WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 05:14 AM EDT

PDB ID	:	3KPR
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)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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.
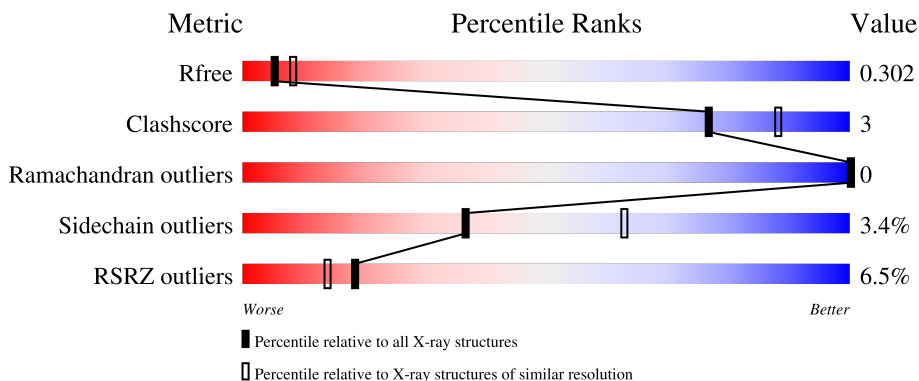
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	8% / 87% / 13%
1	F	276	18% / 89% / 10%
2	B	99	7% / 92% / 8%
2	G	99	3% / 88% / 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	9	78% 22%
3	H	9	78% 22%
4	D	201	5% 89% 10%
4	I	201	3% 90% 10%
5	E	241	2% 90% 10%
5	J	241	% 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			

Continued on next page...

Continued from previous page...

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

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

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

• Molecule 6 is water.

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

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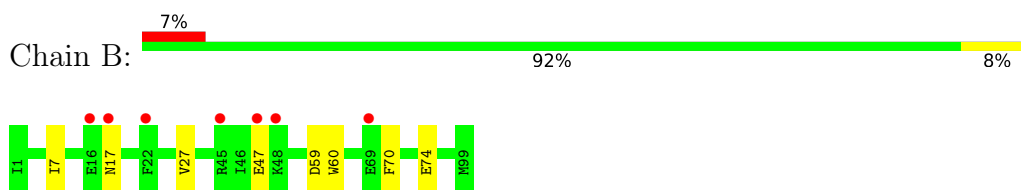
- Molecule 1: HLA class I histocompatibility antigen, B-44 alpha chain
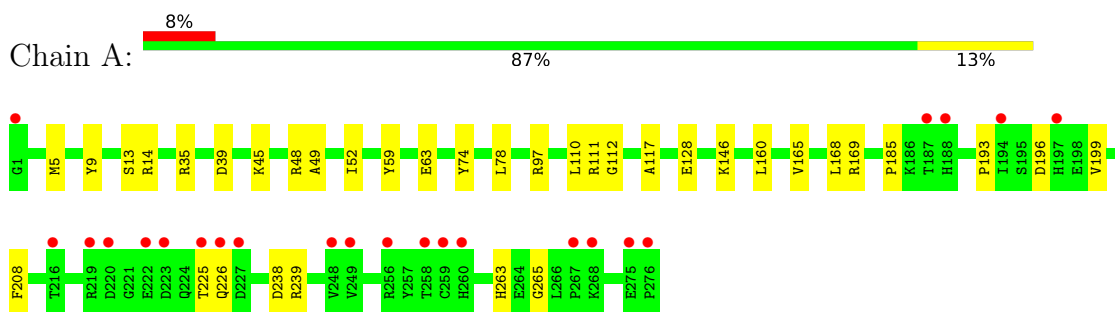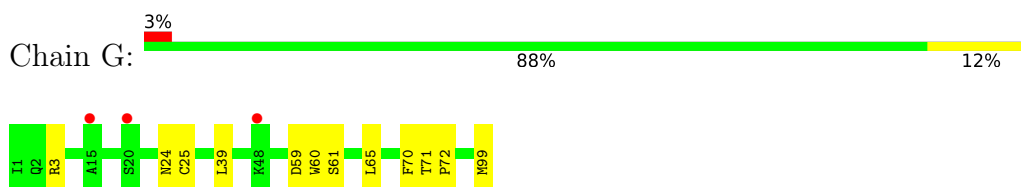
Chain A:

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

Chain F:
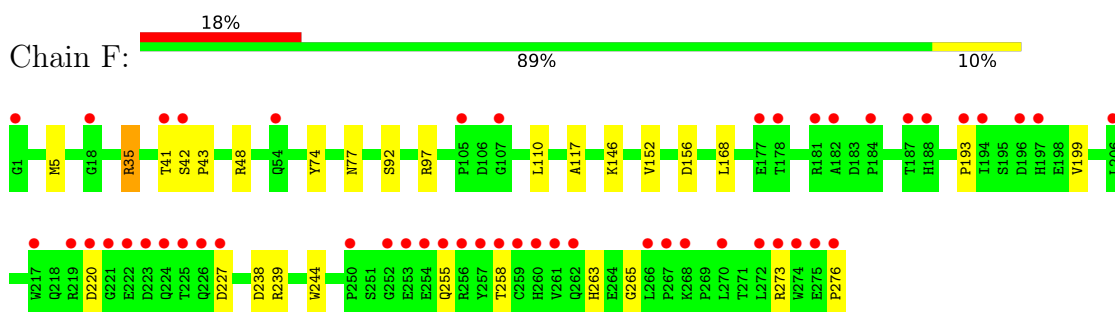
- Molecule 2: Beta-2-microglobulin

Chain B:

- Molecule 2: Beta-2-microglobulin

Chain G:

- Molecule 3: EEYLKAWTF, mimotope peptide

Chain C: 78% 22%

E1 F9

• Molecule 3: EEYLKAWTF, mimotope peptide

Chain H: 78% 22%
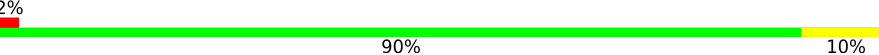
E1 W7 T8 F9

• Molecule 4: LC13 TCR alpha chain

5%

Chain D: 89% 10%

K2 T3 T4 Q5 E11 E15 H24 S28 L50 T51 S52 R58 M61 A62 R70 R79 A86 Y89 F106 G107 I111 L112 S133 S134 D135 K136 S137 V138 K154 L166 S182 N191 S206

• Molecule 4: LC13 TCR alpha chain

3%

Chain I: 90% 10%

K2 D30A Y31 I32 H33 L50 T51 R58 M61 A62 R70 R79 P93 G96 K103 H115 S133 S134 D135 F141 S146 Y159 D162 K163 T164 V165 L166 R169 A180 N191 A192 F193 S206

• Molecule 5: LC13 TCR beta chain

2%

Chain E: 90% 10%

G3 L21 H29 L60 P61 S62 D63 F66 E71 Q84 S87 A88 T112 D119 L120 K121 P133 L146 P155 D156 H157 V158 E159 D176 L180 N187 R196 T202 Q205 N206 P207 R208 D247
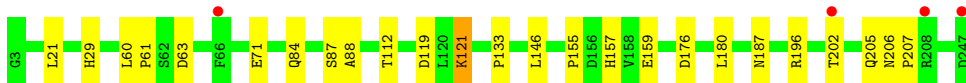
• Molecule 5: LC13 TCR beta chain

%

Chain J: 88% 11%

G3 L21 D24 H29 L39 F45 N51 R69 Q84 A93 Q106 T112 E118 K121 T141 Q142 C148 H157 W162 S174 L180 A185 R196 N206 P207 D224 E225 W226 T227 Q228 D229 A246 D247
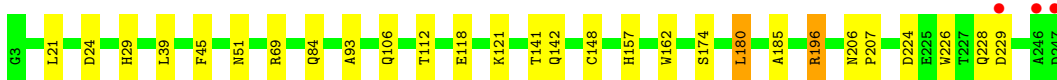
4 Data and refinement statistics (i)

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 49.31 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.60) 97.5 (49.31-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.279 0.257 , 0.302	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)	0.39 , 38.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	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.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.32	0/2320	0.48	0/3154
1	F	0.32	0/2320	0.48	0/3154
2	B	0.33	0/852	0.46	0/1152
2	G	0.33	0/852	0.46	0/1152
3	C	0.34	0/88	0.42	0/117
3	H	0.32	0/88	0.42	0/117
4	D	0.40	0/1603	0.57	1/2181 (0.0%)
4	I	0.33	0/1603	0.51	1/2181 (0.0%)
5	E	0.44	1/1971 (0.1%)	0.49	0/2681
5	J	0.41	0/1971	0.51	1/2681 (0.0%)
All	All	0.36	1/13668 (0.0%)	0.50	3/18570 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	159	GLU	CG-CD	-5.59	1.43	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	185	ALA	CB-CA-C	5.92	118.97	110.10
4	I	166	LEU	CA-CB-CG	5.38	127.68	115.30
4	D	166	LEU	CA-CB-CG	5.32	127.53	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	20	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	3	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	10	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	77	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 (77) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
4:D:3:THR:HG22	4:D:24:HIS:HB3	1.98	0.46
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:119:ASP:CG	5:E:121:LYS:HG2	2.40	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:14:ARG:HH22	1:A:39:ASP:CG	2.23	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   ⓘ

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	274/276 (99%)	264 (96%)	10 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	233 (98%)	4 (2%)	60	81
1	F	237/237 (100%)	230 (97%)	7 (3%)	41	67
2	B	94/94 (100%)	90 (96%)	4 (4%)	29	54
2	G	94/94 (100%)	93 (99%)	1 (1%)	73	88
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%)	172 (96%)	8 (4%)	28	53
4	I	180/180 (100%)	174 (97%)	6 (3%)	38	64
5	E	207/207 (100%)	200 (97%)	7 (3%)	37	63
5	J	207/207 (100%)	195 (94%)	12 (6%)	20	40
All	All	1452/1452 (100%)	1403 (97%)	49 (3%)	37	63

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	LEU
1	A	196	ASP
1	A	225	THR
1	A	226	GLN
2	B	7	ILE
2	B	27	VAL
2	B	47	GLU
2	B	70	PHE
4	D	5	GLN
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	29	HIS
5	E	63	ASP
5	E	71	GLU
5	E	84	GLN
5	E	121	LYS
5	E	180	LEU
5	E	187	ASN
1	F	35	ARG
1	F	42	SER
1	F	92	SER
1	F	110	LEU
1	F	156	ASP
1	F	220	ASP
1	F	227	ASP
2	G	70	PHE
4	I	30(A)	ASP
4	I	32	ILE
4	I	58	ARG
4	I	162	ASP
4	I	166	LEU
4	I	191	ASN
5	J	24	ASP
5	J	29	HIS
5	J	39	LEU
5	J	84	GLN
5	J	118	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	J	121	LYS
5	J	157	HIS
5	J	174	SER
5	J	180	LEU
5	J	196	ARG
5	J	224	ASP
5	J	229	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	77	ASN
1	A	263	HIS
2	B	8	GLN
2	B	17	ASN
4	D	8	ASN
4	D	33	HIS
4	D	191	ASN
5	E	29	HIS
5	E	41	GLN
5	E	51	ASN
5	E	122	ASN
5	E	223	ASN
5	E	236	GLN
1	F	70	ASN
1	F	77	ASN
1	F	255	GLN
1	F	263	HIS
2	G	8	GLN
4	I	8	ASN
4	I	13	ASN
4	I	33	HIS
4	I	191	ASN
5	J	29	HIS
5	J	41	GLN
5	J	157	HIS
5	J	206	ASN
5	J	210	HIS
5	J	236	GLN

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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

There are no ligands in this entry.

5.7   Other polymers ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	276/276 (100%)	0.52	23 (8%)	11	8	24, 36, 44, 50	1 (0%)
1	F	276/276 (100%)	0.81	50 (18%)	1	0	25, 35, 44, 49	1 (0%)
2	B	99/99 (100%)	0.61	7 (7%)	16	11	27, 35, 46, 47	0
2	G	99/99 (100%)	0.50	3 (3%)	50	43	29, 36, 43, 45	0
3	C	9/9 (100%)	0.35	0	100	100	31, 34, 37, 38	0
3	H	9/9 (100%)	0.41	0	100	100	33, 34, 37, 38	0
4	D	201/201 (100%)	0.52	10 (4%)	28	23	26, 36, 44, 57	0
4	I	201/201 (100%)	0.39	7 (3%)	44	36	28, 36, 46, 55	0
5	E	241/241 (100%)	0.23	4 (1%)	70	66	29, 36, 46, 54	0
5	J	241/241 (100%)	0.23	3 (1%)	79	76	28, 36, 44, 57	0
All	All	1652/1652 (100%)	0.47	107 (6%)	18	14	24, 36, 45, 57	2 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	134	SER	6.0
2	B	48	LYS	5.3
1	F	42	SER	4.7
1	A	197	HIS	4.4
4	D	154	LYS	4.2
5	J	247	ASP	4.1
4	D	58	ARG	4.1
4	D	134	SER	4.1
1	F	223	ASP	4.1
4	I	135	ASP	4.1
1	F	275	GLU	3.9
1	A	225	THR	3.8
5	J	246	ALA	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	1	GLY	3.7
1	F	177	GLU	3.6
1	F	225	THR	3.6
4	D	135	ASP	3.5
4	I	133	SER	3.5
1	F	194	ILE	3.5
1	F	197	HIS	3.4
1	F	274	TRP	3.4
1	F	273	ARG	3.3
1	F	268	LYS	3.2
2	G	48	LYS	3.2
5	E	247	ASP	3.2
1	F	227	ASP	3.1
1	F	276	PRO	3.1
1	A	188	HIS	3.0
4	D	79	ARG	2.9
1	F	257	TYR	2.9
1	A	249	VAL	2.9
1	F	193	PRO	2.9
4	D	133	SER	2.8
5	E	202	THR	2.8
1	F	224	GLN	2.8
1	A	223	ASP	2.8
1	F	220	ASP	2.8
1	F	222	GLU	2.8
1	F	188	HIS	2.8
1	F	260	HIS	2.8
1	A	275	GLU	2.7
1	F	196	ASP	2.7
1	F	187	THR	2.7
2	G	15	ALA	2.7
4	D	206	SER	2.7
2	B	22	PHE	2.7
1	A	248	VAL	2.7
1	F	252	GLY	2.7
1	A	258	THR	2.7
1	F	206	LEU	2.7
2	B	17	ASN	2.7
1	F	54	GLN	2.6
4	D	15	GLU	2.6
1	F	181	ARG	2.6
1	A	260	HIS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	266	LEU	2.6
1	F	255	GLN	2.6
1	F	219	ARG	2.6
1	A	226	GLN	2.6
1	F	261	VAL	2.6
1	A	187	THR	2.5
2	G	20	SER	2.5
1	F	258	THR	2.5
1	F	272	LEU	2.5
5	E	66	PHE	2.5
2	B	47	GLU	2.5
1	F	254	GLU	2.4
1	A	276	PRO	2.4
1	A	1	GLY	2.4
1	F	250	PRO	2.4
1	F	226	GLN	2.4
1	A	194	ILE	2.4
5	J	229	ASP	2.4
1	A	220	ASP	2.4
5	E	208	ARG	2.4
1	F	253	GLU	2.4
1	A	227	ASP	2.4
1	F	259	CYS	2.4
1	F	18	GLY	2.3
1	F	256	ARG	2.3
1	F	262	GLN	2.3
1	A	259	CYS	2.3
1	F	221	GLY	2.3
1	F	270	LEU	2.3
1	F	178	THR	2.3
1	A	267	PRO	2.3
4	I	96	GLY	2.2
4	I	206	SER	2.2
1	F	182	ALA	2.2
4	D	137	SER	2.2
1	F	105	PRO	2.2
1	F	184	PRO	2.2
2	B	16	GLU	2.2
4	I	79	ARG	2.2
2	B	69	GLU	2.2
4	I	169	ARG	2.2
2	B	45	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	107	GLY	2.1
1	A	216	THR	2.1
1	F	41	THR	2.1
1	F	267	PRO	2.1
4	D	52	SER	2.1
1	F	217	TRP	2.1
1	A	268	LYS	2.0
1	A	222	GLU	2.0
1	A	256	ARG	2.0
1	A	219	ARG	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.