



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:53 AM UTC

PDB ID : 4JZO / pdb_00004jzo
Title : Three dimensional structure of broadly neutralizing human anti - Hepatitis C virus (HCV) glycoprotein E2 Fab fragment HC84-27
Authors : Krey, T.; Rey, F.A.
Deposited on : 2013-04-03
Resolution : 2.22 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

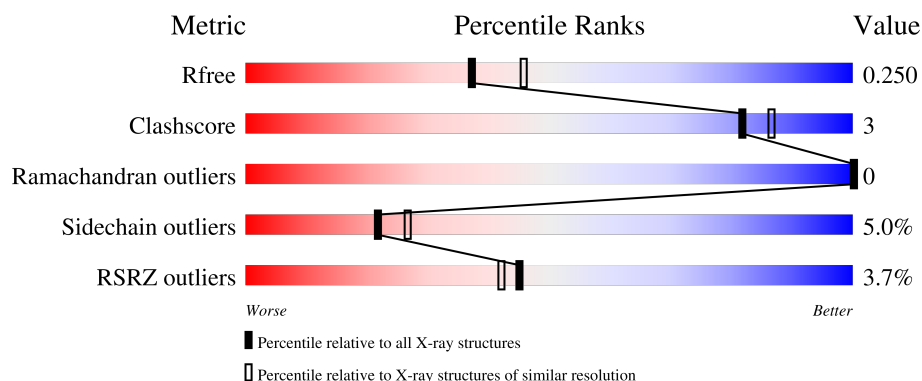
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	261	3% 72% 11% 18%
1	C	261	4% 71% 9% 18%
1	D	261	3% 73% 8% 18%
1	G	261	5% 71% 11% 17%
2	B	215	2% 91% 7% ..

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Mol	Chain	Length	Quality of chain
2	E	215	2% 88% 8% ..
2	F	215	88% 9% ..
2	H	215	% 89% 7% ..
3	I	13	8% 69% 15% 15%
3	J	13	31% 69% 15% 15%
3	K	13	15% 69% 15% 15%
3	L	13	38% 77% 8% 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13544 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 Anti-HCV E2 Fab HC84-27 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	4	0
			1612	1019	265	317	11			
1	C	214	Total	C	N	O	S	0	2	0
			1597	1010	263	315	9			
1	D	214	Total	C	N	O	S	0	2	0
			1600	1012	264	315	9			
1	G	217	Total	C	N	O	S	0	2	0
			1618	1022	267	320	9			

- Molecule 2 is a protein called Anti-HCV E2 Fab HC84-27 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	2	0
			1613	1005	272	329	7			
2	E	211	Total	C	N	O	S	0	2	0
			1613	1005	272	329	7			
2	F	210	Total	C	N	O	S	0	4	0
			1613	1006	271	327	9			
2	H	210	Total	C	N	O	S	0	0	0
			1601	998	271	327	5			

- Molecule 3 is a protein called Envelope glycoprotein E2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	11	Total	C	N	O	0	0	0
			94	65	16	13			
3	J	11	Total	C	N	O	0	0	0
			94	65	16	13			
3	K	11	Total	C	N	O	0	0	0
			94	65	16	13			
3	L	11	Total	C	N	O	0	0	0
			94	65	16	13			

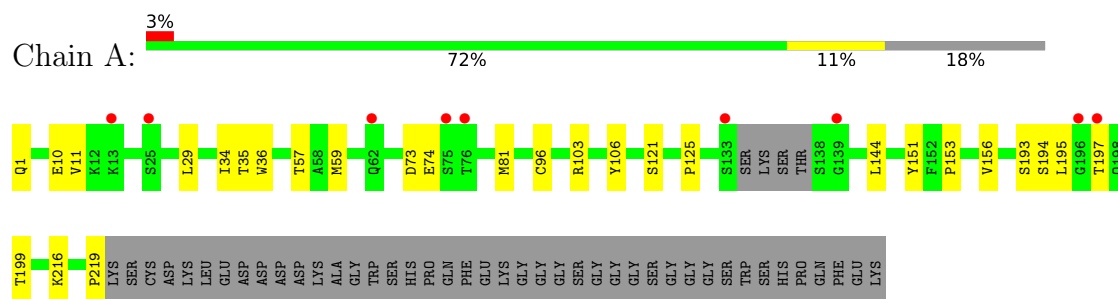
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total 27	O 27	0	0
4	B	48	Total 48	O 48	0	0
4	C	24	Total 24	O 24	0	0
4	D	33	Total 33	O 33	0	0
4	E	50	Total 50	O 50	0	0
4	F	40	Total 40	O 40	0	0
4	G	26	Total 26	O 26	0	0
4	H	52	Total 52	O 52	0	0
4	I	1	Total 1	O 1	0	0

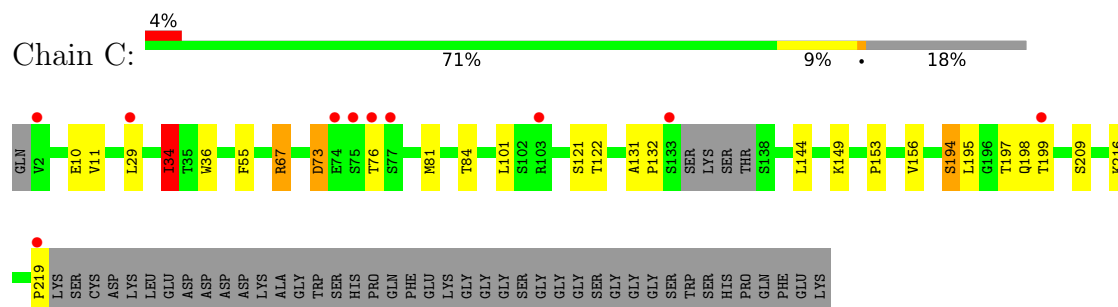
3 Residue-property plots [i](#)

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.

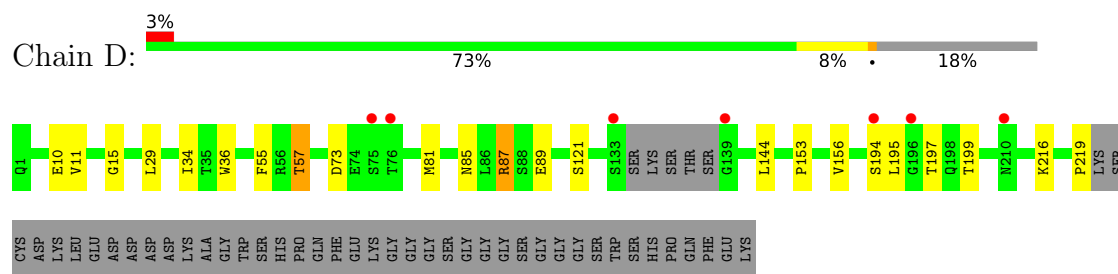
- Molecule 1: Anti-HCV E2 Fab HC84-27 heavy chain



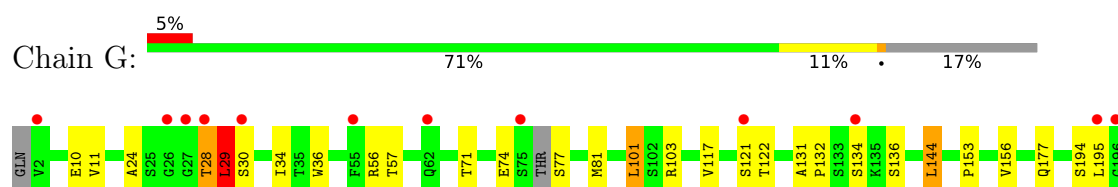
- Molecule 1: Anti-HCV E2 Fab HC84-27 heavy chain

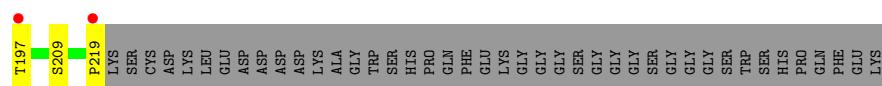


- Molecule 1: Anti-HCV E2 Fab HC84-27 heavy chain

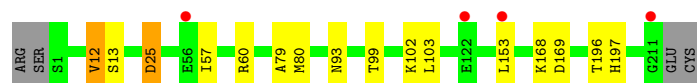
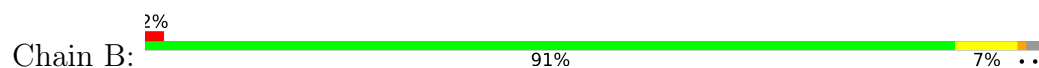


- Molecule 1: Anti-HCV E2 Fab HC84-27 heavy chain

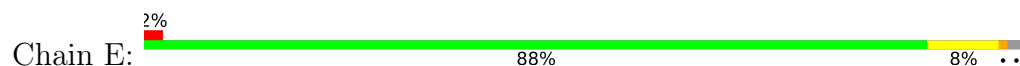




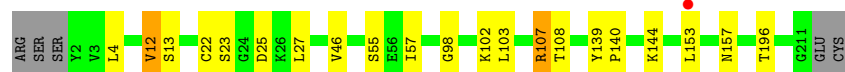
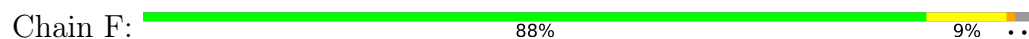
- Molecule 2: Anti-HCV E2 Fab HC84-27 light chain



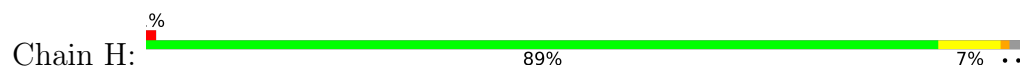
- Molecule 2: Anti-HCV E2 Fab HC84-27 light chain



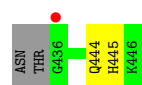
- Molecule 2: Anti-HCV E2 Fab HC84-27 light chain



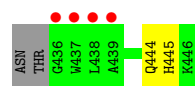
- Molecule 2: Anti-HCV E2 Fab HC84-27 light chain



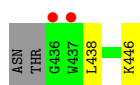
- Molecule 3: Envelope glycoprotein E2



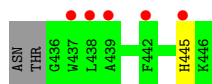
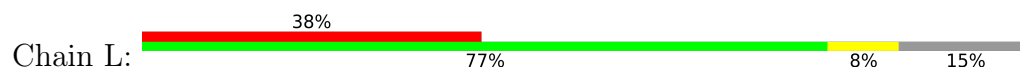
- Molecule 3: Envelope glycoprotein E2



- Molecule 3: Envelope glycoprotein E2



• Molecule 3: Envelope glycoprotein E2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.94Å 77.33Å 85.82Å 92.10° 107.62° 90.24°	Depositor
Resolution (Å)	41.35 – 2.22 41.35 – 2.22	Depositor EDS
% Data completeness (in resolution range)	85.8 (41.35-2.22) 85.8 (41.35-2.22)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.22Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.196 , 0.236 0.209 , 0.250	Depositor DCC
R_{free} test set	3996 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.137 for -h,k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13544	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.50% 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](#)

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	0.81	0/1662	1.10	3/2265 (0.1%)
1	C	0.83	0/1641	1.16	4/2237 (0.2%)
1	D	0.81	0/1644	1.12	2/2241 (0.1%)
1	G	0.85	0/1662	1.16	5/2264 (0.2%)
2	B	0.85	0/1654	1.21	7/2251 (0.3%)
2	E	0.88	0/1654	1.16	3/2251 (0.1%)
2	F	0.87	0/1660	1.13	3/2259 (0.1%)
2	H	0.85	0/1636	1.17	2/2227 (0.1%)
3	I	1.16	1/98 (1.0%)	1.61	1/131 (0.8%)
3	J	1.12	1/98 (1.0%)	1.40	1/131 (0.8%)
3	K	0.78	0/98	1.33	0/131
3	L	0.83	0/98	1.59	1/131 (0.8%)
All	All	0.85	2/13605 (0.0%)	1.16	32/18519 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	445	HIS	ND1-CE1	6.55	1.39	1.32
3	I	445	HIS	ND1-CE1	6.47	1.39	1.32

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57	ILE	N-CA-C	10.09	116.74	107.56
3	L	445	HIS	N-CA-C	8.88	121.03	111.36
2	H	57	ILE	N-CA-C	7.82	115.36	108.63
2	B	57	ILE	N-CA-C	7.70	116.40	107.77
3	I	445	HIS	CB-CG-CD2	-7.33	121.67	131.20
3	J	445	HIS	CB-CG-CD2	-7.21	121.82	131.20
2	B	25	ASP	N-CA-C	7.19	118.81	110.97
1	D	73	ASP	CA-C-N	6.44	129.20	120.38
1	D	73	ASP	C-N-CA	6.44	129.20	120.38
1	G	131	ALA	N-CA-C	6.27	117.98	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	ASP	CA-CB-CG	6.14	118.74	112.60
2	E	197	HIS	CA-C-N	5.89	128.45	120.38
2	E	197	HIS	C-N-CA	5.89	128.45	120.38
1	G	28	THR	N-CA-C	5.89	119.65	112.23
2	B	197	HIS	CA-C-N	5.88	128.44	120.38
2	B	197	HIS	C-N-CA	5.88	128.44	120.38
2	H	57	ILE	CB-CA-C	5.78	116.31	110.94
1	A	74	GLU	N-CA-C	5.71	118.24	111.33
1	C	34	ILE	N-CA-CB	5.67	118.60	111.46
2	B	79	ALA	CA-C-N	5.64	129.63	120.60
2	B	79	ALA	C-N-CA	5.64	129.63	120.60
1	C	131	ALA	N-CA-C	5.64	117.18	110.07
1	C	149	LYS	N-CA-C	5.60	118.60	109.59
1	G	29	LEU	CA-C-N	5.19	128.24	120.87
1	G	29	LEU	C-N-CA	5.19	128.24	120.87
2	F	140	PRO	CA-C-N	5.08	127.60	120.28
2	F	140	PRO	C-N-CA	5.08	127.60	120.28
1	G	117	VAL	N-CA-CB	5.04	118.02	111.67
2	F	23	SER	N-CA-C	5.03	116.60	108.41
1	A	73	ASP	CA-C-N	5.02	127.26	120.38
1	A	73	ASP	C-N-CA	5.02	127.26	120.38
2	B	169	ASP	N-CA-C	5.00	119.36	113.16

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	1612	0	1582	11	0
1	C	1597	0	1563	12	0
1	D	1600	0	1569	10	0
1	G	1618	0	1586	12	0
2	B	1613	0	1562	3	0
2	E	1613	0	1562	6	0
2	F	1613	0	1562	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1601	0	1546	8	0
3	I	94	0	88	0	0
3	J	94	0	88	0	0
3	K	94	0	88	1	0
3	L	94	0	88	0	0
4	A	27	0	0	0	0
4	B	48	0	0	0	0
4	C	24	0	0	0	0
4	D	33	0	0	0	0
4	E	50	0	0	0	0
4	F	40	0	0	0	0
4	G	26	0	0	0	0
4	H	52	0	0	1	0
4	I	1	0	0	0	0
All	All	13544	0	12884	66	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 3.

All (66) 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)
1:G:101:LEU:HD22	1:G:101:LEU:H	1.51	0.74
1:D:15:GLY:HA2	2:H:168:LYS:HD3	1.79	0.62
1:A:29:LEU:HD22	1:A:34:ILE:HD13	1.80	0.62
1:D:85:ASN:HB3	2:H:168:LYS:HG2	1.83	0.61
1:D:87:ARG:HD2	1:D:89:GLU:HB2	1.82	0.61
1:A:34:ILE:HD11	1:A:96[B]:CYS:SG	2.41	0.60
2:B:60:ARG:NH2	2:B:80:MET:SD	2.73	0.60
1:D:29:LEU:HD22	1:D:34:ILE:HD13	1.85	0.58
2:B:12:VAL:HG22	2:B:103:LEU:HD11	1.87	0.57
2:H:107:ARG:HD3	2:H:108:THR:O	2.05	0.56
1:C:55:PHE:HE2	3:K:438:LEU:HD11	1.71	0.54
2:F:12:VAL:HG22	2:F:103:LEU:HD11	1.90	0.54
2:E:12:VAL:HG22	2:E:103:LEU:HD11	1.90	0.53
1:C:29:LEU:HD22	1:C:34:ILE:HD12	1.90	0.53
1:D:11:VAL:HB	1:D:153:PRO:HG3	1.89	0.53
1:A:194:SER:HA	1:A:197:THR:HG22	1.91	0.52
2:F:107:ARG:HD3	2:F:108:THR:O	2.09	0.52
1:G:29:LEU:HB2	1:G:77:SER:HB3	1.91	0.51
1:A:199:THR:HG23	1:A:216:LYS:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:TRP:CE2	1:C:81:MET:HB2	2.46	0.51
2:E:107:ARG:HD3	2:E:108:THR:O	2.10	0.51
1:A:11:VAL:HB	1:A:153:PRO:HG3	1.93	0.50
1:D:36:TRP:CE2	1:D:81:MET:HB2	2.47	0.50
2:F:144:LYS:HB3	2:F:196:THR:OG1	2.12	0.50
1:G:36:TRP:CE2	1:G:81:MET:HB2	2.47	0.49
1:G:194:SER:HA	1:G:197:THR:HG22	1.94	0.49
1:G:29:LEU:HD11	1:G:34:ILE:HD13	1.94	0.48
2:H:189:LYS:HG3	4:H:331:HOH:O	2.12	0.48
2:H:12:VAL:HG22	2:H:103:LEU:HD11	1.96	0.48
1:C:122:THR:HG22	1:C:209:SER:HB3	1.96	0.47
1:G:195:LEU:HB3	1:G:219:PRO:HG3	1.96	0.47
1:G:132:PRO:HG3	1:G:144:LEU:HD23	1.97	0.47
1:G:122:THR:HG22	1:G:209:SER:HB3	1.97	0.47
1:C:11:VAL:HB	1:C:153:PRO:HG3	1.96	0.47
1:D:194:SER:HA	1:D:197:THR:HG22	1.96	0.47
1:D:199:THR:HG23	1:D:216:LYS:HE2	1.98	0.46
1:A:35:THR:HG21	1:A:106:TYR:CE1	2.51	0.46
2:E:4:LEU:HB2	2:E:98:GLY:HA2	1.98	0.46
2:F:4:LEU:HB2	2:F:98:GLY:HA2	1.98	0.46
2:H:4:LEU:HB2	2:H:98:GLY:HA2	1.98	0.45
1:C:195:LEU:HB3	1:C:219:PRO:HG3	1.99	0.45
2:H:107:ARG:HD2	2:H:139:TYR:CB	2.47	0.44
1:D:195:LEU:HB3	1:D:219:PRO:HG3	1.99	0.44
2:H:13:SER:HA	2:H:106:LEU:HB2	2.00	0.44
1:A:195:LEU:HB3	1:A:219:PRO:HG3	2.00	0.43
2:F:107:ARG:HD2	2:F:139:TYR:CB	2.47	0.43
1:G:132:PRO:HA	1:G:136:SER:OG	2.18	0.43
1:C:132:PRO:HG2	1:C:219:PRO:HB3	2.00	0.43
2:E:46:VAL:HA	2:E:57:ILE:HG13	2.00	0.43
1:A:36:TRP:CE2	1:A:81:MET:HB2	2.53	0.43
1:C:194:SER:HA	1:C:197:THR:HG22	2.00	0.43
1:G:24:ALA:HB2	1:G:29:LEU:HD13	2.01	0.42
2:E:107:ARG:HD2	2:E:139:TYR:CB	2.49	0.42
1:C:67:ARG:HD2	1:C:84:THR:O	2.18	0.42
1:G:28:THR:C	1:G:30:SER:H	2.26	0.42
1:G:11:VAL:HB	1:G:153:PRO:HG3	2.01	0.42
1:C:199:THR:HG23	1:C:216:LYS:HE3	2.02	0.42
2:F:46:VAL:HA	2:F:57:ILE:HG13	2.01	0.42
1:A:193:SER:CB	2:F:157:ASN:HB3	2.50	0.41
1:C:73:ASP:HB3	1:C:76:THR:OG1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:PRO:HB3	1:A:151:TYR:HB3	2.02	0.41
2:E:185:TYR:CZ	2:E:210:ARG:HG3	2.56	0.41
1:A:59:MET:SD	2:B:93:ASN:HB3	2.61	0.41
1:C:29:LEU:HB3	1:C:34:ILE:HD11	2.02	0.40
2:F:22[B]:CYS:SG	2:F:27:LEU:HD21	2.61	0.40
1:D:55:PHE:O	1:D:57:THR:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	215/261 (82%)	211 (98%)	4 (2%)	0	100	100
1	C	212/261 (81%)	207 (98%)	5 (2%)	0	100	100
1	D	212/261 (81%)	207 (98%)	5 (2%)	0	100	100
1	G	215/261 (82%)	210 (98%)	5 (2%)	0	100	100
2	B	211/215 (98%)	205 (97%)	6 (3%)	0	100	100
2	E	211/215 (98%)	206 (98%)	5 (2%)	0	100	100
2	F	212/215 (99%)	208 (98%)	4 (2%)	0	100	100
2	H	208/215 (97%)	203 (98%)	5 (2%)	0	100	100
3	I	9/13 (69%)	9 (100%)	0	0	100	100
3	J	9/13 (69%)	9 (100%)	0	0	100	100
3	K	9/13 (69%)	9 (100%)	0	0	100	100
3	L	9/13 (69%)	9 (100%)	0	0	100	100
All	All	1732/1956 (88%)	1693 (98%)	39 (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	A	181/212 (85%)	174 (96%)	7 (4%)	28	37
1	C	178/212 (84%)	169 (95%)	9 (5%)	21	26
1	D	178/212 (84%)	172 (97%)	6 (3%)	32	42
1	G	181/212 (85%)	168 (93%)	13 (7%)	13	14
2	B	184/186 (99%)	176 (96%)	8 (4%)	26	33
2	E	184/186 (99%)	173 (94%)	11 (6%)	17	20
2	F	185/186 (100%)	178 (96%)	7 (4%)	29	38
2	H	181/186 (97%)	171 (94%)	10 (6%)	19	23
3	I	8/10 (80%)	7 (88%)	1 (12%)	4	3
3	J	8/10 (80%)	7 (88%)	1 (12%)	4	3
3	K	8/10 (80%)	7 (88%)	1 (12%)	4	3
3	L	8/10 (80%)	8 (100%)	0	100	100
All	All	1484/1632 (91%)	1410 (95%)	74 (5%)	22	27

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	10	GLU
1	A	57	THR
1	A	103	ARG
1	A	121	SER
1	A	144	LEU
1	A	156	VAL
2	B	12	VAL
2	B	13	SER
2	B	25	ASP
2	B	99	THR
2	B	102	LYS
2	B	153	LEU
2	B	168	LYS

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Mol	Chain	Res	Type
2	B	196	THR
1	C	10	GLU
1	C	34	ILE
1	C	67	ARG
1	C	101	LEU
1	C	121	SER
1	C	144	LEU
1	C	156	VAL
1	C	194	SER
1	C	198	GLN
1	D	10	GLU
1	D	57	THR
1	D	87	ARG
1	D	121	SER
1	D	144	LEU
1	D	156	VAL
2	E	12	VAL
2	E	13	SER
2	E	25	ASP
2	E	27	LEU
2	E	53	ARG
2	E	99	THR
2	E	102	LYS
2	E	107	ARG
2	E	153	LEU
2	E	180	LEU
2	E	196	THR
2	F	12	VAL
2	F	13	SER
2	F	25	ASP
2	F	55	SER
2	F	102	LYS
2	F	107	ARG
2	F	153	LEU
1	G	10	GLU
1	G	29	LEU
1	G	56	ARG
1	G	57	THR
1	G	71	THR
1	G	74	GLU
1	G	101	LEU
1	G	103	ARG

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Mol	Chain	Res	Type
1	G	121	SER
1	G	134	SER
1	G	144	LEU
1	G	156	VAL
1	G	177	GLN
2	H	12	VAL
2	H	13	SER
2	H	25	ASP
2	H	55	SER
2	H	56	GLU
2	H	99	THR
2	H	107	ARG
2	H	153	LEU
2	H	196	THR
2	H	201	SER
3	I	444	GLN
3	J	444	GLN
3	K	446	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
2	B	16	GLN
2	B	51	ASN
2	B	88	GLN
1	C	31	ASN
2	E	16	GLN
2	E	36	GLN
2	E	51	ASN
2	E	65	ASN
2	E	159	GLN
2	F	49	GLN
2	F	51	ASN
2	F	65	ASN
2	F	136	ASN
1	G	205	ASN
2	H	36	GLN
2	H	49	GLN
2	H	51	ASN
2	H	65	ASN
3	I	445	HIS

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Mol	Chain	Res	Type
3	J	445	HIS
3	L	444	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	A	215/261 (82%)	0.40	9 (4%) 40 37	21, 41, 66, 87	4 (1%)
1	C	214/261 (81%)	0.39	10 (4%) 36 33	20, 40, 66, 94	2 (0%)
1	D	214/261 (81%)	0.31	7 (3%) 49 46	20, 38, 63, 78	2 (0%)
1	G	217/261 (83%)	0.49	14 (6%) 25 22	21, 40, 70, 98	2 (0%)
2	B	211/215 (98%)	0.11	4 (1%) 66 64	22, 35, 56, 73	2 (0%)
2	E	211/215 (98%)	0.04	4 (1%) 66 64	20, 34, 54, 74	2 (0%)
2	F	210/215 (97%)	0.06	1 (0%) 87 86	18, 35, 52, 63	4 (1%)
2	H	210/215 (97%)	0.13	3 (1%) 73 72	22, 36, 55, 71	0
3	I	11/13 (84%)	0.73	1 (9%) 15 12	33, 45, 64, 65	0
3	J	11/13 (84%)	1.31	4 (36%) 1 0	37, 60, 91, 93	0
3	K	11/13 (84%)	1.04	2 (18%) 3 2	47, 50, 65, 70	0
3	L	11/13 (84%)	1.92	5 (45%) 0 0	57, 69, 96, 97	0
All	All	1746/1956 (89%)	0.27	64 (3%) 45 42	18, 38, 64, 98	18 (1%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	211	GLY	4.4
1	C	133	SER	4.3
3	L	437	TRP	4.1
3	J	437	TRP	3.6
1	C	76	THR	3.5
1	A	62	GLN	3.4
1	G	26	GLY	3.2
2	B	211	GLY	3.2
1	A	75	SER	3.2
3	L	438	LEU	3.2
1	G	197	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	2	VAL	3.1
1	D	133	SER	2.8
1	C	219	PRO	2.8
3	J	439	ALA	2.8
1	A	196	GLY	2.8
1	G	27	GLY	2.7
1	G	30	SER	2.7
1	G	55	PHE	2.7
2	H	94	THR	2.7
1	D	76	THR	2.6
1	A	133	SER	2.6
1	D	75	SER	2.6
3	K	436	GLY	2.5
1	C	103	ARG	2.5
1	D	196	GLY	2.5
2	E	153	LEU	2.5
1	C	77	SER	2.5
1	G	196	GLY	2.5
1	A	25	SER	2.4
2	B	56	GLU	2.4
1	G	219	PRO	2.4
1	C	199	THR	2.4
1	G	75	SER	2.4
1	A	197	THR	2.3
2	F	153	LEU	2.3
1	D	194	SER	2.3
1	D	210	ASN	2.3
1	A	76	THR	2.3
2	B	122	GLU	2.2
1	G	134	SER	2.2
1	G	121	SER	2.2
1	G	195	LEU	2.2
3	J	438	LEU	2.2
1	C	74	GLU	2.2
1	G	62	GLN	2.2
3	L	445	HIS	2.2
2	B	153	LEU	2.1
3	L	442	PHE	2.1
2	H	3	VAL	2.1
1	A	139	GLY	2.1
1	G	28	THR	2.1
3	L	439	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	125	LYS	2.1
1	C	29	LEU	2.1
1	G	2	VAL	2.1
3	K	437	TRP	2.1
2	H	57	ILE	2.1
1	D	139	GLY	2.1
3	I	436	GLY	2.1
3	J	436	GLY	2.1
1	C	75	SER	2.0
1	A	13	LYS	2.0
2	E	1	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.