Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:01 AM GMT

PDB ID	:	2F74
Title	:	Murine MHC class I H-2Db in complex with human b2-microglobulin and LCMV-derived immunodminant peptide gp33
Authors	:	Achour, A.; Michaelsson, J.; Harris, R.A.; Ljunggren, H.G.; Karre, K.; Schneider, G.; Sandalova, T.
Deposited on	:	2005-11-30
Resolution	:	2.70 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:

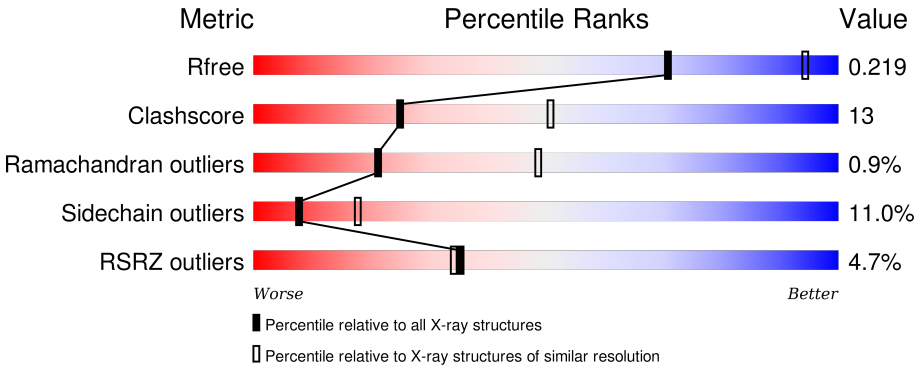
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	276	3% 65% 29% 5%
1	D	276	8% 65% 29% 6%
2	B	100	63% 27% 9%
2	E	100	2% 73% 22%
3	C	9	89% 11%

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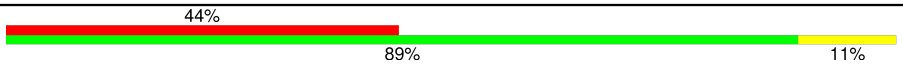
Mol	Chain	Length	Quality of chain
3	F	9	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6419 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2261	1428	399	425	9			
1	D	276	Total	C	N	O	S	0	0	0
			2265	1430	400	426	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			
2	E	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	CLONING ARTIFACT	UNP P61769
E	0	MET	-	CLONING ARTIFACT	UNP P61769

- Molecule 3 is a protein called NONAMERIC PEPTIDE, GP33, DERIVED FROM LYMPHOCYTIC CHORIOMENINGITIS VIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			73	48	11	13	1			
3	F	9	Total	C	N	O	S	0	0	0
			73	48	11	13	1			

- Molecule 4 is water.

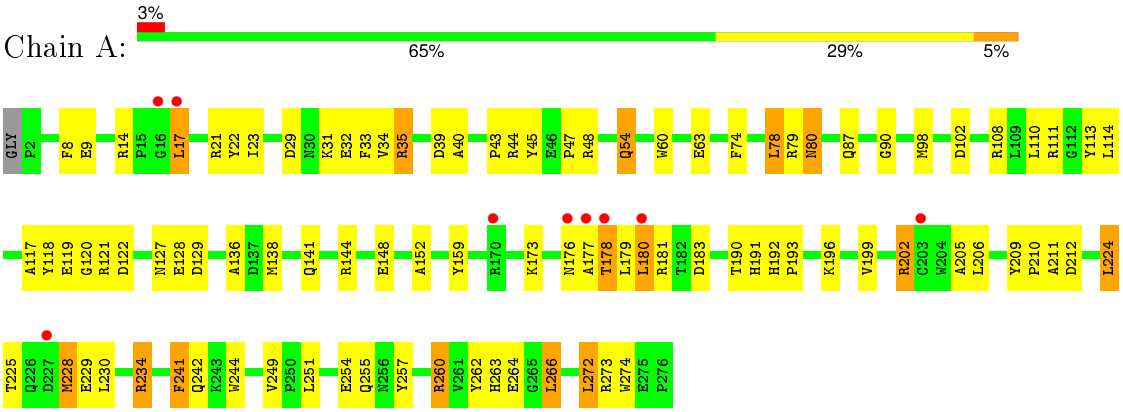
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	28	Total O 28 28	0	0
4	B	17	Total O 17 17	0	0
4	D	25	Total O 25 25	0	0
4	E	11	Total O 11 11	0	0

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.

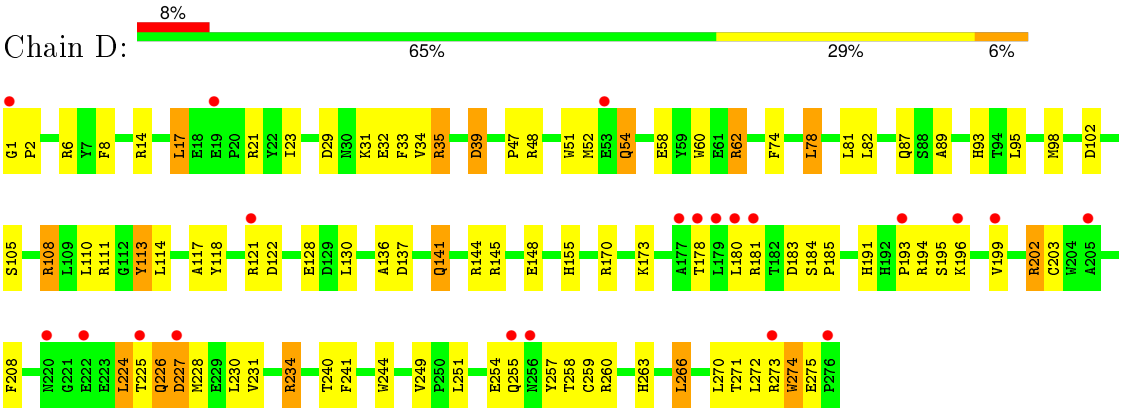
• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain A:



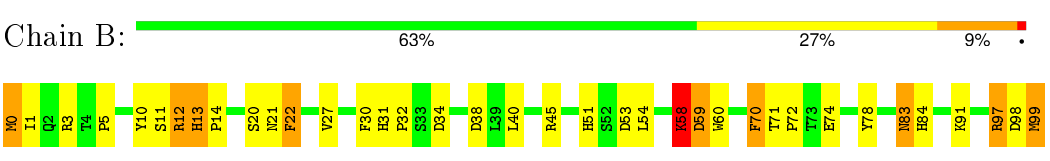
• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain D:



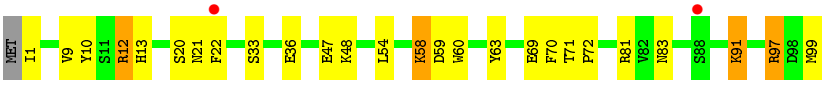
• Molecule 2: Beta-2-microglobulin

Chain B:



• Molecule 2: Beta-2-microglobulin

Chain E:

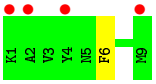


• Molecule 3: NONAMERIC PEPTIDE, GP33, DERIVED FROM LYMPHOCYTIC CHORIOMENINGITIS VIRUS

Chain C:

• Molecule 3: NONAMERIC PEPTIDE, GP33, DERIVED FROM LYMPHOCYTIC CHORIOMENINGITIS VIRUS

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.14Å 65.20Å 101.94Å 90.00° 102.43° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 19.97 – 2.69	Depositor EDS
% Data completeness (in resolution range)	92.5 (30.00-2.70) 92.0 (19.97-2.69)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.223 , 0.298 0.221 , 0.219	Depositor DCC
R_{free} test set	1135 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	62.9	Xtriage
Anisotropy	0.698	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 30.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 22473 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6419	wwPDB-VP
Average B, all atoms (Å^2)	17.0	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 27.75 % 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 2.0802e-03.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, 0.375 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	1.30	9/2328 (0.4%)	1.12	9/3160 (0.3%)
1	D	1.25	9/2332 (0.4%)	1.10	12/3166 (0.4%)
2	B	1.23	3/860 (0.3%)	1.22	7/1162 (0.6%)
2	E	1.16	2/852 (0.2%)	1.12	2/1152 (0.2%)
3	C	1.18	0/74	1.02	0/97
3	F	1.54	0/74	1.28	0/97
All	All	1.26	23/6520 (0.4%)	1.13	30/8834 (0.3%)

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
1	A	0	2
1	D	0	1
All	All	0	3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	113	TYR	CE1-CZ	-15.26	1.18	1.38
1	D	113	TYR	CG-CD2	-14.63	1.20	1.39
1	A	113	TYR	CE2-CZ	-14.27	1.20	1.38
1	A	241	PHE	CE1-CZ	-13.83	1.11	1.37
1	D	113	TYR	CE2-CZ	-13.48	1.21	1.38
1	D	113	TYR	CG-CD1	-13.12	1.22	1.39
1	A	113	TYR	CG-CD2	-12.90	1.22	1.39
1	A	241	PHE	CE2-CZ	-12.71	1.13	1.37
1	A	113	TYR	CE1-CZ	-12.65	1.22	1.38
1	D	241	PHE	CE2-CZ	-12.10	1.14	1.37
1	A	241	PHE	CG-CD2	-11.74	1.21	1.38
1	A	113	TYR	CG-CD1	-11.71	1.24	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	241	PHE	CE1-CZ	-11.27	1.16	1.37
1	A	241	PHE	CG-CD1	-9.89	1.24	1.38
1	D	241	PHE	CG-CD1	-9.68	1.24	1.38
2	E	58	LYS	CD-CE	9.12	1.74	1.51
1	D	241	PHE	CG-CD2	-8.75	1.25	1.38
2	B	99	MET	CG-SD	-7.06	1.62	1.81
2	B	58	LYS	CD-CE	6.42	1.67	1.51
1	A	138	MET	CG-SD	6.28	1.97	1.81
1	D	274	TRP	CB-CG	6.05	1.61	1.50
2	E	63	TYR	CE2-CZ	-5.92	1.30	1.38
2	B	58	LYS	CE-NZ	5.13	1.61	1.49

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	137	ASP	CB-CG-OD2	10.53	127.78	118.30
2	B	12	ARG	NE-CZ-NH2	-8.37	116.11	120.30
2	E	12	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	D	29	ASP	CB-CG-OD2	7.71	125.24	118.30
1	A	122	ASP	CB-CG-OD2	7.27	124.85	118.30
2	B	34	ASP	CB-CG-OD2	7.08	124.67	118.30
1	D	137	ASP	OD1-CG-OD2	-7.04	109.92	123.30
1	A	102	ASP	CB-CG-OD1	7.01	124.61	118.30
1	D	122	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	35	ARG	NE-CZ-NH1	6.87	123.73	120.30
2	B	53	ASP	CB-CG-OD1	6.73	124.36	118.30
2	E	58	LYS	CD-CE-NZ	6.68	127.08	111.70
1	A	180	LEU	CA-CB-CG	6.59	130.46	115.30
1	A	29	ASP	CB-CG-OD2	6.59	124.23	118.30
2	B	98	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	183	ASP	CB-CG-OD2	6.15	123.84	118.30
1	D	180	LEU	CA-CB-CG	5.77	128.56	115.30
2	B	38	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	260	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	102	ASP	CB-CG-OD2	5.58	123.32	118.30
2	B	22	PHE	CB-CG-CD1	5.57	124.70	120.80
1	A	241	PHE	CD1-CG-CD2	-5.42	111.25	118.30
1	D	121	ARG	CB-CA-C	-5.42	99.57	110.40
1	D	113	TYR	CZ-CE2-CD2	5.40	124.66	119.80
2	B	59	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	241	PHE	CB-CG-CD1	5.37	124.56	120.80
1	D	35	ARG	NE-CZ-NH1	5.25	122.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	241	PHE	CB-CG-CD1	5.05	124.33	120.80
1	D	241	PHE	CD1-CG-CD2	-5.04	111.74	118.30
1	D	62	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	ALA	Peptide
1	A	178	THR	Peptide
1	D	89	ALA	Peptide

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	2261	0	2131	54	0
1	D	2265	0	2136	58	0
2	B	837	0	803	34	0
2	E	829	0	794	21	0
3	C	73	0	74	1	0
3	F	73	0	74	3	0
4	A	28	0	0	2	0
4	B	17	0	0	5	0
4	D	25	0	0	2	0
4	E	11	0	0	1	0
All	All	6419	0	6012	157	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 13.

All (157) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:GLN:NE2	1:D:274:TRP:O	1.87	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:12:ARG:HG2	2:E:13:HIS:CE1	2.09	0.88
2:B:58:LYS:NZ	4:B:102:HOH:O	2.10	0.82
1:D:35:ARG:HB2	1:D:48:ARG:HD2	1.63	0.80
1:D:155:HIS:HB3	3:F:6:PHE:CE1	2.16	0.79
1:A:35:ARG:HB2	1:A:48:ARG:HD2	1.66	0.76
2:B:12:ARG:CZ	2:B:22:PHE:CD2	2.70	0.75
1:D:155:HIS:HB3	3:F:6:PHE:CZ	2.21	0.74
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.22	0.74
1:A:32:GLU:OE2	1:A:48:ARG:HD3	1.89	0.73
2:B:12:ARG:NH2	2:B:22:PHE:HD2	1.87	0.73
1:A:229:GLU:OE1	4:A:296:HOH:O	2.09	0.69
1:D:31:LYS:HE2	1:D:178:THR:HG21	1.74	0.69
1:D:144:ARG:O	1:D:148:GLU:HG3	1.93	0.69
2:B:30:PHE:HB2	2:B:84:HIS:CE1	2.29	0.67
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.28	0.67
2:B:83:ASN:HD22	2:B:84:HIS:N	1.92	0.67
2:B:30:PHE:HB2	2:B:84:HIS:HE1	1.59	0.67
2:E:12:ARG:CZ	2:E:22:PHE:CD2	2.77	0.67
2:E:12:ARG:NH2	2:E:22:PHE:HD2	1.93	0.66
2:B:31:HIS:ND1	2:B:32:PRO:HA	2.11	0.66
1:A:119:GLU:HB3	2:B:0:MET:HB3	1.78	0.65
1:D:35:ARG:CB	1:D:48:ARG:HD2	2.26	0.65
1:D:224:LEU:O	1:D:228:MET:CE	2.45	0.65
1:A:63:GLU:HA	1:A:63:GLU:OE1	1.96	0.64
1:A:40:ALA:O	1:A:43:PRO:HD3	1.98	0.63
2:E:12:ARG:CG	2:E:13:HIS:CE1	2.81	0.63
2:B:1:ILE:O	2:B:1:ILE:HG23	1.98	0.63
1:D:8:PHE:CD1	1:D:98:MET:HG2	2.35	0.62
1:A:230:LEU:HD12	1:A:230:LEU:C	2.19	0.62
2:E:21:ASN:O	2:E:22:PHE:HD1	1.83	0.62
1:A:87:GLN:NE2	1:A:118:TYR:OH	2.29	0.62
1:D:74:PHE:O	1:D:78:LEU:HB2	1.99	0.61
2:E:59:ASP:O	2:E:60:TRP:HB2	2.00	0.61
1:D:155:HIS:CD2	3:F:6:PHE:CE2	2.88	0.61
1:A:31:LYS:HD3	1:A:179:LEU:HD23	1.84	0.60
2:B:12:ARG:NH2	2:B:22:PHE:CD2	2.67	0.60
1:A:21:ARG:CZ	1:A:23:ILE:HD11	2.31	0.60
1:D:260:ARG:HA	1:D:270:LEU:O	2.01	0.60
2:E:97:ARG:HH11	2:E:97:ARG:HG2	1.67	0.59
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.38	0.59
1:A:35:ARG:CB	1:A:48:ARG:HD2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:LEU:O	1:D:228:MET:HE3	2.03	0.58
1:D:191:HIS:CE1	1:D:199:VAL:HG11	2.38	0.58
2:E:91:LYS:NZ	4:E:108:HOH:O	2.36	0.58
1:D:234:ARG:NH2	2:E:99:MET:OXT	2.34	0.57
2:B:59:ASP:O	2:B:60:TRP:HB2	2.04	0.56
1:A:190:THR:OG1	1:A:192:HIS:CE1	2.59	0.56
1:A:193:PRO:HA	1:A:199:VAL:HG12	1.86	0.56
2:B:21:ASN:O	2:B:22:PHE:HD1	1.89	0.56
1:D:141:GLN:O	1:D:145:ARG:HG3	2.05	0.55
1:D:191:HIS:HE1	1:D:199:VAL:HG11	1.70	0.55
1:D:47:PRO:HG3	1:D:60:TRP:CZ2	2.41	0.55
1:D:8:PHE:CE1	1:D:98:MET:HG2	2.42	0.55
1:D:21:ARG:CZ	1:D:23:ILE:HD11	2.37	0.55
2:E:12:ARG:CD	2:E:13:HIS:CE1	2.89	0.55
1:D:226:GLN:O	1:D:227:ASP:HB2	2.08	0.54
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.43	0.53
2:B:83:ASN:HD22	2:B:84:HIS:H	1.54	0.53
2:E:12:ARG:NH2	2:E:22:PHE:CD2	2.76	0.53
1:D:259:CYS:O	1:D:271:THR:HA	2.09	0.53
1:D:226:GLN:O	1:D:227:ASP:CB	2.57	0.53
2:E:22:PHE:CE1	2:E:69:GLU:HG2	2.43	0.53
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.44	0.53
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.44	0.52
2:E:12:ARG:CZ	2:E:22:PHE:HD2	2.22	0.52
1:A:173:LYS:O	1:A:176:ASN:HB2	2.09	0.52
1:D:33:PHE:CD2	1:D:34:VAL:HG13	2.44	0.52
2:B:12:ARG:NH1	2:B:22:PHE:CE2	2.78	0.52
2:B:97:ARG:HH11	2:B:97:ARG:HG2	1.75	0.52
1:D:74:PHE:CD2	1:D:95:LEU:HD23	2.46	0.51
1:A:224:LEU:O	1:A:228:MET:HE3	2.11	0.51
1:A:211:ALA:HB2	1:A:241:PHE:CE2	2.45	0.51
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.45	0.51
1:D:82:LEU:HD12	1:D:87:GLN:HE21	1.76	0.51
1:A:47:PRO:HG3	1:A:60:TRP:CZ2	2.46	0.51
1:D:234:ARG:HD3	2:E:10:TYR:CE2	2.47	0.50
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.47	0.49
1:A:79:ARG:O	1:A:80:ASN:C	2.51	0.49
1:D:32:GLU:OE2	1:D:48:ARG:HD3	2.13	0.49
1:D:249:VAL:HG22	1:D:257:TYR:CZ	2.48	0.49
2:B:5:PRO:HD3	2:B:84:HIS:ND1	2.29	0.48
1:A:32:GLU:OE2	1:A:48:ARG:CD	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:LEU:O	2:B:78:TYR:HA	2.13	0.48
1:A:74:PHE:O	1:A:78:LEU:HB2	2.14	0.47
1:A:212:ASP:O	1:A:263:HIS:HD2	1.97	0.47
2:E:59:ASP:O	2:E:60:TRP:CB	2.62	0.47
1:A:190:THR:OG1	1:A:192:HIS:HE1	1.97	0.46
1:A:260:ARG:HD2	1:A:262:TYR:OH	2.15	0.46
2:B:27:VAL:O	2:B:27:VAL:HG23	2.15	0.46
2:B:58:LYS:CE	4:B:102:HOH:O	2.61	0.46
1:A:35:ARG:O	1:A:45:TYR:HA	2.15	0.46
1:A:35:ARG:NH2	2:B:54:LEU:O	2.36	0.46
1:D:87:GLN:NE2	1:D:118:TYR:OH	2.43	0.46
1:A:8:PHE:CD1	1:A:98:MET:HG2	2.50	0.46
1:A:159:TYR:HA	4:A:283:HOH:O	2.16	0.46
2:B:21:ASN:C	2:B:22:PHE:HD1	2.19	0.45
1:D:203:CYS:O	1:D:244:TRP:HB2	2.17	0.45
1:D:181:ARG:HG2	1:D:181:ARG:HH11	1.82	0.45
1:D:108:ARG:CB	1:D:108:ARG:HH11	2.30	0.45
1:A:31:LYS:HB3	1:A:31:LYS:HE3	1.83	0.45
1:A:144:ARG:O	1:A:148:GLU:HG3	2.16	0.45
1:A:181:ARG:NH1	1:A:209:TYR:CD2	2.85	0.45
1:A:230:LEU:C	1:A:230:LEU:CD1	2.85	0.45
1:D:39:ASP:HB3	4:D:297:HOH:O	2.16	0.45
1:D:82:LEU:HD12	1:D:87:GLN:NE2	2.32	0.44
1:D:183:ASP:HA	4:D:299:HOH:O	2.17	0.44
1:D:231:VAL:CG1	1:D:244:TRP:CZ2	3.01	0.44
1:A:54:GLN:H	1:A:54:GLN:HG3	1.59	0.44
1:D:1:GLY:N	1:D:2:PRO:HD2	2.32	0.44
2:B:11:SER:OG	2:B:13:HIS:O	2.21	0.44
1:D:231:VAL:HG11	1:D:244:TRP:CZ2	2.53	0.44
1:D:81:LEU:O	1:D:82:LEU:C	2.56	0.44
1:A:255:GLN:NE2	1:A:274:TRP:O	2.51	0.43
1:A:8:PHE:CE1	1:A:98:MET:HG2	2.53	0.43
1:D:51:TRP:CZ3	1:D:52:MET:SD	3.11	0.43
1:A:180:LEU:O	1:A:181:ARG:C	2.57	0.43
1:A:272:LEU:HD23	1:A:272:LEU:N	2.33	0.43
2:E:12:ARG:HG2	2:E:13:HIS:ND1	2.30	0.43
2:B:74:GLU:HG2	4:B:104:HOH:O	2.18	0.43
1:D:31:LYS:HE2	1:D:178:THR:CG2	2.46	0.42
2:E:71:THR:HA	2:E:72:PRO:HD2	1.94	0.42
2:B:91:LYS:HA	4:B:112:HOH:O	2.18	0.42
1:D:128:GLU:O	1:D:130:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:GLU:OE1	1:A:22:TYR:OH	2.28	0.42
1:A:209:TYR:CD1	1:A:210:PRO:HA	2.54	0.42
1:A:111:ARG:HG3	1:A:128:GLU:HG2	2.02	0.42
1:A:234:ARG:NH2	2:B:99:MET:OXT	2.52	0.42
1:D:208:PHE:O	1:D:240:THR:HB	2.20	0.42
1:D:185:PRO:HD3	1:D:263:HIS:ND1	2.35	0.41
2:B:58:LYS:HE3	4:B:102:HOH:O	2.19	0.41
1:A:228:MET:HE3	1:A:228:MET:HB2	1.88	0.41
1:D:1:GLY:C	1:D:105:SER:HB3	2.41	0.41
1:A:263:HIS:O	1:A:266:LEU:HB2	2.20	0.41
1:D:35:ARG:NH2	2:E:54:LEU:O	2.37	0.41
1:A:120:GLY:C	2:B:1:ILE:CG2	2.89	0.41
2:E:12:ARG:HD2	2:E:13:HIS:CE1	2.55	0.41
1:D:108:ARG:CG	1:D:108:ARG:HH11	2.33	0.41
2:B:71:THR:HA	2:B:72:PRO:HD2	1.94	0.41
1:D:6:ARG:NH2	1:D:113:TYR:CE1	2.89	0.41
1:A:205:ALA:O	1:A:206:LEU:HD23	2.19	0.41
2:E:21:ASN:C	2:E:22:PHE:HD1	2.23	0.41
1:D:58:GLU:O	1:D:62:ARG:HD2	2.19	0.41
1:A:127:ASN:HB2	1:A:129:ASP:OD1	2.20	0.41
1:A:234:ARG:HD2	1:A:242:GLN:HB2	2.01	0.41
1:D:1:GLY:N	1:D:2:PRO:CD	2.84	0.41
1:D:184:SER:HB3	1:D:266:LEU:HD13	2.03	0.41
2:B:3:ARG:HH22	2:B:59:ASP:CG	2.24	0.40
1:D:258:THR:HG22	1:D:273:ARG:HD3	2.03	0.40
1:D:54:GLN:HG3	1:D:54:GLN:H	1.64	0.40
1:A:152:ALA:HA	3:C:6:PHE:HD2	1.86	0.40
2:B:13:HIS:HB3	2:B:14:PRO:HD2	2.02	0.40
1:D:111:ARG:HG3	1:D:128:GLU:HG2	2.04	0.40
2:B:1:ILE:HG21	2:B:1:ILE:HD13	1.72	0.40
1:A:211:ALA:HB2	1:A:241:PHE:CD2	2.56	0.40
1:D:82:LEU:HD11	1:D:93:HIS:NE2	2.37	0.40
2:B:70:PHE:HD2	2:B:78:TYR:CZ	2.39	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	273/276 (99%)	253 (93%)	15 (6%)	5 (2%)	11 27
1	D	274/276 (99%)	246 (90%)	26 (10%)	2 (1%)	26 55
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100 100
2	E	97/100 (97%)	91 (94%)	6 (6%)	0	100 100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100 100
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100 100
All	All	756/770 (98%)	697 (92%)	52 (7%)	7 (1%)	21 49

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	THR
1	A	17	LEU
1	D	17	LEU
1	A	136	ALA
1	A	80	ASN
1	A	90	GLY
1	D	136	ALA

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	234/234 (100%)	210 (90%)	24 (10%)	9 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	234/234 (100%)	207 (88%)	27 (12%)	7 16
2	B	95/95 (100%)	86 (90%)	9 (10%)	11 24
2	E	94/95 (99%)	81 (86%)	13 (14%)	4 10
3	C	7/7 (100%)	6 (86%)	1 (14%)	4 10
3	F	7/7 (100%)	7 (100%)	0	100 100
All	All	671/672 (100%)	597 (89%)	74 (11%)	8 18

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	17	LEU
1	A	39	ASP
1	A	44	ARG
1	A	54	GLN
1	A	78	LEU
1	A	108	ARG
1	A	110	LEU
1	A	114	LEU
1	A	121	ARG
1	A	141	GLN
1	A	191	HIS
1	A	196	LYS
1	A	202	ARG
1	A	224	LEU
1	A	225	THR
1	A	228	MET
1	A	234	ARG
1	A	251	LEU
1	A	254	GLU
1	A	264	GLU
1	A	266	LEU
1	A	272	LEU
1	A	273	ARG
2	B	0	MET
2	B	13	HIS
2	B	20	SER
2	B	45	ARG
2	B	51	HIS
2	B	58	LYS

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Mol	Chain	Res	Type
2	B	70	PHE
2	B	83	ASN
2	B	97	ARG
3	C	6	PHE
1	D	14	ARG
1	D	17	LEU
1	D	39	ASP
1	D	54	GLN
1	D	78	LEU
1	D	108	ARG
1	D	110	LEU
1	D	114	LEU
1	D	141	GLN
1	D	170	ARG
1	D	173	LYS
1	D	193	PRO
1	D	194	ARG
1	D	195	SER
1	D	196	LYS
1	D	202	ARG
1	D	224	LEU
1	D	225	THR
1	D	226	GLN
1	D	227	ASP
1	D	230	LEU
1	D	234	ARG
1	D	251	LEU
1	D	254	GLU
1	D	266	LEU
1	D	272	LEU
1	D	275	GLU
2	E	1	ILE
2	E	9	VAL
2	E	20	SER
2	E	33	SER
2	E	36	GLU
2	E	47	GLU
2	E	48	LYS
2	E	58	LYS
2	E	70	PHE
2	E	81	ARG
2	E	83	ASN

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Mol	Chain	Res	Type
2	E	91	LYS
2	E	97	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	97	GLN
1	A	192	HIS
2	B	2	GLN
2	B	13	HIS
2	B	83	ASN
2	B	89	GLN
3	C	5	ASN
1	D	87	GLN
1	D	97	GLN
1	D	155	HIS
1	D	191	HIS
2	E	2	GLN
2	E	13	HIS
2	E	83	ASN
2	E	89	GLN
3	F	5	ASN

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	275/276 (99%)	-0.00	9 (3%) 50 50	8, 16, 26, 37	0
1	D	276/276 (100%)	0.37	21 (7%) 17 15	9, 16, 26, 39	0
2	B	100/100 (100%)	-0.21	0 100 100	11, 17, 24, 59	0
2	E	99/100 (99%)	0.08	2 (2%) 68 69	11, 17, 24, 47	0
3	C	9/9 (100%)	0.85	0 100 100	15, 16, 18, 24	0
3	F	9/9 (100%)	1.95	4 (44%) 0 0	15, 16, 18, 25	0
All	All	768/770 (99%)	0.15	36 (4%) 35 34	8, 16, 26, 59	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	178	THR	5.6
1	D	177	ALA	5.2
1	D	276	PRO	4.8
1	D	220	ASN	4.4
1	D	227	ASP	4.0
1	A	178	THR	3.9
1	D	180	LEU	3.6
1	D	256	ASN	3.4
3	F	9	MET	3.1
3	F	1	LYS	3.1
1	A	203	CYS	3.1
3	F	4	TYR	3.1
2	E	88	SER	3.0
1	D	193	PRO	3.0
1	A	180	LEU	2.7
1	A	16	GLY	2.7
1	A	170	ARG	2.6
1	D	181	ARG	2.5
1	D	179	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	176	ASN	2.4
1	D	1	GLY	2.3
1	D	222	GLU	2.3
1	D	205	ALA	2.3
1	A	17	LEU	2.3
1	A	227	ASP	2.3
1	D	225	THR	2.3
1	D	19	GLU	2.2
1	D	121	ARG	2.2
1	A	177	ALA	2.2
3	F	2	ALA	2.2
1	D	53	GLU	2.2
1	D	199	VAL	2.2
1	D	273	ARG	2.1
1	D	196	LYS	2.1
1	D	255	GLN	2.1
2	E	22	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates 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.