Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:04 PM GMT

PDB ID	:	3VXM
Title	:	The complex between C1-28 TCR and HLA-A24 bound to HIV-1 Nef134-10(2F) peptide
Authors	:	Shimizu, A.; Fukai, S.; Yamagata, A.; Iwamoto, A.
Deposited on	:	2012-09-20
Resolution	:	2.50 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:

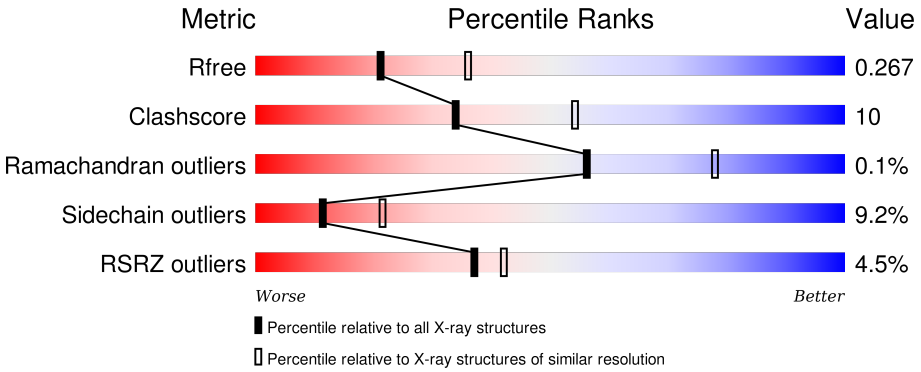
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	81% 15%
2	B	100	2% 78% 18%
3	C	10	80% 20%
4	D	211	11% 68% 19% 6% 6%
5	E	244	4% 81% 15%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6900 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-24 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2222	1382	403	427	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP P05534

- 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			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	EXPRESSION TAG	UNP P61769

- Molecule 3 is a protein called 10-mer peptide from Protein Nef.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	S	0	0	0
			91	64	14	12	1			

- Molecule 4 is a protein called C1-28 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	198	Total	C	N	O	S	0	0	0
			1533	968	254	304	7			

- Molecule 5 is a protein called C1-28 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total	C	N	O	S	0	0	0
			1948	1233	334	370	11			

- Molecule 6 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Co	0	0
			1	1		
6	E	2	Total	Co	0	0
			2	2		

- Molecule 7 is water.

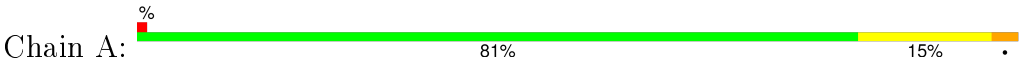
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	112	Total	O	0	0
			112	112		
7	B	48	Total	O	0	0
			48	48		
7	C	3	Total	O	0	0
			3	3		
7	D	52	Total	O	0	0
			52	52		
7	E	59	Total	O	0	0
			59	59		

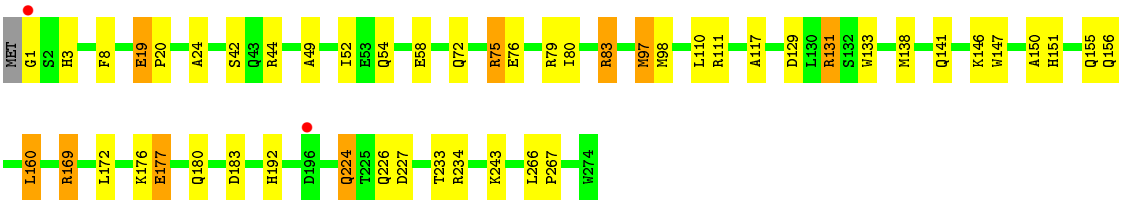
3 Residue-property plots (i)

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-24 alpha chain

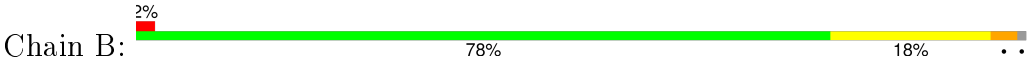
Chain A:

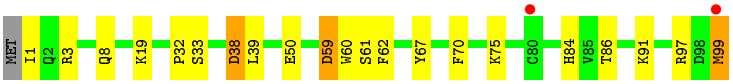




- Molecule 2: Beta-2-microglobulin

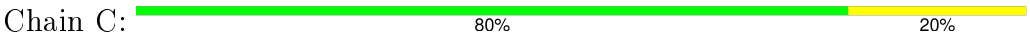
Chain B:

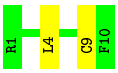




- Molecule 3: 10-mer peptide from Protein Nef

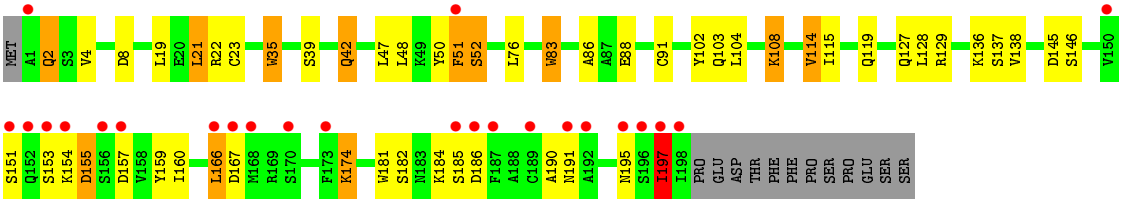
Chain C:





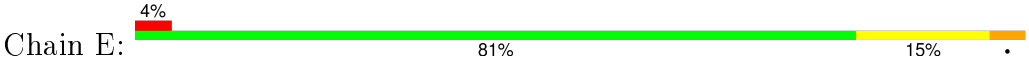
- Molecule 4: C1-28 TCR alpha chain

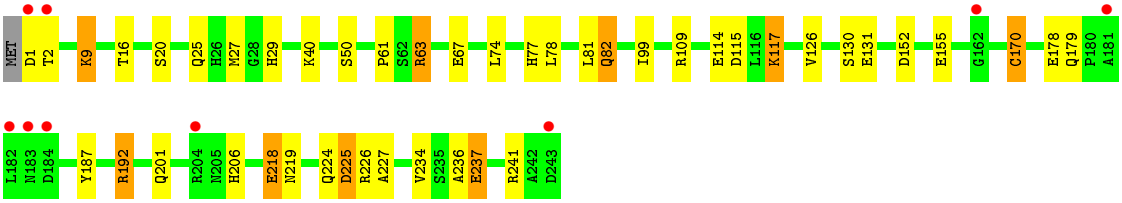
Chain D:



- Molecule 5: C1-28 TCR beta chain

Chain E:




MET D1 T2 K9 T16 S20 Q25 H26 M27 G28 H29 K40 S50 P61 S62 R63 E67 L74 H77 L78 L81 Q82 I99 R109 E114 D115 L116 K117 V126 S130 E131 D152 E155 G162 C170 E178 Q179 P180 A181
L182 N183 D184 Y187 R192 Q201 R204 N205 H206 E218 N219 Q224 D225 R226 A227 V234 S235 A236 E237 R241 A242 D243

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.12Å 86.49Å 234.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 42.53 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.50) 98.3 (42.53-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	6.61 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.209 , 0.267 0.208 , 0.267	Depositor DCC
R_{free} test set	1809 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 35638 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6900	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CO

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	0.54	0/2282	0.54	0/3092
2	B	0.50	0/852	0.51	0/1152
3	C	0.73	0/96	0.54	0/128
4	D	0.50	4/1569 (0.3%)	0.48	0/2127
5	E	0.50	0/2005	0.50	0/2728
All	All	0.52	4/6804 (0.1%)	0.51	0/9227

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	197	ILE	CB-CG1	6.01	1.70	1.54
4	D	197	ILE	CB-CG2	5.32	1.69	1.52
4	D	35	TRP	CD2-CE2	5.12	1.47	1.41
4	D	83	TRP	CD2-CE2	5.02	1.47	1.41

There are no bond angle outliers.

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	2222	0	2082	46	0
2	B	829	0	794	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	91	0	85	2	0
4	D	1533	0	1465	46	0
5	E	1948	0	1871	28	0
6	D	1	0	0	0	0
6	E	2	0	0	0	0
7	A	112	0	0	9	0
7	B	48	0	0	6	0
7	C	3	0	0	0	0
7	D	52	0	0	3	0
7	E	59	0	0	1	0
All	All	6900	0	6297	131	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 (131) 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)
5:E:9:LYS:HD3	5:E:9:LYS:H	0.94	1.11
1:A:169:ARG:HG2	1:A:169:ARG:HH11	0.95	1.08
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.24	1.02
5:E:9:LYS:H	5:E:9:LYS:CD	1.73	1.00
1:A:83:ARG:HH11	1:A:83:ARG:CG	1.75	0.99
5:E:9:LYS:HD3	5:E:9:LYS:N	1.78	0.99
1:A:133:TRP:HH2	1:A:156:GLN:OE1	1.47	0.96
4:D:154:LYS:HG3	4:D:155:ASP:H	1.32	0.93
1:A:169:ARG:HG2	1:A:169:ARG:NH1	1.75	0.91
1:A:133:TRP:CH2	1:A:156:GLN:OE1	2.24	0.91
1:A:169:ARG:CG	1:A:169:ARG:HH11	1.87	0.84
1:A:1:GLY:O	1:A:3:HIS:CD2	2.29	0.84
4:D:127:GLN:HE21	4:D:129:ARG:NH1	1.75	0.84
4:D:190:ALA:HA	7:D:440:HOH:O	1.80	0.82
5:E:63:ARG:HG3	5:E:81:LEU:CD2	2.10	0.82
4:D:154:LYS:CG	4:D:155:ASP:H	1.93	0.81
4:D:166:LEU:HB3	5:E:170:CYS:HB3	1.65	0.79
1:A:233:THR:OG1	1:A:243:LYS:HE2	1.81	0.79
4:D:51:PHE:CD2	4:D:51:PHE:N	2.51	0.78
1:A:72:GLN:HG3	7:D:433:HOH:O	1.85	0.75
4:D:51:PHE:N	4:D:52:SER:HB2	2.02	0.75
1:A:83:ARG:HG3	1:A:83:ARG:NH1	2.00	0.74
1:A:83:ARG:HH11	1:A:83:ARG:CB	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:51:PHE:H	4:D:52:SER:HB2	1.52	0.74
4:D:51:PHE:H	4:D:52:SER:CB	2.04	0.71
4:D:127:GLN:NE2	4:D:129:ARG:NH1	2.38	0.71
4:D:154:LYS:CG	4:D:155:ASP:N	2.54	0.70
4:D:2:GLN:HE21	4:D:2:GLN:H	1.39	0.69
4:D:108:LYS:NZ	4:D:108:LYS:H	1.91	0.69
4:D:191:ASN:HB2	4:D:197:ILE:HG12	1.74	0.69
1:A:138:MET:HG2	7:A:383:HOH:O	1.93	0.69
2:B:84:HIS:HD2	2:B:86:THR:OG1	1.75	0.68
1:A:83:ARG:HH11	1:A:83:ARG:HB2	1.61	0.66
5:E:63:ARG:HG3	5:E:81:LEU:HD22	1.78	0.66
2:B:1:ILE:HG22	7:B:116:HOH:O	1.96	0.66
4:D:138:VAL:HG12	4:D:181:TRP:HB3	1.78	0.65
1:A:49:ALA:O	1:A:52:ILE:HG22	1.96	0.65
1:A:83:ARG:HB2	1:A:83:ARG:NH1	2.11	0.65
1:A:83:ARG:CB	1:A:83:ARG:NH1	2.60	0.64
5:E:63:ARG:HG3	5:E:81:LEU:HD23	1.80	0.63
5:E:25:GLN:HE22	5:E:29:HIS:H	1.47	0.62
5:E:206:HIS:HE1	5:E:237:GLU:OE2	1.82	0.62
2:B:59:ASP:HB3	2:B:61:SER:H	1.64	0.61
4:D:153:SER:O	4:D:154:LYS:HG2	2.00	0.61
1:A:80:ILE:O	1:A:83:ARG:HG2	2.02	0.60
7:A:397:HOH:O	2:B:99:MET:HB2	2.01	0.60
4:D:127:GLN:NE2	4:D:129:ARG:HH12	2.00	0.59
4:D:51:PHE:HD2	4:D:51:PHE:N	2.01	0.58
4:D:86:ALA:HB2	4:D:114:VAL:HG13	1.86	0.57
5:E:61:PRO:HB2	5:E:63:ARG:HD2	1.84	0.57
4:D:159:TYR:HE1	5:E:178:GLU:O	1.88	0.57
2:B:32:PRO:O	2:B:84:HIS:HE1	1.88	0.56
5:E:226:ARG:HG2	5:E:227:ALA:H	1.70	0.56
5:E:152:ASP:HB3	5:E:187:TYR:CE2	2.41	0.56
4:D:191:ASN:HD22	4:D:197:ILE:HG23	1.71	0.55
2:B:97:ARG:HD2	7:B:135:HOH:O	2.06	0.55
2:B:33:SER:HB3	2:B:62:PHE:CE2	2.43	0.54
1:A:58:GLU:HB3	7:A:339:HOH:O	2.08	0.53
3:C:4:LEU:HG	4:D:102:TYR:OH	2.08	0.53
5:E:20:SER:OG	5:E:77:HIS:HD2	1.91	0.53
4:D:157:ASP:O	4:D:182:SER:HB2	2.09	0.53
4:D:39:SER:HB2	4:D:42:GLN:HG2	1.90	0.52
7:A:397:HOH:O	2:B:99:MET:HG3	2.10	0.51
1:A:76:GLU:OE1	1:A:79:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:51:PHE:CG	4:D:52:SER:HA	2.46	0.51
5:E:218:GLU:HG2	5:E:219:ASN:N	2.25	0.51
1:A:110:LEU:O	1:A:111:ARG:HG3	2.11	0.50
4:D:19:LEU:HD11	4:D:21:LEU:HD13	1.92	0.50
4:D:50:TYR:CE1	4:D:52:SER:HB3	2.46	0.50
1:A:129:ASP:O	1:A:131:ARG:HD2	2.12	0.50
1:A:133:TRP:HH2	1:A:156:GLN:CD	2.14	0.50
5:E:224:GLN:HG3	5:E:225:ASP:N	2.28	0.49
4:D:51:PHE:N	4:D:52:SER:CB	2.70	0.49
1:A:19:GLU:HB2	7:A:333:HOH:O	2.13	0.49
2:B:38:ASP:HB3	7:B:120:HOH:O	2.12	0.49
4:D:154:LYS:HG3	4:D:155:ASP:N	2.11	0.48
5:E:192:ARG:HD3	5:E:192:ARG:N	2.28	0.48
1:A:226:GLN:HG3	1:A:227:ASP:OD2	2.14	0.48
5:E:78:LEU:HG	5:E:81:LEU:HD11	1.95	0.48
5:E:114:GLU:HG3	7:E:418:HOH:O	2.14	0.48
4:D:153:SER:HA	4:D:160:ILE:HD12	1.95	0.48
1:A:1:GLY:O	1:A:3:HIS:NE2	2.47	0.47
4:D:8:ASP:OD2	4:D:22:ARG:HD3	2.14	0.47
1:A:80:ILE:HA	1:A:83:ARG:HD3	1.96	0.47
1:A:20:PRO:HD2	1:A:75:ARG:HD2	1.96	0.47
1:A:151:HIS:CE1	7:A:410:HOH:O	2.67	0.47
1:A:192:HIS:HE1	7:B:113:HOH:O	1.97	0.47
1:A:147:TRP:O	1:A:150:ALA:O	2.32	0.47
4:D:23:CYS:HB2	4:D:35:TRP:CZ2	2.50	0.47
5:E:25:GLN:NE2	5:E:29:HIS:H	2.12	0.46
1:A:42:SER:O	1:A:44:ARG:HG2	2.16	0.46
1:A:156:GLN:O	1:A:160:LEU:HD22	2.15	0.46
5:E:152:ASP:HB3	5:E:187:TYR:CD2	2.51	0.45
4:D:157:ASP:HB2	4:D:184:LYS:HE2	1.98	0.45
4:D:83:TRP:HA	4:D:114:VAL:CG2	2.47	0.45
5:E:226:ARG:HG2	5:E:227:ALA:N	2.32	0.45
5:E:82:GLN:HE21	5:E:82:GLN:HB3	1.60	0.45
1:A:192:HIS:CE1	7:B:113:HOH:O	2.70	0.44
5:E:126:VAL:HG23	5:E:236:ALA:HB3	1.99	0.44
1:A:83:ARG:CG	1:A:83:ARG:NH1	2.47	0.44
1:A:146:LYS:NZ	3:C:9:CYS:SG	2.91	0.44
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.53	0.44
5:E:201:GLN:HA	5:E:241:ARG:O	2.18	0.44
4:D:2:GLN:O	4:D:2:GLN:HG2	2.18	0.44
4:D:108:LYS:HZ2	4:D:108:LYS:H	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:157:ASP:HB3	4:D:184:LYS:HB2	2.00	0.43
4:D:167:ASP:HA	4:D:174:LYS:HG3	2.00	0.43
4:D:115:ILE:HG23	4:D:146:SER:HB3	1.99	0.43
4:D:19:LEU:HD11	4:D:21:LEU:CD1	2.48	0.43
4:D:4:VAL:HG11	4:D:91:CYS:SG	2.59	0.43
1:A:176:LYS:HG3	1:A:177:GLU:N	2.33	0.43
5:E:67:GLU:O	5:E:74:LEU:HD12	2.20	0.42
1:A:224:GLN:NE2	1:A:226:GLN:O	2.52	0.42
1:A:97:MET:HB3	1:A:97:MET:HE2	1.98	0.42
1:A:19:GLU:HG3	1:A:20:PRO:N	2.34	0.42
7:A:397:HOH:O	2:B:99:MET:CG	2.67	0.42
5:E:115:ASP:CG	5:E:117:LYS:HD2	2.40	0.42
1:A:234:ARG:HH11	2:B:8:GLN:NE2	2.18	0.42
1:A:8:PHE:O	1:A:24:ALA:HA	2.20	0.42
4:D:128:LEU:O	4:D:137:SER:HB2	2.20	0.42
5:E:25:GLN:HE21	5:E:27:MET:H	1.67	0.41
4:D:50:TYR:CD1	4:D:52:SER:CB	3.04	0.41
4:D:4:VAL:CG1	4:D:91:CYS:SG	3.08	0.41
2:B:50:GLU:HB2	2:B:67:TYR:CZ	2.56	0.41
2:B:75:LYS:HB3	2:B:75:LYS:HE2	1.94	0.41
4:D:108:LYS:HZ1	4:D:108:LYS:H	1.68	0.41
1:A:192:HIS:HD2	7:A:311:HOH:O	2.04	0.40
1:A:54:GLN:HB3	7:A:403:HOH:O	2.20	0.40
4:D:51:PHE:HB2	7:D:444:HOH:O	2.22	0.40
1:A:266:LEU:HA	1:A:267:PRO:HD2	1.93	0.40
2:B:3:ARG:NE	7:B:128:HOH:O	2.54	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	272/275 (99%)	267 (98%)	5 (2%)	0	100 100
2	B	97/100 (97%)	95 (98%)	2 (2%)	0	100 100
3	C	8/10 (80%)	7 (88%)	1 (12%)	0	100 100
4	D	196/211 (93%)	180 (92%)	15 (8%)	1 (0%)	34 55
5	E	241/244 (99%)	232 (96%)	9 (4%)	0	100 100
All	All	814/840 (97%)	781 (96%)	32 (4%)	1 (0%)	56 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	197	ILE

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	230/231 (100%)	215 (94%)	15 (6%)	21 39
2	B	94/95 (99%)	87 (93%)	7 (7%)	17 31
3	C	9/9 (100%)	9 (100%)	0	100 100
4	D	171/184 (93%)	148 (86%)	23 (14%)	5 9
5	E	217/218 (100%)	196 (90%)	21 (10%)	10 19
All	All	721/737 (98%)	655 (91%)	66 (9%)	11 21

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	75	ARG
1	A	83	ARG
1	A	97	MET
1	A	98	MET
1	A	131	ARG
1	A	141	GLN

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Mol	Chain	Res	Type
1	A	155	GLN
1	A	160	LEU
1	A	169	ARG
1	A	172	LEU
1	A	177	GLU
1	A	180	GLN
1	A	183	ASP
1	A	224	GLN
2	B	19	LYS
2	B	38	ASP
2	B	39	LEU
2	B	59	ASP
2	B	70	PHE
2	B	91	LYS
2	B	99	MET
4	D	2	GLN
4	D	21	LEU
4	D	42	GLN
4	D	47	LEU
4	D	48	LEU
4	D	51	PHE
4	D	52	SER
4	D	76	LEU
4	D	88	GLU
4	D	103	GLN
4	D	104	LEU
4	D	108	LYS
4	D	114	VAL
4	D	119	GLN
4	D	136	LYS
4	D	145	ASP
4	D	151	SER
4	D	155	ASP
4	D	166	LEU
4	D	174	LYS
4	D	185	SER
4	D	186	ASP
4	D	195	ASN
5	E	1	ASP
5	E	2	THR
5	E	9	LYS
5	E	16	THR

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Mol	Chain	Res	Type
5	E	40	LYS
5	E	50	SER
5	E	63	ARG
5	E	82	GLN
5	E	99	ILE
5	E	109	ARG
5	E	117	LYS
5	E	130	SER
5	E	131	GLU
5	E	155	GLU
5	E	170	CYS
5	E	179	GLN
5	E	192	ARG
5	E	218	GLU
5	E	225	ASP
5	E	234	VAL
5	E	237	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	156	GLN
1	A	192	HIS
2	B	8	GLN
2	B	84	HIS
4	D	2	GLN
4	D	82	HIS
4	D	119	GLN
4	D	127	GLN
4	D	194	ASN
4	D	195	ASN
5	E	25	GLN
5	E	77	HIS
5	E	82	GLN
5	E	179	GLN
5	E	206	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	274/275 (99%)	-0.13	2 (0%) 89 90	16, 24, 45, 68	0
2	B	99/100 (99%)	-0.12	2 (2%) 68 72	17, 30, 44, 53	0
3	C	10/10 (100%)	0.08	0 100 100	21, 23, 27, 27	0
4	D	198/211 (93%)	0.57	24 (12%) 6 5	19, 36, 101, 140	0
5	E	243/244 (99%)	0.07	9 (3%) 45 50	21, 33, 68, 100	2 (0%)
All	All	824/840 (98%)	0.10	37 (4%) 37 42	16, 29, 77, 140	2 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	196	SER	9.5
4	D	198	ILE	9.4
4	D	170	SER	7.9
4	D	197	ILE	7.4
4	D	195	ASN	7.4
4	D	152	GLN	5.6
4	D	167	ASP	5.2
4	D	153	SER	4.7
1	A	1	GLY	4.7
5	E	2	THR	4.5
4	D	151	SER	4.3
4	D	1	ALA	4.3
5	E	1	ASP	3.9
4	D	150	VAL	3.5
5	E	181	ALA	3.5
4	D	186	ASP	3.4
5	E	162	GLY	3.2
4	D	51	PHE	3.1
4	D	166	LEU	3.1
5	E	183	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
4	D	168	MET	2.9
5	E	204	ARG	2.9
5	E	182	LEU	2.8
5	E	243	ASP	2.8
4	D	191	ASN	2.7
2	B	99	MET	2.7
4	D	173	PHE	2.6
5	E	184	ASP	2.6
4	D	187	PHE	2.4
4	D	157	ASP	2.4
4	D	185	SER	2.4
4	D	154	LYS	2.4
4	D	156	SER	2.4
2	B	80	CYS	2.3
4	D	189	CYS	2.2
1	A	196	ASP	2.2
4	D	192	ALA	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	CO	E	302	1/1	0.92	0.05	-	61,61,61,61	0
6	CO	E	301	1/1	0.99	0.18	-	55,55,55,55	0
6	CO	D	301	1/1	0.94	0.17	-	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.