



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:52 PM GMT

PDB ID : 3TBT
Title : CRYSTAL STRUCTURE OF THE MURINE CLASS I MAJOR HISTO-COMPATIBILITY COMPLEX H-2DB IN COMPLEX WITH THE LCMV-DERIVED GP33 ALTERED PEPTIDE ligand (V3P, Y4S)
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Deposited on : 2011-08-08
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

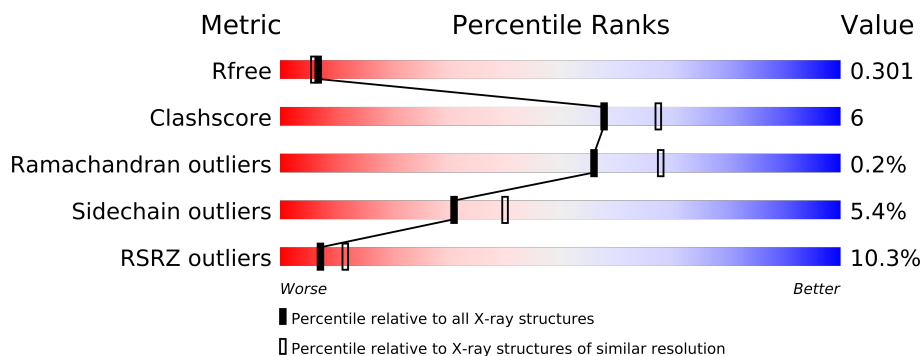
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	338	
1	D	338	
1	G	338	
1	J	338	
2	B	99	
2	E	99	
2	H	99	
2	K	99	
3	C	9	
3	F	9	
3	I	9	
3	L	9	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13045 atoms, of which 0 are hydrogen and 0 are deuterium.

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	263	Total	C	N	O	S	0	0	0
			2168	1369	384	406	9			
1	D	263	Total	C	N	O	S	0	0	0
			2170	1373	384	404	9			
1	G	269	Total	C	N	O	S	0	0	0
			2214	1399	392	414	9			
1	J	268	Total	C	N	O	S	0	0	0
			2204	1394	390	411	9			

- 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
			821	524	138	152	7			
2	E	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	H	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	K	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

- Molecule 3 is a protein called GLYCOPROTEIN G1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			66	42	11	12	1			
3	F	9	Total	C	N	O	S	0	0	0
			63	39	10	13	1			
3	I	9	Total	C	N	O	S	0	0	0
			67	42	11	13	1			
3	L	9	Total	C	N	O	S	0	0	0
			67	42	11	13	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	PRO	VAL	ENGINEERED MUTATION	UNP P07399
C	4	SER	TYR	ENGINEERED MUTATION	UNP P07399
C	9	MET	CYS	ENGINEERED MUTATION	UNP P07399
F	3	PRO	VAL	ENGINEERED MUTATION	UNP P07399
F	4	SER	TYR	ENGINEERED MUTATION	UNP P07399
F	9	MET	CYS	ENGINEERED MUTATION	UNP P07399
I	3	PRO	VAL	ENGINEERED MUTATION	UNP P07399
I	4	SER	TYR	ENGINEERED MUTATION	UNP P07399
I	9	MET	CYS	ENGINEERED MUTATION	UNP P07399
L	3	PRO	VAL	ENGINEERED MUTATION	UNP P07399
L	4	SER	TYR	ENGINEERED MUTATION	UNP P07399
L	9	MET	CYS	ENGINEERED MUTATION	UNP P07399

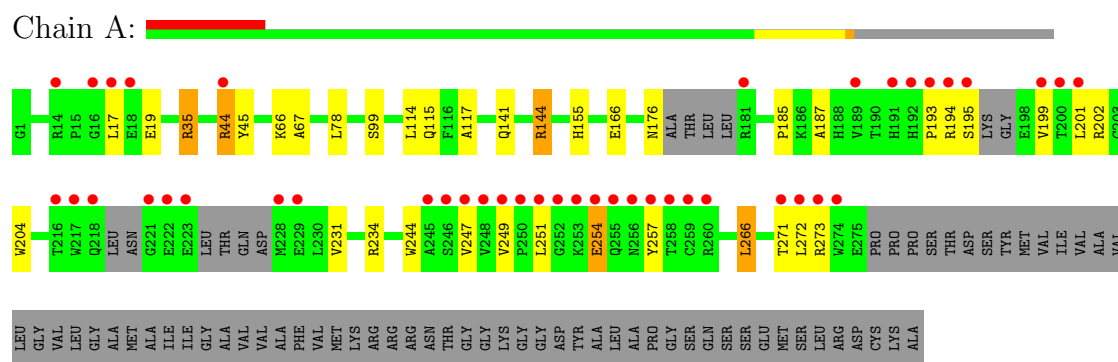
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	115	Total O 115 115	0	0
4	B	60	Total O 60 60	0	0
4	C	7	Total O 7 7	0	0
4	D	93	Total O 93 93	0	0
4	E	65	Total O 65 65	0	0
4	F	2	Total O 2 2	0	0
4	G	131	Total O 131 131	0	0
4	H	65	Total O 65 65	0	0
4	I	3	Total O 3 3	0	0
4	J	130	Total O 130 130	0	0
4	K	66	Total O 66 66	0	0
4	L	5	Total O 5 5	0	0

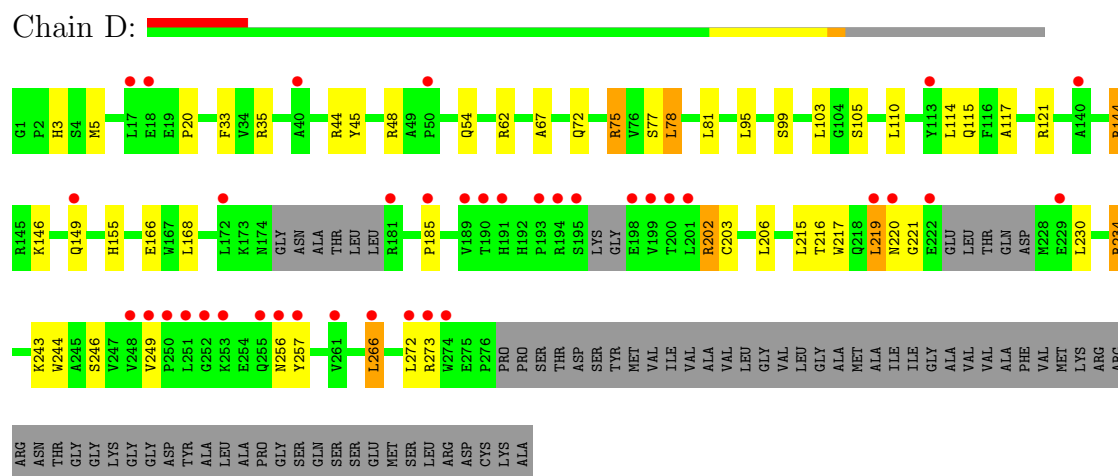
3 Residue-property plots

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.

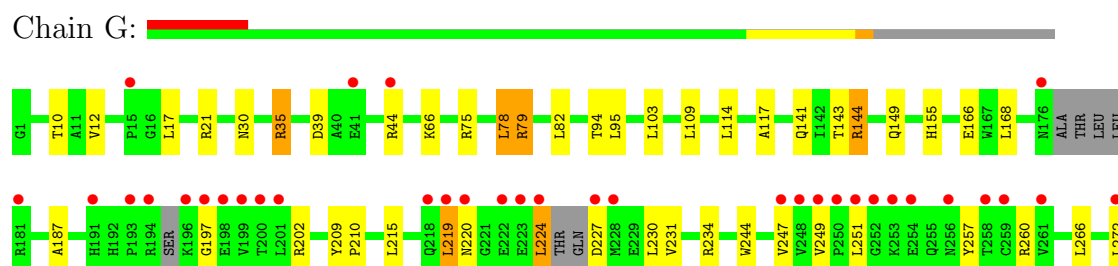
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

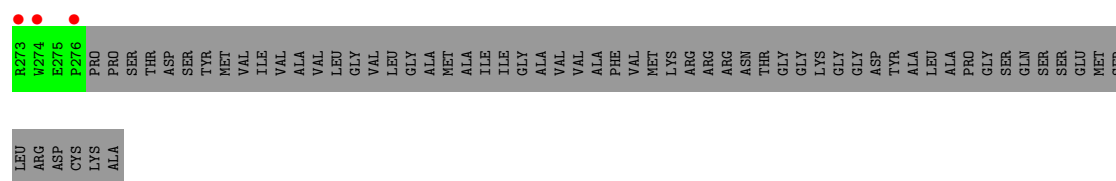


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



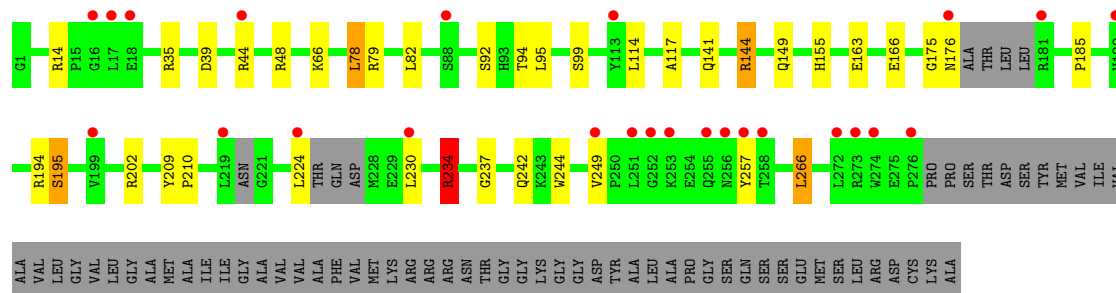
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain





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

Chain J:



- Molecule 2: Beta-2-microglobulin

Chain B:



- Molecule 2: Beta-2-microglobulin

Chain E:



- Molecule 2: Beta-2-microglobulin

Chain H:



- Molecule 2: Beta-2-microglobulin

Chain K:



- Molecule 3: GLYCOPROTEIN G1

Chain C:



- Molecule 3: GLYCOPROTEIN G1

Chain F: 



- Molecule 3: GLYCOPROTEIN G1

Chain I: 



- Molecule 3: GLYCOPROTEIN G1

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.67Å 123.80Å 99.59Å 90.00° 103.34° 90.00°	Depositor
Resolution (Å)	42.37 – 2.30 42.36 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.37-2.30) 99.5 (42.36-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.242 , 0.295 0.254 , 0.301	Depositor DCC
R_{free} test set	4821 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 96531 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13045	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.58	0/2230	0.73	3/3021 (0.1%)
1	D	0.56	0/2234	0.72	4/3030 (0.1%)
1	G	0.57	0/2278	0.74	6/3088 (0.2%)
1	J	0.55	0/2268	0.69	3/3074 (0.1%)
2	B	0.60	0/847	0.70	0/1148
2	E	0.61	0/847	0.68	0/1148
2	H	0.65	0/847	0.71	1/1148 (0.1%)
2	K	0.60	0/847	0.69	0/1148
3	C	0.81	0/67	0.84	0/89
3	F	0.68	0/64	0.73	0/85
3	I	0.90	0/68	0.77	0/89
3	L	0.72	0/68	0.76	0/89
All	All	0.59	0/12665	0.72	17/17157 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	220	ASN	N-CA-CB	-7.40	97.27	110.60
1	G	219	LEU	N-CA-C	7.29	130.67	111.00
1	D	219	LEU	N-CA-C	6.76	129.25	111.00
1	J	35	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	D	220	ASN	N-CA-CB	-6.39	99.10	110.60
1	A	144	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	35	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	G	220	ASN	N-CA-C	-6.06	94.64	111.00
1	J	35	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	D	220	ASN	N-CA-C	-5.70	95.61	111.00
1	J	234	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	A	144	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	G	35	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	35	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	H	60	TRP	CB-CA-C	-5.21	99.99	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	35	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	G	79	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2168	0	2028	26	0
1	D	2170	0	2038	36	0
1	G	2214	0	2079	32	0
1	J	2204	0	2074	24	0
2	B	821	0	796	11	0
2	E	821	0	796	16	0
2	H	821	0	796	6	0
2	K	821	0	796	11	0
3	C	66	0	68	2	0
3	F	63	0	57	4	0
3	I	67	0	68	3	0
3	L	67	0	68	4	0
4	A	115	0	0	3	0
4	B	60	0	0	2	0
4	C	7	0	0	1	0
4	D	93	0	0	4	0
4	E	65	0	0	2	0
4	F	2	0	0	0	0
4	G	131	0	0	3	0
4	H	65	0	0	0	0
4	I	3	0	0	0	0
4	J	130	0	0	6	0
4	K	66	0	0	4	0
4	L	5	0	0	0	0
All	All	13045	0	11664	150	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (150) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:219:LEU:O	1:G:219:LEU:HD12	1.30	1.27
1:D:219:LEU:O	1:D:219:LEU:HD12	1.61	0.99
1:G:219:LEU:O	1:G:219:LEU:CD1	2.22	0.86
2:B:39:MET:CE	2:B:49:VAL:HG13	2.08	0.83
1:J:144:ARG:NH2	4:J:1467:HOH:O	2.13	0.81
1:D:115:GLN:NE2	4:D:1186:HOH:O	2.18	0.75
2:K:4:THR:HB	4:K:1433:HOH:O	1.85	0.75
1:G:187:ALA:HB3	1:G:272:LEU:HD11	1.70	0.73
2:E:7:ILE:HG21	2:E:93:VAL:HG11	1.70	0.71
2:E:7:ILE:CG2	2:E:93:VAL:HG11	2.20	0.71
2:E:4:THR:HG23	2:E:87:MET:HE3	1.72	0.69
1:A:193:PRO:HA	1:A:199:VAL:HG12	1.73	0.69
1:J:66:LYS:NZ	3:L:2:ALA:O	2.25	0.69
1:A:144:ARG:HH11	1:A:144:ARG:HG2	1.56	0.68
2:K:4:THR:CB	4:K:1433:HOH:O	2.40	0.68
1:D:155:HIS:HB3	3:F:6:PHE:CZ	2.29	0.68
2:B:60:TRP:O	4:B:1211:HOH:O	2.12	0.68
1:D:103:LEU:HD11	1:D:168:LEU:HD23	1.76	0.67
1:J:234:ARG:HD3	2:K:10:TYR:CE2	2.30	0.67
1:G:249:VAL:HG13	1:G:257:TYR:CE2	2.32	0.65
1:J:94:THR:HG22	4:J:339:HOH:O	1.95	0.65
1:A:66:LYS:HD3	4:C:1382:HOH:O	1.97	0.64
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.32	0.63
1:D:206:LEU:HD12	4:D:660:HOH:O	1.99	0.63
1:A:199:VAL:HG13	1:A:251:LEU:HD21	1.81	0.62
2:B:4:THR:HB	4:B:1309:HOH:O	2.00	0.61
1:G:230:LEU:C	1:G:230:LEU:HD12	2.21	0.61
1:A:115:GLN:NE2	4:A:1152:HOH:O	2.34	0.60
1:G:94:THR:HG22	4:G:1207:HOH:O	2.00	0.60
1:J:44:ARG:NE	4:J:1056:HOH:O	2.29	0.60
1:G:103:LEU:HD11	1:G:168:LEU:HD23	1.84	0.60
1:A:231:VAL:HG13	1:A:244:TRP:CZ2	2.36	0.59
2:B:39:MET:CE	2:B:49:VAL:CG1	2.78	0.59
1:D:215:LEU:HD13	1:D:243:LYS:HD3	1.84	0.59
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.38	0.59
1:J:14:ARG:NH1	4:J:1654:HOH:O	2.36	0.58
1:D:219:LEU:C	1:D:219:LEU:HD12	2.22	0.58
1:A:199:VAL:CG1	1:A:251:LEU:HD21	2.34	0.58
1:D:219:LEU:HD13	1:D:257:TYR:CE2	2.39	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:39:MET:HE1	2:B:49:VAL:HG13	1.86	0.58
1:D:185:PRO:HD2	1:D:266:LEU:HD13	1.85	0.57
1:A:44:ARG:NH1	4:A:1508:HOH:O	2.27	0.57
1:G:35:ARG:NH2	2:H:54:MET:O	2.33	0.57
1:A:249:VAL:HG22	1:A:257:TYR:CE2	2.41	0.56
1:D:103:LEU:HD11	1:D:168:LEU:CD2	2.35	0.56
1:D:216:THR:HG22	4:D:996:HOH:O	2.06	0.56
1:D:81:LEU:HD11	3:F:9:MET:HG3	1.88	0.56
1:J:155:HIS:HB3	3:L:6:PHE:CZ	2.41	0.56
2:K:4:THR:HG22	2:K:86:SER:OG	2.07	0.55
1:G:187:ALA:CB	1:G:272:LEU:HD11	2.35	0.55
1:A:19:GLU:CD	4:A:1475:HOH:O	2.43	0.55
1:J:141:GLN:OE1	1:J:144:ARG:NH1	2.40	0.55
1:G:219:LEU:HD12	1:G:219:LEU:C	2.15	0.54
1:J:249:VAL:HG22	1:J:257:TYR:CE2	2.42	0.54
1:D:121:ARG:CZ	2:E:1:ILE:HD12	2.37	0.54
1:A:35:ARG:NH2	2:B:54:MET:O	2.38	0.54
1:J:185:PRO:HD2	1:J:266:LEU:HD13	1.89	0.54
1:J:78:LEU:HD13	1:J:95:LEU:HB2	1.89	0.53
1:G:155:HIS:HB3	3:I:6:PHE:CZ	2.44	0.53
1:A:141:GLN:OE1	1:A:144:ARG:NH2	2.42	0.53
2:K:4:THR:HG22	2:K:86:SER:HB2	1.91	0.53
1:J:79:ARG:NH1	4:J:1361:HOH:O	2.40	0.53
1:D:234:ARG:HD3	2:E:10:TYR:CE2	2.43	0.53
2:K:4:THR:HG22	2:K:86:SER:CB	2.38	0.52
2:E:7:ILE:HG21	2:E:93:VAL:CG1	2.38	0.52
1:D:219:LEU:HD13	1:D:257:TYR:CZ	2.45	0.52
2:B:39:MET:HE2	2:B:49:VAL:CG1	2.40	0.52
1:D:77:SER:HB3	3:F:9:MET:HG2	1.92	0.52
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.45	0.52
1:A:185:PRO:HD2	1:A:266:LEU:HD13	1.92	0.51
1:D:144:ARG:NH2	4:D:1117:HOH:O	2.43	0.51
1:J:249:VAL:HG22	1:J:257:TYR:CZ	2.45	0.51
1:D:219:LEU:O	1:D:256:ASN:O	2.28	0.51
1:G:141:GLN:OE1	1:G:144:ARG:NH1	2.44	0.50
1:A:194:ARG:NE	1:A:195:SER:OG	2.44	0.50
1:G:10:THR:HG22	1:G:12:VAL:HG23	1.93	0.50
1:D:20:PRO:HD2	1:D:75:ARG:HD3	1.94	0.49
1:G:30:ASN:ND2	4:G:1402:HOH:O	2.37	0.49
1:G:78:LEU:HD13	1:G:95:LEU:HB2	1.95	0.49
1:A:271:THR:O	1:A:272:LEU:HD12	2.13	0.49
1:D:33:PHE:C	1:D:48:ARG:HB2	2.33	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.47	0.48
2:E:1:ILE:CG2	2:E:2:GLN:N	2.75	0.48
1:D:72:GLN:HE22	1:D:75:ARG:NH2	2.11	0.48
1:G:103:LEU:CD1	1:G:168:LEU:HD23	2.44	0.48
1:G:224:LEU:HD23	1:G:247:VAL:HG21	1.94	0.48
2:E:59:ASP:O	2:E:60:TRP:HB2	2.13	0.48
1:J:163:GLU:OE1	3:L:1:LYS:NZ	2.43	0.48
1:G:219:LEU:HD13	1:G:257:TYR:CZ	2.49	0.48
1:A:201:LEU:HD11	1:A:254:GLU:HB2	1.95	0.48
2:K:94:TYR:O	4:K:1592:HOH:O	2.20	0.47
1:D:121:ARG:NH2	2:E:1:ILE:HD12	2.28	0.47
1:G:197:GLY:CA	1:G:251:LEU:HD12	2.44	0.47
1:J:234:ARG:HD2	1:J:242:GLN:HB2	1.95	0.47
1:G:95:LEU:HD12	1:G:117:ALA:O	2.14	0.47
1:A:144:ARG:NH1	1:A:144:ARG:HG2	2.28	0.46
1:G:231:VAL:HG13	1:G:244:TRP:CZ2	2.50	0.46
1:A:199:VAL:HG13	1:A:251:LEU:CD2	2.44	0.46
2:H:12:ARG:CZ	2:H:22:ILE:HD13	2.46	0.46
1:D:45:TYR:CE2	1:D:67:ALA:HB2	2.51	0.45
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.51	0.45
2:E:1:ILE:CG2	2:E:2:GLN:H	2.28	0.45
1:J:202:ARG:HD3	1:J:244:TRP:CE3	2.50	0.45
1:J:209:TYR:CD1	1:J:210:PRO:HA	2.51	0.45
2:K:32:PRO:HB2	2:K:33:PRO:HD2	1.99	0.45
1:D:202:ARG:HD3	1:D:246:SER:HB3	1.97	0.45
1:G:230:LEU:C	1:G:230:LEU:CD1	2.84	0.45
1:A:45:TYR:CE2	1:A:67:ALA:HB2	2.52	0.45
2:E:1:ILE:HG23	2:E:2:GLN:N	2.33	0.44
2:E:3:LYS:CE	4:E:1329:HOH:O	2.65	0.44
2:E:59:ASP:O	2:E:60:TRP:CB	2.65	0.44
2:E:3:LYS:HE2	4:E:1329:HOH:O	2.18	0.44
2:H:51:MET:SD	2:H:66:ALA:HB2	2.58	0.43
1:D:72:GLN:HE22	1:D:75:ARG:HH22	1.64	0.43
2:H:12:ARG:NH1	2:H:22:ILE:HD13	2.32	0.43
1:J:237:GLY:HA3	4:K:1179:HOH:O	2.19	0.43
1:G:21:ARG:HD2	1:G:39:ASP:OD2	2.18	0.43
1:J:175:GLY:O	1:J:176:ASN:C	2.57	0.43
1:D:249:VAL:HG22	1:D:257:TYR:CZ	2.53	0.43
1:A:155:HIS:HB3	3:C:6:PHE:CZ	2.54	0.43
2:H:3:LYS:HE3	2:H:31:HIS:HB2	2.01	0.43
1:J:66:LYS:HZ1	3:L:1:LYS:HG2	1.83	0.43
1:G:103:LEU:HD23	1:G:109:LEU:HA	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:143:THR:HG21	3:I:9:MET:HG2	2.01	0.42
2:K:10:TYR:CD1	2:K:10:TYR:N	2.86	0.42
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.54	0.42
1:G:260:ARG:NH1	4:G:1483:HOH:O	2.41	0.42
1:A:187:ALA:HA	1:A:204:TRP:O	2.20	0.42
1:J:194:ARG:O	1:J:195:SER:O	2.38	0.42
1:A:244:TRP:CH2	2:B:99:MET:HE1	2.55	0.41
1:D:5:MET:HB2	1:D:168:LEU:HD13	2.01	0.41
1:D:202:ARG:HD2	1:D:244:TRP:CE3	2.56	0.41
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.55	0.41
1:A:66:LYS:HE3	3:C:2:ALA:HB3	2.02	0.41
1:D:78:LEU:HD13	1:D:95:LEU:HB2	2.03	0.41
2:B:54:MET:CE	2:B:64:ILE:HD12	2.51	0.41
2:E:15:PRO:HG3	2:E:97:ARG:HB2	2.01	0.41
1:D:230:LEU:HD12	1:D:230:LEU:C	2.41	0.41
1:D:103:LEU:CD1	1:D:168:LEU:HD23	2.46	0.41
1:D:203:CYS:HB2	1:D:217:TRP:CZ2	2.55	0.41
1:D:3:HIS:HB2	1:D:103:LEU:HD12	2.03	0.41
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.56	0.41
1:G:21:ARG:CZ	1:G:39:ASP:OD2	2.69	0.41
1:D:146:LYS:NZ	3:F:9:MET:OXT	2.50	0.41
1:G:66:LYS:HG2	3:I:4:SER:HB3	2.03	0.41
1:G:209:TYR:CD1	1:G:210:PRO:HA	2.56	0.40
1:J:202:ARG:NH2	4:J:1345:HOH:O	2.55	0.40
1:J:48:ARG:NH2	2:K:53:ASP:OD2	2.54	0.40
1:G:219:LEU:HD22	1:G:257:TYR:OH	2.22	0.40
2:B:4:THR:HG22	2:B:86:SER:OG	2.21	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	253/338 (75%)	247 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	255/338 (75%)	244 (96%)	9 (4%)	2 (1%)	27	30
1	G	261/338 (77%)	255 (98%)	6 (2%)	0	100	100
1	J	260/338 (77%)	254 (98%)	5 (2%)	1 (0%)	43	52
2	B	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	E	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	H	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	K	97/99 (98%)	96 (99%)	1 (1%)	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
3	I	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	L	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1445/1784 (81%)	1404 (97%)	38 (3%)	3 (0%)	56	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	195	SER
1	D	54	GLN
1	D	221	GLY

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	223/280 (80%)	211 (95%)	12 (5%)	31	40
1	D	224/280 (80%)	208 (93%)	16 (7%)	21	26
1	G	228/280 (81%)	213 (93%)	15 (7%)	24	29
1	J	227/280 (81%)	214 (94%)	13 (6%)	29	37
2	B	94/94 (100%)	91 (97%)	3 (3%)	51	67
2	E	94/94 (100%)	91 (97%)	3 (3%)	51	67
2	H	94/94 (100%)	89 (95%)	5 (5%)	32	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	94/94 (100%)	90 (96%)	4 (4%)	40	52
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	6/7 (86%)	6 (100%)	0	100	100
3	I	7/7 (100%)	7 (100%)	0	100	100
3	L	7/7 (100%)	7 (100%)	0	100	100
All	All	1305/1524 (86%)	1234 (95%)	71 (5%)	31	40

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	44	ARG
1	A	78	LEU
1	A	99	SER
1	A	114	LEU
1	A	166	GLU
1	A	176	ASN
1	A	234	ARG
1	A	247	VAL
1	A	254	GLU
1	A	266	LEU
1	A	273	ARG
2	B	1	ILE
2	B	70	PHE
2	B	77	THR
1	D	44	ARG
1	D	62	ARG
1	D	75	ARG
1	D	78	LEU
1	D	99	SER
1	D	105	SER
1	D	110	LEU
1	D	114	LEU
1	D	144	ARG
1	D	149	GLN
1	D	166	GLU
1	D	202	ARG
1	D	234	ARG
1	D	266	LEU
1	D	272	LEU

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Mol	Chain	Res	Type
1	D	273	ARG
2	E	1	ILE
2	E	44	LYS
2	E	98	ASP
1	G	17	LEU
1	G	44	ARG
1	G	75	ARG
1	G	78	LEU
1	G	79	ARG
1	G	82	LEU
1	G	114	LEU
1	G	144	ARG
1	G	149	GLN
1	G	166	GLU
1	G	215	LEU
1	G	224	LEU
1	G	227	ASP
1	G	234	ARG
1	G	266	LEU
2	H	1	ILE
2	H	19	LYS
2	H	48	LYS
2	H	64	ILE
2	H	70	PHE
1	J	39	ASP
1	J	78	LEU
1	J	82	LEU
1	J	92	SER
1	J	99	SER
1	J	114	LEU
1	J	144	ARG
1	J	149	GLN
1	J	166	GLU
1	J	224	LEU
1	J	230	LEU
1	J	234	ARG
1	J	266	LEU
2	K	19	LYS
2	K	45	LYS
2	K	70	PHE
2	K	74	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	192	HIS
1	A	256	ASN
2	B	31	HIS
2	B	38	GLN
3	C	5	ASN
1	D	42	ASN
1	D	54	GLN
1	D	72	GLN
1	D	97	GLN
1	D	192	HIS
1	D	256	ASN
2	E	31	HIS
3	F	5	ASN
1	G	97	GLN
1	G	220	ASN
2	H	2	GLN
2	H	31	HIS
3	I	5	ASN
1	J	97	GLN
1	J	192	HIS
1	J	256	ASN
2	K	2	GLN
3	L	5	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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, 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	263/338 (77%)	0.99	43 (16%)	2 4	40, 56, 88, 98	0
1	D	263/338 (77%)	1.04	38 (14%)	3 5	40, 57, 88, 97	0
1	G	269/338 (79%)	1.00	38 (14%)	3 6	40, 57, 89, 97	0
1	J	268/338 (79%)	0.79	25 (9%)	9 14	40, 57, 86, 96	0
2	B	99/99 (100%)	0.52	3 (3%)	48 58	43, 55, 64, 67	0
2	E	99/99 (100%)	0.45	1 (1%)	79 87	43, 51, 64, 73	0
2	H	99/99 (100%)	0.46	3 (3%)	48 58	39, 51, 63, 67	0
2	K	99/99 (100%)	0.49	3 (3%)	48 58	41, 53, 64, 70	0
3	C	9/9 (100%)	0.24	0	100 100	38, 41, 45, 49	0
3	F	9/9 (100%)	0.51	0	100 100	44, 48, 52, 53	0
3	I	9/9 (100%)	0.35	0	100 100	42, 43, 48, 51	0
3	L	9/9 (100%)	0.10	0	100 100	44, 46, 49, 52	0
All	All	1495/1784 (83%)	0.81	154 (10%)	7 11	38, 55, 86, 98	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	17	LEU	9.9
1	A	17	LEU	7.3
1	D	251	LEU	7.2
1	A	257	TYR	6.9
1	G	248	VAL	6.9
1	D	219	LEU	6.8
1	G	253	LYS	6.7
1	D	250	PRO	6.3
1	D	193	PRO	6.3
1	D	249	VAL	6.3
1	D	199	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	248	VAL	5.8
1	G	256	ASN	5.7
1	J	176	ASN	5.7
1	D	257	TYR	5.6
1	J	181	ARG	5.5
1	J	219	LEU	5.3
1	J	249	VAL	5.1
1	J	272	LEU	5.1
1	G	274	TRP	5.1
1	A	253	LYS	5.0
1	G	251	LEU	5.0
1	A	195	SER	5.0
1	D	195	SER	5.0
1	G	252	GLY	5.0
1	D	189	VAL	5.0
1	G	196	LYS	4.8
1	D	256	ASN	4.8
1	J	255	GLN	4.7
1	A	256	ASN	4.7
1	D	201	LEU	4.6
1	J	16	GLY	4.6
1	A	251	LEU	4.6
1	G	249	VAL	4.5
1	G	191	HIS	4.5
1	D	248	VAL	4.4
1	D	200	THR	4.4
1	G	223	GLU	4.4
1	A	18	GLU	4.3
1	A	221	GLY	4.3
1	G	276	PRO	4.3
1	G	197	GLY	4.2
2	E	99	MET	4.1
1	J	251	LEU	4.1
1	G	199	VAL	4.1
1	G	219	LEU	4.1
1	A	272	LEU	4.0
1	A	199	VAL	4.0
1	G	258	THR	4.0
1	A	218	GLN	4.0
1	G	250	PRO	4.0
1	A	258	THR	3.9
2	H	48	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	201	LEU	3.8
1	G	181	ARG	3.8
1	G	228	MET	3.8
1	A	250	PRO	3.8
1	A	245	ALA	3.7
1	G	227	ASP	3.7
1	D	17	LEU	3.7
1	J	18	GLU	3.7
1	G	198	GLU	3.7
1	G	200	THR	3.6
1	A	201	LEU	3.6
1	G	254	GLU	3.6
1	J	257	TYR	3.5
1	D	190	THR	3.5
1	A	228	MET	3.5
1	A	249	VAL	3.5
1	G	222	GLU	3.5
1	G	259	CYS	3.4
1	A	16	GLY	3.4
1	J	252	GLY	3.4
1	D	191	HIS	3.4
1	G	41	GLU	3.4
1	A	255	GLN	3.4
1	D	181	ARG	3.3
1	J	274	TRP	3.3
1	A	217	TRP	3.2
1	D	274	TRP	3.2
1	A	247	VAL	3.2
1	D	273	ARG	3.1
1	A	252	GLY	3.1
2	K	48	LYS	3.1
1	A	273	ARG	3.1
1	D	252	GLY	3.1
1	G	194	ARG	3.0
2	B	48	LYS	3.0
1	A	274	TRP	3.0
1	A	259	CYS	3.0
2	K	47	PRO	3.0
1	G	44	ARG	3.0
1	J	224	LEU	2.9
1	D	198	GLU	2.9
1	J	256	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	194	ARG	2.9
1	A	193	PRO	2.9
1	J	44	ARG	2.8
1	G	224	LEU	2.8
2	K	22	ILE	2.8
1	D	222	GLU	2.8
1	D	220	ASN	2.8
1	J	273	ARG	2.7
1	A	191	HIS	2.7
1	D	255	GLN	2.7
1	G	193	PRO	2.7
1	J	276	PRO	2.6
1	D	272	LEU	2.6
1	D	18	GLU	2.6
1	A	200	THR	2.6
1	A	246	SER	2.6
1	D	229	GLU	2.6
1	A	181	ARG	2.5
2	H	49	VAL	2.5
1	G	15	PRO	2.5
1	A	192	HIS	2.5
1	J	230	LEU	2.4
1	G	218	GLN	2.4
1	D	185	PRO	2.4
1	D	40	ALA	2.4
1	J	258	THR	2.4
2	B	47	PRO	2.4
1	G	272	LEU	2.3
1	A	271	THR	2.3
1	G	220	ASN	2.3
1	D	50	PRO	2.3
1	J	253	LYS	2.3
2	B	93	VAL	2.3
1	A	44	ARG	2.3
1	A	260	ARG	2.2
1	D	253	LYS	2.2
1	D	194	ARG	2.2
2	H	92	THR	2.2
1	G	247	VAL	2.2
1	A	216	THR	2.1
1	D	172	LEU	2.1
1	D	266	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	222	GLU	2.1
1	G	176	ASN	2.1
1	J	189	VAL	2.1
1	D	140	ALA	2.1
1	A	14	ARG	2.1
1	J	113	TYR	2.1
1	A	189	VAL	2.1
1	J	199	VAL	2.1
1	A	229	GLU	2.1
1	D	113	TYR	2.1
1	G	273	ARG	2.0
1	D	261	VAL	2.0
1	J	88	SER	2.0
1	D	149	GLN	2.0
1	A	223	GLU	2.0
1	G	261	VAL	2.0
1	A	254	GLU	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.