



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:32 AM UTC

PDB ID : 5TJE / pdb_00005tje
Title : Murine class I major histocompatibility complex H-2Db in complex with LCMV-derived gp33 and T cell receptor P14
Authors : Achour, A.; Sandalova, T.; Allerbring, E.; Popov, A.
Deposited on : 2016-10-04
Resolution : 3.20 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

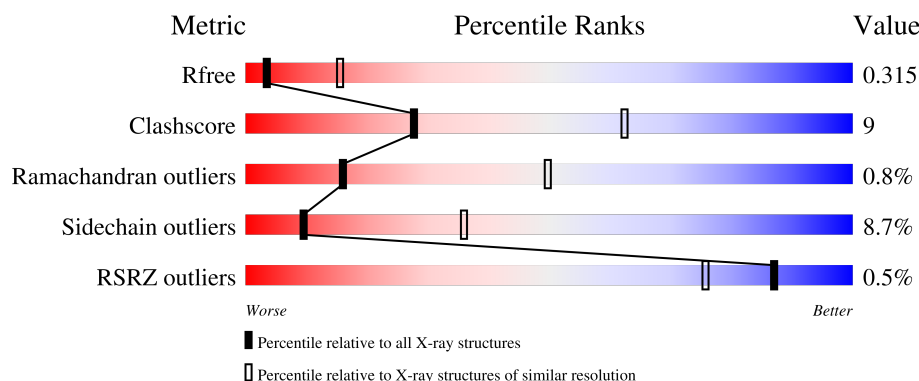
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



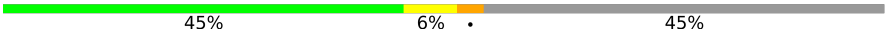
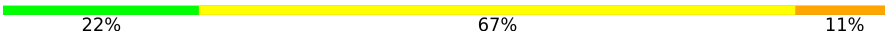
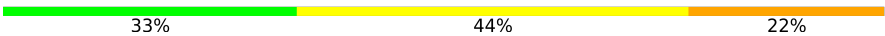
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	276	
1	C	276	
2	B	99	
2	D	99	
3	E	205	

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Mol	Chain	Length	Quality of chain
3	G	205	 45% 6% . 45%
4	F	238	 72% 24% .
4	H	238	 73% 20% . .
5	I	9	 22% 67% 11%
5	J	9	 33% 44% 22%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11784 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	1	0	0
			2256	1425	398	424	9			
1	C	274	Total	C	N	O	S	1	0	0
			2248	1420	396	423	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			813	518	137	151	7			
2	D	98	Total	C	N	O	S	0	0	0
			813	518	137	151	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ASP	ALA	conflict	UNP P01887
D	85	ASP	ALA	conflict	UNP P01887

- Molecule 3 is a protein called ALPHA CHAIN OF MURINE T CELL RECEPTOR p14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	112	Total	C	N	O	S	0	0	0
			880	567	140	171	2			
3	E	116	Total	C	N	O	S	0	0	0
			903	581	147	173	2			

- Molecule 4 is a protein called BETA CHAIN OF MURINE T CELL RECEPTOR p14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	232	Total	C	N	O	S	0	0	0
			1826	1146	326	348	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	237	Total	C	N	O	S	0	0	0
			1872	1176	333	357	6			

- Molecule 5 is a protein called Peptide gp33-41 from LCMV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	9	Total	C	N	O	S	0	0	0
			73	48	11	13	1			
5	J	9	Total	C	N	O	S	0	0	0
			73	48	11	13	1			

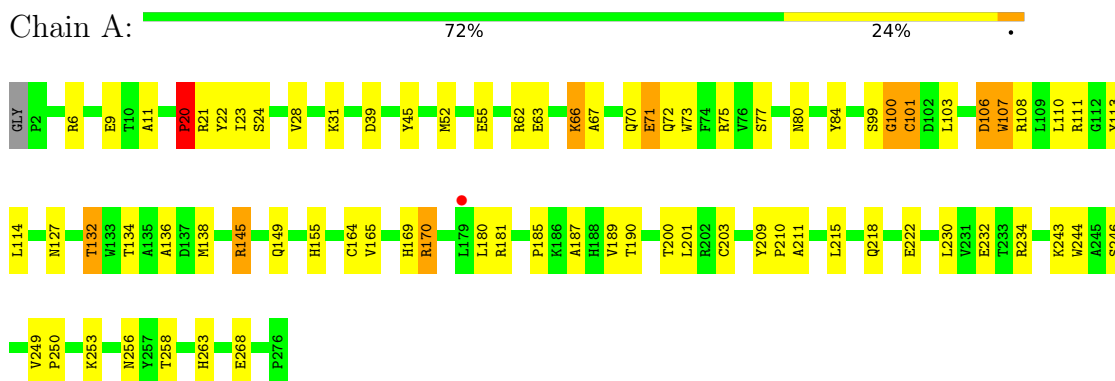
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	O	0	0
			9	9		
6	B	4	Total	O	0	0
			4	4		
6	C	8	Total	O	0	0
			8	8		
6	H	2	Total	O	0	0
			2	2		
6	F	4	Total	O	0	0
			4	4		

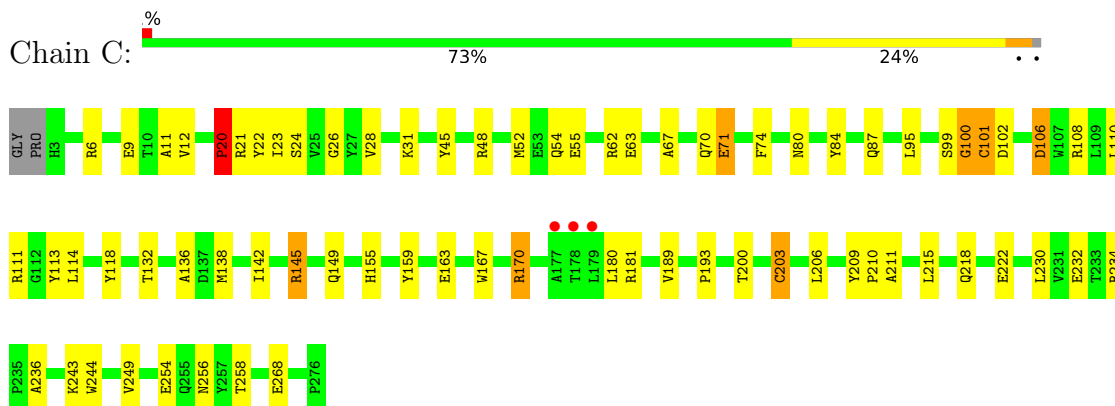
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

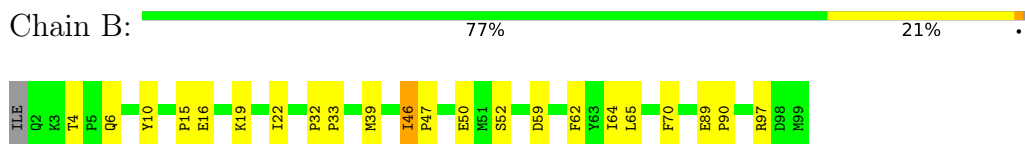
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



- Molecule 2: Beta-2-microglobulin



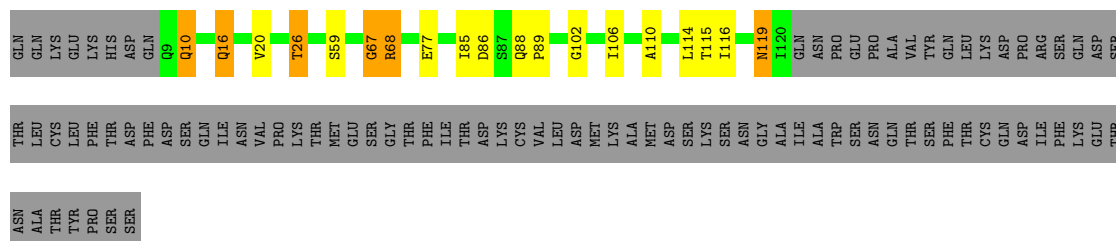
- Molecule 2: Beta-2-microglobulin





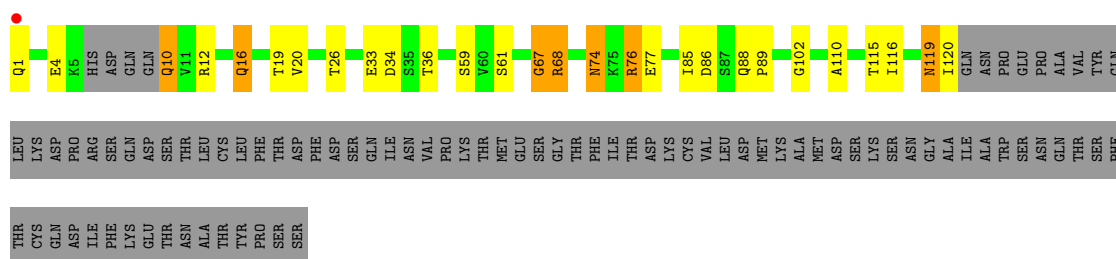
• Molecule 3: ALPHA CHAIN OF MURINE T CELL RECEPTOR p14

Chain G: 45% 6% 45%



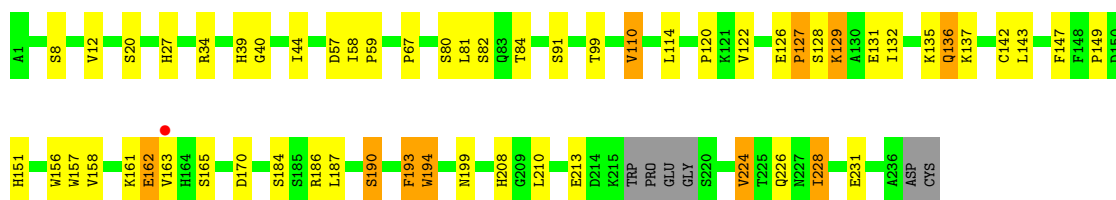
• Molecule 3: ALPHA CHAIN OF MURINE T CELL RECEPTOR p14

Chain E: 43% 10% 43%



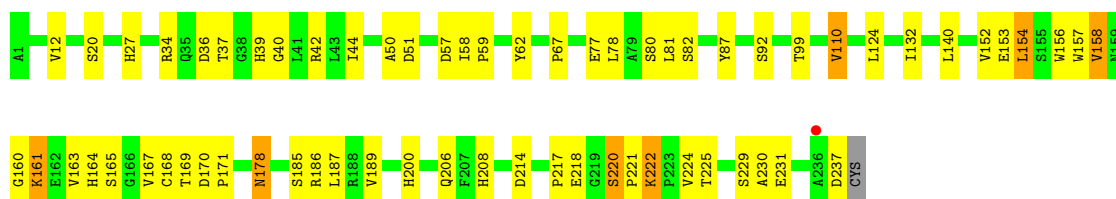
• Molecule 4: BETA CHAIN OF MURINE T CELL RECEPTOR p14

Chain H: 73% 20% 7%

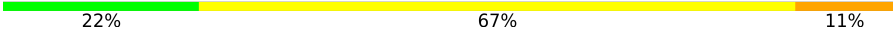


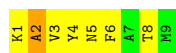
• Molecule 4: BETA CHAIN OF MURINE T CELL RECEPTOR p14

Chain F: 72% 24% 4%



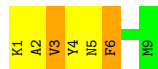
• Molecule 5: Peptide gp33-41 from LCMV

Chain I:  22% 67% 11%



● Molecule 5: Peptide gp33-41 from LCMV

Chain J:  33% 44% 22%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.17Å 66.94Å 525.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.88 – 3.20 38.88 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.7 (38.88-3.20) 94.7 (38.88-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.228 , 0.314 0.234 , 0.315	Depositor DCC
R_{free} test set	1825 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11784	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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	A	0.93	2/2323 (0.1%)	1.10	6/3156 (0.2%)
1	C	0.91	2/2313 (0.1%)	1.09	7/3141 (0.2%)
2	B	0.98	0/839	1.12	1/1137 (0.1%)
2	D	0.95	1/839 (0.1%)	1.08	1/1137 (0.1%)
3	E	0.97	1/925 (0.1%)	1.11	3/1254 (0.2%)
3	G	0.95	0/903	1.16	2/1226 (0.2%)
4	F	0.96	0/1924	1.04	3/2615 (0.1%)
4	H	0.93	0/1873	1.12	14/2542 (0.6%)
5	I	1.08	0/74	1.37	1/97 (1.0%)
5	J	1.39	1/74 (1.4%)	1.41	2/97 (2.1%)
All	All	0.94	7/12087 (0.1%)	1.10	40/16402 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	H	0	2
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	6	PHE	CA-C	-8.20	1.48	1.52
1	A	6	ARG	CA-C	-6.60	1.44	1.52
3	E	4	GLU	CA-C	5.33	1.59	1.52
1	C	20	PRO	N-CD	5.24	1.55	1.47
1	A	20	PRO	N-CD	5.23	1.55	1.47
2	D	94	TYR	CA-C	-5.08	1.46	1.52
1	C	26	GLY	CA-C	-5.02	1.48	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	194	TRP	CB-CA-C	-12.69	91.79	110.06
3	G	68	ARG	CB-CA-C	-9.75	95.32	110.04
4	H	193	PHE	N-CA-C	-9.16	96.22	109.96
4	H	128	SER	CB-CA-C	8.31	123.93	110.88
3	E	68	ARG	CB-CA-C	-7.16	96.67	110.35
1	C	142	ILE	CB-CA-C	-6.80	103.13	112.24
2	D	58	LYS	N-CA-C	6.58	120.41	112.38
2	B	65	LEU	N-CA-C	6.26	119.07	107.99
5	J	3	VAL	CB-CA-C	-6.23	101.43	111.59
4	H	122	VAL	N-CA-C	6.23	117.96	107.18
1	C	136	ALA	N-CA-C	6.14	123.88	110.80
4	H	190	SER	N-CA-C	6.09	123.78	110.80
4	H	193	PHE	CB-CA-C	6.04	119.55	109.89
1	A	136	ALA	N-CA-C	5.98	123.54	110.80
1	C	211	ALA	N-CA-C	5.89	117.79	111.36
4	H	136	GLN	N-CA-C	5.77	119.53	111.74
4	F	229	SER	N-CA-C	5.72	117.92	109.69
3	G	67	GLY	N-CA-C	5.71	126.72	113.18
4	H	194	TRP	CA-C-N	5.66	130.17	120.71
4	H	194	TRP	C-N-CA	5.66	130.17	120.71
4	H	128	SER	N-CA-C	-5.57	105.11	111.07
5	J	2	ALA	N-CA-C	5.52	118.23	110.23
4	H	129	LYS	CB-CA-C	-5.45	99.58	110.42
1	C	100	GLY	N-CA-C	5.43	118.45	110.80
4	H	190	SER	CB-CA-C	-5.39	99.69	110.42
1	C	106	ASP	N-CA-C	-5.39	102.22	110.30
1	A	106	ASP	N-CA-C	-5.36	102.36	110.24
5	I	2	ALA	N-CA-C	5.36	118.00	110.23
1	A	211	ALA	N-CA-C	5.35	117.19	111.36
1	A	187	ALA	N-CA-C	5.28	117.98	108.48
4	H	231	GLU	N-CA-C	5.27	117.89	110.14
4	H	194	TRP	N-CA-C	5.25	121.53	113.28
3	E	67	GLY	N-CA-C	5.25	125.62	113.18
1	C	54	GLN	N-CA-C	5.19	117.34	111.11
1	A	246	SER	N-CA-C	5.12	117.04	108.99
3	E	74	ASN	N-CA-C	5.12	116.66	107.80
1	A	100	GLY	N-CA-C	5.09	117.98	110.80
4	F	222	LYS	CA-C-N	5.02	128.69	121.91
4	F	222	LYS	C-N-CA	5.02	128.69	121.91
1	C	12	VAL	N-CA-C	5.02	115.07	107.75

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	TRP	Peptide
4	H	129	LYS	Peptide
4	H	135	LYS	Peptide

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	2256	0	2120	43	1
1	C	2248	0	2118	35	0
2	B	813	0	782	16	0
2	D	813	0	782	16	1
3	E	903	0	864	16	0
3	G	880	0	845	12	0
4	F	1872	0	1784	36	0
4	H	1826	0	1741	40	0
5	I	73	0	74	15	0
5	J	73	0	74	9	0
6	A	9	0	0	0	0
6	B	4	0	0	0	0
6	C	8	0	0	2	0
6	F	4	0	0	1	0
6	H	2	0	0	0	0
All	All	11784	0	11184	207	1

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 9.

All (207) 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)
4:H:157:TRP:CE3	4:H:162:GLU:HB2	1.56	1.41
4:H:194:TRP:O	4:H:194:TRP:CG	2.08	1.05
4:F:158:VAL:O	4:F:200:HIS:O	1.76	1.00
4:H:157:TRP:CZ3	4:H:162:GLU:HB2	1.99	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:PRO:HG2	2:B:97:ARG:CG	2.01	0.91
4:H:157:TRP:CE3	4:H:162:GLU:CB	2.52	0.91
2:B:15:PRO:CG	2:B:97:ARG:HG3	2.01	0.90
4:H:157:TRP:HE3	4:H:162:GLU:HB2	1.28	0.87
1:A:66:LYS:CE	5:I:2:ALA:O	2.22	0.87
2:B:15:PRO:HG2	2:B:97:ARG:HG3	1.57	0.86
1:A:63:GLU:OE2	1:A:66:LYS:NZ	2.11	0.83
1:C:159:TYR:OH	5:J:1:LYS:O	1.98	0.82
1:A:11:ALA:HA	1:A:21:ARG:O	1.80	0.81
4:H:157:TRP:CZ3	4:H:162:GLU:CB	2.65	0.79
2:D:33:PRO:HB3	2:D:62:PHE:CE2	2.19	0.78
4:H:194:TRP:O	4:H:194:TRP:CD2	2.37	0.77
1:C:145:ARG:HG3	6:C:307:HOH:O	1.84	0.76
1:C:209:TYR:CD1	1:C:210:PRO:HA	2.22	0.75
4:H:190:SER:O	4:H:193:PHE:O	2.05	0.74
1:A:66:LYS:HZ3	5:I:2:ALA:HB3	1.52	0.74
1:C:99:SER:HB3	5:J:3:VAL:HG21	1.70	0.73
2:B:15:PRO:HG3	2:B:97:ARG:HG3	1.71	0.71
1:A:66:LYS:HE3	5:I:2:ALA:O	1.90	0.71
4:H:194:TRP:O	4:H:194:TRP:CD1	2.45	0.69
1:A:99:SER:HB3	5:I:3:VAL:HG21	1.75	0.69
1:A:209:TYR:CD1	1:A:210:PRO:HA	2.28	0.68
2:B:33:PRO:HB3	2:B:62:PHE:CE2	2.27	0.68
1:A:63:GLU:CD	5:I:1:LYS:HG2	2.20	0.67
3:E:88:GLN:C	3:E:116:ILE:HG21	2.21	0.66
1:A:66:LYS:HE2	5:I:2:ALA:O	1.96	0.66
3:G:20:VAL:HG23	3:G:116:ILE:HD13	1.77	0.66
3:E:20:VAL:HG23	3:E:116:ILE:HD13	1.79	0.65
1:A:66:LYS:HD2	5:I:4:TYR:HD2	1.62	0.65
3:G:102:GLY:HA2	5:I:4:TYR:CE2	2.34	0.63
1:A:66:LYS:NZ	5:I:2:ALA:HB3	2.13	0.63
2:D:4:THR:O	2:D:6:GLN:NE2	2.31	0.63
4:F:222:LYS:HB3	4:F:224:VAL:HG13	1.81	0.62
3:G:88:GLN:C	3:G:116:ILE:HG21	2.24	0.62
1:A:107:TRP:HB3	1:A:169:HIS:CE1	2.35	0.61
1:A:107:TRP:HB3	1:A:169:HIS:NE2	2.17	0.60
4:H:126:GLU:HB3	4:H:127:PRO:HD2	1.84	0.58
1:C:45:TYR:HE2	1:C:67:ALA:HB2	1.68	0.58
4:H:80:SER:O	4:H:110:VAL:HG11	2.03	0.58
1:C:11:ALA:HA	1:C:21:ARG:O	2.04	0.57
4:H:163:VAL:HG13	4:H:163:VAL:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:89:PRO:HA	3:E:116:ILE:HB	1.87	0.57
1:A:180:LEU:HD12	1:A:181:ARG:N	2.20	0.56
2:B:15:PRO:HG2	2:B:97:ARG:CD	2.36	0.56
3:G:119:ASN:OD1	3:G:119:ASN:C	2.48	0.56
3:E:1:GLN:HA	3:E:19:THR:O	2.06	0.56
1:C:180:LEU:HD12	1:C:181:ARG:N	2.20	0.55
2:B:15:PRO:HG2	2:B:97:ARG:HD2	1.89	0.55
4:H:8:SER:HB3	4:H:208:HIS:CD2	2.42	0.54
3:E:119:ASN:OD1	3:E:119:ASN:C	2.51	0.54
4:F:154:LEU:C	4:F:154:LEU:HD23	2.32	0.54
1:A:52:MET:HE1	1:A:55:GLU:HG3	1.91	0.53
3:G:89:PRO:HA	3:G:116:ILE:HB	1.91	0.53
1:A:9:GLU:HG2	1:A:24:SER:OG	2.08	0.53
2:D:89:GLU:HB2	2:D:90:PRO:HD2	1.90	0.53
4:H:137:LYS:HG2	4:H:190:SER:HA	1.91	0.53
4:H:120:PRO:HG2	4:H:228:ILE:HD13	1.90	0.53
4:H:114:LEU:HD13	4:H:210:LEU:HG	1.91	0.53
3:E:10:GLN:NE2	3:E:10:GLN:HA	2.25	0.52
1:C:52:MET:HE1	1:C:55:GLU:HG3	1.92	0.52
3:E:74:ASN:OD1	3:E:76:ARG:NH1	2.43	0.52
4:H:186:ARG:C	4:H:187:LEU:N	2.68	0.52
4:F:62:TYR:HH	4:F:87:TYR:HH	1.46	0.52
4:F:81:LEU:N	6:F:301:HOH:O	2.42	0.51
1:A:111:ARG:HD3	1:A:113:TYR:CE1	2.45	0.51
2:B:32:PRO:CB	2:B:33:PRO:CD	2.88	0.51
2:B:89:GLU:HB2	2:B:90:PRO:HD2	1.92	0.51
4:H:57:ASP:C	4:H:59:PRO:HD3	2.35	0.51
3:E:16:GLN:N	3:E:16:GLN:OE1	2.43	0.51
4:F:58:ILE:O	4:F:58:ILE:HG22	2.09	0.51
2:B:16:GLU:O	2:B:19:LYS:HB2	2.11	0.51
4:F:158:VAL:HG23	4:F:163:VAL:HG21	1.93	0.51
4:F:158:VAL:HG23	4:F:163:VAL:CG2	2.41	0.51
1:A:63:GLU:HG2	5:I:1:LYS:HE2	1.93	0.50
3:G:16:GLN:N	3:G:16:GLN:OE1	2.44	0.50
3:E:102:GLY:HA2	5:J:4:TYR:CE2	2.46	0.50
3:E:67:GLY:O	3:E:68:ARG:HB2	2.12	0.50
4:F:169:THR:HA	4:F:185:SER:CB	2.42	0.50
3:E:68:ARG:HA	3:E:85:ILE:HD12	1.94	0.50
4:F:62:TYR:OH	4:F:87:TYR:OH	2.19	0.50
1:A:66:LYS:HD2	5:I:4:TYR:CD2	2.46	0.49
1:C:106:ASP:O	1:C:108:ARG:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:153:GLU:OE1	4:F:208:HIS:HE1	1.95	0.49
1:C:234:ARG:HD3	2:D:10:TYR:CZ	2.47	0.49
4:H:132:ILE:O	4:H:136:GLN:HG2	2.13	0.49
1:A:127:ASN:HD21	1:A:134:THR:HG1	1.60	0.49
1:C:167:TRP:CZ2	5:J:1:LYS:HD2	2.48	0.49
1:C:234:ARG:HD3	2:D:10:TYR:CE1	2.48	0.49
4:F:27:HIS:HB3	4:F:92:SER:O	2.12	0.49
1:A:70:GLN:HE22	5:I:5:ASN:HB2	1.79	0.48
4:H:142:CYS:HB2	4:H:156:TRP:CH2	2.49	0.48
4:F:124:LEU:HB3	4:F:230:ALA:HB1	1.95	0.48
1:A:31:LYS:HD3	1:A:209:TYR:OH	2.14	0.48
1:C:111:ARG:HD3	1:C:113:TYR:CE1	2.49	0.48
4:F:220:SER:CB	4:F:221:PRO:CD	2.92	0.48
4:F:220:SER:HB3	4:F:221:PRO:CD	2.43	0.48
1:C:80:ASN:O	1:C:84:TYR:CD1	2.67	0.47
2:D:16:GLU:O	2:D:19:LYS:HB2	2.14	0.47
1:A:106:ASP:O	1:A:108:ARG:N	2.48	0.47
4:H:27:HIS:ND1	4:H:91:SER:OG	2.36	0.47
4:F:152:VAL:HA	4:F:206:GLN:O	2.14	0.47
1:A:66:LYS:HZ1	5:I:2:ALA:N	2.12	0.47
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.49	0.47
1:C:163:GLU:O	1:C:167:TRP:HD1	1.98	0.47
2:D:32:PRO:CB	2:D:33:PRO:CD	2.91	0.47
3:G:110:ALA:O	4:H:40:GLY:N	2.47	0.47
4:H:143:LEU:HD12	4:H:184:SER:HB3	1.96	0.47
1:C:48:ARG:NH2	2:D:53:ASP:OD2	2.48	0.47
4:F:167:VAL:HG12	4:F:168:CYS:N	2.29	0.47
1:C:215:LEU:HD11	1:C:243:LYS:HG2	1.97	0.47
4:H:80:SER:C	4:H:110:VAL:HG11	2.40	0.47
4:F:50:ALA:HB1	4:F:51:ASP:OD1	2.14	0.46
1:A:55:GLU:OE1	1:A:170:ARG:NH1	2.49	0.46
4:H:58:ILE:HG22	4:H:58:ILE:O	2.15	0.46
3:E:110:ALA:O	4:F:40:GLY:N	2.48	0.46
4:F:156:TRP:N	4:F:156:TRP:CD1	2.83	0.46
1:C:203:CYS:O	1:C:244:TRP:HA	2.16	0.46
4:H:131:GLU:O	4:H:136:GLN:N	2.48	0.46
4:H:151:HIS:HB3	4:H:208:HIS:HB2	1.98	0.46
1:A:185:PRO:HD3	1:A:263:HIS:CD2	2.51	0.46
1:C:55:GLU:OE1	1:C:170:ARG:NH1	2.48	0.46
1:C:70:GLN:HE22	5:J:5:ASN:HB2	1.81	0.46
4:H:157:TRP:CZ3	4:H:162:GLU:HB3	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLN:OE1	1:A:75:ARG:NH1	2.49	0.45
1:C:155:HIS:HB3	5:J:6:PHE:CZ	2.51	0.45
1:A:21:ARG:HH21	1:A:39:ASP:HB2	1.81	0.45
1:A:22:TYR:HB3	1:A:71:GLU:HG3	1.97	0.45
1:A:100:GLY:C	1:A:101:CYS:SG	2.99	0.45
1:C:45:TYR:CE2	1:C:67:ALA:HB2	2.49	0.45
1:A:218:GLN:HA	1:A:222:GLU:O	2.17	0.45
4:H:114:LEU:HD13	4:H:210:LEU:CG	2.46	0.45
2:D:21:ASN:OD1	2:D:22:ILE:N	2.44	0.45
1:A:80:ASN:O	1:A:84:TYR:CD1	2.69	0.44
1:A:190:THR:O	1:A:201:LEU:HA	2.16	0.44
1:C:63:GLU:CD	5:J:1:LYS:HG2	2.42	0.44
1:C:87:GLN:NE2	1:C:118:TYR:OH	2.49	0.44
1:A:103:LEU:HD11	1:A:165:VAL:HG22	1.98	0.44
4:H:156:TRP:CE3	4:H:187:LEU:HD23	2.52	0.44
3:E:10:GLN:HA	3:E:10:GLN:HE21	1.83	0.44
3:G:10:GLN:NE2	3:G:10:GLN:HA	2.32	0.44
3:G:26:THR:HG21	3:G:114:LEU:HD11	1.98	0.44
2:D:33:PRO:HB3	2:D:62:PHE:CD2	2.53	0.44
1:A:203:CYS:O	1:A:244:TRP:HA	2.18	0.44
4:F:77:GLU:C	4:F:78:LEU:HD23	2.43	0.44
1:C:70:GLN:O	1:C:71:GLU:C	2.60	0.43
3:G:67:GLY:O	3:G:68:ARG:HB2	2.18	0.43
1:A:45:TYR:HE2	1:A:67:ALA:HB2	1.82	0.43
4:F:80:SER:O	4:F:110:VAL:HG11	2.18	0.43
1:A:215:LEU:HD11	1:A:243:LYS:HG2	1.99	0.43
1:C:22:TYR:HB3	1:C:71:GLU:HG3	2.01	0.43
3:G:106:ILE:HG23	3:G:106:ILE:O	2.19	0.43
4:F:57:ASP:C	4:F:59:PRO:HD3	2.43	0.43
4:F:169:THR:HA	4:F:185:SER:HB3	1.99	0.43
2:B:52:SER:HB3	2:B:64:ILE:HG13	2.01	0.43
4:H:84:THR:HG23	4:H:84:THR:O	2.18	0.43
3:E:34:ASP:OD1	3:E:36:THR:OG1	2.26	0.43
2:B:32:PRO:CB	2:B:33:PRO:HD2	2.48	0.42
2:D:19:LYS:O	2:D:72:PRO:HD2	2.19	0.42
2:D:32:PRO:CB	2:D:33:PRO:HD2	2.49	0.42
4:F:158:VAL:CG2	4:F:163:VAL:HG11	2.49	0.42
4:F:178:ASN:OD1	4:F:178:ASN:N	2.50	0.42
1:C:9:GLU:HG2	1:C:24:SER:OG	2.20	0.42
1:C:218:GLN:HA	1:C:222:GLU:O	2.20	0.42
4:F:34:ARG:HB2	4:F:44:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:36:ASP:OD2	4:F:42:ARG:NH1	2.52	0.42
3:G:68:ARG:HA	3:G:85:ILE:HD12	2.02	0.42
1:A:155:HIS:HB3	5:I:6:PHE:CE2	2.55	0.42
2:B:4:THR:O	2:B:6:GLN:NE2	2.53	0.42
4:H:149:PRO:O	4:H:151:HIS:N	2.53	0.42
3:E:12:ARG:NH2	3:E:33:GLU:OE1	2.53	0.42
4:F:152:VAL:HG23	4:F:152:VAL:O	2.20	0.42
1:A:155:HIS:CB	5:I:6:PHE:CE2	3.03	0.42
2:B:59:ASP:OD1	2:B:59:ASP:N	2.53	0.42
2:D:82:VAL:HG12	2:D:87:MET:HE1	2.02	0.42
4:H:224:VAL:HG23	4:H:226:GLN:NE2	2.35	0.42
1:A:127:ASN:HB2	1:A:132:THR:HG22	2.02	0.42
4:F:158:VAL:CG2	4:F:163:VAL:HG21	2.49	0.42
2:D:21:ASN:HB3	2:D:70:PHE:CE1	2.55	0.41
4:H:156:TRP:CD2	4:H:187:LEU:HD23	2.54	0.41
2:B:39:MET:O	2:B:46:ILE:HG13	2.20	0.41
1:C:236:ALA:O	2:D:24:ASN:ND2	2.52	0.41
4:H:34:ARG:HB2	4:H:44:ILE:HD11	2.01	0.41
1:C:6:ARG:NH1	1:C:102:ASP:OD1	2.53	0.41
1:C:31:LYS:HD3	1:C:209:TYR:OH	2.21	0.41
4:H:57:ASP:O	4:H:59:PRO:HD3	2.20	0.41
4:F:36:ASP:O	4:F:37:THR:OG1	2.35	0.41
1:A:73:TRP:O	1:A:77:SER:OG	2.35	0.41
1:C:74:PHE:CD2	1:C:95:LEU:HD23	2.56	0.41
1:C:100:GLY:C	1:C:101:CYS:SG	3.03	0.41
6:C:302:HOH:O	2:D:58:LYS:HE2	2.20	0.41
4:H:190:SER:HB3	4:H:193:PHE:HB2	2.03	0.41
4:F:80:SER:C	4:F:110:VAL:HG11	2.46	0.41
1:A:250:PRO:HG2	1:A:253:LYS:HG3	2.03	0.40
1:C:155:HIS:CB	5:J:6:PHE:CE2	3.05	0.40
4:H:158:VAL:HG23	4:H:161:LYS:O	2.22	0.40
3:E:119:ASN:O	3:E:120:ILE:HB	2.22	0.40
4:F:157:TRP:HE3	4:F:160:GLY:C	2.29	0.40
4:F:220:SER:HB3	4:F:221:PRO:HD3	2.04	0.40
4:H:81:LEU:O	4:H:84:THR:HG22	2.22	0.40
4:H:120:PRO:HB3	4:H:147:PHE:HB3	2.03	0.40
1:C:167:TRP:CE2	5:J:1:LYS:HD2	2.57	0.40
4:F:161:LYS:HA	4:F:161:LYS:HD3	1.65	0.40
4:F:170:ASP:HB3	4:F:171:PRO:CD	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ARG:NH2	2:D:20:PRO:O[1_565]	2.05	0.15

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	273/276 (99%)	253 (93%)	19 (7%)	1 (0%)	30	62
1	C	272/276 (99%)	253 (93%)	17 (6%)	2 (1%)	18	52
2	B	96/99 (97%)	86 (90%)	9 (9%)	1 (1%)	12	45
2	D	96/99 (97%)	88 (92%)	8 (8%)	0	100	100
3	E	112/205 (55%)	101 (90%)	11 (10%)	0	100	100
3	G	110/205 (54%)	98 (89%)	12 (11%)	0	100	100
4	F	235/238 (99%)	211 (90%)	20 (8%)	4 (2%)	7	35
4	H	226/238 (95%)	197 (87%)	25 (11%)	4 (2%)	6	34
5	I	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
5	J	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
All	All	1434/1654 (87%)	1297 (90%)	125 (9%)	12 (1%)	16	50

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	217	PRO
1	A	20	PRO
4	H	67	PRO
4	F	67	PRO
4	F	220	SER
4	H	213	GLU
4	H	127	PRO
1	C	20	PRO
4	H	224	VAL

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Mol	Chain	Res	Type
4	F	158	VAL
1	C	193	PRO
2	B	47	PRO

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	233/234 (100%)	210 (90%)	23 (10%)	7	31
1	C	232/234 (99%)	208 (90%)	24 (10%)	7	28
2	B	93/94 (99%)	89 (96%)	4 (4%)	26	59
2	D	93/94 (99%)	86 (92%)	7 (8%)	12	42
3	E	96/184 (52%)	86 (90%)	10 (10%)	7	28
3	G	96/184 (52%)	88 (92%)	8 (8%)	10	38
4	F	203/204 (100%)	182 (90%)	21 (10%)	7	28
4	H	198/204 (97%)	187 (94%)	11 (6%)	19	52
5	I	7/7 (100%)	6 (86%)	1 (14%)	3	16
5	J	7/7 (100%)	7 (100%)	0	100	100
All	All	1258/1446 (87%)	1149 (91%)	109 (9%)	9	36

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	PRO
1	A	23	ILE
1	A	28	VAL
1	A	62	ARG
1	A	66	LYS
1	A	71	GLU
1	A	101	CYS
1	A	110	LEU
1	A	114	LEU
1	A	132	THR

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Mol	Chain	Res	Type
1	A	138	MET
1	A	145	ARG
1	A	149	GLN
1	A	164	CYS
1	A	170	ARG
1	A	189	VAL
1	A	200	THR
1	A	230	LEU
1	A	232	GLU
1	A	249	VAL
1	A	256	ASN
1	A	258	THR
1	A	268	GLU
2	B	22	ILE
2	B	46	ILE
2	B	50	GLU
2	B	70	PHE
1	C	20	PRO
1	C	23	ILE
1	C	28	VAL
1	C	62	ARG
1	C	71	GLU
1	C	101	CYS
1	C	110	LEU
1	C	114	LEU
1	C	132	THR
1	C	138	MET
1	C	145	ARG
1	C	149	GLN
1	C	170	ARG
1	C	189	VAL
1	C	200	THR
1	C	203	CYS
1	C	206	LEU
1	C	230	LEU
1	C	232	GLU
1	C	249	VAL
1	C	254	GLU
1	C	256	ASN
1	C	258	THR
1	C	268	GLU
2	D	2	GLN

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Mol	Chain	Res	Type
2	D	22	ILE
2	D	29	GLN
2	D	46	ILE
2	D	50	GLU
2	D	52	SER
2	D	70	PHE
3	G	10	GLN
3	G	16	GLN
3	G	26	THR
3	G	59	SER
3	G	77	GLU
3	G	86	ASP
3	G	115	THR
3	G	119	ASN
4	H	12	VAL
4	H	20	SER
4	H	39	HIS
4	H	82	SER
4	H	99	THR
4	H	110	VAL
4	H	162	GLU
4	H	165	SER
4	H	170	ASP
4	H	199	ASN
4	H	228	ILE
3	E	10	GLN
3	E	16	GLN
3	E	26	THR
3	E	59	SER
3	E	61	SER
3	E	76	ARG
3	E	77	GLU
3	E	86	ASP
3	E	115	THR
3	E	119	ASN
4	F	12	VAL
4	F	20	SER
4	F	39	HIS
4	F	82	SER
4	F	99	THR
4	F	110	VAL
4	F	132	ILE

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Mol	Chain	Res	Type
4	F	140	LEU
4	F	154	LEU
4	F	161	LYS
4	F	164	HIS
4	F	165	SER
4	F	178	ASN
4	F	186	ARG
4	F	187	LEU
4	F	189	VAL
4	F	214	ASP
4	F	218	GLU
4	F	225	THR
4	F	231	GLU
4	F	237	ASP
5	I	8	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	96	GLN
1	A	97	GLN
1	A	127	ASN
1	A	242	GLN
1	A	263	HIS
2	B	8	GLN
2	B	13	HIS
2	B	67	HIS
1	C	70	GLN
1	C	93	HIS
1	C	97	GLN
1	C	242	GLN
2	D	8	GLN
2	D	13	HIS
3	G	10	GLN
3	G	44	GLN
4	H	199	ASN
4	H	206	GLN
4	H	208	HIS
4	H	226	GLN
3	E	10	GLN
4	F	69	GLN

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Mol	Chain	Res	Type
4	F	172	GLN
4	F	208	HIS
5	I	5	ASN
5	J	5	ASN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	186:ARG	C	187:LEU	N	2.68

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	275/276 (99%)	-0.23	1 (0%) 88 79	36, 72, 119, 153	1 (0%)
1	C	274/276 (99%)	-0.18	3 (1%) 78 61	39, 76, 115, 195	1 (0%)
2	B	98/99 (98%)	-0.33	0 100 100	41, 64, 90, 113	0
2	D	98/99 (98%)	-0.28	0 100 100	43, 71, 104, 128	0
3	E	116/205 (56%)	-0.26	1 (0%) 81 64	50, 74, 106, 129	0
3	G	112/205 (54%)	-0.37	0 100 100	41, 71, 102, 117	0
4	F	237/238 (99%)	-0.19	1 (0%) 88 79	49, 83, 117, 142	0
4	H	232/238 (97%)	-0.09	1 (0%) 88 79	44, 85, 141, 188	0
5	I	9/9 (100%)	-0.09	0 100 100	48, 52, 66, 72	0
5	J	9/9 (100%)	-0.44	0 100 100	39, 51, 67, 69	0
All	All	1460/1654 (88%)	-0.22	7 (0%) 87 76	36, 75, 119, 195	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	179	LEU	2.7
1	C	178	THR	2.6
4	H	163	VAL	2.5
3	E	1	GLN	2.2
4	F	236	ALA	2.2
1	C	177	ALA	2.1
1	A	179	LEU	2.0

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

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.