Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2024 – 06:32 PM EDT

PDB ID	:	2UWE
Title	:	Large CDR3a loop alteration as a function of MHC mutation
Authors	:	Miller, P.J.; Pazy, Y.; Conti, B.; Riddle, D.; Biddison, W.E.; Appella, E.; Collins, E.J.
Deposited on	:	2007-03-20
Resolution	:	2.40 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:

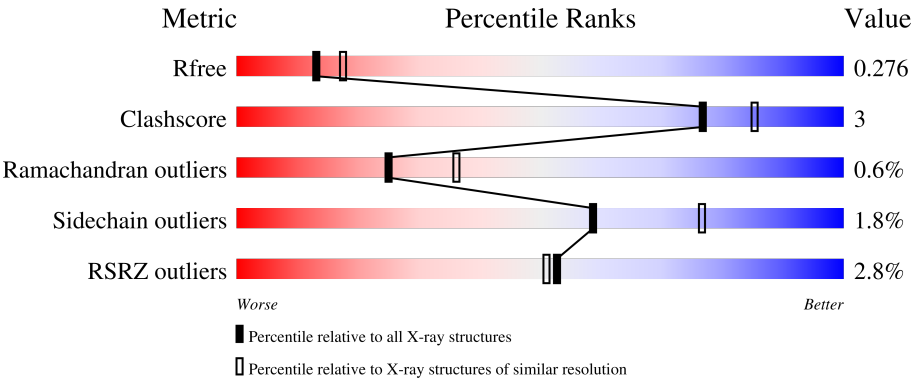
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	275	92% 7%
1	H	275	94% 5%
2	B	100	2% 95% 5%
2	I	100	2% 95% 5%
3	C	9	67% 33%

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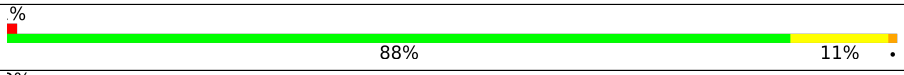
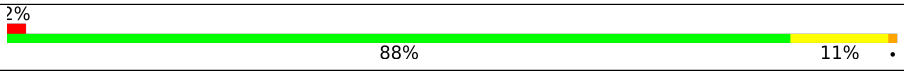
Mol	Chain	Length	Quality of chain
3	J	9	
4	E	194	
4	L	194	
5	F	238	
5	M	238	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13366 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	19	1	0
			2249	1404	410	426	9			
1	H	275	Total	C	N	O	S	6	1	0
			2252	1406	412	425	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	163	ALA	THR	engineered mutation	UNP P01892
H	163	ALA	THR	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	3	0	0
			837	533	141	159	4			
2	I	100	Total	C	N	O	S	3	0	0
			837	533	141	159	4			

- Molecule 3 is a protein called UNCHARACTERIZED PROTEIN C15ORF24.

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	75	1	0
			1523	966	245	303	9			
4	L	194	Total	C	N	O	S	84	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	13	1	0
			1894	1195	331	363	5			
5	M	237	Total	C	N	O	S	3	0	0
			1891	1194	331	361	5			

- Molecule 6 is water.

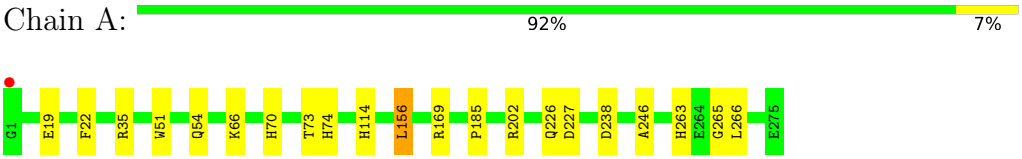
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	37	Total	O	0	0
			37	37		
6	B	9	Total	O	0	0
			9	9		
6	C	2	Total	O	0	0
			2	2		
6	E	25	Total	O	0	0
			25	25		
6	F	33	Total	O	0	0
			33	33		
6	H	36	Total	O	0	0
			36	36		
6	I	16	Total	O	0	0
			16	16		
6	J	2	Total	O	0	0
			2	2		
6	L	28	Total	O	0	0
			28	28		
6	M	22	Total	O	0	0
			22	22		

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.

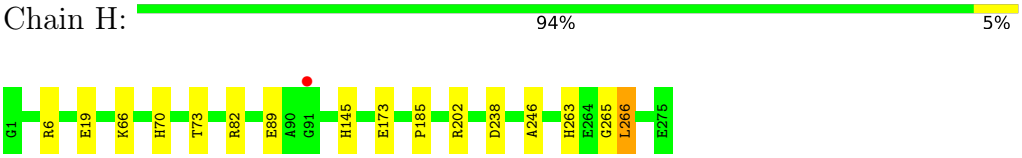
• Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN

Chain A:



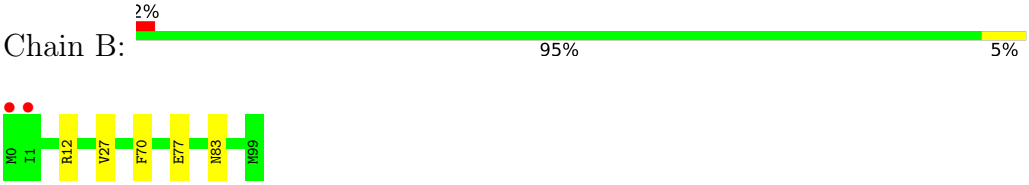
• Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN

Chain H:



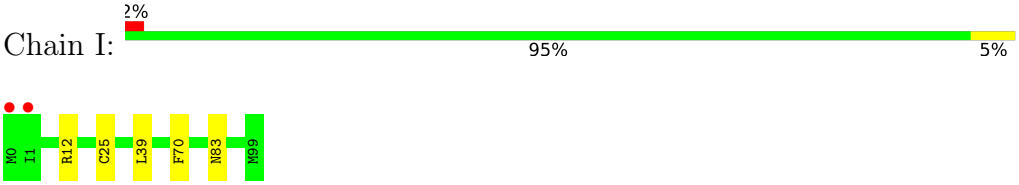
• Molecule 2: BETA-2-MICROGLOBULIN

Chain B:



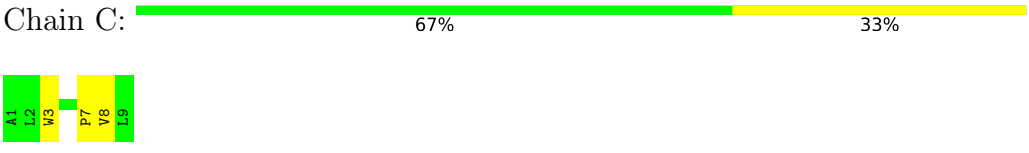
• Molecule 2: BETA-2-MICROGLOBULIN

Chain I:



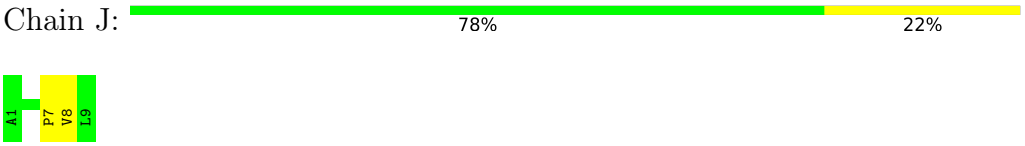
• Molecule 3: UNCHARACTERIZED PROTEIN C15ORF24

Chain C:



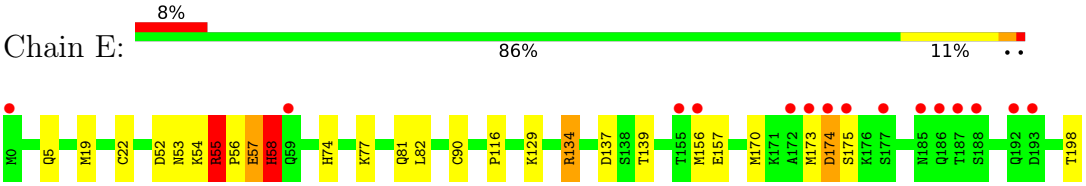
• Molecule 3: UNCHARACTERIZED PROTEIN C15ORF24

Chain J:



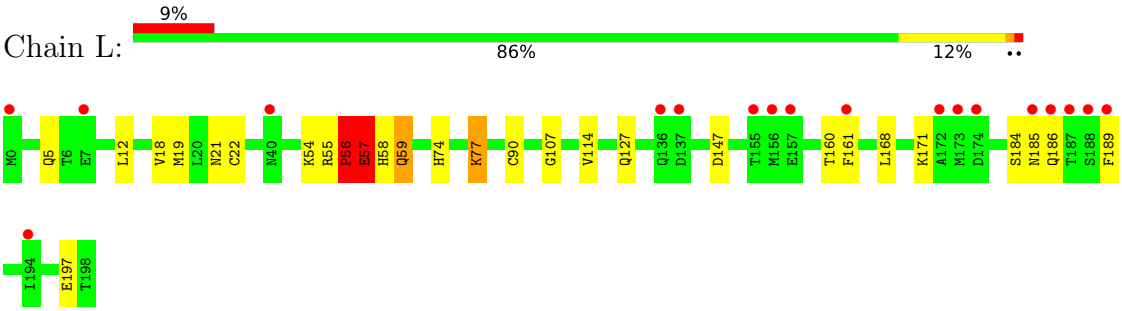
• Molecule 4: AHIII TCR ALPHA CHAIN

Chain E:



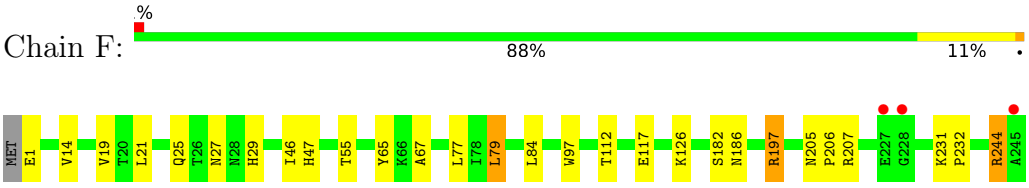
• Molecule 4: AHIII TCR ALPHA CHAIN

Chain L:



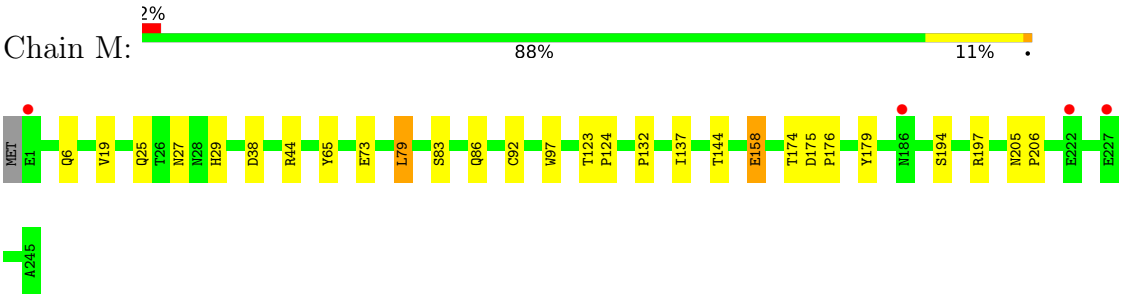
• Molecule 5: AHIII TCR BETA CHAIN

Chain F:



• Molecule 5: AHIII TCR BETA CHAIN

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.49Å 84.18Å 121.77Å 90.00° 92.05° 90.00°	Depositor
Resolution (Å)	121.00 – 2.40 49.31 – 2.10	Depositor EDS
% Data completeness (in resolution range)	84.8 (121.00-2.40) 69.9 (49.31-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.290 0.231 , 0.276	Depositor DCC
R_{free} test set	3839 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	38.5	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13366	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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 46.09 % 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 1.2027e-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

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	0.55	2/2319 (0.1%)	0.59	6/3146 (0.2%)
1	H	0.38	2/2321 (0.1%)	0.52	2/3148 (0.1%)
2	B	0.39	1/860 (0.1%)	0.45	0/1162
2	I	0.33	0/860	0.45	0/1162
3	C	0.45	0/80	0.50	0/108
3	J	0.46	0/80	0.46	0/108
4	E	0.53	2/1562 (0.1%)	0.84	7/2117 (0.3%)
4	L	0.66	3/1556 (0.2%)	0.90	15/2109 (0.7%)
5	F	0.66	3/1955 (0.2%)	0.71	5/2660 (0.2%)
5	M	0.42	1/1947 (0.1%)	0.50	1/2649 (0.0%)
All	All	0.52	14/13540 (0.1%)	0.65	36/18369 (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	4
4	L	0	1
5	F	0	1
5	M	0	1
All	All	0	7

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1	GLU	CG-CD	-19.97	1.22	1.51
1	A	226	GLN	CA-CB	-19.36	1.11	1.53
4	L	189	PHE	CA-CB	14.91	1.86	1.53
5	F	126	LYS	CD-CE	12.80	1.83	1.51
5	M	158	GLU	CG-CD	11.87	1.69	1.51
4	E	174	ASP	CB-CG	-11.63	1.27	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	244	ARG	NE-CZ	10.11	1.46	1.33
1	A	227	ASP	CB-CG	-9.43	1.31	1.51
4	L	59	GLN	C-N	-9.33	1.16	1.33
1	H	19	GLU	CG-CD	-8.13	1.39	1.51
4	E	58	HIS	C-N	6.34	1.48	1.34
4	L	56	PRO	N-CA	-6.26	1.36	1.47
1	H	173	GLU	CG-CD	-5.82	1.43	1.51
2	B	77	GLU	CG-CD	-5.78	1.43	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	244	ARG	NE-CZ-NH1	-20.79	109.90	120.30
4	E	198	THR	CA-C-O	19.92	161.92	120.10
4	E	52	ASP	N-CA-CB	12.34	132.81	110.60
5	F	244	ARG	NE-CZ-NH2	11.42	126.01	120.30
4	L	56	PRO	CA-N-CD	-10.78	96.40	111.50
4	L	59	GLN	C-N-CA	-9.48	102.39	122.30
4	L	57	GLU	CA-C-N	8.97	136.93	117.20
1	A	227	ASP	CA-CB-CG	8.67	132.47	113.40
4	E	58	HIS	O-C-N	-8.63	108.89	122.70
4	L	58	HIS	C-N-CA	8.61	143.22	121.70
1	A	19	GLU	CG-CD-OE1	-7.84	102.62	118.30
1	A	19	GLU	CG-CD-OE2	7.82	133.93	118.30
4	L	57	GLU	O-C-N	-7.51	110.69	122.70
5	F	1	GLU	CB-CG-CD	-6.91	95.53	114.20
4	L	58	HIS	N-CA-C	6.81	129.39	111.00
4	L	189	PHE	N-CA-CB	-6.80	98.35	110.60
4	L	58	HIS	CA-CB-CG	-6.78	102.08	113.60
5	M	158	GLU	CG-CD-OE1	-6.74	104.82	118.30
4	L	56	PRO	CB-CA-C	-6.70	95.24	112.00
4	L	127	GLN	CG-CD-NE2	6.48	132.24	116.70
1	A	227	ASP	CB-CG-OD1	-6.46	112.49	118.30
1	H	19	GLU	CG-CD-OE1	6.43	131.16	118.30
1	H	19	GLU	CG-CD-OE2	-6.36	105.57	118.30
1	A	19	GLU	CB-CG-CD	6.14	130.77	114.20
5	F	1	GLU	CG-CD-OE2	-5.86	106.58	118.30
4	L	57	GLU	N-CA-C	5.81	126.70	111.00
4	L	58	HIS	CA-C-N	-5.80	104.44	117.20
4	E	53	ASN	N-CA-C	5.78	126.60	111.00
5	F	1	GLU	CG-CD-OE1	5.67	129.64	118.30
4	E	174	ASP	CA-CB-CG	5.61	125.74	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	56	PRO	CA-C-N	-5.58	104.91	117.20
4	E	174	ASP	CB-CG-OD2	5.25	123.03	118.30
4	E	174	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	A	227	ASP	CB-CG-OD2	5.17	122.96	118.30
4	L	168	LEU	CA-CB-CG	5.07	126.96	115.30
4	L	58	HIS	CB-CA-C	-5.02	100.36	110.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	137	ASP	Sidechain
4	E	55	ARG	Peptide
4	E	56	PRO	Peptide
4	E	58	HIS	Mainchain
5	F	244	ARG	Sidechain
4	L	59	GLN	Mainchain
5	M	158	GLU	Sidechain

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	2249	0	2098	12	1
1	H	2252	0	2103	11	0
2	B	837	0	803	1	0
2	I	837	0	803	2	0
3	C	76	0	76	3	0
3	J	76	0	76	2	0
4	E	1523	0	1474	12	1
4	L	1521	0	1473	11	2
5	F	1894	0	1794	15	0
5	M	1891	0	1794	17	0
6	A	37	0	0	0	0
6	B	9	0	0	0	0
6	C	2	0	0	0	0
6	E	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	33	0	0	0	0
6	H	36	0	0	0	0
6	I	16	0	0	0	0
6	J	2	0	0	0	0
6	L	28	0	0	0	0
6	M	22	0	0	0	0
All	All	13366	0	12494	76	2

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 (76) 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	1.23	0.83
4:E:22:CYS:H	4:E:74:HIS:HD2	1.31	0.78
4:E:134:ARG:HH11	4:E:134:ARG:HG3	1.49	0.77
5:F:186:ASN:HB3	4:L:171:LYS:O	1.88	0.72
4:E:170:MET:HB2	4:E:175:SER:HB2	1.72	0.70
5:F:55:THR:HG21	5:F:67:ALA:HB3	1.73	0.68
4:E:134:ARG:HH11	4:E:134:ARG:CG	2.08	0.66
1:A:66:LYS:O	1:A:70:HIS:HD2	1.80	0.64
5:F:25:GLN:HE22	5:F:29:HIS:H	1.45	0.62
1:H:6:ARG:HH11	1:H:6:ARG:HG3	1.68	0.59
5:F:25:GLN:HE21	5:F:27:ASN:H	1.51	0.58
1:A:22:PHE:HE1	1:A:74:HIS:HD2	1.52	0.56
5:M:25:GLN:HE21	5:M:27:ASN:H	1.54	0.55
5:M:25:GLN:HE22	5:M:29:HIS:H	1.54	0.54
5:M:25:GLN:NE2	5:M:29:HIS:H	2.06	0.53
1:H:66:LYS:O	1:H:70:HIS:HD2	1.92	0.53
1:H:263:HIS:CD2	1:H:265:GLY:H	2.27	0.52
1:A:114:HIS:CG	1:A:156:LEU:HD11	2.45	0.52
4:E:170:MET:SD	5:F:197:ARG:HG2	2.50	0.52
4:E:82:LEU:HD21	4:E:116:PRO:HG3	1.92	0.51
1:H:185:PRO:HD2	1:H:266:LEU:HD13	1.92	0.51
3:J:7:PRO:HA	5:M:97:TRP:CE3	2.48	0.49
4:E:77:LYS:NZ	4:E:81:GLN:HE21	2.10	0.49
4:E:77:LYS:HZ1	4:E:81:GLN:HE21	1.61	0.49
2:I:25:CYS:HB2	2:I:39:LEU:HD21	1.95	0.48
4:E:156:MET:HG3	4:E:157:GLU:HG2	1.96	0.48
5:M:83:SER:H	5:M:86:GLN:HE21	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:21:LEU:HD22	5:F:112:THR:HG21	1.96	0.48
1:H:202:ARG:HG3	1:H:246:ALA:HB2	1.96	0.47
4:L:160:THR:HG23	4:L:184:SER:HB3	1.95	0.47
4:E:5:GLN:NE2	4:E:90:CYS:H	2.12	0.47
5:M:144:THR:OG1	5:M:197:ARG:HD3	2.15	0.47
1:A:22:PHE:CE1	1:A:74:HIS:HD2	2.31	0.46
3:C:7:PRO:HA	5:F:97:TRP:CE3	2.50	0.46
1:A:263:HIS:CD2	1:A:265:GLY:H	2.34	0.46
1:A:185:PRO:HD2	1:A:266:LEU:HD13	1.97	0.46
5:M:132:PRO:HB2	5:M:137:ILE:HD11	1.98	0.46
5:M:6:GLN:HG2	5:M:92:CYS:SG	2.56	0.46
4:L:5:GLN:NE2	4:L:90:CYS:H	2.14	0.46
5:M:38:ASP:OD2	5:M:44:ARG:NH2	2.48	0.46
4:E:129:LYS:HG2	4:E:139:THR:HG22	1.98	0.46
4:L:21:ASN:HA	4:L:74:HIS:CD2	2.51	0.46
1:H:73:THR:HG23	3:J:8:VAL:HG12	1.97	0.45
4:L:22:CYS:H	4:L:74:HIS:CD2	2.15	0.45
4:L:160:THR:OG1	4:L:186:GLN:NE2	2.49	0.45
5:M:174:THR:HG23	5:M:194:SER:HB2	1.99	0.45
4:E:134:ARG:CG	4:E:134:ARG:NH1	2.71	0.45
5:F:46:ILE:HG22	5:F:47:HIS:CD2	2.52	0.45
1:A:238:ASP:HB3	2:B:12:ARG:HD3	1.99	0.45
5:F:84:LEU:HD21	5:F:117:GLU:HG3	1.97	0.44
5:F:19:VAL:HB	5:F:79:LEU:HG	1.99	0.43
1:H:6:ARG:HG3	1:H:6:ARG:NH1	2.32	0.43
4:L:161:PHE:HZ	5:M:179:TYR:CD1	2.36	0.43
5:M:19:VAL:HB	5:M:79:LEU:HG	2.01	0.43
4:L:5:GLN:HE21	4:L:107:GLY:HA3	1.84	0.43
5:M:65:TYR:CD1	5:M:79:LEU:HD22	2.53	0.43
1:A:51:TRP:O	1:A:54:GLN:HG2	2.19	0.43
1:H:82:ARG:HD3	1:H:89:GLU:HG3	2.01	0.43
1:A:156:LEU:HG	3:C:3:TRP:CH2	2.53	0.43
1:A:202:ARG:HG3	1:A:246:ALA:HB2	2.01	0.42
4:L:12:LEU:O	4:L:114:VAL:HA	2.19	0.42
1:H:66:LYS:O	1:H:70:HIS:CD2	2.72	0.42
5:F:21:LEU:HD12	5:F:77:LEU:HD23	2.02	0.42
5:M:205:ASN:HA	5:M:206:PRO:HD3	1.93	0.42
5:F:231:LYS:HA	5:F:232:PRO:HD3	1.86	0.42
5:M:25:GLN:HE21	5:M:27:ASN:N	2.18	0.42
1:A:73:THR:HG23	3:C:8:VAL:HG12	2.01	0.42
5:M:123:THR:HA	5:M:124:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:238:ASP:HB3	2:I:12:ARG:HD3	2.02	0.41
5:F:25:GLN:NE2	5:F:29:HIS:H	2.15	0.41
5:F:205:ASN:HA	5:F:206:PRO:HD3	1.90	0.41
5:F:65:TYR:CD1	5:F:79:LEU:HD22	2.56	0.41
4:L:18:VAL:HB	4:L:77:LYS:HB3	2.02	0.41
1:H:263:HIS:HD2	1:H:265:GLY:H	1.69	0.40
1:A:263:HIS:HD2	1:A:265:GLY:H	1.69	0.40
5:M:175:ASP:HA	5:M:176:PRO:HD3	1.96	0.40

All (2) 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:173:MET:CE	4:L:185:ASN:OD1[1_545]	2.04	0.16
1:A:169:ARG:NH2	4:L:197:GLU:OE2[2_645]	2.11	0.09

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	274/275 (100%)	268 (98%)	6 (2%)	0	100 100
1	H	274/275 (100%)	267 (97%)	7 (3%)	0	100 100
2	B	98/100 (98%)	98 (100%)	0	0	100 100
2	I	98/100 (98%)	94 (96%)	4 (4%)	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	191/194 (98%)	176 (92%)	10 (5%)	5 (3%)	5 5
4	L	190/194 (98%)	176 (93%)	10 (5%)	4 (2%)	7 8
5	F	236/238 (99%)	229 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	M	235/238 (99%)	228 (97%)	7 (3%)	0	100 100
All	All	1610/1632 (99%)	1550 (96%)	51 (3%)	9 (1%)	25 36

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	55	ARG
4	E	58	HIS
4	L	54	LYS
4	L	55	ARG
4	L	56	PRO
4	L	57	GLU
4	E	54	LYS
4	E	174	ASP
4	E	57	GLU

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	231/230 (100%)	229 (99%)	2 (1%)	78 90
1	H	231/230 (100%)	229 (99%)	2 (1%)	78 90
2	B	95/95 (100%)	92 (97%)	3 (3%)	39 59
2	I	95/95 (100%)	93 (98%)	2 (2%)	53 72
3	C	7/7 (100%)	7 (100%)	0	100 100
3	J	7/7 (100%)	7 (100%)	0	100 100
4	E	178/177 (101%)	174 (98%)	4 (2%)	52 71
4	L	177/177 (100%)	172 (97%)	5 (3%)	43 63
5	F	206/206 (100%)	201 (98%)	5 (2%)	49 68
5	M	205/206 (100%)	203 (99%)	2 (1%)	76 88
All	All	1432/1430 (100%)	1407 (98%)	25 (2%)	59 78

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	156	LEU
2	B	27	VAL
2	B	70	PHE
2	B	83	ASN
4	E	19	MET
4	E	55	ARG
4	E	57	GLU
4	E	134	ARG
5	F	14	VAL
5	F	79	LEU
5	F	182	SER
5	F	197	ARG
5	F	207	ARG
1	H	145	HIS
1	H	266	LEU
2	I	70	PHE
2	I	83	ASN
4	L	19	MET
4	L	56	PRO
4	L	57	GLU
4	L	77	LYS
4	L	147	ASP
5	M	73	GLU
5	M	79	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	74	HIS
1	A	87	GLN
1	A	141	GLN
1	A	263	HIS
2	B	2	GLN
2	B	31	HIS
2	B	83	ASN
4	E	5	GLN
4	E	74	HIS
4	E	81	GLN
5	F	24	HIS

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Mol	Chain	Res	Type
5	F	25	GLN
5	F	28	ASN
1	H	70	HIS
1	H	87	GLN
1	H	263	HIS
2	I	2	GLN
2	I	83	ASN
4	L	5	GLN
4	L	74	HIS
4	L	185	ASN
4	L	186	GLN
5	M	24	HIS
5	M	25	GLN
5	M	74	ASN
5	M	86	GLN
5	M	217	HIS

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 (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	L	2
4	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	51:THR	C	52:ASP	N	3.54
1	E	51:THR	C	52:ASP	N	3.11
1	L	59:GLN	C	61:GLY	N	1.16

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, 95^{th} 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%)	-0.15	1 (0%) 92 91	33, 38, 42, 47	6 (2%)
1	H	275/275 (100%)	-0.12	1 (0%) 92 91	30, 37, 42, 46	3 (1%)
2	B	100/100 (100%)	-0.15	2 (2%) 65 63	34, 37, 45, 48	1 (1%)
2	I	100/100 (100%)	-0.10	2 (2%) 65 63	31, 36, 43, 47	1 (1%)
3	C	9/9 (100%)	-0.17	0 100 100	32, 32, 36, 37	0
3	J	9/9 (100%)	-0.16	0 100 100	35, 35, 38, 38	0
4	E	187/194 (96%)	0.15	15 (8%) 12 11	30, 38, 46, 52	4 (2%)
4	L	186/194 (95%)	0.19	18 (9%) 7 7	32, 38, 46, 54	3 (1%)
5	F	237/238 (99%)	-0.20	3 (1%) 77 75	31, 36, 42, 44	5 (2%)
5	M	237/238 (99%)	-0.21	4 (1%) 70 68	31, 36, 43, 47	1 (0%)
All	All	1615/1632 (98%)	-0.09	46 (2%) 53 51	30, 37, 44, 54	24 (1%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	0	MET	9.5
4	L	187	THR	8.1
4	E	173	MET	7.1
4	L	188	SER	6.4
4	E	156	MET	6.2
4	E	187	THR	5.9
4	L	173	MET	5.8
4	L	185	ASN	4.8
4	L	156	MET	4.5
4	E	0	MET	4.5
4	E	59	GLN	4.1
4	E	188	SER	4.0
4	L	0	MET	3.7

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Mol	Chain	Res	Type	RSRZ
4	E	192	GLN	3.3
4	L	186	GLN	3.3
5	F	245	ALA	3.3
4	E	177[A]	SER	3.2
4	E	155	THR	3.2
4	E	186	GLN	3.2
2	B	1	ILE	2.9
4	L	136	GLN	2.9
5	M	227	GLU	2.8
4	E	175	SER	2.6
4	L	40	ASN	2.5
1	A	1	GLY	2.5
4	L	161	PHE	2.4
4	L	189	PHE	2.4
4	E	193	ASP	2.4
4	L	157	GLU	2.4
1	H	91	GLY	2.4
5	M	222	GLU	2.4
2	B	0	MET	2.4
5	F	228	GLY	2.3
4	E	185	ASN	2.3
4	E	174	ASP	2.2
4	L	174	ASP	2.2
5	F	227	GLU	2.2
4	L	137	ASP	2.2
5	M	186	ASN	2.2
4	L	155	THR	2.2
4	L	172	ALA	2.2
4	L	7	GLU	2.1
2	I	1	ILE	2.1
5	M	1	GLU	2.1
4	E	172	ALA	2.0
4	L	194	ILE	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 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.