



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:23 am GMT

PDB ID : 2J8U
Title : LARGE CDR3A LOOP ALTERATION AS A FUNCTION OF MHC MUTATION.
Authors : Miller, P.J.; Benhar, Y.P.; Biddison, W.; Collins, E.J.
Deposited on : 2006-10-27
Resolution : 2.88 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

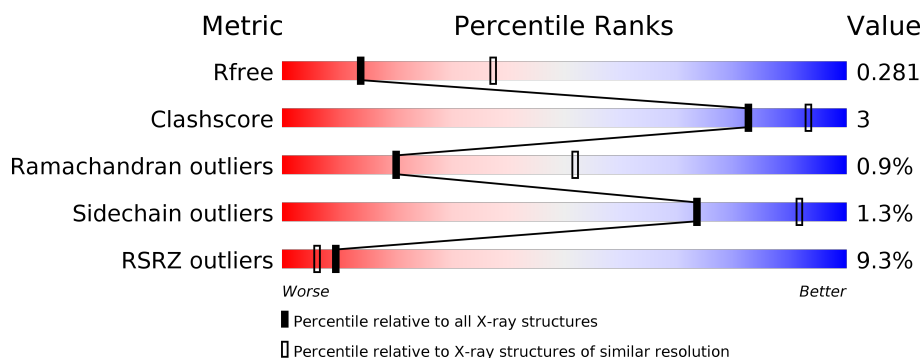
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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}	100719	2135 (2.90-2.86)
Clashscore	112137	2400 (2.90-2.86)
Ramachandran outliers	110173	2346 (2.90-2.86)
Sidechain outliers	110143	2349 (2.90-2.86)
RSRZ outliers	101464	2149 (2.90-2.86)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	275	<div> <div>7%</div> <div>92%</div> <div>7%</div> </div>
1	H	275	<div> <div>6%</div> <div>91%</div> <div>9%</div> </div>
2	B	100	<div> <div>6%</div> <div>98%</div> <div></div> </div>
2	I	100	<div> <div>7%</div> <div>96%</div> <div></div> </div>
3	C	9	<div> <div></div> <div>89%</div> <div>11%</div> </div>
3	J	9	<div> <div></div> <div>100%</div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
4	E	194	<div><div></div><div>13%</div><div>84%</div><div>15%</div><div>..</div></div>
4	L	194	<div><div></div><div>15%</div><div>80%</div><div>16%</div><div>..</div></div>
5	F	238	<div><div></div><div>11%</div><div>88%</div><div>11%</div><div>.</div></div>
5	M	238	<div><div></div><div>8%</div><div>93%</div><div>6%</div><div></div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13128 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, A-2 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2243	1400	408	426	9			
1	H	275	Total	C	N	O	S	0	0	0
			2243	1400	408	426	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	ALA	LYS	ENGINEERED MUTATION	UNP P01892
H	66	ALA	LYS	ENGINEERED MUTATION	UNP P01892

- Molecule 2 is a protein called BETA-2-MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	I	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

- Molecule 3 is a protein called SELF-PEPTIDE P1049.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			76	56	10	10			
3	J	9	Total	C	N	O	0	0	0
			76	56	10	10			

- Molecule 4 is a protein called AHIII TCR ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	194	Total	C	N	O	S	86	0	0
			1521	965	245	302	9			
4	L	194	Total	C	N	O	S	86	0	0
			1521	965	245	302	9			

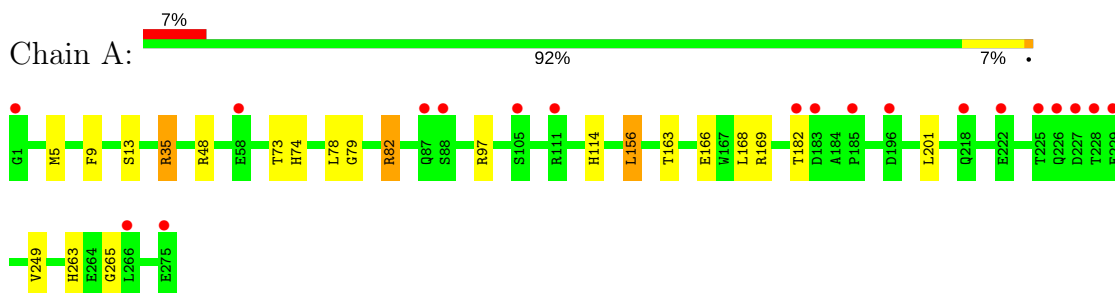
- Molecule 5 is a protein called AHIII TCR BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	237	Total	C	N	O	S	0	0	0
			1887	1192	331	359	5			
5	M	237	Total	C	N	O	S	0	0	0
			1887	1192	331	359	5			

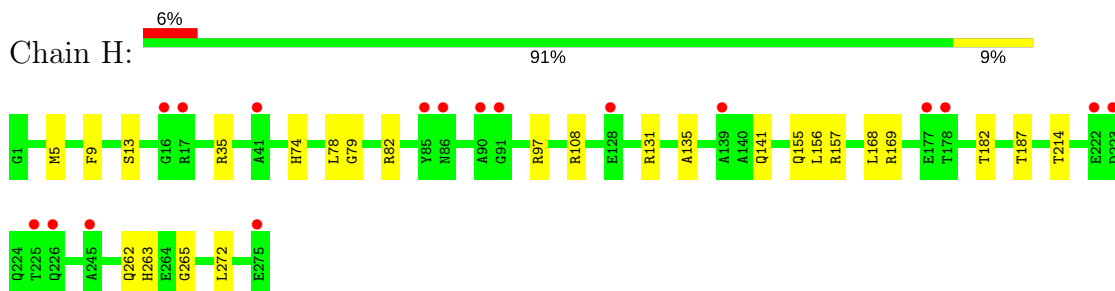
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

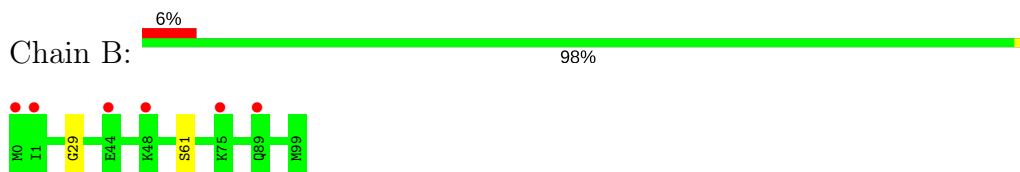
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN



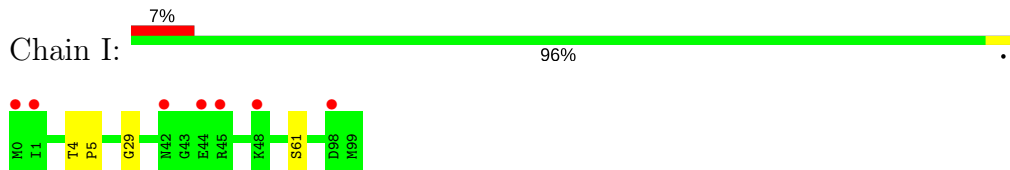
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN



- Molecule 2: BETA-2-MICROGLOBULIN



- Molecule 2: BETA-2-MICROGLOBULIN



- Molecule 3: SELF-PEPTIDE P1049





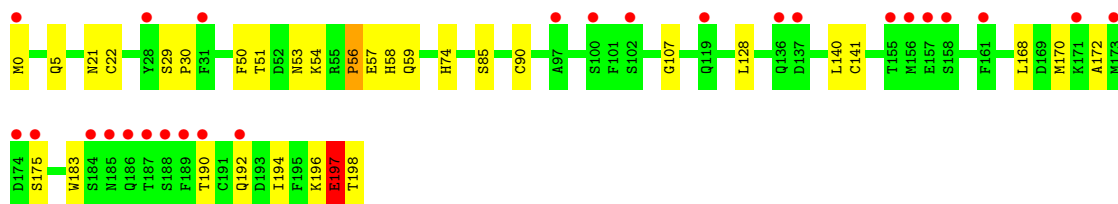
- Molecule 3: SELF-PEPTIDE P1049

Chain J: 100%

There are no outlier residues recorded for this chain.

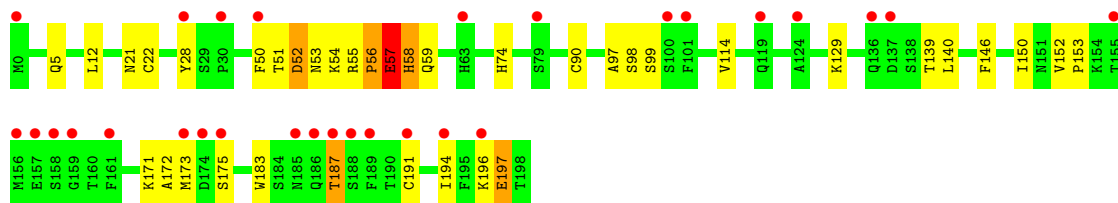
- Molecule 4: AHIII TCR ALPHA CHAIN

Chain E: 13% 84% 15% ..



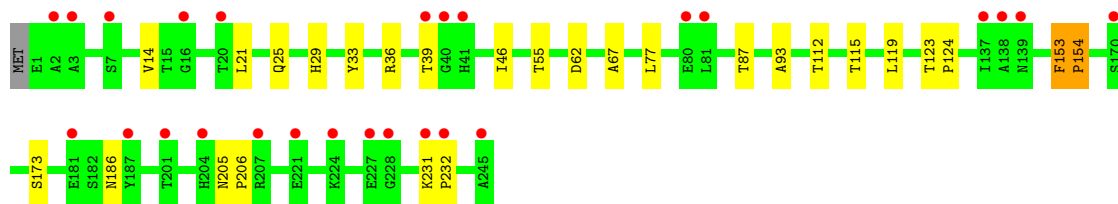
- Molecule 4: AHIII TCR ALPHA CHAIN

Chain L: 15% 80% 16% ..



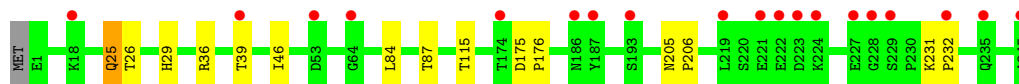
- Molecule 5: AHIII TCR BETA CHAIN

Chain F: 11% 88% 11% .



- Molecule 5: AHIII TCR BETA CHAIN

Chain M: 8% 93% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.42Å 83.89Å 122.27Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	122.17 – 2.88 39.67 – 2.88	Depositor EDS
% Data completeness (in resolution range)	94.8 (122.17-2.88) 94.9 (39.67-2.88)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.268 , 0.293 0.259 , 0.281	Depositor DCC
R_{free} test set	2007 reflections (5.19%)	DCC
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13128	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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 45.67 % 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 1.2779e-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	0.29	0/2308	0.43	0/3133
1	H	0.29	0/2308	0.43	0/3133
2	B	0.31	0/860	0.41	0/1162
2	I	0.30	0/860	0.41	0/1162
3	C	0.43	0/80	0.41	0/108
3	J	0.43	0/80	0.41	0/108
4	E	0.58	2/1556 (0.1%)	0.72	5/2109 (0.2%)
4	L	1.17	12/1556 (0.8%)	1.27	24/2109 (1.1%)
5	F	0.30	0/1943	0.43	0/2644
5	M	0.30	0/1942	0.43	0/2641
All	All	0.52	14/13493 (0.1%)	0.62	29/18309 (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
4	E	0	1
4	L	1	1
5	F	0	1
All	All	1	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	58	HIS	C-N	22.04	1.84	1.34
4	L	59	GLN	CA-CB	18.42	1.94	1.53
4	L	50	PHE	C-N	15.50	1.69	1.34
4	L	197	GLU	C-N	15.12	1.68	1.34
4	L	56	PRO	CG-CD	-14.70	1.02	1.50
4	E	50	PHE	C-N	14.17	1.66	1.34
4	E	197	GLU	C-N	8.65	1.53	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	58	HIS	N-CA	7.12	1.60	1.46
4	L	57	GLU	N-CA	6.80	1.59	1.46
4	L	58	HIS	CA-C	6.05	1.68	1.52
4	L	57	GLU	CA-C	5.97	1.68	1.52
4	L	57	GLU	C-N	5.49	1.46	1.34
4	L	51	THR	C-N	-5.44	1.21	1.34
4	L	56	PRO	CA-C	5.41	1.63	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	50	PHE	CA-C-N	-21.21	70.53	117.20
4	E	50	PHE	CA-C-N	-15.65	82.76	117.20
4	L	56	PRO	N-CA-CB	-14.70	85.66	103.30
4	L	57	GLU	O-C-N	-14.28	99.85	122.70
4	L	59	GLN	N-CA-CB	14.06	135.91	110.60
4	L	197	GLU	O-C-N	-13.61	100.92	122.70
4	L	50	PHE	O-C-N	12.68	142.98	122.70
4	L	50	PHE	C-N-CA	-12.45	90.57	121.70
4	L	57	GLU	N-CA-C	11.55	142.18	111.00
4	L	58	HIS	CA-CB-CG	10.98	132.26	113.60
4	E	50	PHE	C-N-CA	-9.65	97.58	121.70
4	L	52	ASP	CA-C-N	-9.62	96.03	117.20
4	E	56	PRO	CA-N-CD	-9.10	98.76	111.50
4	L	58	HIS	N-CA-C	9.07	135.49	111.00
4	L	59	GLN	CB-CA-C	-8.49	93.42	110.40
4	L	57	GLU	N-CA-CB	-8.38	95.52	110.60
4	L	56	PRO	N-CD-CG	7.62	114.63	103.20
4	L	53	ASN	C-N-CA	-6.98	104.25	121.70
4	L	56	PRO	N-CA-C	6.71	129.55	112.10
4	L	52	ASP	O-C-N	6.70	133.43	122.70
4	L	54	LYS	CB-CA-C	6.50	123.41	110.40
4	E	58	HIS	CB-CA-C	6.13	122.66	110.40
4	L	57	GLU	CA-C-N	6.00	130.41	117.20
4	L	58	HIS	O-C-N	5.74	131.89	122.70
4	L	55	ARG	N-CA-C	5.55	125.98	111.00
4	L	57	GLU	CA-CB-CG	5.43	125.34	113.40
4	L	57	GLU	C-N-CA	5.42	135.26	121.70
4	L	57	GLU	CB-CA-C	5.42	121.24	110.40
4	E	197	GLU	CA-C-N	-5.07	106.05	117.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	L	57	GLU	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	197	GLU	Mainchain
5	F	153	PHE	Peptide
4	L	57	GLU	Mainchain

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	2243	0	2088	13	0
1	H	2243	0	2088	11	2
2	B	837	0	803	1	0
2	I	837	0	803	2	0
3	C	76	0	76	1	0
3	J	76	0	76	0	0
4	E	1521	0	1474	13	3
4	L	1521	0	1473	14	0
5	F	1887	0	1790	16	0
5	M	1887	0	1789	6	1
All	All	13128	0	12460	73	3

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 (73) 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:L:22:CYS:H	4:L:74:HIS:HD2	1.33	0.74
4:E:22:CYS:H	4:E:74:HIS:HD2	1.36	0.73
1:A:97:ARG:HH21	1:A:114:HIS:HE1	1.45	0.65
5:F:25:GLN:HE22	5:F:29:HIS:H	1.43	0.63
1:A:79:GLY:HA2	1:A:82:ARG:HD2	1.81	0.61
2:B:29:GLY:HA2	2:B:61:SER:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:HG2	1:A:48:ARG:HD3	1.87	0.56
4:E:140:LEU:HD12	4:E:183:TRP:HB3	1.86	0.56
5:F:55:THR:HG21	5:F:67:ALA:HB3	1.89	0.54
1:H:79:GLY:HA2	1:H:82:ARG:HD2	1.89	0.52
4:E:141:CYS:HB2	4:E:194:ILE:HD11	1.92	0.52
1:H:9:PHE:HB2	1:H:97:ARG:HB3	1.92	0.52
4:E:128:LEU:HD12	4:E:140:LEU:HD23	1.92	0.52
1:H:5:MET:HB2	1:H:168:LEU:HD13	1.92	0.51
4:E:170:MET:HB2	4:E:175:SER:HB2	1.91	0.51
4:E:196:LYS:O	4:E:197:GLU:HG2	2.11	0.50
4:L:196:LYS:O	4:L:197:GLU:HB2	2.12	0.50
1:A:9:PHE:HB2	1:A:97:ARG:HB3	1.94	0.49
5:M:25:GLN:NE2	5:M:29:HIS:H	2.11	0.49
5:M:87:THR:HG23	5:M:115:THR:HA	1.94	0.49
5:M:36:ARG:HB3	5:M:46:ILE:HD11	1.94	0.49
1:A:74:HIS:NE2	1:A:97:ARG:HD2	2.28	0.48
4:L:22:CYS:H	4:L:74:HIS:CD2	2.22	0.48
5:F:186:ASN:HB2	4:L:171:LYS:O	2.13	0.48
4:L:12:LEU:O	4:L:114:VAL:HA	2.13	0.47
4:E:22:CYS:H	4:E:74:HIS:CD2	2.24	0.47
1:A:166:GLU:HG2	1:A:169:ARG:HH12	1.80	0.46
4:L:146:PHE:HB2	4:L:150:ILE:HD11	1.97	0.46
4:L:140:LEU:HD12	4:L:183:TRP:HB3	1.97	0.45
1:A:73:THR:HG23	3:C:8:VAL:HG12	1.97	0.45
5:F:87:THR:HG23	5:F:115:THR:HA	1.98	0.45
2:I:29:GLY:HA2	2:I:61:SER:HB2	1.99	0.45
1:H:155:GLN:HE22	4:L:97:ALA:HA	1.81	0.45
1:A:114:HIS:CG	1:A:156:LEU:HD11	2.52	0.45
5:F:21:LEU:HD12	5:F:77:LEU:HD23	1.99	0.44
5:F:36:ARG:HB3	5:F:46:ILE:HD11	1.98	0.44
4:L:21:ASN:HA	4:L:74:HIS:CD2	2.53	0.44
5:M:205:ASN:HA	5:M:206:PRO:HD3	1.88	0.44
1:H:131:ARG:HE	1:H:157:ARG:HH12	1.65	0.44
4:E:5:GLN:HE21	4:E:107:GLY:HA3	1.83	0.43
4:L:191:CYS:HA	4:L:194:ILE:CD1	2.48	0.43
4:L:129:LYS:HG2	4:L:139:THR:HG22	2.01	0.43
5:F:153:PHE:CG	5:F:154:PRO:CD	3.01	0.43
5:F:33:TYR:HB2	5:F:93:ALA:HB3	2.01	0.43
1:H:135:ALA:HB3	1:H:141:GLN:HE21	1.83	0.43
1:H:13:SER:HB3	1:H:78:LEU:HD22	2.00	0.43
4:L:5:GLN:NE2	4:L:90:CYS:H	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:190:THR:HG22	4:E:192:GLN:H	1.83	0.43
5:F:25:GLN:NE2	5:F:29:HIS:H	2.13	0.43
1:A:166:GLU:HG2	1:A:169:ARG:NH1	2.33	0.43
5:F:231:LYS:HA	5:F:232:PRO:HD3	1.84	0.42
1:A:13:SER:HB3	1:A:78:LEU:HD22	2.01	0.42
4:E:168:LEU:HB3	5:F:173:SER:HB2	2.00	0.42
4:E:5:GLN:NE2	4:E:90:CYS:H	2.18	0.42
1:H:187:THR:HB	1:H:272:LEU:HD11	2.01	0.42
2:I:4:THR:HA	2:I:5:PRO:HD3	1.91	0.41
1:A:201:LEU:HD12	1:A:249:VAL:HG21	2.01	0.41
1:H:214:THR:HB	1:H:262:GLN:HB2	2.01	0.41
1:H:263:HIS:CD2	1:H:265:GLY:H	2.38	0.41
1:H:74:HIS:NE2	1:H:97:ARG:HD2	2.35	0.41
1:A:5:MET:HB2	1:A:168:LEU:HD13	2.02	0.41
5:F:14:VAL:HG22	5:F:119:LEU:HD21	2.02	0.41
4:L:28:TYR:CD1	4:L:98:SER:HB3	2.55	0.41
5:M:175:ASP:HA	5:M:176:PRO:HD3	1.93	0.41
4:E:21:ASN:HA	4:E:74:HIS:CD2	2.56	0.41
5:M:231:LYS:HA	5:M:232:PRO:HD3	1.87	0.41
4:L:152:VAL:HA	4:L:153:PRO:HD3	1.87	0.40
1:A:263:HIS:CD2	1:A:265:GLY:H	2.39	0.40
5:F:153:PHE:CD2	5:F:154:PRO:HD3	2.57	0.40
4:E:29:SER:HA	4:E:30:PRO:HD3	1.88	0.40
5:F:123:THR:HA	5:F:124:PRO:HD3	1.90	0.40
5:F:205:ASN:HA	5:F:206:PRO:HD3	1.94	0.40
5:F:21:LEU:HD22	5:F:112:THR:HG21	2.03	0.40

All (3) 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)
4:E:198:THR:O	1:H:169:ARG:NH2[2_645]	1.71	0.49
4:E:59:GLN:NE2	5:M:84:LEU:CD1[1_545]	1.79	0.41
4:E:198:THR:OG1	1:H:108:ARG:NE[2_645]	2.12	0.08

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	273/275 (99%)	268 (98%)	5 (2%)	0	100	100
1	H	273/275 (99%)	267 (98%)	6 (2%)	0	100	100
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	I	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	J	7/9 (78%)	7 (100%)	0	0	100	100
4	E	190/194 (98%)	174 (92%)	9 (5%)	7 (4%)	4	14
4	L	190/194 (98%)	169 (89%)	14 (7%)	7 (4%)	4	14
5	F	235/238 (99%)	227 (97%)	7 (3%)	1 (0%)	38	70
5	M	233/238 (98%)	228 (98%)	5 (2%)	0	100	100
All	All	1604/1632 (98%)	1539 (96%)	50 (3%)	15 (1%)	20	52

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	51	THR
4	E	53	ASN
4	E	56	PRO
4	E	57	GLU
5	F	154	PRO
4	L	56	PRO
4	L	58	HIS
4	E	54	LYS
4	E	172	ALA
4	L	57	GLU
4	L	172	ALA
4	L	187	THR
4	L	99	SER
4	E	85	SER

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Mol	Chain	Res	Type
4	L	52	ASP

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	230/230 (100%)	225 (98%)	5 (2%)	57	84
1	H	230/230 (100%)	227 (99%)	3 (1%)	73	91
2	B	95/95 (100%)	95 (100%)	0	100	100
2	I	95/95 (100%)	95 (100%)	0	100	100
3	C	7/7 (100%)	7 (100%)	0	100	100
3	J	7/7 (100%)	7 (100%)	0	100	100
4	E	177/177 (100%)	176 (99%)	1 (1%)	89	97
4	L	177/177 (100%)	173 (98%)	4 (2%)	56	84
5	F	204/206 (99%)	202 (99%)	2 (1%)	80	94
5	M	204/206 (99%)	201 (98%)	3 (2%)	70	89
All	All	1426/1430 (100%)	1408 (99%)	18 (1%)	73	91

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	82	ARG
1	A	156	LEU
1	A	163	THR
1	A	182	THR
4	E	0	MET
5	F	39	THR
5	F	62	ASP
1	H	35	ARG
1	H	156	LEU
1	H	182	THR
4	L	57	GLU

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Mol	Chain	Res	Type
4	L	173	MET
4	L	175	SER
4	L	187	THR
5	M	25	GLN
5	M	26	THR
5	M	39	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	87	GLN
1	A	93	HIS
1	A	114	HIS
1	A	141	GLN
1	A	263	HIS
4	E	5	GLN
4	E	25	GLN
4	E	74	HIS
5	F	25	GLN
1	H	87	GLN
1	H	93	HIS
1	H	141	GLN
1	H	155	GLN
1	H	263	HIS
2	I	2	GLN
2	I	83	ASN
4	L	5	GLN
4	L	25	GLN
4	L	74	HIS
5	M	25	GLN
5	M	156	HIS
5	M	215	GLN

5.3.3 RNA ⓘ

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 carbohydrates 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	275/275 (100%)	0.62	19 (6%) 18 13	44, 49, 51, 52	0
1	H	275/275 (100%)	0.61	17 (6%) 21 17	42, 47, 49, 50	0
2	B	100/100 (100%)	0.69	6 (6%) 23 18	44, 45, 48, 49	0
2	I	100/100 (100%)	0.65	7 (7%) 17 13	44, 45, 49, 50	0
3	C	9/9 (100%)	-0.21	0 100 100	35, 36, 37, 37	0
3	J	9/9 (100%)	-0.07	0 100 100	38, 38, 40, 40	0
4	E	184/194 (94%)	0.93	26 (14%) 3 2	39, 47, 51, 52	0
4	L	184/194 (94%)	1.05	29 (15%) 2 2	42, 47, 50, 52	0
5	F	237/238 (99%)	0.83	26 (10%) 6 4	44, 49, 52, 52	0
5	M	237/238 (99%)	0.75	19 (8%) 13 10	43, 47, 55, 56	0
All	All	1610/1632 (98%)	0.75	149 (9%) 9 6	35, 47, 51, 56	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	245	ALA	7.0
5	M	245	ALA	6.8
4	L	173	MET	6.7
4	E	173	MET	6.2
4	L	189	PHE	6.1
4	L	187	THR	6.0
4	L	0	MET	5.6
4	E	156	MET	5.5
5	M	227	GLU	5.5
4	L	188	SER	5.3
4	E	171	LYS	5.0
4	L	174	ASP	4.8
2	B	48	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
4	E	175	SER	4.5
1	A	1	GLY	4.4
1	A	226	GLN	4.3
2	I	0	MET	4.1
5	F	228	GLY	4.1
4	L	186	GLN	4.1
4	L	175	SER	4.0
4	E	188	SER	4.0
4	L	161	PHE	4.0
4	E	192	GLN	3.9
5	M	221	GLU	3.9
5	F	227	GLU	3.9
4	L	156	MET	3.7
4	L	119	GLN	3.6
2	I	48	LYS	3.5
1	A	227	ASP	3.5
1	H	91	GLY	3.5
5	F	3	ALA	3.4
5	F	181	GLU	3.4
4	E	137	ASP	3.3
4	E	155	THR	3.3
1	A	105	SER	3.3
2	B	1	ILE	3.3
4	L	194	ILE	3.3
5	M	228	GLY	3.3
4	E	161	PHE	3.3
4	E	187	THR	3.3
5	M	229	SER	3.2
5	M	222	GLU	3.2
5	F	138	ALA	3.2
2	B	0	MET	3.2
5	F	39	THR	3.2
5	M	223	ASP	3.2
5	F	201	THR	3.1
5	F	2	ALA	3.1
5	F	221	GLU	3.1
5	F	232	PRO	3.1
1	H	90	ALA	3.1
4	L	155	THR	3.1
1	A	58	GLU	3.1
5	F	204	HIS	3.0
4	E	184	SER	3.0

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Mol	Chain	Res	Type	RSRZ
5	M	186	ASN	3.0
5	M	64	GLY	3.0
4	L	137	ASP	2.9
4	L	157	GLU	2.9
4	E	0	MET	2.9
1	A	88	SER	2.9
1	A	185	PRO	2.9
4	L	28	TYR	2.9
5	M	224	LYS	2.9
4	E	189	PHE	2.8
5	M	39	THR	2.8
1	A	228	THR	2.8
4	E	190	THR	2.7
5	M	232	PRO	2.7
4	L	63	HIS	2.7
5	F	187	TYR	2.7
4	E	119	GLN	2.7
5	F	80	GLU	2.7
4	L	158	SER	2.6
1	A	111	ARG	2.6
4	E	31	PHE	2.6
4	L	159	GLY	2.6
4	E	100	SER	2.6
1	H	225	THR	2.6
5	M	18	LYS	2.6
5	M	219	LEU	2.6
1	H	222	GLU	2.6
1	H	177	GLU	2.6
5	F	207	ARG	2.6
5	F	40	GLY	2.6
4	E	174	ASP	2.5
1	H	41	ALA	2.5
4	L	185	ASN	2.5
5	F	41	HIS	2.5
1	H	275	GLU	2.5
4	L	124	ALA	2.5
2	I	44	GLU	2.5
1	H	85	TYR	2.5
4	E	158	SER	2.4
2	B	89	GLN	2.4
1	A	229	GLU	2.4
5	F	139	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	I	98	ASP	2.4
1	A	266	LEU	2.4
5	F	137	ILE	2.4
4	L	136	GLN	2.4
4	L	101	PHE	2.4
1	H	139	ALA	2.4
1	H	16	GLY	2.4
4	E	97	ALA	2.4
4	L	79	SER	2.4
2	I	1	ILE	2.4
1	A	275	GLU	2.4
4	L	50	PHE	2.4
5	F	16	GLY	2.4
5	F	20	THR	2.4
4	L	191	CYS	2.3
5	M	174	THR	2.3
4	L	30	PRO	2.3
2	I	45	ARG	2.3
1	A	218	GLN	2.3
5	M	187	TYR	2.3
1	H	17	ARG	2.3
4	E	102	SER	2.3
1	A	222	GLU	2.3
5	F	81	LEU	2.2
5	M	235	GLN	2.2
1	A	196	ASP	2.2
4	E	28	TYR	2.2
1	A	183	ASP	2.2
1	H	245	ALA	2.2
5	F	224	LYS	2.2
1	H	86	ASN	2.2
4	E	185	ASN	2.2
4	E	136	GLN	2.2
5	M	53	ASP	2.1
1	H	128	GLU	2.1
4	E	157	GLU	2.1
2	I	42	ASN	2.1
5	F	170	SER	2.1
5	M	193	SER	2.1
4	L	100	SER	2.1
1	A	182	THR	2.1
1	H	226	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	44	GLU	2.1
1	A	87	GLN	2.1
5	F	7	SER	2.1
2	B	75	LYS	2.0
1	A	225	THR	2.0
5	F	231	LYS	2.0
4	L	196	LYS	2.0
1	H	178	THR	2.0
1	H	223	ASP	2.0
4	E	186	GLN	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 carbohydrates 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.