



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:44 PM UTC

PDB ID : 2F74 / pdb_00002f74
Title : Murine MHC class I H-2Db in complex with human b2-microglobulin and LCMV-derived immunodominant 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

<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:

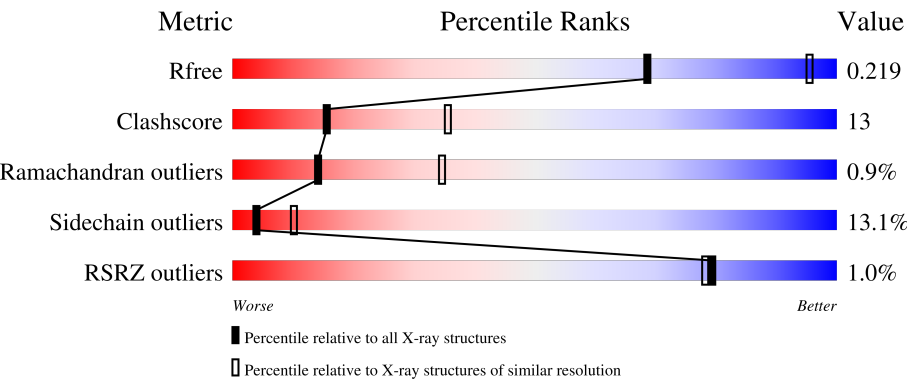
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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 $\leq 5\%$. 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	60%33%5%.
1	D	276	% 59%34%6%
2	B	100	63%28%9%
2	E	100	% 68%27%. .
3	C	9	11% 89%11%

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Mol	Chain	Length	Quality of chain
3	F	9	33% 78% 22%

2 Entry composition [i](#)

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			

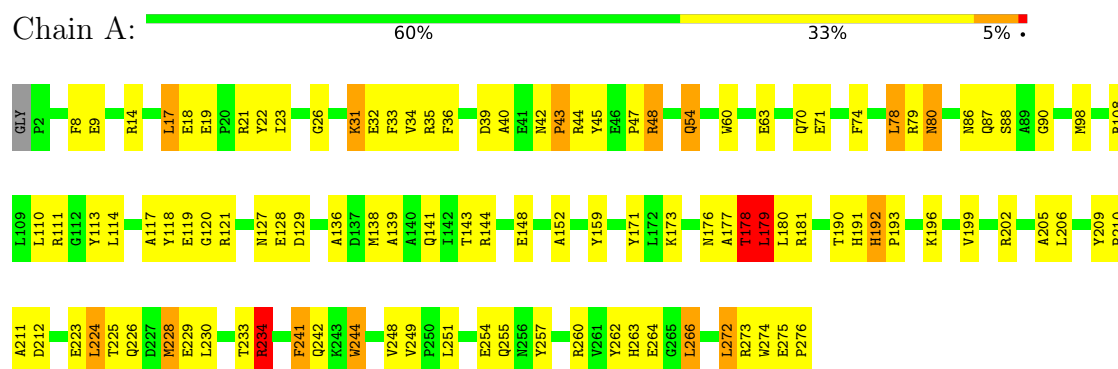
- Molecule 4 is water.

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

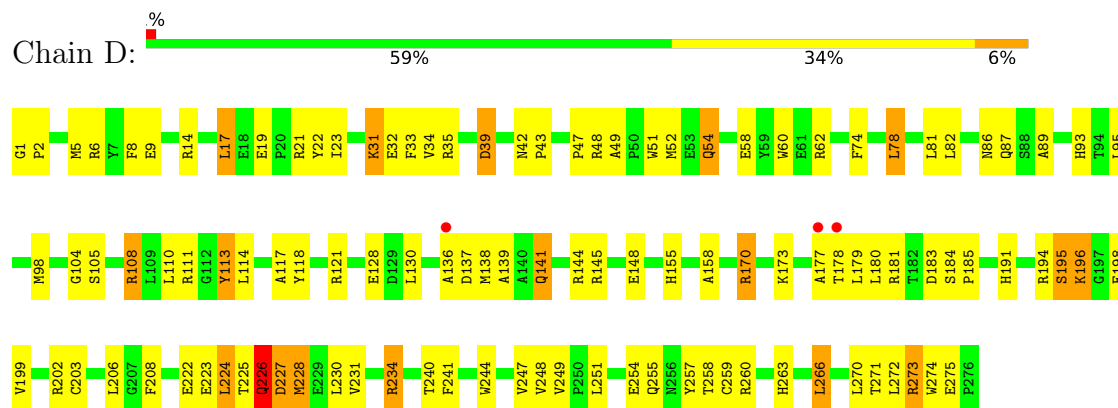
3 Residue-property plots

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.

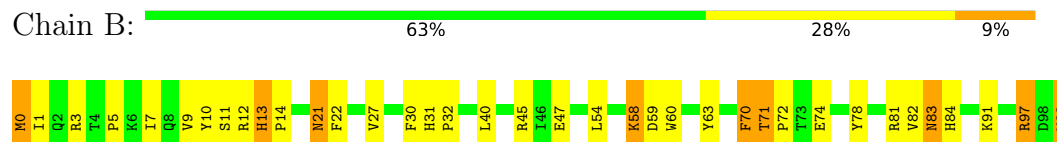
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



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- Molecule 2: Beta-2-microglobulin

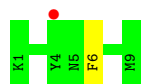
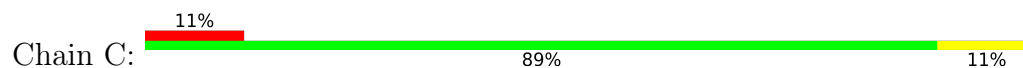


- Molecule 2: Beta-2-microglobulin

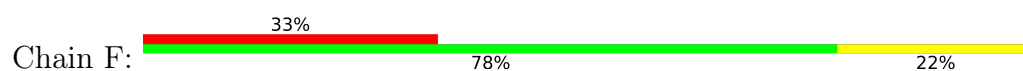




- Molecule 3: NONAMERIC PEPTIDE, GP33, DERIVED FROM LYMPHOCYTIC CHORIOMENINGITIS VIRUS



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



4 Data and refinement statistics

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 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.5 (30.00-2.70) 92.4 (30.00-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.698	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	16/2328 (0.7%)	1.28	10/3160 (0.3%)
1	D	1.34	12/2332 (0.5%)	1.24	13/3166 (0.4%)
2	B	1.45	2/860 (0.2%)	1.38	5/1162 (0.4%)
2	E	1.34	2/852 (0.2%)	1.32	3/1152 (0.3%)
3	C	1.43	0/74	1.11	0/97
3	F	1.66	1/74 (1.4%)	1.43	0/97
All	All	1.39	33/6520 (0.5%)	1.29	31/8834 (0.4%)

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 (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	PHE	CE1-CZ	-9.19	1.11	1.38
1	D	113	TYR	CG-CD2	-9.15	1.20	1.39
1	A	241	PHE	CE2-CZ	-8.48	1.13	1.38
1	A	241	PHE	CG-CD2	-8.43	1.21	1.38
1	D	5	MET	SD-CE	-8.34	1.58	1.79
1	D	113	TYR	CG-CD1	-8.22	1.22	1.39
1	D	113	TYR	CE1-CZ	-8.14	1.18	1.38
1	D	241	PHE	CE2-CZ	-8.10	1.14	1.38
1	A	113	TYR	CG-CD2	-8.08	1.22	1.39
1	D	138	MET	SD-CE	7.89	1.99	1.79
1	A	113	TYR	CE2-CZ	-7.60	1.20	1.38
1	D	241	PHE	CE1-CZ	-7.57	1.16	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	TYR	CG-CD1	-7.34	1.24	1.39
2	E	58	LYS	CD-CE	7.20	1.74	1.52
2	B	99	MET	CG-SD	-7.18	1.62	1.80
1	D	113	TYR	CE2-CZ	-7.17	1.21	1.38
1	A	241	PHE	CG-CD1	-7.11	1.24	1.38
1	D	241	PHE	CG-CD1	-6.96	1.24	1.38
1	A	113	TYR	CE1-CZ	-6.73	1.22	1.38
1	A	138	MET	CG-SD	6.69	1.97	1.80
1	A	244	TRP	C-O	-6.45	1.15	1.23
1	D	241	PHE	CG-CD2	-6.30	1.25	1.38
3	F	9	MET	SD-CE	-6.09	1.64	1.79
1	A	234	ARG	CA-C	-5.79	1.46	1.52
1	A	178	THR	CA-C	5.67	1.60	1.52
1	A	178	THR	CA-CB	5.55	1.62	1.53
1	A	233	THR	C-O	-5.46	1.17	1.23
2	B	71	THR	CA-CB	-5.41	1.45	1.53
2	E	8	GLN	CA-C	-5.40	1.46	1.52
1	A	26	GLY	CA-C	-5.39	1.48	1.52
1	D	49	ALA	CA-CB	-5.38	1.46	1.54
1	D	177	ALA	CA-CB	5.23	1.59	1.53
1	A	18	GLU	N-CA	5.02	1.52	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	226	GLN	OE1-CD-NE2	-9.64	112.96	122.60
1	A	226	GLN	OE1-CD-NE2	-9.31	113.29	122.60
1	D	19	GLU	CA-C-O	7.80	125.09	119.32
2	B	47	GLU	N-CA-C	6.88	118.56	111.14
1	A	226	GLN	CG-CD-NE2	6.74	126.51	116.40
1	D	226	GLN	CG-CD-NE2	6.63	126.35	116.40
1	A	139	ALA	N-CA-C	6.57	118.10	111.07
2	E	51	HIS	N-CA-C	6.52	119.08	109.24
1	A	19	GLU	CA-C-O	6.22	123.93	119.32
1	D	206	LEU	N-CA-C	6.22	119.33	109.50
1	D	121	ARG	CB-CA-C	-6.20	99.57	109.80
2	B	82	VAL	N-CA-C	6.19	116.75	108.27
2	E	76	ASP	N-CA-C	6.14	119.91	110.20
1	D	43	PRO	CB-CA-C	-6.05	103.31	111.12
1	A	179	LEU	CA-C-N	5.89	128.98	120.38
1	A	179	LEU	C-N-CA	5.89	128.98	120.38
1	D	42	ASN	CA-C-N	5.88	126.21	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	42	ASN	C-N-CA	5.88	126.21	119.92
2	B	21	ASN	N-CA-C	-5.74	100.67	108.24
1	D	158	ALA	N-CA-C	-5.67	105.01	111.14
2	B	7	ILE	CB-CA-C	-5.59	102.52	110.12
2	E	21	ASN	N-CA-C	-5.59	101.41	108.45
1	D	139	ALA	N-CA-C	5.56	117.02	111.07
1	A	171	TYR	N-CA-C	-5.46	105.87	112.54
1	D	137	ASP	OD1-CG-OD2	-5.41	109.92	122.90
1	A	43	PRO	N-CA-C	5.25	119.33	111.14
1	A	192	HIS	CB-CA-C	-5.20	103.84	111.01
1	D	104	GLY	N-CA-C	-5.18	104.39	112.58
1	A	88	SER	N-CA-C	5.12	117.90	109.76
2	B	63	TYR	N-CA-C	5.04	117.04	109.23
1	D	170	ARG	CB-CA-C	-5.00	102.81	110.81

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	57	0
1	D	2265	0	2136	61	0
2	B	837	0	803	34	0
2	E	829	0	794	23	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6419	0	6012	165	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 (165) 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
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
1:A:230:LEU:HD12	1:A:230:LEU:C	2.19	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:B:31:HIS:ND1	2:B:32:PRO:HA	2.11	0.66
2:E:12:ARG:NH2	2:E:22:PHE:HD2	1.93	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:HG23	2:B:1:ILE:O	1.98	0.63
1:D:8:PHE:CD1	1:D:98:MET:HG2	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:59:ASP:O	2:E:60:TRP:HB2	2.00	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
1:A:224:LEU:O	1:A: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
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:59:ASP:O	2:B:60:TRP:HB2	2.04	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:D:224:LEU:O	1:D:228:MET:HE3	2.07	0.54
1:A:79:ARG:O	1:A:80:ASN:C	2.51	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
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.44	0.53
2:E:22:PHE:CE1	2:E:69:GLU:HG2	2.43	0.53
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.44	0.52
1:D:9:GLU:OE1	1:D:22:TYR:OH	2.28	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:A:9:GLU:OE1	1:A:22:TYR:OH	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:PHE:CD2	1:D:95:LEU:HD23	2.46	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:A:47:PRO:HG3	1:A:60:TRP:CZ2	2.46	0.51
1:D:82:LEU:HD12	1:D:87:GLN:HE21	1.76	0.51
2:B:21:ASN:C	2:B:22:PHE:HD1	2.19	0.50
1:A:230:LEU:C	1:A:230:LEU:CD1	2.85	0.50
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: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
1:D:81:LEU:O	1:D:82:LEU:C	2.56	0.48
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
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
1:A:180:LEU:O	1:A:181:ARG:C	2.57	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:1:GLY:C	1:D:105:SER:HB3	2.41	0.46
1:A:120:GLY:C	2:B:1:ILE:CG2	2.89	0.46
1:A:8:PHE:CD1	1:A:98:MET:HG2	2.50	0.46
1:D:87:GLN:NE2	1:D:118:TYR:OH	2.43	0.46
2:E:21:ASN:C	2:E:22:PHE:HD1	2.23	0.46
1:A:159:TYR:HA	4:A:283:HOH:O	2.16	0.46
2:B:11:SER:OG	2:B:13:HIS:O	2.21	0.45
2:B:3:ARG:HH22	2:B:59:ASP:CG	2.24	0.45
1:D:181:ARG:HH11	1:D:181:ARG:HG2	1.82	0.45
1:D:203:CYS:O	1:D:244:TRP:HB2	2.17	0.45
1:D:108:ARG:HH11	1:D:108:ARG:CB	2.30	0.45
1:A:31:LYS:HE3	1:A:31:LYS:HB3	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:275:GLU:C	1:A:276:PRO:O	2.59	0.45
1:D:39:ASP:HB3	4:D:297:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:231:VAL:HG11	1:D:244:TRP:CZ2	2.53	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:272:LEU:N	1:A:272:LEU:HD23	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
1:A:70:GLN:O	1:A:71:GLU:C	2.62	0.42
1:A:209:TYR:CD1	1:A:210:PRO:HA	2.54	0.42
2:E:4:THR:O	2:E:5:PRO:C	2.62	0.42
2:E:16:GLU:O	2:E:17:ASN:C	2.61	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:A:275:GLU:O	1:A:276:PRO:C	2.62	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: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:205:ALA:O	1:A:206:LEU:HD23	2.19	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:D:108:ARG:HH11	1:D:108:ARG:CG	2.33	0.41
2:E:12:ARG:HD2	2:E:13:HIS:CE1	2.55	0.41
1:D:58:GLU:O	1:D:62:ARG:HD2	2.19	0.41
1:D:228:MET:HE2	1:D:228:MET:HB2	1.75	0.41
1:A:127:ASN:HB2	1:A:129:ASP:OD1	2.20	0.41
1:A:36:PHE:CD1	1:A:36:PHE:C	2.99	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
1:D:195:SER:O	1:D:196:LYS:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:GLN:H	1:D:54:GLN:HG3	1.64	0.40
1:D:258:THR:HG22	1:D:273:ARG:HD3	2.03	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
1:A:211:ALA:HB2	1:A:241:PHE:CD2	2.56	0.40
2:B:1:ILE:HD13	2:B:1:ILE:HG21	1.72	0.40
2:B:70:PHE:HD2	2:B:78:TYR:CZ	2.39	0.40
1:D:82:LEU:HD11	1:D:93:HIS:NE2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	6	18
1	D	274/276 (99%)	246 (90%)	26 (10%)	2 (1%)	18	41
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%)	14	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	THR
1	A	17	LEU
1	D	17	LEU

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Mol	Chain	Res	Type
1	A	136	ALA
1	A	80	ASN
1	A	90	GLY
1	D	136	ALA

5.3.2 Protein sidechains ⓘ

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%)	203 (87%)	31 (13%)	4	10
1	D	234/234 (100%)	198 (85%)	36 (15%)	2	7
2	B	95/95 (100%)	86 (90%)	9 (10%)	8	20
2	E	94/95 (99%)	82 (87%)	12 (13%)	4	11
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	7 (100%)	0	100	100
All	All	671/672 (100%)	583 (87%)	88 (13%)	4	10

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	17	LEU
1	A	31	LYS
1	A	39	ASP
1	A	42	ASN
1	A	44	ARG
1	A	48	ARG
1	A	54	GLN
1	A	78	LEU
1	A	86	ASN
1	A	108	ARG
1	A	110	LEU
1	A	114	LEU
1	A	121	ARG

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Mol	Chain	Res	Type
1	A	141	GLN
1	A	143	THR
1	A	179	LEU
1	A	191	HIS
1	A	196	LYS
1	A	223	GLU
1	A	224	LEU
1	A	225	THR
1	A	228	MET
1	A	234	ARG
1	A	248	VAL
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	9	VAL
2	B	13	HIS
2	B	45	ARG
2	B	58	LYS
2	B	70	PHE
2	B	81	ARG
2	B	83	ASN
2	B	97	ARG
1	D	14	ARG
1	D	17	LEU
1	D	31	LYS
1	D	39	ASP
1	D	54	GLN
1	D	78	LEU
1	D	86	ASN
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	179	LEU
1	D	180	LEU
1	D	194	ARG

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Mol	Chain	Res	Type
1	D	195	SER
1	D	196	LYS
1	D	198	GLU
1	D	222	GLU
1	D	223	GLU
1	D	224	LEU
1	D	225	THR
1	D	226	GLN
1	D	227	ASP
1	D	228	MET
1	D	230	LEU
1	D	234	ARG
1	D	247	VAL
1	D	248	VAL
1	D	251	LEU
1	D	254	GLU
1	D	266	LEU
1	D	272	LEU
1	D	273	ARG
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	91	LYS
2	E	97	ARG

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

Mol	Chain	Res	Type
1	A	42	ASN
1	A	87	GLN
1	A	97	GLN
1	A	192	HIS
2	B	83	ASN
2	B	89	GLN

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Mol	Chain	Res	Type
3	C	5	ASN
1	D	87	GLN
1	D	97	GLN
1	D	155	HIS
1	D	188	HIS
1	D	191	HIS
2	E	13	HIS
2	E	83	ASN
2	E	89	GLN
3	F	5	ASN

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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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%)	-0.27	0 100 100	8, 16, 26, 37	0
1	D	276/276 (100%)	-0.19	3 (1%) 78 76	9, 16, 26, 39	0
2	B	100/100 (100%)	-0.15	0 100 100	11, 17, 24, 59	0
2	E	99/100 (99%)	-0.25	1 (1%) 79 78	11, 17, 24, 47	0
3	C	9/9 (100%)	0.66	1 (11%) 10 8	15, 16, 18, 24	0
3	F	9/9 (100%)	1.50	3 (33%) 1 1	15, 16, 18, 25	0
All	All	768/770 (99%)	-0.19	8 (1%) 79 78	8, 16, 26, 59	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	4	TYR	5.2
3	C	4	TYR	3.1
2	E	1	ILE	2.7
3	F	6	PHE	2.3
3	F	7	ALA	2.2
1	D	178	THR	2.1
1	D	136	ALA	2.1
1	D	177	ALA	2.1

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 oligosaccharides 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.