Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 06:16 PM GMT

PDB ID	:	4L3E
Title	:	The complex between high affinity TCR DMF5(alpha-D26Y,beta-L98W) and human Class I MHC HLA-A2 with the bound MART-1(26-35)(A27L) peptide
Authors	:	Hellman, L.M.
Deposited on	:	2013-06-05
Resolution	:	2.56 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

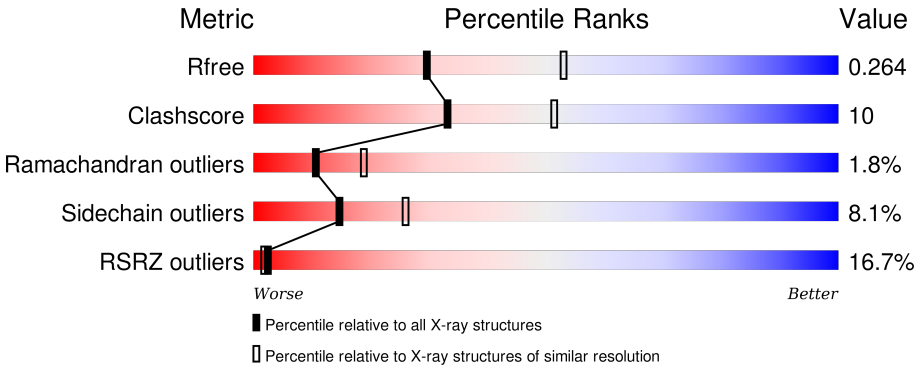
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.56 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}	91344	3324 (2.60-2.52)
Clashscore	102246	3729 (2.60-2.52)
Ramachandran outliers	100387	3673 (2.60-2.52)
Sidechain outliers	100360	3673 (2.60-2.52)
RSRZ outliers	91569	3333 (2.60-2.52)

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 <=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	15% 78% 19% ·
2	B	100	3% 78% 20% ·
3	C	10	90% 10%
4	D	199	30% 63% 31% 6%
5	E	242	14% 76% 21% ·

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6615 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
			2246	1403	409	425	9			

- 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			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	INITIATING METHIONINE	UNP P61769

- Molecule 3 is a protein called Melanoma antigen recognized by T-cells 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			69	45	10	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	LEU	ALA	ENGINEERED MUTATION	UNP Q16655

- Molecule 4 is a protein called DMF5 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	199	Total	C	N	O	S	0	0	0
			1549	970	255	316	8			

- Molecule 5 is a protein called DMF5 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	0	0
			1902	1196	334	364	8			

- Molecule 6 is water.

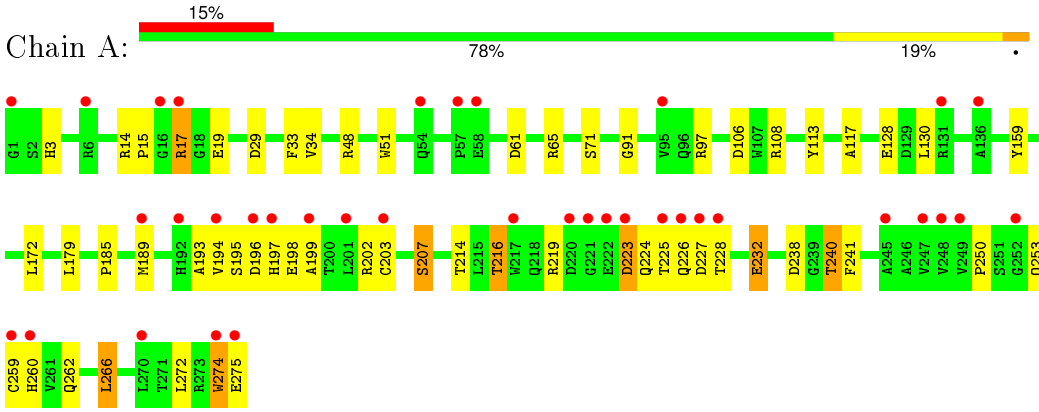
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	O	0	0
			4	4		
6	B	2	Total	O	0	0
			2	2		
6	C	1	Total	O	0	0
			1	1		
6	D	3	Total	O	0	0
			3	3		
6	E	2	Total	O	0	0
			2	2		

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 errors 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.

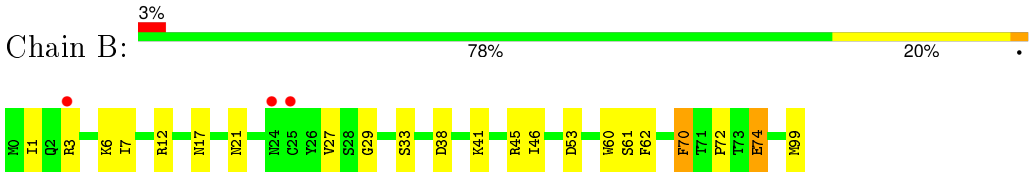
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain A:



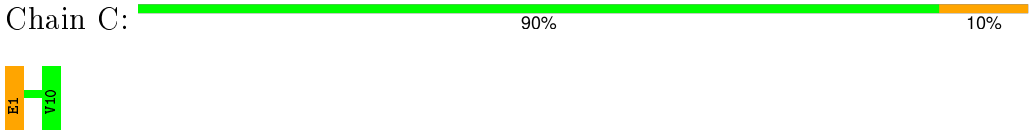
- Molecule 2: Beta-2-microglobulin

Chain B:



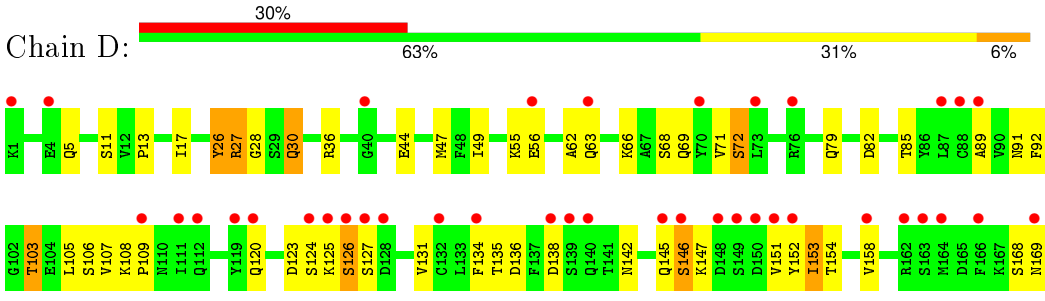
- Molecule 3: Melanoma antigen recognized by T-cells 1

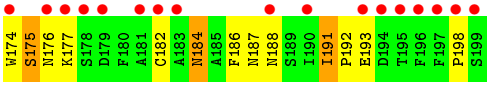
Chain C:



- Molecule 4: DMF5 alpha chain

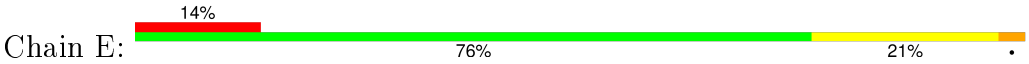
Chain D:

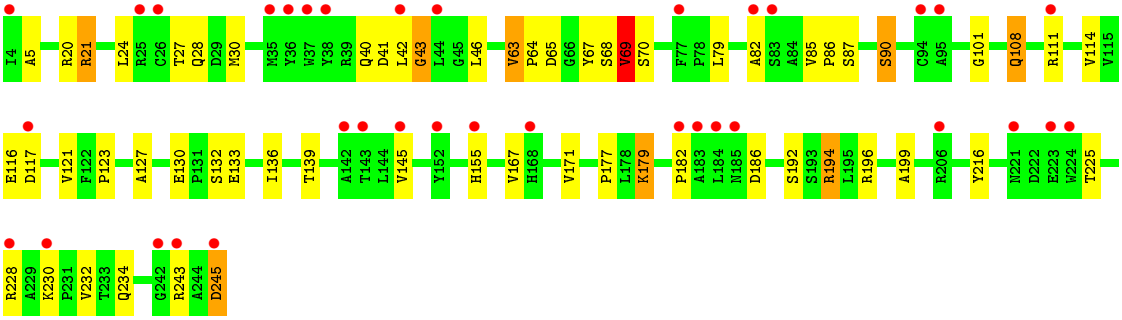




• Molecule 5: DMF5 beta chain

Chain E:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	227.04Å 49.32Å 92.89Å 90.00° 94.82° 90.00°	Depositor
Resolution (Å)	20.05 – 2.56 20.05 – 2.56	Depositor EDS
% Data completeness (in resolution range)	94.6 (20.05-2.56) 94.8 (20.05-2.56)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.229 , 0.266 0.226 , 0.264	Depositor DCC
R_{free} test set	1625 reflections (5.11%)	DCC
Wilson B-factor (Å^2)	58.8	Xtriage
Anisotropy	0.862	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 31904 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6615	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.43	0/2311	0.60	0/3137
2	B	0.44	0/860	0.58	0/1162
3	C	0.79	0/68	0.78	0/90
4	D	0.49	0/1583	0.59	0/2142
5	E	0.45	1/1953 (0.1%)	0.60	1/2663 (0.0%)
All	All	0.46	1/6775 (0.0%)	0.59	1/9194 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	64	PRO	N-CD	5.33	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	63	VAL	C-N-CD	5.52	139.99	128.40

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	2246	0	2096	38	0
2	B	837	0	803	15	0
3	C	69	0	79	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1549	0	1467	58	0
5	E	1902	0	1807	34	0
6	A	4	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	3	0	0	0	0
6	E	2	0	0	0	0
All	All	6615	0	6252	132	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 10.

All (132) 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:D:26:TYR:HE1	4:D:28:GLY:HA3	1.16	1.07
4:D:26:TYR:HE1	4:D:28:GLY:CA	1.81	0.93
4:D:26:TYR:CE1	4:D:28:GLY:CA	2.55	0.88
4:D:26:TYR:CE1	4:D:28:GLY:HA3	2.07	0.88
1:A:274:TRP:HE3	1:A:275:GLU:H	1.24	0.85
4:D:109:PRO:HG2	4:D:158:VAL:HG21	1.61	0.80
1:A:250:PRO:O	1:A:253:GLN:NE2	2.15	0.80
4:D:26:TYR:HD1	4:D:28:GLY:H	1.29	0.79
4:D:26:TYR:CD1	4:D:28:GLY:N	2.51	0.78
5:E:41:ASP:OD1	5:E:90:SER:OG	2.01	0.78
5:E:136:ILE:HD11	5:E:199:ALA:HA	1.67	0.76
5:E:130:GLU:OE2	5:E:243:ARG:NH1	2.19	0.75
4:D:26:TYR:HD1	4:D:28:GLY:N	1.85	0.74
4:D:91:ASN:HD22	5:E:101:GLY:HA2	1.53	0.73
4:D:147:LYS:NZ	4:D:187:ASN:OD1	2.22	0.72
1:A:202:ARG:NH1	2:B:99:MET:O	2.23	0.71
5:E:245:ASP:OD1	5:E:245:ASP:N	2.23	0.70
4:D:123:ASP:OD1	4:D:124:SER:N	2.27	0.68
4:D:184:ASN:OD1	4:D:184:ASN:N	2.27	0.68
1:A:216:THR:HG23	1:A:260:HIS:HB2	1.76	0.68
4:D:27:ARG:NH1	4:D:27:ARG:HB2	2.08	0.68
1:A:238:ASP:OD1	1:A:240:THR:HG23	1.94	0.67
5:E:86:PRO:HA	5:E:114:VAL:HB	1.77	0.66
4:D:146:SER:O	4:D:188:ASN:ND2	2.29	0.65
1:A:219:ARG:HB3	1:A:224:GLN:NE2	2.11	0.65
4:D:158:VAL:HG22	4:D:169:ASN:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:121:VAL:O	5:E:228:ARG:NH2	2.27	0.62
5:E:155:HIS:HB3	5:E:216:TYR:HB2	1.81	0.62
1:A:185:PRO:HD2	1:A:266:LEU:HD13	1.80	0.62
4:D:172:VAL:HG23	5:E:194:ARG:HE	1.65	0.61
4:D:134:PHE:HB2	4:D:186:PHE:CZ	2.35	0.61
5:E:68:SER:O	5:E:69:VAL:HB	2.00	0.61
5:E:63:VAL:HG23	5:E:63:VAL:O	2.00	0.61
4:D:153:ILE:HD11	4:D:171:ALA:HB1	1.83	0.60
4:D:26:TYR:CE1	4:D:28:GLY:N	2.70	0.59
4:D:154:THR:OG1	5:E:194:ARG:NH2	2.36	0.59
2:B:38:ASP:OD2	2:B:45:ARG:HD2	2.04	0.58
1:A:15:PRO:HG3	1:A:91:GLY:O	2.03	0.57
2:B:41:LYS:HB2	2:B:46:ILE:HD11	1.86	0.57
4:D:91:ASN:ND2	5:E:101:GLY:HA2	2.19	0.57
5:E:85:VAL:HG13	5:E:87:SER:H	1.68	0.56
5:E:41:ASP:O	5:E:43:GLY:N	2.33	0.56
4:D:13:PRO:HA	4:D:108:LYS:HG2	1.87	0.56
1:A:240:THR:OG1	1:A:241:PHE:N	2.38	0.55
1:A:224:GLN:HE22	1:A:257:TYR:HE2	1.54	0.55
5:E:68:SER:OG	5:E:69:VAL:N	2.40	0.55
1:A:51:TRP:CE2	1:A:179:LEU:HD11	2.42	0.55
4:D:151:VAL:HA	4:D:175:SER:HB3	1.88	0.54
1:A:172:LEU:HD23	1:A:179:LEU:HD23	1.89	0.54
1:A:232:GLU:OE2	2:B:6:LYS:HE3	2.08	0.54
4:D:5:GLN:O	4:D:101:GLN:NE2	2.41	0.54
1:A:195:SER:O	1:A:197:HIS:N	2.41	0.54
4:D:27:ARG:HH11	4:D:27:ARG:HB2	1.73	0.53
5:E:123:PRO:HB3	5:E:234:GLN:HE21	1.74	0.53
5:E:133:GLU:O	5:E:136:ILE:HG22	2.09	0.53
4:D:27:ARG:CB	4:D:27:ARG:NH1	2.73	0.52
5:E:40:GLN:HB2	5:E:46:LEU:HD23	1.92	0.52
4:D:105:LEU:HD21	4:D:107:VAL:HG23	1.92	0.52
4:D:66:LYS:O	4:D:69:GLN:NE2	2.42	0.52
4:D:27:ARG:CZ	4:D:27:ARG:CB	2.88	0.51
1:A:194:VAL:HG13	1:A:198:GLU:HB3	1.93	0.51
1:A:159:TYR:HD1	4:D:30:GLN:OE1	1.93	0.51
4:D:49:ILE:HD13	4:D:55:LYS:HB2	1.92	0.50
1:A:203:CYS:SG	1:A:272:LEU:HD11	2.52	0.50
5:E:5:ALA:HB1	5:E:30:MET:HG2	1.94	0.49
5:E:111:ARG:NH1	5:E:155:HIS:HA	2.27	0.49
5:E:24:LEU:HD12	5:E:79:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:SER:HA	1:A:240:THR:OG1	2.13	0.49
4:D:5:GLN:HB3	4:D:103:THR:HG22	1.94	0.49
4:D:89:ALA:HB1	4:D:97:LEU:HD11	1.94	0.49
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.48	0.49
1:A:48:ARG:NH2	2:B:53:ASP:OD2	2.46	0.49
5:E:108:GLN:CD	5:E:108:GLN:H	2.17	0.49
4:D:26:TYR:C	4:D:26:TYR:CD1	2.85	0.48
4:D:26:TYR:CE1	4:D:28:GLY:C	2.86	0.48
4:D:131:VAL:HG22	4:D:174:TRP:HB3	1.95	0.48
1:A:65:ARG:NH1	4:D:92:PHE:O	2.47	0.48
1:A:15:PRO:HG3	1:A:91:GLY:C	2.35	0.47
2:B:29:GLY:HA2	2:B:61:SER:OG	2.14	0.47
4:D:26:TYR:C	4:D:26:TYR:HD1	2.18	0.47
4:D:27:ARG:CZ	4:D:27:ARG:HB3	2.45	0.47
1:A:214:THR:HB	1:A:262:GLN:HB2	1.97	0.47
5:E:123:PRO:HB3	5:E:234:GLN:NE2	2.30	0.47
1:A:223:ASP:N	1:A:223:ASP:OD1	2.48	0.47
2:B:74:GLU:CD	2:B:74:GLU:H	2.18	0.47
4:D:125:LYS:HD2	5:E:127:ALA:HB2	1.96	0.46
1:A:167:TRP:CD2	3:C:1:GLU:HG3	2.51	0.46
2:B:33:SER:HB3	2:B:62:PHE:CE2	2.50	0.46
4:D:120:GLN:HB2	4:D:182:CYS:SG	2.55	0.46
4:D:30:GLN:HB2	4:D:30:GLN:HE21	1.65	0.46
5:E:139:THR:HG21	5:E:196:ARG:NH2	2.31	0.46
1:A:219:ARG:HB3	1:A:224:GLN:HE21	1.79	0.45
1:A:51:TRP:CZ2	1:A:179:LEU:HD11	2.51	0.45
4:D:82:ASP:O	4:D:105:LEU:HD22	2.17	0.45
4:D:47:MET:SD	4:D:62:ALA:HB2	2.57	0.45
1:A:238:ASP:HB3	2:B:12:ARG:HD3	1.99	0.45
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.52	0.45
5:E:63:VAL:C	5:E:65:ASP:H	2.20	0.45
1:A:14:ARG:O	1:A:17:ARG:HG3	2.17	0.44
1:A:219:ARG:HD2	1:A:224:GLN:HE21	1.82	0.44
4:D:145:GLN:HA	4:D:153:ILE:CG2	2.48	0.44
1:A:128:GLU:O	1:A:130:LEU:HD13	2.18	0.44
2:B:1:ILE:HG13	2:B:1:ILE:H	1.64	0.44
4:D:153:ILE:HD12	4:D:154:THR:N	2.34	0.43
1:A:61:ASP:HB3	1:A:65:ARG:NH2	2.33	0.43
4:D:138:ASP:N	4:D:138:ASP:OD1	2.52	0.43
2:B:6:LYS:HB2	2:B:6:LYS:HE2	1.74	0.43
4:D:176:ASN:OD1	4:D:177:LYS:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:91:ASN:HD22	5:E:101:GLY:CA	2.25	0.42
5:E:179:LYS:HD2	5:E:182:PRO:HA	2.01	0.42
1:A:193:ALA:HA	1:A:199:ALA:HA	2.01	0.42
4:D:124:SER:O	4:D:126:SER:N	2.52	0.42
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.54	0.42
1:A:3:HIS:HD2	1:A:29:ASP:OD2	2.03	0.42
4:D:153:ILE:HD12	4:D:154:THR:H	1.84	0.42
4:D:145:GLN:HA	4:D:153:ILE:HG23	2.02	0.42
5:E:20:ARG:NH1	5:E:21:ARG:O	2.53	0.42
2:B:7:ILE:HG12	2:B:27:VAL:HG12	2.02	0.42
5:E:243:ARG:HG3	5:E:245:ASP:H	1.85	0.42
1:A:106:ASP:OD1	1:A:106:ASP:N	2.49	0.41
4:D:145:GLN:O	4:D:147:LYS:N	2.53	0.41
4:D:135:THR:HG22	4:D:136:ASP:CG	2.41	0.41
5:E:230:LYS:HG2	5:E:232:VAL:HG13	2.02	0.41
5:E:63:VAL:C	5:E:65:ASP:N	2.73	0.41
1:A:15:PRO:C	1:A:17:ARG:H	2.23	0.41
1:A:189:MET:SD	1:A:272:LEU:HD13	2.61	0.41
4:D:152:TYR:O	4:D:173:ALA:HA	2.21	0.41
5:E:111:ARG:HE	5:E:111:ARG:HB3	1.53	0.41
4:D:36:ARG:O	4:D:44:GLU:HG2	2.21	0.40
4:D:191:ILE:H	4:D:191:ILE:HG13	1.40	0.40
4:D:63:GLN:HB3	4:D:72:SER:HB2	2.02	0.40
2:B:17:ASN:HA	2:B:72:PRO:O	2.21	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	273/275 (99%)	260 (95%)	9 (3%)	4 (2%)	13 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100 100
3	C	8/10 (80%)	8 (100%)	0	0	100 100
4	D	197/199 (99%)	177 (90%)	14 (7%)	6 (3%)	5 7
5	E	240/242 (99%)	221 (92%)	14 (6%)	5 (2%)	9 15
All	All	816/826 (99%)	762 (93%)	39 (5%)	15 (2%)	11 19

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
4	D	126	SER
5	E	42	LEU
1	A	196	ASP
1	A	227	ASP
5	E	69	VAL
4	D	146	SER
4	D	175	SER
4	D	192	PRO
5	E	82	ALA
1	A	19	GLU
4	D	193	GLU
4	D	198	PRO
5	E	177	PRO
5	E	43	GLY

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	231/231 (100%)	216 (94%)	15 (6%)	21 38
2	B	95/95 (100%)	92 (97%)	3 (3%)	46 71
3	C	7/7 (100%)	6 (86%)	1 (14%)	4 6
4	D	176/176 (100%)	157 (89%)	19 (11%)	8 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	E	204/204 (100%)	184 (90%)	20 (10%)	10 17
All	All	713/713 (100%)	655 (92%)	58 (8%)	15 26

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	71	SER
1	A	97	ARG
1	A	108	ARG
1	A	113	TYR
1	A	207	SER
1	A	216	THR
1	A	223	ASP
1	A	225	THR
1	A	228	THR
1	A	232	GLU
1	A	240	THR
1	A	259	CYS
1	A	266	LEU
1	A	274	TRP
2	B	3	ARG
2	B	70	PHE
2	B	74	GLU
3	C	1	GLU
4	D	11	SER
4	D	17	ILE
4	D	26	TYR
4	D	27	ARG
4	D	30	GLN
4	D	56	GLU
4	D	68	SER
4	D	71	VAL
4	D	72	SER
4	D	79	GLN
4	D	85	THR
4	D	103	THR
4	D	106	SER
4	D	127	SER
4	D	142	ASN
4	D	153	ILE
4	D	168	SER

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Mol	Chain	Res	Type
4	D	184	ASN
4	D	191	ILE
5	E	21	ARG
5	E	27	THR
5	E	28	GLN
5	E	67	TYR
5	E	69	VAL
5	E	70	SER
5	E	90	SER
5	E	108	GLN
5	E	116	GLU
5	E	117	ASP
5	E	132	SER
5	E	145	VAL
5	E	167	VAL
5	E	171	VAL
5	E	179	LYS
5	E	186	ASP
5	E	192	SER
5	E	194	ARG
5	E	225	THR
5	E	245	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	ASN
1	A	192	HIS
1	A	197	HIS
1	A	224	GLN
4	D	37	GLN
4	D	113	ASN
5	E	33	ASN
5	E	40	GLN
5	E	234	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 carbohydrates 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, 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%)	0.79	41 (14%) 3 2	14, 44, 112, 129	0
2	B	100/100 (100%)	0.35	3 (3%) 54 52	15, 33, 67, 78	0
3	C	10/10 (100%)	0.23	0 100 100	13, 19, 27, 34	0
4	D	199/199 (100%)	1.49	59 (29%) 1 0	31, 72, 130, 159	0
5	E	242/242 (100%)	0.88	35 (14%) 3 3	18, 62, 109, 135	0
All	All	826/826 (100%)	0.93	138 (16%) 2 2	13, 53, 116, 159	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	127	SER	7.3
4	D	126	SER	7.0
5	E	184	LEU	6.5
1	A	16	GLY	6.0
1	A	275	GLU	6.0
4	D	190	ILE	5.6
4	D	128	ASP	5.5
5	E	42	LEU	5.5
4	D	149	SER	5.3
4	D	173	ALA	5.2
5	E	245	ASP	5.2
1	A	248	VAL	5.1
1	A	225	THR	4.7
4	D	132	CYS	4.7
1	A	257	TYR	4.6
1	A	223	ASP	4.6
4	D	150	ASP	4.5
4	D	179	ASP	4.5
4	D	163	SER	4.5
4	D	111	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
5	E	185	ASN	4.4
1	A	203	CYS	4.4
4	D	1	LYS	4.4
4	D	193	GLU	4.3
4	D	112	GLN	4.2
1	A	270	LEU	4.2
4	D	177	LYS	4.1
4	D	194	ASP	4.1
4	D	199	SER	4.1
5	E	94	CYS	4.1
4	D	182	CYS	3.9
1	A	249	VAL	3.9
4	D	169	ASN	3.8
1	A	252	GLY	3.7
4	D	162	ARG	3.7
1	A	274	TRP	3.7
1	A	222	GLU	3.7
1	A	220	ASP	3.6
5	E	182	PRO	3.6
4	D	196	PHE	3.6
4	D	152	TYR	3.6
1	A	227	ASP	3.5
4	D	176	ASN	3.5
5	E	44	LEU	3.5
1	A	245	ALA	3.5
5	E	206	ARG	3.4
5	E	168	HIS	3.4
4	D	198	PRO	3.4
4	D	164	MET	3.4
4	D	195	THR	3.3
5	E	223	GLU	3.3
4	D	134	PHE	3.3
4	D	171	ALA	3.3
1	A	194	VAL	3.3
4	D	88	CYS	3.3
4	D	70	TYR	3.3
5	E	142	ALA	3.3
4	D	166	PHE	3.2
1	A	17	ARG	3.2
2	B	3	ARG	3.2
5	E	38	TYR	3.1
5	E	155	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
4	D	178	SER	3.1
1	A	226	GLN	3.1
1	A	189	MET	3.0
1	A	221	GLY	3.0
1	A	259	CYS	3.0
4	D	148	ASP	2.9
4	D	125	LYS	2.9
1	A	197	HIS	2.9
1	A	260	HIS	2.9
1	A	192	HIS	2.9
4	D	151	VAL	2.9
5	E	143	THR	2.9
5	E	82	ALA	2.9
5	E	36	TYR	2.8
1	A	54	GLN	2.8
5	E	4	ILE	2.8
5	E	183	ALA	2.8
4	D	139	SER	2.8
1	A	57	PRO	2.7
4	D	89	ALA	2.7
5	E	37	TRP	2.7
5	E	152	TYR	2.7
1	A	1	GLY	2.7
4	D	109	PRO	2.7
1	A	254	GLU	2.7
4	D	56	GLU	2.7
1	A	136	ALA	2.7
4	D	76	ARG	2.6
5	E	25	ARG	2.6
1	A	201	LEU	2.6
5	E	242	GLY	2.6
5	E	221	ASN	2.6
4	D	140	GLN	2.6
4	D	124	SER	2.5
1	A	199	ALA	2.5
4	D	170	SER	2.5
5	E	145	VAL	2.5
5	E	228	ARG	2.5
1	A	196	ASP	2.5
4	D	87	LEU	2.5
5	E	35	MET	2.5
1	A	58	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	119	TYR	2.4
4	D	4	GLU	2.4
1	A	217	TRP	2.3
4	D	120	GLN	2.3
1	A	247	VAL	2.3
4	D	73	LEU	2.3
5	E	243	ARG	2.3
4	D	197	PHE	2.3
4	D	138	ASP	2.3
4	D	174	TRP	2.3
4	D	63	GLN	2.2
4	D	40	GLY	2.2
1	A	166	GLU	2.2
4	D	183	ALA	2.2
2	B	24	ASN	2.2
5	E	111	ARG	2.2
5	E	77	PHE	2.2
5	E	117	ASP	2.2
5	E	83	SER	2.2
4	D	188	ASN	2.2
1	A	95	VAL	2.1
2	B	25	CYS	2.1
1	A	228	THR	2.1
4	D	158	VAL	2.1
1	A	131	ARG	2.1
4	D	181	ALA	2.1
5	E	95	ALA	2.1
4	D	145	GLN	2.1
4	D	146	SER	2.1
1	A	169	ARG	2.1
5	E	26	CYS	2.1
5	E	230	LYS	2.0
1	A	6	ARG	2.0
5	E	224	TRP	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.