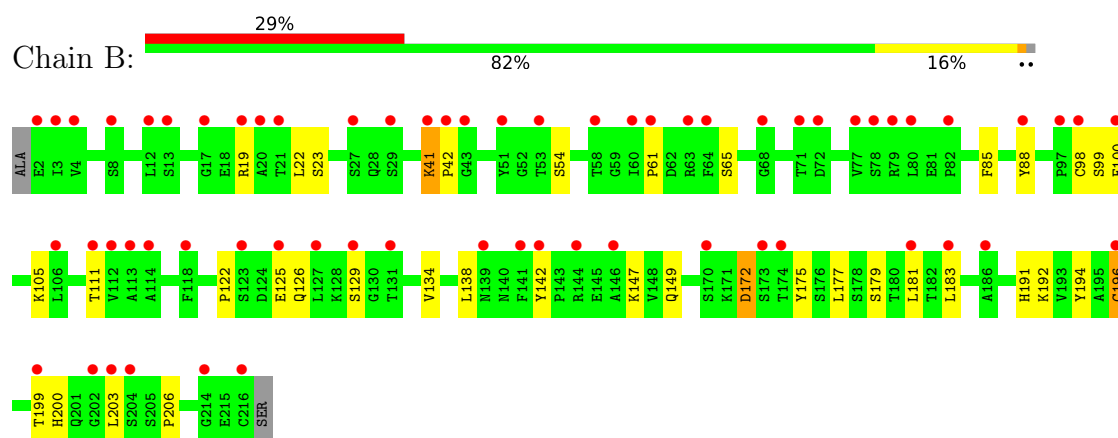
3 Residue-property plots [i](#)

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.

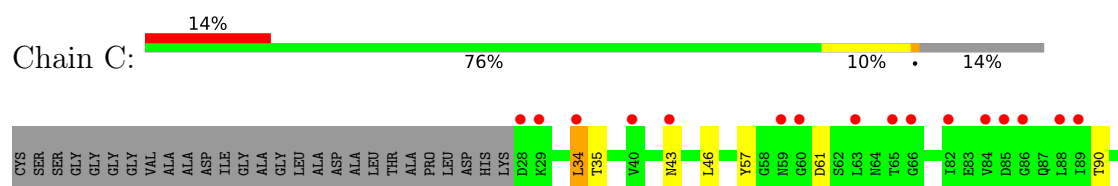
- Molecule 1: Immunoglobulin heavy chain Fd fragment

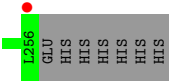
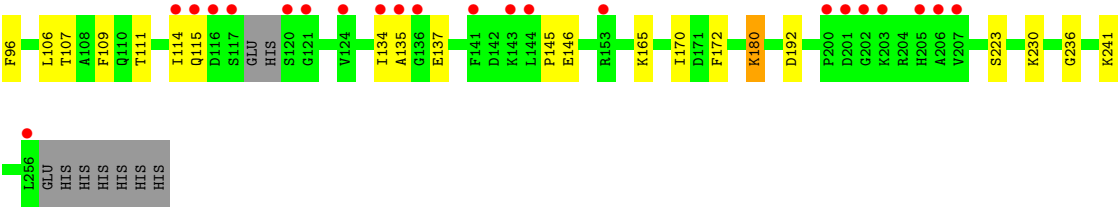


- Molecule 2: Immunoglobulin kappa light chain



- Molecule 3: Factor H binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	39.47Å 52.37Å 84.56Å 73.78° 84.48° 74.17°	Depositor
Resolution (Å)	81.18 – 1.70 81.18 – 1.70	Depositor EDS
% Data completeness (in resolution range)	93.1 (81.18-1.70) 78.6 (81.18-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.75 (at 1.23Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.239 , 0.270 0.242 , 0.271	Depositor DCC
R_{free} test set	1120 reflections (0.94%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9631	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.89% 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:
CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.29	16/1412 (1.1%)	1.37	8/1921 (0.4%)
2	B	1.26	23/1681 (1.4%)	1.42	18/2284 (0.8%)
3	C	0.95	7/1730 (0.4%)	1.13	8/2319 (0.3%)
All	All	1.17	46/4823 (1.0%)	1.31	34/6524 (0.5%)

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	CYS	CA-C	14.03	1.68	1.52
1	A	22	CYS	N-CA	13.21	1.62	1.46
3	C	137	GLU	C-O	-9.30	1.13	1.23
1	A	18	LEU	C-O	-8.75	1.13	1.23
2	B	142	TYR	C-O	-8.42	1.12	1.24
1	A	116	THR	C-O	-8.37	1.14	1.24
3	C	34	LEU	C-O	-8.00	1.14	1.24
2	B	177	LEU	C-O	-7.97	1.14	1.23
2	B	99	SER	C-O	-7.96	1.14	1.23
1	A	22	CYS	C-O	-7.78	1.15	1.23
3	C	145	PRO	C-O	-7.66	1.14	1.23
2	B	125	GLU	C-O	-7.58	1.15	1.24
2	B	179	SER	C-O	-7.39	1.15	1.24
2	B	88	TYR	C-O	-7.03	1.15	1.24
2	B	149	GLN	C-O	-7.02	1.15	1.24
2	B	196[A]	CYS	C-O	6.77	1.31	1.24
2	B	196[B]	CYS	C-O	6.77	1.31	1.24
1	A	111	VAL	C-O	-6.75	1.17	1.24
2	B	111	THR	C-O	-6.71	1.15	1.23
1	A	71	SER	C-O	-6.63	1.16	1.23
1	A	16	GLY	C-O	-6.54	1.17	1.23
1	A	64	VAL	C-O	-6.50	1.14	1.24
2	B	192	LYS	C-O	-6.40	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	GLY	C-O	-6.22	1.17	1.23
3	C	114	ILE	C-O	-6.22	1.17	1.23
2	B	175	TYR	C-O	-6.15	1.16	1.23
1	A	14	PRO	C-O	-6.13	1.16	1.23
2	B	196[A]	CYS	N-CA	6.05	1.53	1.46
2	B	196[B]	CYS	N-CA	6.05	1.53	1.46
1	A	176	PRO	C-O	-6.03	1.16	1.23
2	B	181	LEU	C-O	-6.01	1.16	1.23
1	A	102	SER	C-O	-5.86	1.16	1.24
3	C	241	LYS	CE-NZ	5.76	1.66	1.49
2	B	183	LEU	C-O	-5.75	1.16	1.23
3	C	241	LYS	CD-CE	5.68	1.69	1.52
1	A	132	PRO	C-O	-5.56	1.17	1.23
2	B	191	HIS	C-O	-5.49	1.17	1.23
2	B	138	LEU	C-O	-5.48	1.17	1.24
2	B	147	LYS	C-O	-5.43	1.17	1.24
3	C	241	LYS	CB-CG	5.40	1.68	1.52
1	A	69	THR	C-O	-5.38	1.18	1.24
2	B	194	TYR	C-O	-5.37	1.17	1.24
2	B	196[A]	CYS	CA-C	5.36	1.58	1.52
2	B	196[B]	CYS	CA-C	5.36	1.58	1.52
2	B	172	ASP	C-O	-5.13	1.17	1.24
1	A	131	PHE	C-O	-5.03	1.17	1.23

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	241	LYS	CB-CG-CD	-8.63	91.45	111.30
2	B	99	SER	O-C-N	8.28	133.35	123.33
2	B	126	GLN	CA-C-O	-8.21	110.53	119.97
1	A	148	GLY	CA-C-O	-8.11	112.53	121.21
2	B	85	PHE	CB-CA-C	7.24	122.47	110.88
3	C	35	THR	CA-CB-OG1	-6.85	99.33	109.60
3	C	180	LYS	CD-CE-NZ	6.19	131.71	111.90
2	B	196[A]	CYS	O-C-N	-6.03	116.28	123.27
2	B	196[B]	CYS	O-C-N	-6.03	116.28	123.27
3	C	61	ASP	CA-CB-CG	5.96	118.56	112.60
2	B	200	HIS	CA-CB-CG	-5.83	107.97	113.80
2	B	100	PHE	CA-CB-CG	5.68	119.48	113.80
1	A	105	TYR	CA-C-O	-5.67	115.38	121.45
2	B	41	LYS	CB-CA-C	5.62	117.21	108.61
1	A	2	VAL	N-CA-CB	5.60	117.45	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	241	LYS	CD-CE-NZ	-5.49	94.34	111.90
1	A	125	THR	CB-CA-C	5.47	118.05	109.84
2	B	61	PRO	CB-CA-C	-5.42	103.84	110.95
3	C	61	ASP	CA-C-O	-5.41	115.43	121.81
1	A	160	THR	CA-C-O	-5.39	115.07	121.16
2	B	196[A]	CYS	CA-C-O	5.34	126.01	120.30
2	B	196[B]	CYS	CA-C-O	5.34	126.01	120.30
3	C	145	PRO	CB-CA-C	5.29	118.31	111.64
1	A	147	LEU	CA-C-O	-5.28	115.63	121.33
2	B	126	GLN	N-CA-C	-5.28	105.70	111.82
2	B	172	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	155	PHE	CA-CB-CG	5.17	118.97	113.80
1	A	71	SER	CA-C-O	-5.12	115.95	121.38
2	B	142	TYR	O-C-N	-5.11	116.71	121.72
2	B	105	LYS	CA-C-O	-5.08	114.74	120.43
2	B	88	TYR	CA-C-O	-5.07	115.23	120.70
2	B	138	LEU	CA-C-O	-5.06	115.05	120.46
3	C	146	GLU	N-CA-C	-5.02	107.15	113.28
2	B	98	CYS	CA-C-O	-5.01	116.23	121.55

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	A	1380	1327	1327	23	0
2	B	1640	1576	1576	10	0
3	C	1709	1696	1694	21	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	65	0	0	2	0
5	B	109	0	0	2	0
5	C	127	0	0	12	0
All	All	5032	4599	4597	54	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 (54) 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)
3:C:115:GLN:OE1	5:C:401:HOH:O	1.77	1.00
3:C:34:LEU:CD1	3:C:135:ALA:HB3	2.03	0.89
3:C:57:TYR:HD1	5:C:403:HOH:O	1.63	0.81
1:A:154:TYR:O	1:A:155:PHE:O	2.04	0.74
3:C:57:TYR:CD1	5:C:403:HOH:O	2.40	0.69
1:A:184:LEU:HD22	1:A:184:LEU:N	2.08	0.68
3:C:34:LEU:HD12	3:C:135:ALA:HB3	1.74	0.67
1:A:73:ASP:OD2	5:A:301:HOH:O	2.12	0.66
3:C:46:LEU:O	5:C:403:HOH:O	2.15	0.66
2:B:203:LEU:O	5:B:401:HOH:O	2.13	0.65
3:C:192:ASP:OD1	5:C:402:HOH:O	2.14	0.65
2:B:41:LYS:CG	2:B:42:PRO:HD2	2.30	0.61
1:A:65:LYS:HD2	5:A:333:HOH:O	1.99	0.61
3:C:115:GLN:CD	5:C:401:HOH:O	2.36	0.58
2:B:41:LYS:HG2	2:B:42:PRO:HD2	1.88	0.56
2:B:22:LEU:HD12	2:B:22:LEU:N	2.20	0.56
3:C:43:ASN:ND2	5:C:405:HOH:O	2.35	0.55
3:C:34:LEU:HD21	3:C:107:THR:HG23	1.91	0.52
1:A:154:TYR:C	1:A:155:PHE:O	2.55	0.50
1:A:130:VAL:HG21	1:A:207:VAL:HG11	1.95	0.49
2:B:199:THR:HG22	2:B:206:PRO:HG3	1.95	0.48
1:A:184:LEU:HD22	1:A:184:LEU:H	1.77	0.48
1:A:127:GLY:HA2	1:A:155:PHE:CD2	2.49	0.48
3:C:90:THR:O	5:C:401:HOH:O	2.20	0.47
3:C:106:LEU:HD13	5:C:428:HOH:O	2.12	0.47
3:C:180:LYS:HD2	5:C:402:HOH:O	2.13	0.47
3:C:46:LEU:HG	5:C:403:HOH:O	2.14	0.47
1:A:2:VAL:HG11	1:A:111:VAL:HG21	1.97	0.47
1:A:184:LEU:N	1:A:184:LEU:CD2	2.76	0.46
3:C:96:PHE:HD1	3:C:109:PHE:CE1	2.34	0.46
1:A:128:PRO:HD3	1:A:155:PHE:CE2	2.51	0.46
2:B:41:LYS:HG3	2:B:42:PRO:HD2	1.97	0.46
1:A:182:SER:HB2	1:A:184:LEU:HD23	1.98	0.44
1:A:207:VAL:HG22	1:A:208:ASN:N	2.32	0.44
3:C:134:ILE:HD13	3:C:236:GLY:HA2	1.99	0.44
1:A:180:GLN:C	1:A:182:SER:H	2.26	0.43
3:C:111:THR:HG23	5:C:463:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLN:C	1:A:182:SER:N	2.76	0.43
1:A:83:MET:HE1	1:A:94:TYR:CZ	2.54	0.43
1:A:155:PHE:HB2	1:A:156:PRO:CD	2.49	0.42
2:B:19:ARG:HG3	2:B:19:ARG:NH1	2.33	0.42
1:A:91:THR:HG23	1:A:119:THR:HA	2.01	0.42
1:A:161:VAL:HG11	1:A:189:SER:HB3	2.01	0.42
1:A:159:VAL:CG2	1:A:187:LEU:HD21	2.49	0.42
2:B:122:PRO:HD3	2:B:134:VAL:HG22	2.01	0.42
3:C:34:LEU:HD12	3:C:135:ALA:CB	2.47	0.41
1:A:36:TRP:NE1	1:A:81:LEU:HB2	2.36	0.41
3:C:170:ILE:HG21	3:C:172:PHE:CE1	2.55	0.41
1:A:184:LEU:H	1:A:184:LEU:CD2	2.34	0.41
1:A:12:VAL:HG22	1:A:13:GLN:H	1.85	0.41
2:B:19:ARG:HG3	2:B:19:ARG:HH11	1.86	0.41
3:C:165:LYS:HA	3:C:165:LYS:HD3	1.85	0.40
2:B:23:SER:HB3	5:B:441:HOH:O	2.22	0.40
3:C:223:SER:O	3:C:236:GLY:HA3	2.21	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	A	178/227 (78%)	164 (92%)	11 (6%)	3 (2%)	7	1
2	B	215/217 (99%)	203 (94%)	12 (6%)	0	100	100
3	C	223/263 (85%)	216 (97%)	7 (3%)	0	100	100
All	All	616/707 (87%)	583 (95%)	30 (5%)	3 (0%)	24	12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	PHE
1	A	207	VAL
1	A	181	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	154/190 (81%)	145 (94%)	9 (6%)	18 5
2	B	187/188 (100%)	181 (97%)	6 (3%)	34 17
3	C	175/202 (87%)	174 (99%)	1 (1%)	78 72
All	All	516/580 (89%)	500 (97%)	16 (3%)	37 18

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ASP
1	A	64	VAL
1	A	104	TYR
1	A	147	LEU
1	A	160	THR
1	A	162	SER
1	A	193	VAL
1	A	195	SER
1	A	207	VAL
2	B	54	SER
2	B	65	SER
2	B	129	SER
2	B	172	ASP
2	B	196[A]	CYS
2	B	196[B]	CYS
3	C	230	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
2	B	162	GLN
3	C	32	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	A	186/227 (81%)	2.06	80 (43%) 0 0	30, 53, 80, 102	0
2	B	215/217 (99%)	1.58	63 (29%) 1 1	22, 50, 68, 86	2 (0%)
3	C	227/263 (86%)	1.20	38 (16%) 4 4	29, 44, 69, 87	0
All	All	628/707 (88%)	1.59	181 (28%) 1 1	22, 49, 74, 102	2 (0%)

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	PHE	6.3
1	A	128	PRO	6.0
1	A	145	ALA	5.6
3	C	256	LEU	5.5
1	A	130	VAL	5.1
1	A	207	VAL	5.1
3	C	34	LEU	5.0
1	A	193	VAL	5.0
1	A	144	THR	5.0
1	A	162	SER	4.9
1	A	125	THR	4.8
2	B	112	VAL	4.8
1	A	136	SER	4.4
2	B	127	LEU	4.4
1	A	158	PRO	4.3
1	A	205	CYS	4.3
2	B	216	CYS	4.3
1	A	154	TYR	4.2
1	A	192	THR	4.2
1	A	194	PRO	4.2
1	A	149	CYS	4.2
3	C	117	SER	4.1
1	A	208	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	147	LEU	4.1
1	A	123	ALA	4.0
1	A	159	VAL	4.0
2	B	77	VAL	3.9
2	B	114	ALA	3.9
1	A	126	LYS	3.9
1	A	11	LEU	3.8
1	A	1	GLU	3.8
1	A	197	SER	3.7
3	C	60	GLY	3.7
1	A	127	GLY	3.6
2	B	71	THR	3.6
1	A	172	VAL	3.6
3	C	114	ILE	3.6
1	A	190	VAL	3.5
3	C	29	LYS	3.5
1	A	196	SER	3.4
1	A	179	LEU	3.4
1	A	151	VAL	3.4
1	A	129	SER	3.4
3	C	121	GLY	3.3
1	A	2	VAL	3.3
1	A	86	LEU	3.2
1	A	68	PHE	3.2
1	A	12	VAL	3.2
2	B	113	ALA	3.2
1	A	184	LEU	3.2
2	B	144	ARG	3.2
1	A	153	ASP	3.2
1	A	195	SER	3.2
1	A	88	ALA	3.2
1	A	131	PHE	3.2
1	A	161	VAL	3.2
2	B	61	PRO	3.1
1	A	146	ALA	3.1
3	C	207	VAL	3.1
3	C	120	SER	3.1
1	A	60	TYR	3.1
1	A	185	TYR	3.1
1	A	171	GLY	3.0
1	A	64	VAL	3.0
1	A	191	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	28	ASP	3.0
1	A	134	ALA	3.0
2	B	170	SER	2.9
2	B	80	LEU	2.9
3	C	88	LEU	2.9
1	A	124	SER	2.9
3	C	84	VAL	2.9
1	A	69	THR	2.9
1	A	178	VAL	2.9
2	B	183	LEU	2.9
3	C	82	ILE	2.9
2	B	58	THR	2.8
1	A	42	GLY	2.8
3	C	43	ASN	2.8
1	A	47	TRP	2.8
1	A	66	GLY	2.8
1	A	133	LEU	2.8
2	B	60	ILE	2.8
1	A	160	THR	2.8
1	A	23	ALA	2.7
2	B	41	LYS	2.7
1	A	105	TYR	2.7
2	B	20	ALA	2.7
3	C	153	ARG	2.7
1	A	148	GLY	2.7
2	B	139	ASN	2.7
2	B	64	PHE	2.6
1	A	183	GLY	2.6
1	A	65	LYS	2.6
2	B	68	GLY	2.6
2	B	141	PHE	2.6
2	B	43	GLY	2.5
2	B	21	THR	2.5
2	B	131	THR	2.5
3	C	65	THR	2.5
1	A	13	GLN	2.5
3	C	116	ASP	2.5
1	A	206	ASN	2.5
2	B	63	ARG	2.5
2	B	203	LEU	2.5
3	C	63	LEU	2.5
1	A	18	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	118	PHE	2.5
2	B	51	TYR	2.5
2	B	202	GLY	2.5
3	C	124	VAL	2.5
3	C	59	ASN	2.4
2	B	214	GLY	2.4
3	C	85	ASP	2.4
1	A	152	LYS	2.4
3	C	205	HIS	2.4
1	A	80	TRP	2.4
2	B	199	THR	2.4
1	A	121	SER	2.4
2	B	42	PRO	2.4
2	B	123	SER	2.4
2	B	196[A]	CYS	2.4
3	C	144	LEU	2.4
3	C	141	PHE	2.4
2	B	142	TYR	2.4
3	C	40	VAL	2.4
2	B	204	SER	2.3
3	C	203	LYS	2.3
1	A	87	ARG	2.3
2	B	19	ARG	2.3
2	B	82	PRO	2.3
2	B	53	THR	2.3
2	B	12	LEU	2.3
2	B	2	GLU	2.3
3	C	86	GLY	2.3
1	A	59	HIS	2.3
1	A	85	SER	2.3
3	C	202	GLY	2.2
3	C	206	ALA	2.2
2	B	29	SER	2.2
1	A	156	PRO	2.2
2	B	4	VAL	2.2
2	B	8	SER	2.2
2	B	13	SER	2.2
2	B	146	ALA	2.2
2	B	181	LEU	2.2
3	C	143	LYS	2.2
1	A	41	PRO	2.2
1	A	48	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	97	PRO	2.1
2	B	111	THR	2.1
3	C	200	PRO	2.1
2	B	186	ALA	2.1
3	C	66	GLY	2.1
2	B	98	CYS	2.1
1	A	150	LEU	2.1
2	B	106	LEU	2.1
2	B	78	SER	2.1
3	C	201	ASP	2.1
2	B	100	PHE	2.1
2	B	3	ILE	2.1
1	A	92	ALA	2.1
1	A	77	ASN	2.1
3	C	115	GLN	2.1
1	A	58	SER	2.1
1	A	187	LEU	2.1
2	B	79	ARG	2.1
3	C	134	ILE	2.1
3	C	136	GLY	2.0
3	C	135	ALA	2.0
1	A	3	GLN	2.0
2	B	173	SER	2.0
2	B	174	THR	2.0
1	A	135	PRO	2.0
2	B	125	GLU	2.0
2	B	17	GLY	2.0
2	B	88	TYR	2.0
3	C	89	ILE	2.0
2	B	72	ASP	2.0
2	B	27	SER	2.0
2	B	129	SER	2.0

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

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

6.3 Carbohydrates [i](#)

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
4	CL	B	301	1/1	0.94	0.12	51,51,51,51	0
4	CL	C	301	1/1	0.96	0.08	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.