



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:56 PM UTC

PDB ID : 3KPR / pdb_00003kpr
Title : Crystal Structure of the LC13 TCR in complex with HLA B*4405 bound to EEYLKAWTF a mimotope
Authors : Macdonald, W.A.; Chen, Z.; Gras, S.; Archbold, J.K.; Tynan, F.E.; Clements, C.S.; Bharadwaj, M.; Kjer-Nielsen, L.; Saunders, P.M.; Wilce, M.C.; Crawford, F.; Stadinsky, B.; Jackson, D.; Brooks, A.G.; Purcell, A.W.; Kappler, J.W.; Burrows, S.R.; Rossjohn, J.; McCluskey, J.
Deposited on : 2009-11-16
Resolution : 2.60 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

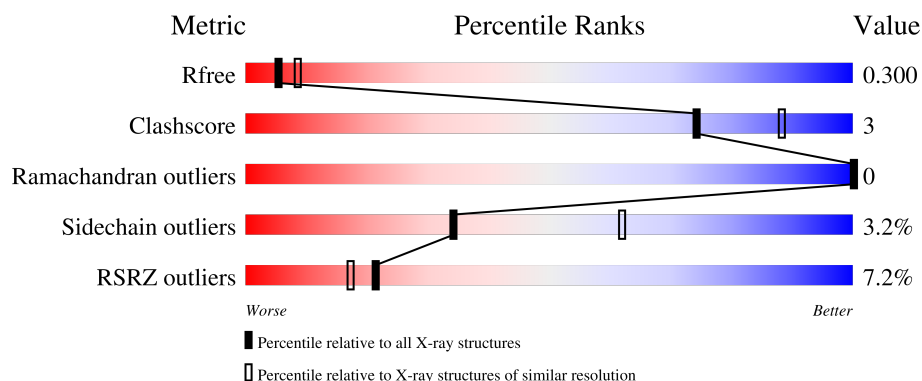
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	5% 87% 13%
1	F	276	16% 89% 11%
2	B	99	4% 91% 9%
2	G	99	3% 88% 12%

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Mol	Chain	Length	Quality of chain
3	C	9	78% 22%
3	H	9	78% 22%
4	D	201	9% 89% 9%
4	I	201	7% 90% 10%
5	E	241	4% 89% 11%
5	J	241	5% 88% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13434 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 HLA class I histocompatibility antigen, B-44 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2259	1408	407	437	7			
1	F	276	Total	C	N	O	S	0	0	0
			2259	1408	407	437	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	TYR	ASP	variant	UNP P30481
F	116	TYR	ASP	variant	UNP P30481

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	G	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

- Molecule 3 is a protein called EEYLKAWTF, mimotope peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			85	58	11	16			
3	H	9	Total	C	N	O	0	0	0
			85	58	11	16			

- Molecule 4 is a protein called LC13 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	201	Total	C	N	O	S	0	0	0
			1567	975	267	317	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	201	Total	C	N	O	S	0	0	0
			1567	975	267	317	8			

- Molecule 5 is a protein called LC13 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	241	Total	C	N	O	S	0	0	0
			1919	1209	335	371	4			
5	J	241	Total	C	N	O	S	0	0	0
			1919	1209	335	371	4			

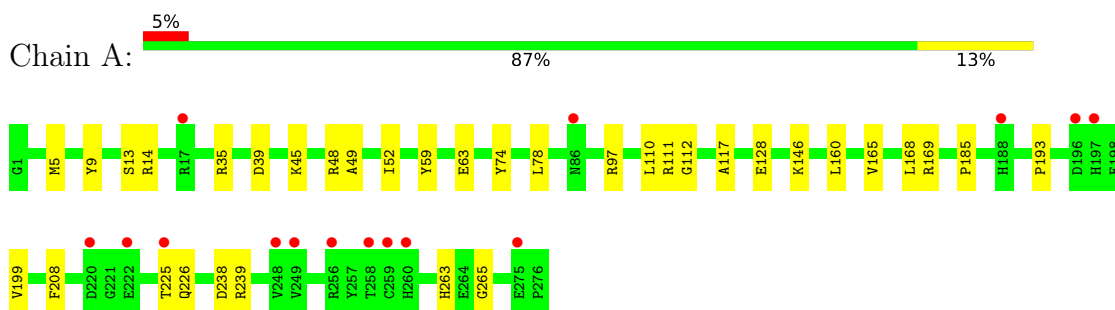
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total	O	0	0
			19	19		
6	B	4	Total	O	0	0
			4	4		
6	C	1	Total	O	0	0
			1	1		
6	D	16	Total	O	0	0
			16	16		
6	E	19	Total	O	0	0
			19	19		
6	F	26	Total	O	0	0
			26	26		
6	G	10	Total	O	0	0
			10	10		
6	H	3	Total	O	0	0
			3	3		
6	I	9	Total	O	0	0
			9	9		
6	J	9	Total	O	0	0
			9	9		

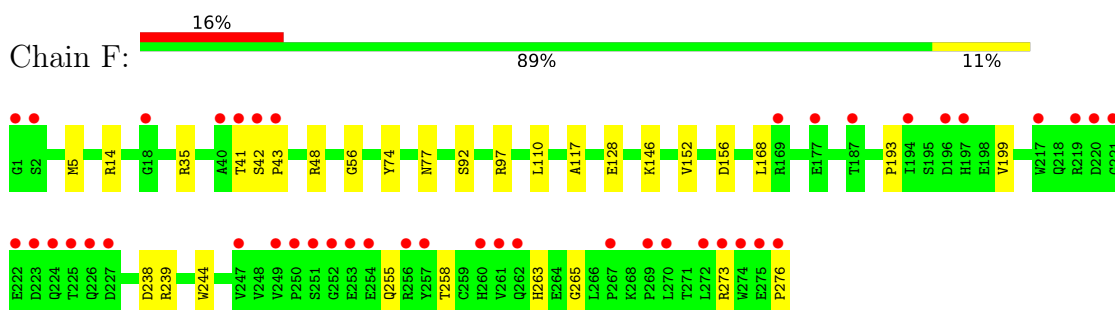
3 Residue-property plots [i](#)

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.

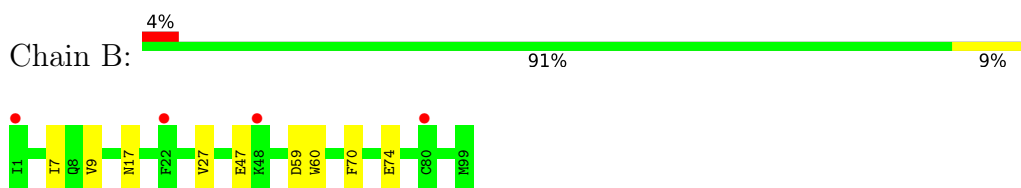
- Molecule 1: HLA class I histocompatibility antigen, B-44 alpha chain



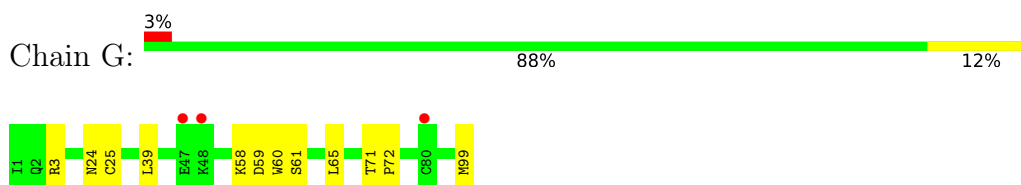
- Molecule 1: HLA class I histocompatibility antigen, B-44 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



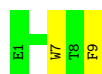
- Molecule 3: EEYLKAWTF, mimotope peptide

Chain C:  78% 22%



- Molecule 3: EEYLKAWTF, mimotope peptide

Chain H:  78% 22%



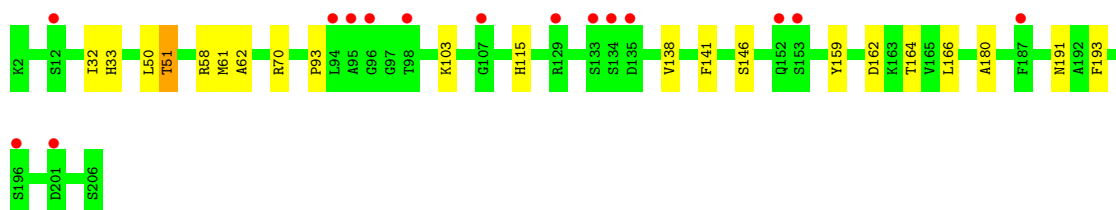
- Molecule 4: LC13 TCR alpha chain

Chain D:  9% 89% 9%



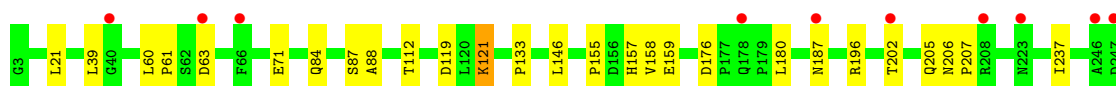
- Molecule 4: LC13 TCR alpha chain

Chain I:  7% 90% 10%



- Molecule 5: LC13 TCR beta chain

Chain E:  4% 89% 11%



- Molecule 5: LC13 TCR beta chain

Chain J:  5% 88% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	223.12Å 53.22Å 143.20Å 90.00° 102.39° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.60) 97.7 (50.00-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.279 0.255 , 0.300	Depositor DCC
R_{free} test set	2538 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13434	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.4962e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.41	0/2320	0.73	0/3154
1	F	0.41	0/2320	0.75	4/3154 (0.1%)
2	B	0.38	0/852	0.67	0/1152
2	G	0.39	0/852	0.66	0/1152
3	C	0.33	0/88	0.51	0/117
3	H	0.32	0/88	0.50	0/117
4	D	0.57	5/1603 (0.3%)	0.82	5/2181 (0.2%)
4	I	0.42	0/1603	0.70	0/2181
5	E	0.54	4/1971 (0.2%)	0.71	0/2681
5	J	0.52	2/1971 (0.1%)	0.73	0/2681
All	All	0.47	11/13668 (0.1%)	0.73	9/18570 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	159	GLU	CA-C	-7.16	1.44	1.52
5	J	158	VAL	C-O	-6.67	1.16	1.24
5	E	158	VAL	CA-CB	-6.34	1.45	1.54
4	D	112	LEU	CA-C	6.14	1.60	1.52
5	J	158	VAL	CA-C	-5.80	1.45	1.52
4	D	111	ILE	CA-CB	-5.66	1.47	1.53
4	D	112	LEU	N-CA	5.55	1.52	1.46
5	E	158	VAL	N-CA	-5.29	1.39	1.46
4	D	110	THR	N-CA	-5.21	1.39	1.46
5	E	159	GLU	C-O	-5.15	1.17	1.23
4	D	110	THR	CA-C	-5.15	1.46	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	112	LEU	N-CA-C	9.22	123.79	109.96
4	D	111	ILE	CB-CA-C	-6.37	102.79	111.33
4	D	106	PHE	N-CA-C	5.46	116.92	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	14	ARG	CA-C-N	5.29	124.95	119.56
1	F	14	ARG	C-N-CA	5.29	124.95	119.56
4	D	112	LEU	CA-C-N	-5.11	115.78	122.99
4	D	112	LEU	C-N-CA	-5.11	115.78	122.99
1	F	56	GLY	CA-C-N	5.08	124.87	119.28
1	F	56	GLY	C-N-CA	5.08	124.87	119.28

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	2259	0	2128	21	0
1	F	2259	0	2128	14	0
2	B	829	0	794	4	0
2	G	829	0	794	7	0
3	C	85	0	78	4	0
3	H	85	0	78	3	0
4	D	1567	0	1492	10	0
4	I	1567	0	1492	10	0
5	E	1919	0	1820	9	0
5	J	1919	0	1820	11	0
6	A	19	0	0	0	0
6	B	4	0	0	0	0
6	C	1	0	0	0	0
6	D	16	0	0	1	0
6	E	19	0	0	0	0
6	F	26	0	0	0	0
6	G	10	0	0	0	0
6	H	3	0	0	0	0
6	I	9	0	0	0	0
6	J	9	0	0	0	0
All	All	13434	0	12624	79	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 (79) 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:A:59:TYR:HE1	3:C:1:GLU:HG2	1.56	0.70
1:A:263:HIS:CD2	1:A:265:GLY:H	2.16	0.64
4:D:51:THR:HG22	4:D:70:ARG:HD3	1.79	0.62
5:E:21:LEU:HD22	5:E:112:THR:HG21	1.81	0.62
1:A:13:SER:HB3	1:A:78:LEU:HD13	1.81	0.61
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.37	0.60
4:D:86:ALA:O	4:D:112:LEU:N	2.28	0.58
4:I:50:LEU:HD23	4:I:51:THR:HG23	1.86	0.58
1:A:59:TYR:CE1	3:C:1:GLU:HG2	2.38	0.57
4:D:50:LEU:HD23	4:D:51:THR:HG23	1.87	0.56
2:B:17:ASN:HD21	2:B:74:GLU:HB2	1.71	0.56
1:F:263:HIS:CD2	1:F:265:GLY:H	2.23	0.55
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.88	0.55
1:A:35:ARG:HG2	1:A:48:ARG:HE	1.73	0.54
1:A:146:LYS:HD2	3:C:9:PHE:O	2.07	0.54
1:F:41:THR:O	1:F:43:PRO:HD3	2.08	0.53
1:A:193:PRO:HA	1:A:199:VAL:HG12	1.90	0.53
5:E:176:ASP:OD1	5:E:196:ARG:NH1	2.41	0.53
4:D:61:MET:HG3	4:D:62:ALA:N	2.24	0.52
5:J:159:GLU:OE1	5:J:218:TYR:OH	2.25	0.52
1:F:77:ASN:ND2	3:H:9:PHE:H	2.07	0.52
1:F:193:PRO:HA	1:F:199:VAL:HG12	1.91	0.52
4:D:86:ALA:H	4:D:112:LEU:HB3	1.74	0.51
4:D:28:SER:O	4:D:70:ARG:NH2	2.43	0.51
4:D:89:TYR:CD2	4:D:106:PHE:HB3	2.46	0.51
4:I:61:MET:HG3	4:I:62:ALA:N	2.24	0.50
1:A:112:GLY:HA3	1:A:160:LEU:HD13	1.93	0.50
5:J:51:ASN:O	5:J:69:ARG:HD3	2.11	0.50
1:F:255:GLN:HE22	1:F:276:PRO:HG3	1.77	0.50
1:A:49:ALA:O	1:A:52:ILE:HG22	2.13	0.48
4:I:103:LYS:HD2	5:J:45:PHE:CD2	2.48	0.48
4:I:164:THR:HG21	5:J:196:ARG:CZ	2.43	0.48
1:A:74:TYR:OH	1:A:97:ARG:HD2	2.14	0.48
2:G:3:ARG:HE	2:G:61:SER:HB3	1.80	0.47
1:A:185:PRO:HB3	1:A:208:PHE:HB3	1.97	0.47
4:I:33:HIS:CD2	4:I:93:PRO:HG2	2.50	0.47
5:E:155:PRO:HG2	5:E:157:HIS:CD2	2.50	0.47
1:F:5:MET:HB2	1:F:168:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:119:ASP:CG	5:E:121:LYS:HG2	2.40	0.46
1:A:9:TYR:HB2	1:A:97:ARG:HB3	1.98	0.46
5:E:133:PRO:HD3	5:E:146:LEU:HG	1.96	0.46
1:A:14:ARG:HH22	1:A:39:ASP:CG	2.23	0.46
4:D:3:THR:HG22	4:D:24:HIS:HB3	1.98	0.46
1:A:146:LYS:NZ	3:C:9:PHE:OXT	2.46	0.45
1:F:146:LYS:NZ	3:H:9:PHE:OXT	2.41	0.45
1:A:45:LYS:HG3	1:A:63:GLU:HB3	1.98	0.45
5:J:141:THR:O	5:J:142:GLN:HB2	2.17	0.45
4:D:106:PHE:HB2	4:D:107:GLY:HA2	1.98	0.45
1:A:165:VAL:O	1:A:169:ARG:HG3	2.17	0.45
5:E:60:LEU:HA	5:E:61:PRO:HD3	1.85	0.45
5:E:202:THR:HA	5:E:205:GLN:HB2	1.98	0.44
1:F:152:VAL:HG22	3:H:7:TRP:CD1	2.52	0.44
5:J:21:LEU:HD22	5:J:112:THR:HG21	1.99	0.44
4:I:115:HIS:HB3	4:I:146:SER:OG	2.17	0.43
4:I:159:TYR:HB3	5:J:180:LEU:HD23	1.99	0.43
1:F:258:THR:HG22	1:F:273:ARG:HG2	1.99	0.43
5:J:93:ALA:HB1	5:J:106:GLN:HB3	2.00	0.43
2:B:59:ASP:O	2:B:60:TRP:HB2	2.19	0.43
5:J:148:CYS:HB2	5:J:162:TRP:CZ2	2.54	0.42
2:G:25:CYS:HB2	2:G:39:LEU:HD21	2.00	0.42
2:G:59:ASP:O	2:G:60:TRP:HB2	2.19	0.42
1:F:238:ASP:O	1:F:239:ARG:HB2	2.20	0.42
5:E:206:ASN:HA	5:E:207:PRO:HD2	1.94	0.41
1:F:244:TRP:NE1	2:G:99:MET:OXT	2.53	0.41
4:D:2:LYS:N	6:D:209:HOH:O	2.52	0.41
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.55	0.41
1:A:117:ALA:HB2	2:B:60:TRP:CD2	2.56	0.41
1:F:35:ARG:HG2	1:F:48:ARG:HH11	1.85	0.41
2:G:24:ASN:HB3	2:G:65:LEU:HD11	2.03	0.41
1:A:111:ARG:HD2	1:A:128:GLU:OE2	2.21	0.41
1:A:238:ASP:O	1:A:239:ARG:HB2	2.21	0.41
5:J:226:TRP:CE2	5:J:228:GLN:HB2	2.56	0.41
2:G:71:THR:HA	2:G:72:PRO:HD2	1.99	0.41
4:I:141:PHE:HB2	4:I:193:PHE:CE1	2.56	0.41
4:I:159:TYR:O	4:I:180:ALA:HA	2.21	0.40
4:I:50:LEU:O	4:I:70:ARG:NH1	2.54	0.40
5:E:87:SER:O	5:E:88:ALA:HB2	2.22	0.40
1:F:74:TYR:OH	1:F:97:ARG:HD2	2.22	0.40
5:J:206:ASN:HA	5:J:207:PRO:HD2	1.88	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	274/276 (99%)	264 (96%)	10 (4%)	0	100	100
1	F	274/276 (99%)	264 (96%)	10 (4%)	0	100	100
2	B	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	G	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	H	7/9 (78%)	7 (100%)	0	0	100	100
4	D	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
4	I	199/201 (99%)	185 (93%)	14 (7%)	0	100	100
5	E	239/241 (99%)	229 (96%)	10 (4%)	0	100	100
5	J	239/241 (99%)	226 (95%)	13 (5%)	0	100	100
All	All	1632/1652 (99%)	1565 (96%)	67 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	237/237 (100%)	234 (99%)	3 (1%)	61	82
1	F	237/237 (100%)	232 (98%)	5 (2%)	47	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	94/94 (100%)	89 (95%)	5 (5%)	20	43
2	G	94/94 (100%)	93 (99%)	1 (1%)	65	84
3	C	8/8 (100%)	8 (100%)	0	100	100
3	H	8/8 (100%)	8 (100%)	0	100	100
4	D	180/180 (100%)	173 (96%)	7 (4%)	28	55
4	I	180/180 (100%)	173 (96%)	7 (4%)	28	55
5	E	207/207 (100%)	199 (96%)	8 (4%)	28	55
5	J	207/207 (100%)	197 (95%)	10 (5%)	23	47
All	All	1452/1452 (100%)	1406 (97%)	46 (3%)	34	62

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	LEU
1	A	225	THR
1	A	226	GLN
2	B	7	ILE
2	B	9	VAL
2	B	27	VAL
2	B	47	GLU
2	B	70	PHE
4	D	11	GLU
4	D	111	ILE
4	D	135	ASP
4	D	138	VAL
4	D	166	LEU
4	D	182	SER
4	D	191	ASN
5	E	39	LEU
5	E	63	ASP
5	E	71	GLU
5	E	84	GLN
5	E	121	LYS
5	E	180	LEU
5	E	187	ASN
5	E	237	ILE
1	F	42	SER
1	F	92	SER
1	F	110	LEU

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Mol	Chain	Res	Type
1	F	128	GLU
1	F	156	ASP
2	G	58	LYS
4	I	32	ILE
4	I	51	THR
4	I	58	ARG
4	I	138	VAL
4	I	162	ASP
4	I	166	LEU
4	I	191	ASN
5	J	24	ASP
5	J	39	LEU
5	J	84	GLN
5	J	118	GLU
5	J	121	LYS
5	J	159	GLU
5	J	174	SER
5	J	180	LEU
5	J	224	ASP
5	J	229	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	77	ASN
1	A	191	HIS
1	A	226	GLN
1	A	263	HIS
2	B	8	GLN
2	B	13	HIS
2	B	17	ASN
4	D	8	ASN
4	D	33	HIS
4	D	37	GLN
4	D	120	ASN
4	D	127	GLN
4	D	191	ASN
5	E	37	GLN
5	E	41	GLN
5	E	51	ASN
5	E	106	GLN

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Mol	Chain	Res	Type
5	E	122	ASN
5	E	157	HIS
5	E	223	ASN
1	F	70	ASN
1	F	77	ASN
1	F	115	GLN
1	F	155	GLN
1	F	255	GLN
1	F	263	HIS
2	G	8	GLN
2	G	13	HIS
4	I	8	ASN
4	I	23	ASN
4	I	33	HIS
5	J	51	ASN
5	J	106	GLN
5	J	122	ASN
5	J	157	HIS
5	J	187	ASN
5	J	206	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 [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	276/276 (100%)	0.69	15 (5%)	31 26	24, 36, 44, 50	1 (0%)
1	F	276/276 (100%)	0.96	43 (15%)	5 4	25, 35, 44, 49	1 (0%)
2	B	99/99 (100%)	0.64	4 (4%)	42 37	27, 35, 46, 47	0
2	G	99/99 (100%)	0.61	3 (3%)	52 47	29, 36, 43, 45	0
3	C	9/9 (100%)	0.62	0	100 100	31, 34, 37, 38	0
3	H	9/9 (100%)	0.63	0	100 100	33, 34, 37, 38	0
4	D	201/201 (100%)	0.78	18 (8%)	15 11	26, 36, 44, 57	0
4	I	201/201 (100%)	0.71	15 (7%)	20 16	28, 36, 46, 55	0
5	E	241/241 (100%)	0.64	10 (4%)	41 36	29, 36, 46, 54	0
5	J	241/241 (100%)	0.71	11 (4%)	37 32	28, 36, 44, 57	0
All	All	1652/1652 (100%)	0.73	119 (7%)	21 17	24, 36, 45, 57	2 (0%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	247	ASP	4.0
4	I	135	ASP	4.0
1	F	42	SER	3.9
5	J	246	ALA	3.8
1	F	18	GLY	3.8
1	A	197	HIS	3.5
1	F	260	HIS	3.4
5	E	66	PHE	3.4
1	F	197	HIS	3.2
5	J	171	SER	3.2
4	D	58	ARG	3.2
1	F	273	ARG	3.1
1	F	177	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	276	PRO	3.1
4	I	134	SER	3.1
4	I	152	GLN	3.1
5	E	247	ASP	3.1
1	A	188	HIS	3.0
1	F	275	GLU	3.0
4	I	133	SER	3.0
1	A	220	ASP	3.0
5	E	40	GLY	3.0
1	F	254	GLU	2.9
4	D	201	ASP	2.9
5	J	63	ASP	2.9
1	F	41	THR	2.9
2	G	80	CYS	2.9
5	E	63	ASP	2.9
1	F	250	PRO	2.8
5	E	187	ASN	2.8
1	F	223	ASP	2.8
5	J	227	THR	2.8
1	A	259	CYS	2.8
5	E	208	ARG	2.8
4	D	51	THR	2.8
1	F	220	ASP	2.7
1	F	221	GLY	2.7
4	I	196	SER	2.7
1	F	253	GLU	2.7
2	G	48	LYS	2.7
1	F	247	VAL	2.7
4	D	135	ASP	2.7
5	J	184	PRO	2.6
1	F	269	PRO	2.6
1	F	219	ARG	2.6
1	F	270	LEU	2.6
4	D	112	LEU	2.6
4	D	186	ASP	2.5
1	F	222	GLU	2.5
1	A	249	VAL	2.5
5	E	202	THR	2.5
1	F	194	ILE	2.5
1	F	274	TRP	2.5
4	D	15	GLU	2.5
4	I	95	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
4	D	154	LYS	2.4
1	A	225	THR	2.4
2	B	80	CYS	2.4
4	I	153	SER	2.4
1	F	169	ARG	2.4
2	B	48	LYS	2.4
4	I	98	THR	2.4
1	F	1	GLY	2.4
1	F	225	THR	2.4
4	I	187	PHE	2.4
2	B	1	ILE	2.3
4	D	30	THR	2.3
1	F	272	LEU	2.3
1	A	260	HIS	2.3
1	A	86	ASN	2.3
1	A	17	ARG	2.3
5	J	178	GLN	2.3
1	A	258	THR	2.3
2	G	47	GLU	2.3
4	I	12	SER	2.3
1	F	249	VAL	2.3
4	D	187	PHE	2.3
1	F	40	ALA	2.3
1	F	187	THR	2.3
1	F	257	TYR	2.3
4	D	8	ASN	2.3
4	D	195	ASN	2.3
5	J	229	ASP	2.3
1	A	222	GLU	2.2
5	E	223	ASN	2.2
1	F	2	SER	2.2
1	F	224	GLN	2.2
1	F	227	ASP	2.2
4	D	206	SER	2.2
1	F	217	TRP	2.2
5	J	225	GLU	2.2
1	F	261	VAL	2.2
4	I	129	ARG	2.2
5	E	178	GLN	2.2
1	F	196	ASP	2.2
1	F	251	SER	2.2
4	I	94	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	22	PHE	2.2
1	A	275	GLU	2.1
1	F	256	ARG	2.1
4	D	2	LYS	2.1
1	F	262	GLN	2.1
4	D	170	SER	2.1
1	F	43	PRO	2.1
4	I	96	GLY	2.1
5	J	59	GLY	2.1
1	A	248	VAL	2.1
4	D	196	SER	2.1
1	A	256	ARG	2.1
1	F	267	PRO	2.1
5	J	228	GLN	2.1
1	F	252	GLY	2.1
1	A	196	ASP	2.0
5	E	246	ALA	2.0
4	D	61	MET	2.0
1	F	226	GLN	2.0
4	I	201	ASP	2.0
4	I	107	GLY	2.0
4	D	169	ARG	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.