Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 11:53 PM EDT

PDB ID	:	5W6A
Title	:	HLA-C*06:02 presenting ARTELYRSL
Authors	:	Mobbs, J.I.; Vivian, J.P.; Rossjohn, J.
Deposited on	:	2017-06-16
Resolution	:	1.74 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:

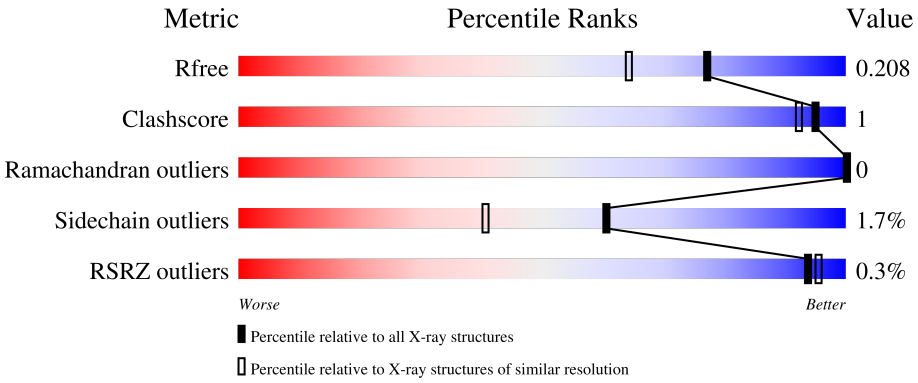
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	276	% 84% 13%
1	C	276	85% 14%
2	B	100	87% 12%
2	D	100	87% 12%
3	E	9	78% 11% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	9	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7031 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, Cw-6 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2221	1384	408	423	6			
1	C	273	Total	C	N	O	S	0	0	0
			2235	1392	410	427	6			

- 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
			817	520	138	155	4			
2	D	100	Total	C	N	O	S	0	0	0
			817	520	138	155	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
D	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called ALA-ARG-THR-GLU-LEU-TYR-ARG-SER-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	9	Total	C	N	O	0	0	0
			78	48	15	15			
3	F	9	Total	C	N	O	0	0	0
			78	48	15	15			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	292	Total	O	0	0
			292	292		

Continued on next page...

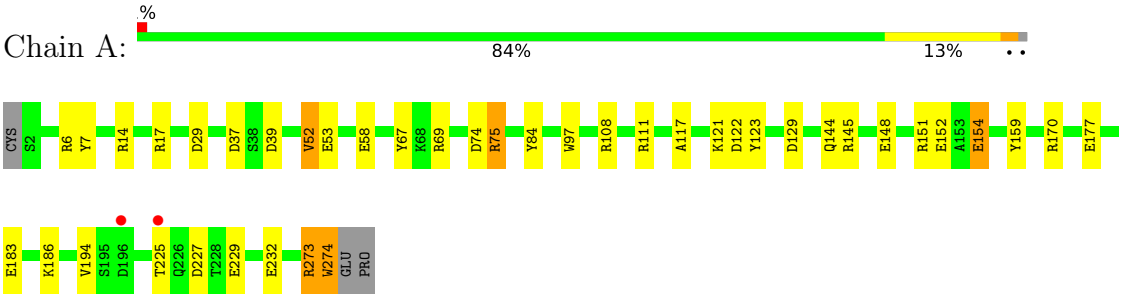
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	107	Total O 107 107	0	0
4	C	268	Total O 268 268	0	0
4	D	100	Total O 100 100	0	0
4	E	9	Total O 9 9	0	0
4	F	9	Total O 9 9	0	0

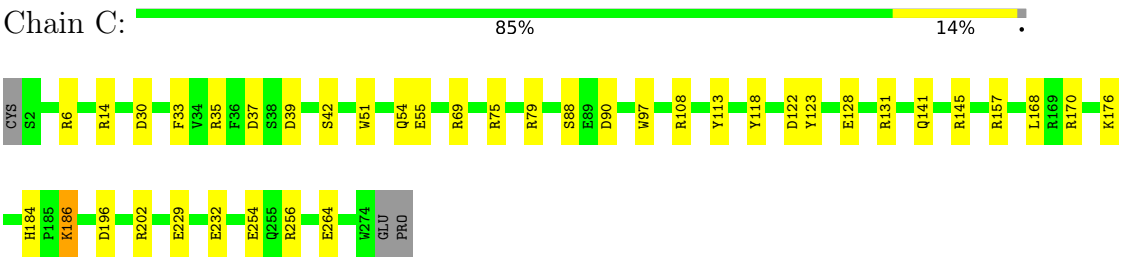
3 Residue-property plots (i)

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.

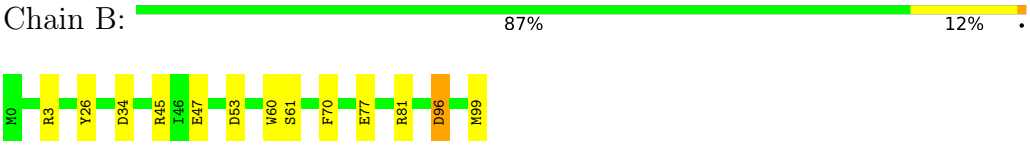
• Molecule 1: HLA class I histocompatibility antigen, Cw-6 alpha chain



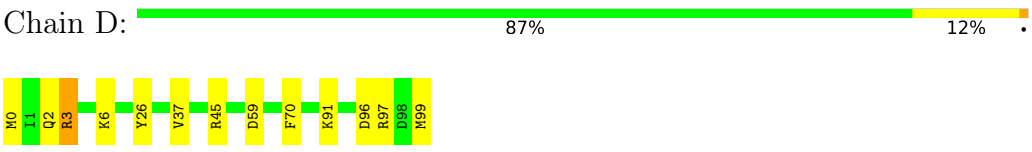
• Molecule 1: HLA class I histocompatibility antigen, Cw-6 alpha chain



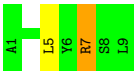
• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin

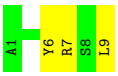


• Molecule 3: ALA-ARG-THR-GLU-LEU-TYR-ARG-SER-LEU



• Molecule 3: ALA-ARG-THR-GLU-LEU-TYR-ARG-SER-LEU

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	46.19Å 136.95Å 70.96Å 90.00° 107.06° 90.00°	Depositor
Resolution (Å)	68.47 – 1.74 44.16 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.5 (68.47-1.74) 99.6 (44.16-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.161 , 0.201 0.171 , 0.208	Depositor DCC
R_{free} test set	4391 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	20.1	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7031	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.16% 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, 0.333 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	1.42	16/2285 (0.7%)	1.44	36/3108 (1.2%)
1	C	1.43	11/2299 (0.5%)	1.31	23/3126 (0.7%)
2	B	1.29	3/840 (0.4%)	1.23	7/1140 (0.6%)
2	D	1.22	0/840	1.28	10/1140 (0.9%)
3	E	1.92	1/78 (1.3%)	1.70	1/102 (1.0%)
3	F	1.78	1/78 (1.3%)	1.37	1/102 (1.0%)
All	All	1.40	32/6420 (0.5%)	1.35	78/8718 (0.9%)

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

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5	LEU	C-O	8.23	1.39	1.23
1	C	229	GLU	CD-OE1	7.64	1.34	1.25
1	A	154	GLU	CD-OE2	7.53	1.33	1.25
1	A	229	GLU	CD-OE1	7.31	1.33	1.25
1	A	177	GLU	CD-OE1	7.14	1.33	1.25
1	A	6	ARG	NE-CZ	-6.99	1.24	1.33
1	C	254	GLU	CD-OE2	6.97	1.33	1.25
2	B	26	TYR	CE2-CZ	-6.28	1.30	1.38
1	C	88	SER	CB-OG	-6.25	1.34	1.42
1	A	159	TYR	CG-CD1	6.22	1.47	1.39
1	C	118	TYR	CG-CD1	-6.22	1.31	1.39
1	C	232	GLU	CD-OE1	6.13	1.32	1.25
1	A	274	TRP	CE3-CZ3	6.07	1.48	1.38
3	F	9	LEU	C-OXT	5.95	1.34	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	90	ASP	CB-CG	5.90	1.64	1.51
1	A	183	GLU	CD-OE2	5.85	1.32	1.25
2	B	47	GLU	CG-CD	5.70	1.60	1.51
1	A	148	GLU	CD-OE1	5.66	1.31	1.25
1	A	154	GLU	CG-CD	5.63	1.60	1.51
1	A	123	TYR	CE1-CZ	5.62	1.45	1.38
1	C	113	TYR	CB-CG	-5.62	1.43	1.51
1	A	145	ARG	CZ-NH2	5.60	1.40	1.33
1	A	53	GLU	CD-OE1	5.41	1.31	1.25
1	A	232	GLU	CD-OE2	5.33	1.31	1.25
2	B	61	SER	CB-OG	-5.31	1.35	1.42
1	C	55	GLU	CD-OE1	-5.30	1.19	1.25
1	A	183	GLU	CD-OE1	5.30	1.31	1.25
1	C	196	ASP	C-O	5.15	1.33	1.23
1	C	123	TYR	CE1-CZ	5.10	1.45	1.38
1	C	264	GLU	CG-CD	5.09	1.59	1.51
1	A	84	TYR	CE1-CZ	-5.07	1.31	1.38
1	A	7	TYR	CG-CD2	-5.05	1.32	1.39

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	145	ARG	NE-CZ-NH1	-13.63	113.49	120.30
1	A	129	ASP	CB-CG-OD1	13.30	130.27	118.30
1	C	256	ARG	NE-CZ-NH1	12.18	126.39	120.30
1	C	170	ARG	NE-CZ-NH1	11.73	126.16	120.30
1	A	152	GLU	OE1-CD-OE2	9.74	134.99	123.30
2	B	34	ASP	CB-CG-OD1	9.62	126.96	118.30
1	A	151	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	C	108	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	A	129	ASP	CB-CG-OD2	-8.97	110.23	118.30
2	D	6	LYS	CD-CE-NZ	8.89	132.15	111.70
1	A	37	ASP	CB-CG-OD1	8.64	126.08	118.30
1	A	37	ASP	CB-CG-OD2	-8.53	110.62	118.30
1	A	194	VAL	CB-CA-C	-8.29	95.65	111.40
1	A	108	ARG	NE-CZ-NH1	8.25	124.42	120.30
2	B	81	ARG	NE-CZ-NH1	8.21	124.40	120.30
2	D	45	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	A	273	ARG	NE-CZ-NH1	8.03	124.31	120.30
2	B	45	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	170	ARG	NE-CZ-NH1	-7.99	116.30	120.30
1	A	69	ARG	NE-CZ-NH1	7.97	124.28	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	37	ASP	CB-CG-OD2	-7.85	111.23	118.30
1	A	14	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	C	37	ASP	CB-CG-OD1	7.77	125.30	118.30
1	A	151	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	C	39	ASP	CB-CG-OD1	7.71	125.24	118.30
2	D	99	MET	CG-SD-CE	7.49	112.19	100.20
1	A	75	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	111	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	39	ASP	CB-CG-OD1	7.35	124.91	118.30
1	A	6	ARG	NE-CZ-NH1	-7.19	116.71	120.30
1	C	157	ARG	NE-CZ-NH1	-7.02	116.79	120.30
2	D	3	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	A	69	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	A	75	ARG	CG-CD-NE	-6.77	97.59	111.80
1	A	14	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	C	35	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	A	67	TYR	CB-CG-CD2	-6.59	117.05	121.00
1	A	152	GLU	CG-CD-OE1	-6.53	105.24	118.30
2	D	45	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	C	108	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	58	GLU	OE1-CD-OE2	6.39	130.97	123.30
1	A	186	LYS	CD-CE-NZ	6.37	126.34	111.70
1	C	256	ARG	NE-CZ-NH2	-6.26	117.17	120.30
2	D	91	LYS	CD-CE-NZ	6.22	126.02	111.70
1	C	186	LYS	CD-CE-NZ	6.18	125.91	111.70
1	A	29	ASP	CB-CG-OD1	-6.15	112.77	118.30
1	A	74	ASP	CB-CG-OD1	6.15	123.83	118.30
1	C	30	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	A	17	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	A	227	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	273	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	52	VAL	CG1-CB-CG2	5.92	120.37	110.90
2	B	34	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	C	168	LEU	CB-CG-CD2	-5.79	101.16	111.00
1	C	202	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	84	TYR	CZ-CE2-CD2	-5.77	114.61	119.80
1	C	79	ARG	NE-CZ-NH2	5.70	123.15	120.30
2	B	53	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	145	ARG	NH1-CZ-NH2	5.54	125.50	119.40
1	C	128	GLU	OE1-CD-OE2	5.40	129.78	123.30
1	A	108	ARG	NE-CZ-NH2	-5.37	117.61	120.30
3	E	5	LEU	CB-CA-C	-5.37	100.01	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	122	ASP	CB-CG-OD1	5.32	123.09	118.30
1	C	14	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	C	170	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	229	GLU	CG-CD-OE2	-5.28	107.74	118.30
2	B	45	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	69	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	75	ARG	NE-CZ-NH2	-5.23	117.69	120.30
2	D	26	TYR	CZ-CE2-CD2	-5.23	115.09	119.80
2	D	3	ARG	NE-CZ-NH1	-5.21	117.69	120.30
3	F	6	TYR	CB-CG-CD1	-5.15	117.91	121.00
2	D	96	ASP	CB-CG-OD1	5.14	122.93	118.30
1	C	131	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	122	ASP	CB-CG-OD1	5.08	122.88	118.30
1	C	6	ARG	CG-CD-NE	-5.07	101.15	111.80
2	B	96	ASP	CB-CG-OD1	5.05	122.84	118.30
2	D	97	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	GLN	Sidechain
1	A	75	ARG	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	2221	0	2049	3	0
1	C	2235	0	2072	5	0
2	B	817	0	762	4	0
2	D	817	0	762	3	0
3	E	78	0	82	1	0
3	F	78	0	82	0	0
4	A	292	0	0	0	0
4	B	107	0	0	2	0
4	C	268	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	100	0	0	1	0
4	E	9	0	0	0	0
4	F	9	0	0	0	0
All	All	7031	0	5809	14	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 1.

All (14) 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:C:184:HIS:ND1	4:C:302:HOH:O	2.24	0.70
1:A:273:ARG:HG2	1:A:274:TRP:N	2.13	0.62
2:B:77:GLU:HG2	4:B:160:HOH:O	2.06	0.54
2:B:3:ARG:NE	4:B:103:HOH:O	2.43	0.52
2:D:37:VAL:O	4:D:101:HOH:O	2.19	0.50
1:C:141:GLN:O	1:C:145:ARG:HG2	2.14	0.48
1:C:54:GLN:H	1:C:54:GLN:CD	2.17	0.47
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.53	0.44
2:B:96:ASP:HB3	2:B:99:MET:HE2	1.98	0.44
2:D:3:ARG:NH1	2:D:59:ASP:OD2	2.52	0.43
1:A:97:TRP:CZ2	3:E:7:ARG:HG2	2.55	0.42
1:C:176:LYS:HE2	4:C:308:HOH:O	2.21	0.41
2:D:0:MET:CE	2:D:2:GLN:HE21	2.34	0.40
1:C:33:PHE:HB3	1:C:51:TRP:CH2	2.56	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	271/276 (98%)	267 (98%)	4 (2%)	0	100	100
1	C	271/276 (98%)	266 (98%)	5 (2%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	D	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	E	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	752/770 (98%)	741 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	224/233 (96%)	220 (98%)	4 (2%)	59	38
1	C	228/233 (98%)	225 (99%)	3 (1%)	69	52
2	B	90/95 (95%)	89 (99%)	1 (1%)	73	59
2	D	90/95 (95%)	89 (99%)	1 (1%)	73	59
3	E	8/8 (100%)	7 (88%)	1 (12%)	4	0
3	F	8/8 (100%)	7 (88%)	1 (12%)	4	0
All	All	648/672 (96%)	637 (98%)	11 (2%)	60	41

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	121	LYS
1	A	154	GLU
1	A	225	THR
2	B	70	PHE
1	C	42	SER
1	C	97	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	186	LYS
2	D	70	PHE
3	E	7	ARG
3	F	7	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	2	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	273/276 (98%)	-0.34	2 (0%) 87 91	11, 23, 41, 60	4 (1%)
1	C	273/276 (98%)	-0.25	0 100 100	12, 24, 41, 51	0
2	B	100/100 (100%)	-0.33	0 100 100	12, 29, 49, 57	0
2	D	100/100 (100%)	-0.22	0 100 100	13, 29, 49, 54	0
3	E	9/9 (100%)	-0.47	0 100 100	14, 19, 22, 32	0
3	F	9/9 (100%)	-0.45	0 100 100	15, 19, 25, 32	0
All	All	764/770 (99%)	-0.29	2 (0%) 94 95	11, 24, 46, 60	4 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	ASP	3.1
1	A	225	THR	2.4

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.