Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 08:59 AM JST

PDB ID	:	6LF9
Title	:	Crystal structure of pSLA-1*1301 complex with dodecapeptide RVEDVT-NTAEYW
Authors	:	Wei, X.H.; Wang, S.; Zhang, N.Z.; Xia, C.
Deposited on	:	2019-11-30
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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:

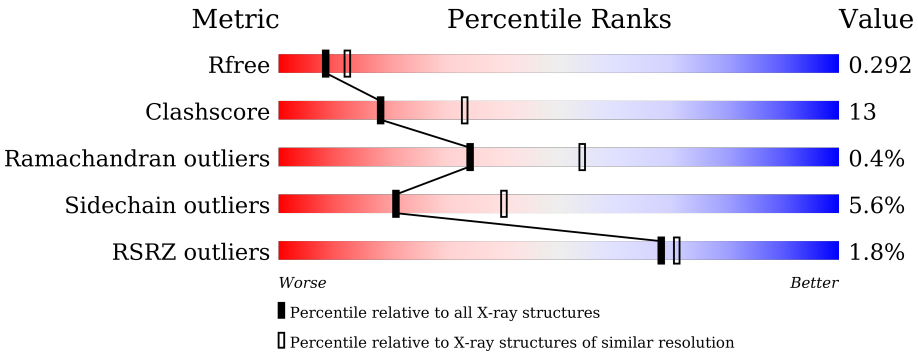
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	273	79% 19% .
1	D	273	82% 15% .
1	G	273	3% 64% 32% . .
1	J	273	3% 76% 21% .
2	B	97	95% 5%
2	E	97	93% 7%

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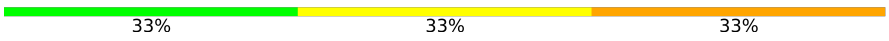
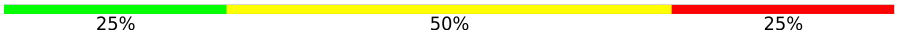
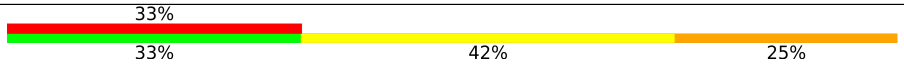
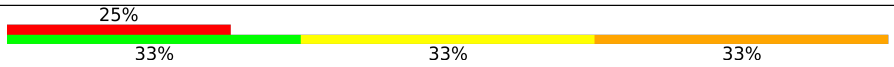
Mol	Chain	Length	Quality of chain
2	H	97	
2	K	97	
3	C	12	
3	F	12	
3	I	12	
3	L	12	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12718 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	273	Total	C	N	O	S	0	0	0
			2205	1378	394	424	9			
1	A	273	Total	C	N	O	S	0	0	0
			2205	1378	394	424	9			
1	G	273	Total	C	N	O	S	0	0	0
			2205	1378	394	424	9			
1	J	273	Total	C	N	O	S	0	0	0
			2205	1378	394	424	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	97	Total	C	N	O	S	0	0	0
			799	510	140	146	3			
2	B	97	Total	C	N	O	S	0	0	0
			799	510	140	146	3			
2	H	97	Total	C	N	O	S	0	0	0
			799	510	140	146	3			
2	K	97	Total	C	N	O	S	0	0	0
			799	510	140	146	3			

- Molecule 3 is a protein called ARG-VAL-GLU-ASP-VAL-THR-ASN-THR-ALA-GLU-TYR-TRP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	12	Total	C	N	O	0	0	0
			104	65	17	22			
3	C	12	Total	C	N	O	0	0	0
			104	65	17	22			
3	I	12	Total	C	N	O	0	0	0
			95	57	16	22			
3	L	12	Total	C	N	O	0	0	0
			104	65	17	22			

- Molecule 4 is water.

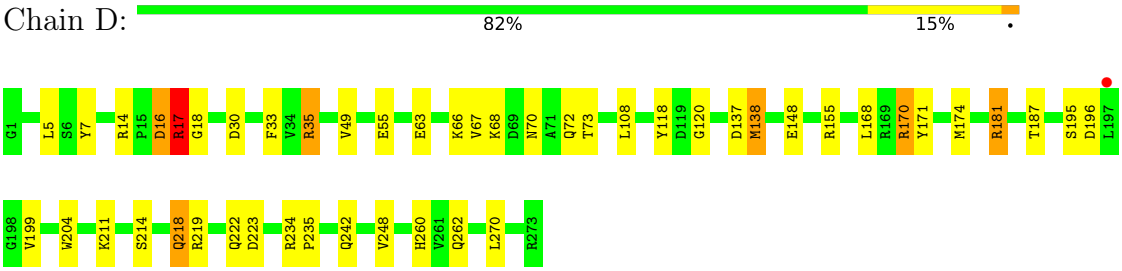
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	62	Total O 62 62	0	0
4	E	29	Total O 29 29	0	0
4	A	76	Total O 76 76	0	0
4	B	28	Total O 28 28	0	0
4	C	1	Total O 1 1	0	0
4	G	26	Total O 26 26	0	0
4	H	13	Total O 13 13	0	0
4	I	1	Total O 1 1	0	0
4	J	39	Total O 39 39	0	0
4	K	19	Total O 19 19	0	0
4	L	1	Total O 1 1	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.

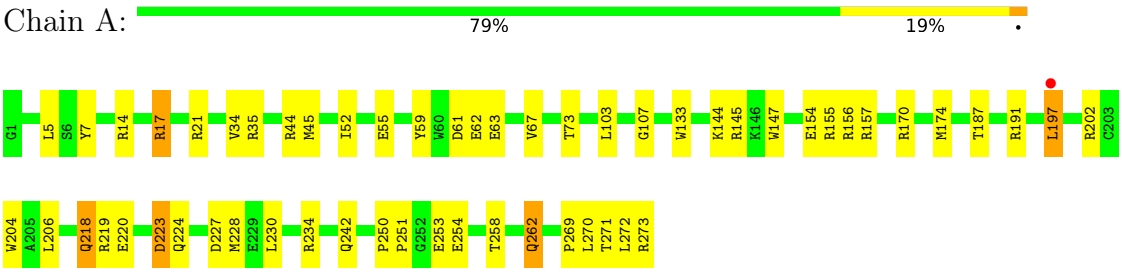
• Molecule 1: MHC class I antigen

Chain D:



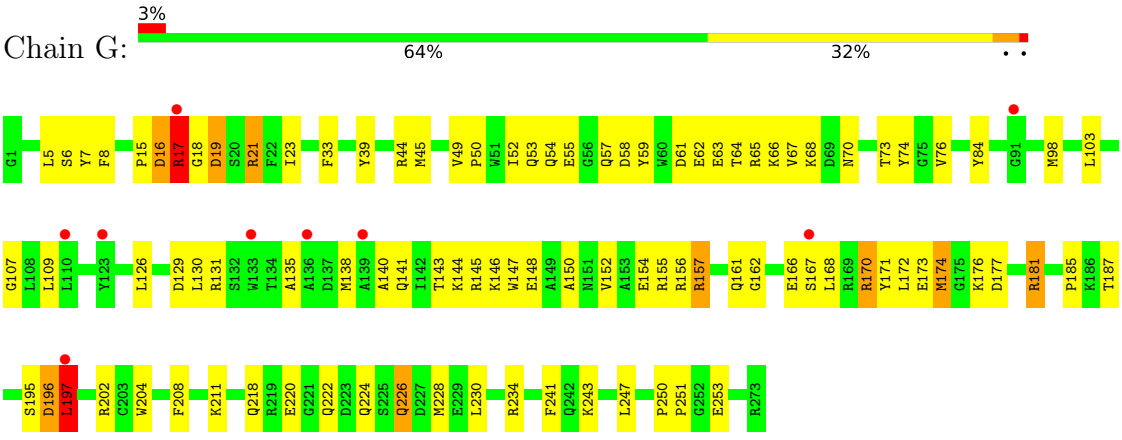
• Molecule 1: MHC class I antigen

Chain A:



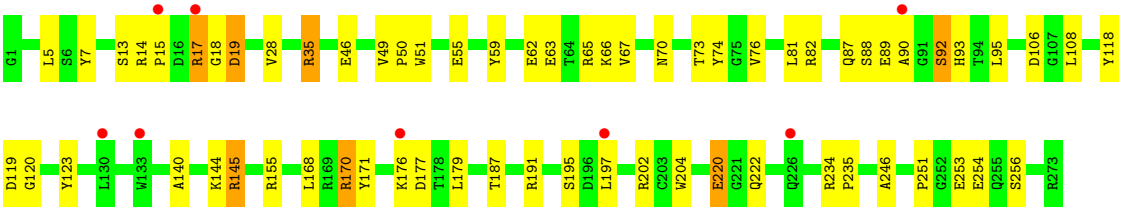
• Molecule 1: MHC class I antigen

Chain G:

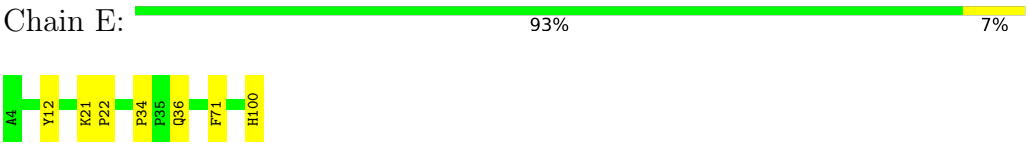


• Molecule 1: MHC class I antigen

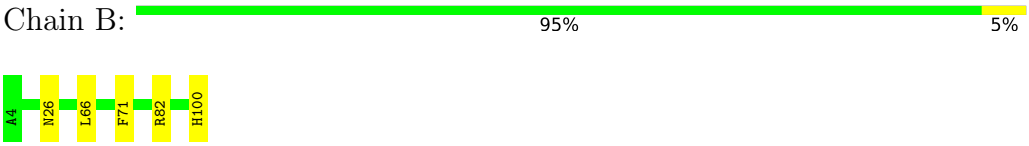
Chain J:



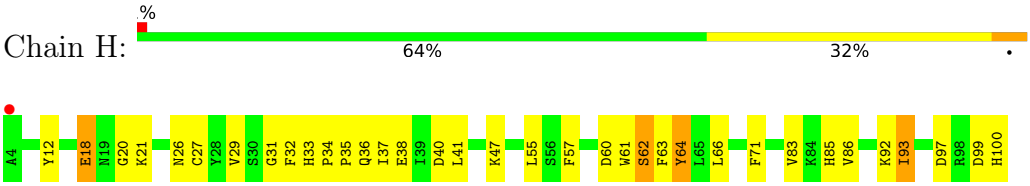
• Molecule 2: Beta-2-microglobulin



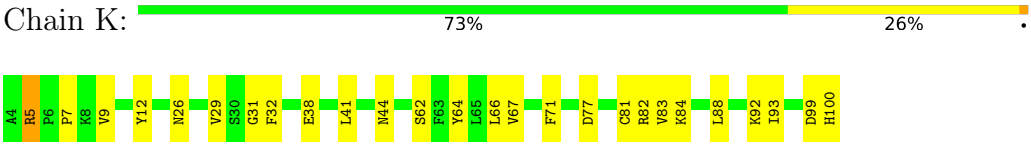
• Molecule 2: Beta-2-microglobulin



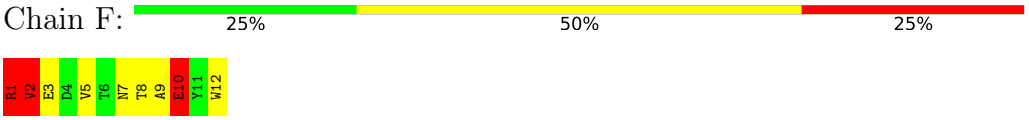
• Molecule 2: Beta-2-microglobulin



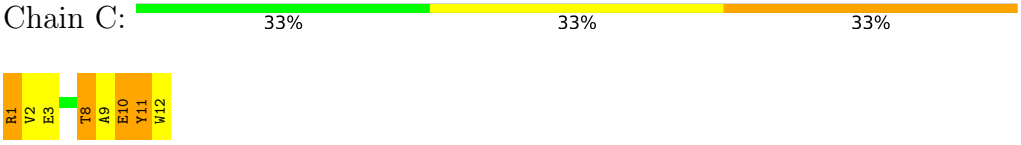
• Molecule 2: Beta-2-microglobulin



• Molecule 3: ARG-VAL-GLU-ASP-VAL-THR-ASN-THR-ALA-GLU-TYR-TRP

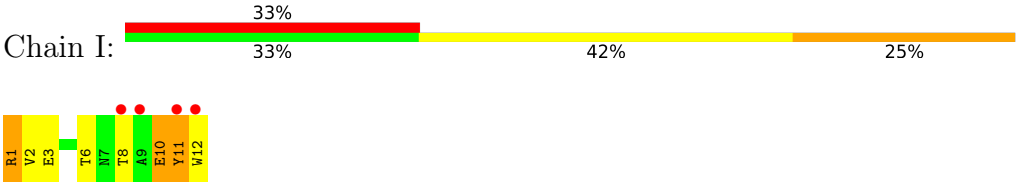


• Molecule 3: ARG-VAL-GLU-ASP-VAL-THR-ASN-THR-ALA-GLU-TYR-TRP



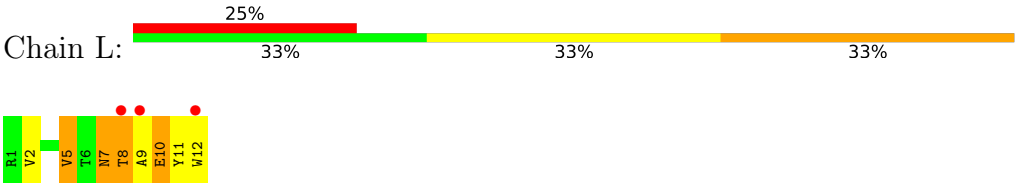
• Molecule 3: ARG-VAL-GLU-ASP-VAL-THR-ASN-THR-ALA-GLU-TYR-TRP

Chain I:



• Molecule 3: ARG-VAL-GLU-ASP-VAL-THR-ASN-THR-ALA-GLU-TYR-TRP

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.17Å 44.24Å 199.63Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	199.63 – 2.50 29.64 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (199.63-2.50) 99.6 (29.64-2.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.251 , 0.291 0.249 , 0.292	Depositor DCC
R_{free} test set	2920 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 17.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.139 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	12718	wwPDB-VP
Average B, all atoms (Å^2)	35.0	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 54.79 % 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 3.4706e-05. 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, 0.333 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	0.48	0/2263	0.63	2/3073 (0.1%)
1	D	0.77	3/2263 (0.1%)	0.66	3/3073 (0.1%)
1	G	0.64	1/2263 (0.0%)	0.79	2/3073 (0.1%)
1	J	0.50	0/2263	0.76	3/3073 (0.1%)
2	B	0.24	0/824	0.46	0/1119
2	E	0.38	0/824	0.47	0/1119
2	H	0.63	1/824 (0.1%)	0.72	1/1119 (0.1%)
2	K	0.26	0/824	0.47	0/1119
3	C	1.46	1/106 (0.9%)	1.33	2/145 (1.4%)
3	F	1.11	1/106 (0.9%)	1.55	3/145 (2.1%)
3	I	0.91	0/95	1.23	0/129
3	L	0.97	0/106	1.28	0/145
All	All	0.59	7/12761 (0.1%)	0.70	16/17332 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	148	GLU	CD-OE2	-5.87	1.19	1.25
1	D	120	GLY	C-O	-5.84	1.14	1.23
3	C	12	TRP	CE3-CZ3	-5.81	1.28	1.38
3	F	2	VAL	C-O	-5.65	1.12	1.23
1	G	84	TYR	CE1-CZ	-5.26	1.31	1.38
2	H	64	TYR	CE1-CZ	-5.06	1.31	1.38
1	D	118	TYR	C-O	-5.06	1.13	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	14	ARG	C-N-CD	-11.65	94.96	120.60
3	F	10	GLU	N-CA-C	-9.85	84.40	111.00
1	G	18	GLY	N-CA-C	9.70	137.34	113.10
1	J	18	GLY	N-CA-C	9.68	137.29	113.10
1	J	14	ARG	C-N-CA	7.66	154.19	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	17	ARG	N-CA-C	7.30	130.71	111.00
1	D	18	GLY	N-CA-C	6.86	130.25	113.10
1	A	223	ASP	CB-CG-OD1	6.84	124.45	118.30
1	G	197	LEU	CA-CB-CG	6.56	130.39	115.30
3	C	10	GLU	N-CA-C	-6.52	93.40	111.00
3	F	9	ALA	C-N-CA	5.90	136.44	121.70
3	C	9	ALA	N-CA-C	5.83	126.75	111.00
1	D	137	ASP	CB-CG-OD1	5.70	123.43	118.30
2	H	18	GLU	CA-CB-CG	5.26	124.97	113.40
3	F	1	ARG	CA-CB-CG	5.18	124.80	113.40
1	D	17	ARG	N-CA-C	5.13	124.86	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2205	0	2082	54	0
1	D	2205	0	2082	49	0
1	G	2205	0	2082	108	0
1	J	2205	0	2082	64	0
2	B	799	0	770	6	0
2	E	799	0	770	8	0
2	H	799	0	770	28	0
2	K	799	0	770	18	0
3	C	104	0	93	19	0
3	F	104	0	93	32	0
3	I	95	0	85	29	0
3	L	104	0	93	18	0
4	A	76	0	0	2	0
4	B	28	0	0	1	0
4	C	1	0	0	0	0
4	D	62	0	0	1	0
4	E	29	0	0	0	0
4	G	26	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	13	0	0	0	0
4	I	1	0	0	0	0
4	J	39	0	0	1	0
4	K	19	0	0	0	0
4	L	1	0	0	0	0
All	All	12718	0	11772	325	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 (325) 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:7:TYR:OH	3:F:2:VAL:CG1	1.82	1.27
1:J:171:TYR:OH	3:L:2:VAL:CG2	1.88	1.22
1:J:13:SER:O	1:J:92:SER:HB3	1.46	1.13
1:G:147:TRP:NE1	3:I:11:TYR:O	1.83	1.11
1:D:7:TYR:OH	3:F:2:VAL:HG11	1.53	1.09
1:J:171:TYR:OH	3:L:2:VAL:HG22	1.54	1.05
1:D:7:TYR:OH	3:F:2:VAL:HG12	1.50	1.05
1:G:155:ARG:HH22	3:I:6:THR:HA	1.17	1.03
3:F:1:ARG:HH11	3:F:1:ARG:HB3	1.31	0.95
1:G:155:ARG:NH1	3:I:8:THR:HG22	1.81	0.95
2:H:36:GLN:HE22	1:J:106:ASP:HB3	1.32	0.95
1:G:16:ASP:OD2	1:J:108:LEU:HD22	1.66	0.94
1:A:218:GLN:OE1	1:A:223:ASP:O	1.85	0.93
1:G:150:ALA:HB2	3:I:11:TYR:CE1	2.05	0.91
1:J:13:SER:O	1:J:92:SER:CB	2.20	0.90
1:G:15:PRO:O	1:G:17:ARG:N	2.08	0.86
1:J:145:ARG:O	1:J:145:ARG:NE	2.08	0.85
1:D:7:TYR:CZ	3:F:2:VAL:HG12	2.12	0.83
1:D:171:TYR:OH	3:F:2:VAL:CG2	2.27	0.83
1:G:155:ARG:NH2	3:I:6:THR:HA	1.92	0.83
1:G:150:ALA:CB	3:I:11:TYR:CE1	2.61	0.82
1:D:7:TYR:CE2	3:F:2:VAL:HG12	2.14	0.81
1:J:170:ARG:HH21	1:J:170:ARG:HG3	1.45	0.81
3:F:1:ARG:HB3	3:F:1:ARG:NH1	1.94	0.81
1:D:7:TYR:CE1	3:F:3:GLU:OE2	2.33	0.81
1:G:17:ARG:CZ	1:G:17:ARG:HB3	2.12	0.78
1:J:95:LEU:HD21	3:L:12:TRP:CZ2	2.18	0.77
1:J:170:ARG:HG3	1:J:170:ARG:NH2	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:157:ARG:HB3	1:G:157:ARG:NH1	2.00	0.77
3:F:1:ARG:HH11	3:F:1:ARG:CB	1.97	0.77
1:G:168:LEU:O	1:G:172:LEU:HG	1.86	0.75
1:G:155:ARG:NH1	3:I:8:THR:CG2	2.48	0.75
1:J:19:ASP:OD1	1:J:19:ASP:N	2.15	0.74
3:I:3:GLU:OE1	3:I:3:GLU:N	2.20	0.74
1:G:17:ARG:HB3	1:G:17:ARG:NH2	2.04	0.73
1:A:59:TYR:HD1	3:C:1:ARG:HD3	1.53	0.73
1:G:152:VAL:HG13	1:G:156:ARG:NH1	2.03	0.73
1:G:44:ARG:NH1	4:G:301:HOH:O	2.20	0.73
1:G:171:TYR:OH	3:I:2:VAL:CG2	2.37	0.73
1:J:93:HIS:ND1	1:J:119:ASP:OD2	2.16	0.72
1:A:155:ARG:HH21	1:A:156:ARG:HH22	1.38	0.71
2:H:36:GLN:NE2	1:J:106:ASP:HB3	2.03	0.71
1:G:62:GLU:HG2	1:G:66:LYS:HE2	1.72	0.71
1:G:181:ARG:HH11	1:G:181:ARG:HG3	1.53	0.71
1:G:197:LEU:O	1:G:251:PRO:HD3	1.91	0.70
1:J:171:TYR:OH	3:L:2:VAL:HG21	1.87	0.70
1:G:19:ASP:OD1	1:G:19:ASP:N	2.26	0.69
1:G:157:ARG:HH11	1:G:157:ARG:HG2	1.58	0.69
1:A:191:ARG:NH1	1:A:254:GLU:OE2	2.26	0.69
1:G:150:ALA:HB2	3:I:11:TYR:HE1	1.58	0.68
1:G:155:ARG:NH2	3:I:6:THR:HG22	2.08	0.68
1:G:54:GLN:OE1	1:G:174:MET:HB3	1.93	0.68
1:J:62:GLU:HG2	1:J:66:LYS:HE2	1.76	0.68
1:G:57:GLN:NE2	1:G:61:ASP:OD2	2.26	0.68
2:K:82:ARG:HD3	2:K:84:LYS:HE2	1.75	0.67
1:G:181:ARG:HG3	1:G:181:ARG:NH1	2.09	0.66
1:G:181:ARG:HH11	1:G:181:ARG:CG	2.09	0.66
1:A:234:ARG:HH22	2:B:100:HIS:CE1	2.14	0.66
1:G:154:GLU:HA	1:G:157:ARG:HH12	1.61	0.66
1:G:162:GLY:O	1:G:166:GLU:HG2	1.96	0.66
1:G:171:TYR:OH	3:I:2:VAL:HG22	1.97	0.65
2:H:12:TYR:HB3	2:H:100:HIS:HE1	1.61	0.65
1:A:44:ARG:NH2	1:A:61:ASP:OD1	2.24	0.65
1:A:197:LEU:HB3	1:A:251:PRO:HG3	1.79	0.64
2:H:18:GLU:OE2	2:H:21:LYS:HE3	1.97	0.64
1:A:250:PRO:HB2	1:A:253:GLU:HG3	1.78	0.64
2:E:12:TYR:HB3	2:E:100:HIS:HE1	1.62	0.64
1:G:7:TYR:OH	3:I:2:VAL:HG11	1.98	0.64
1:A:7:TYR:HE2	3:C:2:VAL:HG12	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:59:TYR:O	1:J:63:GLU:HG2	1.98	0.63
1:G:250:PRO:HB2	1:G:253:GLU:OE1	1.98	0.63
1:G:155:ARG:HH21	3:I:6:THR:HG22	1.62	0.63
1:J:197:LEU:HD12	1:J:251:PRO:HG3	1.80	0.63
1:G:157:ARG:HH11	1:G:157:ARG:CG	2.11	0.62
1:G:147:TRP:CD1	3:I:11:TYR:O	2.53	0.62
1:D:35:ARG:NH1	4:D:303:HOH:O	2.32	0.62
1:G:167:SER:HB3	3:I:1:ARG:O	1.99	0.62
1:D:66:LYS:HE3	3:F:3:GLU:O	1.99	0.62
1:G:131:ARG:NH1	1:G:157:ARG:HE	1.97	0.62
1:G:17:ARG:HG2	1:G:17:ARG:HH21	1.65	0.62
1:G:157:ARG:HB3	1:G:157:ARG:CZ	2.29	0.61
1:A:63:GLU:OE1	3:C:1:ARG:N	2.23	0.60
1:G:135:ALA:HB1	1:G:140:ALA:HB3	1.82	0.60
1:J:55:GLU:HG2	1:J:59:TYR:CB	2.31	0.60
1:D:214:SER:HB3	1:D:262:GLN:HB2	1.84	0.60
1:G:131:ARG:NH1	1:G:157:ARG:NE	2.49	0.60
3:F:1:ARG:HH11	3:F:1:ARG:N	1.99	0.60
1:D:155:ARG:HH12	3:F:8:THR:HG22	1.66	0.59
1:A:170:ARG:NH1	3:C:1:ARG:HH11	2.00	0.59
1:G:17:ARG:HH21	1:G:17:ARG:CG	2.14	0.59
1:J:171:TYR:CZ	3:L:2:VAL:HG22	2.38	0.59
1:G:7:TYR:CZ	3:I:2:VAL:HG11	2.37	0.59
1:D:73:THR:HA	3:F:10:GLU:CG	2.34	0.58
1:G:5:LEU:HB2	1:G:168:LEU:HD13	1.84	0.58
1:A:147:TRP:NE1	3:C:11:TYR:HB3	2.19	0.58
2:K:44:ASN:ND2	2:K:77:ASP:OD1	2.36	0.58
1:D:187:THR:HA	1:D:204:TRP:O	2.04	0.57
1:A:14:ARG:NH1	1:A:21:ARG:HD3	2.18	0.57
1:A:133:TRP:O	1:A:144:LYS:NZ	2.33	0.57
1:A:34:VAL:HB	1:A:45:MET:SD	2.45	0.57
2:B:82:ARG:NH2	4:B:202:HOH:O	2.37	0.57
1:D:7:TYR:HH	3:F:2:VAL:HG11	1.67	0.56
2:H:27:CYS:HB2	2:H:41:LEU:HD21	1.88	0.56
1:G:23:ILE:HG21	2:H:55:LEU:HB3	1.87	0.56
1:J:155:ARG:NH1	4:J:303:HOH:O	2.37	0.56
1:J:191:ARG:NH2	1:J:254:GLU:OE2	2.38	0.55
1:J:73:THR:HG23	3:L:10:GLU:HG3	1.88	0.55
2:H:31:GLY:CA	2:H:62:SER:OG	2.55	0.55
2:H:31:GLY:HA2	2:H:62:SER:OG	2.07	0.55
1:G:64:THR:HA	1:G:67:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:15:PRO:C	1:G:17:ARG:N	2.57	0.54
1:A:262:GLN:OE1	1:A:269:PRO:HG3	2.07	0.54
1:J:82:ARG:HD2	1:J:88:SER:O	2.08	0.54
1:A:7:TYR:CE2	3:C:2:VAL:HG12	2.42	0.54
1:D:16:ASP:N	1:D:16:ASP:OD1	2.40	0.54
1:J:170:ARG:HH21	1:J:170:ARG:CG	2.17	0.54
1:A:35:ARG:NH2	4:A:302:HOH:O	2.40	0.53
1:G:45:MET:CE	1:G:67:VAL:HG11	2.39	0.53
1:G:76:VAL:HG21	3:I:10:GLU:OE2	2.09	0.53
1:G:147:TRP:HE1	3:I:11:TYR:C	2.05	0.53
1:G:204:TRP:HH2	2:H:100:HIS:CD2	2.26	0.53
1:J:187:THR:HA	1:J:204:TRP:O	2.09	0.53
1:J:55:GLU:HG2	1:J:59:TYR:CG	2.43	0.53
1:G:202:ARG:NH1	2:H:99:ASP:O	2.41	0.53
1:G:70:ASN:O	1:G:74:TYR:HD1	1.92	0.53
2:H:29:VAL:O	2:H:64:TYR:HA	2.09	0.53
1:A:270:LEU:HD11	2:H:20:GLY:HA3	1.91	0.53
1:G:155:ARG:HH12	3:I:8:THR:HG22	1.68	0.53
1:A:197:LEU:N	1:A:197:LEU:CD2	2.73	0.52
1:G:62:GLU:HG3	1:G:65:ARG:HH12	1.74	0.52
2:H:34:PRO:HD2	2:H:86:VAL:HG11	1.91	0.52
1:G:145:ARG:HA	1:G:148:GLU:HG3	1.90	0.52
1:D:171:TYR:OH	3:F:2:VAL:HG21	2.06	0.52
3:F:7:ASN:O	3:F:8:THR:HB	2.09	0.52
1:J:234:ARG:HH22	2:K:100:HIS:CE1	2.27	0.52
1:A:73:THR:HG23	3:C:10:GLU:CG	2.40	0.52
1:G:131:ARG:NH1	1:G:157:ARG:CD	2.72	0.52
1:J:70:ASN:O	1:J:74:TYR:HD1	1.92	0.52
1:A:228:MET:CE	1:A:230:LEU:HD12	2.40	0.52
1:G:170:ARG:O	1:G:174:MET:HG2	2.10	0.52
1:G:147:TRP:CD1	1:G:147:TRP:N	2.76	0.52
1:J:82:ARG:HG3	1:J:87:GLN:HB2	1.91	0.51
1:G:7:TYR:CE1	3:I:2:VAL:HG11	2.45	0.51
1:J:15:PRO:HB3	1:J:92:SER:N	2.26	0.51
2:K:9:VAL:HG22	2:K:29:VAL:HG22	1.91	0.51
1:D:66:LYS:CD	3:F:5:VAL:HG22	2.40	0.51
1:J:5:LEU:HD21	3:L:2:VAL:CG1	2.41	0.51
1:A:197:LEU:N	1:A:197:LEU:HD23	2.26	0.51
1:D:73:THR:HA	3:F:10:GLU:HG3	1.92	0.51
1:A:206:LEU:HD23	1:A:242:GLN:HB2	1.92	0.51
1:J:5:LEU:HD21	3:L:2:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:7:PRO:HB3	2:K:32:PHE:HB3	1.92	0.51
1:D:5:LEU:HB2	1:D:168:LEU:HD13	1.92	0.50
2:H:32:PHE:CE2	2:H:63:PHE:O	2.65	0.50
1:J:66:LYS:HD3	3:L:5:VAL:HG22	1.93	0.50
1:A:197:LEU:O	1:A:251:PRO:HD3	2.11	0.50
1:G:17:ARG:NH2	1:G:17:ARG:CB	2.72	0.50
1:D:7:TYR:HE2	3:F:2:VAL:HG12	1.70	0.50
1:D:108:LEU:HD11	1:A:14:ARG:HB3	1.93	0.50
1:D:138:MET:HE2	1:D:138:MET:H	1.76	0.50
1:A:45:MET:CE	1:A:67:VAL:HG11	2.41	0.50
1:G:98:MET:HG2	2:H:61:TRP:CH2	2.46	0.50
1:G:157:ARG:NH1	1:G:157:ARG:CG	2.73	0.50
1:G:141:GLN:NE2	1:G:144:LYS:HD2	2.26	0.50
1:G:59:TYR:O	1:G:63:GLU:HG2	2.12	0.50
1:J:95:LEU:HD21	3:L:12:TRP:CE2	2.47	0.50
1:G:63:GLU:OE2	3:I:1:ARG:N	2.44	0.50
1:A:14:ARG:NH2	4:A:301:HOH:O	2.25	0.49
1:G:21:ARG:HD2	1:G:39:TYR:HB2	1.94	0.49
1:G:230:LEU:HD21	1:G:243:LYS:HE3	1.94	0.49
1:J:171:TYR:OH	3:L:2:VAL:HG23	2.01	0.49
1:G:157:ARG:NH1	1:G:157:ARG:CB	2.72	0.49
1:D:234:ARG:HH12	2:E:100:HIS:CE1	2.30	0.49
1:A:187:THR:HA	1:A:204:TRP:O	2.12	0.49
3:L:7:ASN:HD22	3:L:7:ASN:C	2.15	0.49
1:A:234:ARG:HH22	2:B:100:HIS:HE1	1.58	0.49
2:H:40:ASP:OD1	2:H:47:LYS:HE3	2.13	0.49
2:K:31:GLY:HA2	2:K:62:SER:HB2	1.94	0.49
3:F:1:ARG:HH11	3:F:1:ARG:H3	1.61	0.48
1:G:103:LEU:HD11	1:G:107:GLY:HA2	1.95	0.48
1:A:147:TRP:HE1	3:C:11:TYR:HB3	1.78	0.48
1:G:143:THR:HG23	3:I:12:TRP:HA	1.95	0.48
1:J:93:HIS:HD1	1:J:119:ASP:CG	2.10	0.48
1:D:66:LYS:HG2	3:F:5:VAL:HG22	1.95	0.48
1:A:147:TRP:CD1	3:C:11:TYR:HB3	2.48	0.48
1:G:17:ARG:NH2	1:G:17:ARG:CG	2.73	0.48
1:D:55:GLU:HG2	1:D:174:MET:HE1	1.96	0.48
1:D:66:LYS:HD2	3:F:5:VAL:HG22	1.95	0.48
1:D:181:ARG:CG	1:D:181:ARG:HH11	2.27	0.48
1:G:129:ASP:O	1:G:131:ARG:HG2	2.13	0.48
1:D:73:THR:HA	3:F:10:GLU:HG2	1.96	0.48
1:A:14:ARG:HH11	1:A:21:ARG:HD3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3:GLU:N	3:I:3:GLU:CD	2.67	0.48
1:G:144:LYS:O	1:G:148:GLU:HG3	2.14	0.48
1:J:202:ARG:HE	1:J:246:ALA:HB2	1.77	0.48
2:K:41:LEU:HD12	2:K:67:VAL:HG12	1.96	0.47
1:D:170:ARG:NH1	3:F:1:ARG:HH21	2.12	0.47
1:D:234:ARG:HD3	2:E:12:TYR:CZ	2.49	0.47
1:G:16:ASP:CG	1:J:108:LEU:HD22	2.35	0.47
1:G:63:GLU:OE1	3:I:3:GLU:OE1	2.33	0.47
2:H:37:ILE:HD12	2:H:85:HIS:CD2	2.49	0.47
1:A:197:LEU:HD23	1:A:197:LEU:H	1.79	0.47
1:J:202:ARG:NH1	2:K:99:ASP:O	2.48	0.47
1:J:62:GLU:OE2	1:J:65:ARG:NH1	2.47	0.47
1:G:196:ASP:OD1	1:G:196:ASP:N	2.46	0.47
1:G:228:MET:CE	1:G:230:LEU:HD12	2.45	0.46
1:A:7:TYR:HE2	3:C:2:VAL:CG1	2.26	0.46
1:A:202:ARG:HG2	1:A:204:TRP:NE1	2.30	0.46
1:G:157:ARG:CZ	1:G:157:ARG:CB	2.91	0.46
2:H:97:ASP:OD2	2:H:100:HIS:N	2.47	0.46
1:J:5:LEU:HB2	1:J:168:LEU:HD13	1.97	0.46
1:J:7:TYR:HE2	3:L:2:VAL:HG11	1.80	0.46
1:D:68:LYS:O	1:D:72:GLN:HG2	2.15	0.46
1:G:234:ARG:HH22	2:H:100:HIS:CE1	2.33	0.46
1:D:138:MET:HE3	1:D:138:MET:HB2	1.60	0.46
2:K:9:VAL:HG21	2:K:83:VAL:HG21	1.97	0.46
2:H:32:PHE:CD2	2:H:63:PHE:O	2.68	0.46
2:H:33:HIS:ND1	2:H:34:PRO:HA	2.31	0.46
1:A:271:THR:O	1:A:272:LEU:HD23	2.16	0.45
1:A:7:TYR:CZ	3:C:3:GLU:OE1	2.70	0.45
1:A:59:TYR:CD1	3:C:1:ARG:HD3	2.43	0.45
1:G:6:SER:HB3	1:G:8:PHE:HE1	1.82	0.45
1:G:63:GLU:O	1:G:67:VAL:HG13	2.16	0.45
1:G:15:PRO:HD2	1:J:108:LEU:HD11	1.98	0.45
1:J:202:ARG:HG2	1:J:204:TRP:NE1	2.31	0.45
2:H:32:PHE:HE1	2:H:35:PRO:HA	1.81	0.45
1:D:17:ARG:HD2	1:D:17:ARG:N	2.32	0.45
1:J:7:TYR:HE2	3:L:2:VAL:CG1	2.30	0.45
1:J:253:GLU:HB3	1:J:256:SER:OG	2.17	0.45
2:K:38:GLU:O	2:K:83:VAL:HA	2.17	0.45
1:A:133:TRP:HB2	1:A:144:LYS:HG3	1.99	0.44
1:G:73:THR:HG23	3:I:10:GLU:HG3	1.99	0.44
1:G:155:ARG:HH11	3:I:8:THR:CG2	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:220:GLU:O	1:J:220:GLU:HG2	2.17	0.44
2:K:81:CYS:O	2:K:93:ILE:HA	2.17	0.44
1:G:211:LYS:HB3	1:G:211:LYS:HE3	1.79	0.44
1:J:93:HIS:HB3	1:J:119:ASP:OD1	2.18	0.44
1:G:17:ARG:CZ	1:G:17:ARG:CB	2.85	0.44
1:G:187:THR:HA	1:G:204:TRP:O	2.17	0.44
1:D:63:GLU:OE2	3:F:3:GLU:HG2	2.17	0.44
1:A:55:GLU:HG2	1:A:174:MET:HE3	1.99	0.44
1:G:109:LEU:HD22	1:G:161:GLN:HG3	1.98	0.44
1:A:155:ARG:NH1	3:C:8:THR:CG2	2.81	0.44
1:G:33:PHE:HD2	1:G:52:ILE:HG12	1.82	0.44
1:D:234:ARG:HG3	1:D:242:GLN:HG3	1.99	0.44
1:D:260:HIS:HA	1:D:270:LEU:O	2.18	0.44
1:A:234:ARG:NH2	2:B:100:HIS:HE1	2.15	0.44
1:J:28:VAL:HG11	1:J:179:LEU:HD13	1.99	0.44
1:J:49:VAL:HG11	1:J:51:TRP:CE2	2.52	0.44
1:D:7:TYR:CE2	3:F:2:VAL:CG1	2.96	0.43
1:G:131:ARG:HH11	1:G:157:ARG:HE	1.63	0.43
1:D:199:VAL:O	1:D:248:VAL:HA	2.17	0.43
1:G:171:TYR:HA	1:G:174:MET:HG3	2.00	0.43
1:A:197:LEU:CD2	1:A:197:LEU:H	2.30	0.43
1:J:63:GLU:O	1:J:67:VAL:HG22	2.17	0.43
2:K:38:GLU:HB2	2:K:84:LYS:HB2	2.00	0.43
1:D:66:LYS:O	1:D:70:ASN:ND2	2.52	0.43
1:A:73:THR:HG23	3:C:10:GLU:HA	1.99	0.43
1:J:49:VAL:HG22	1:J:50:PRO:HD2	2.01	0.43
1:D:33:PHE:HA	1:D:49:VAL:HG22	2.01	0.43
2:B:100:HIS:N	2:B:100:HIS:CD2	2.85	0.43
1:D:63:GLU:O	1:D:67:VAL:HG22	2.18	0.43
1:A:5:LEU:HD21	3:C:2:VAL:HG13	2.01	0.43
1:A:52:ILE:HA	1:A:174:MET:HE1	2.01	0.43
1:G:50:PRO:O	1:G:53:GLN:HB2	2.19	0.43
3:L:7:ASN:C	3:L:7:ASN:ND2	2.72	0.43
1:G:49:VAL:O	1:G:52:ILE:HG22	2.18	0.43
1:G:126:LEU:HD11	1:G:130:LEU:O	2.19	0.43
1:D:235:PRO:O	2:E:12:TYR:OH	2.29	0.42
1:J:177:ASP:OD1	1:J:177:ASP:N	2.50	0.42
1:D:181:ARG:CG	1:D:181:ARG:NH1	2.81	0.42
1:G:129:ASP:O	1:G:131:ARG:NH1	2.52	0.42
1:J:35:ARG:NH2	1:J:46:GLU:OE1	2.53	0.42
1:J:123:TYR:CZ	1:J:140:ALA:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:TYR:CZ	3:F:2:VAL:CG2	3.02	0.42
1:D:218:GLN:OE1	1:D:223:ASP:O	2.37	0.42
1:J:81:LEU:HD23	1:J:118:TYR:CD1	2.54	0.42
1:A:63:GLU:OE2	3:C:3:GLU:HG2	2.20	0.42
1:A:59:TYR:HB2	3:C:1:ARG:NH2	2.35	0.42
1:G:226:GLN:OE1	1:G:226:GLN:N	2.53	0.42
2:H:26:ASN:HB3	2:H:66:LEU:HD11	2.01	0.42
1:D:66:LYS:CG	3:F:5:VAL:HG22	2.50	0.42
1:J:17:ARG:NH2	1:J:89:GLU:OE1	2.48	0.42
2:K:26:ASN:HB3	2:K:66:LEU:HD11	2.01	0.42
1:D:30:ASP:OD1	1:D:211:LYS:HE2	2.20	0.42
1:A:154:GLU:CD	1:A:157:ARG:HH12	2.23	0.42
1:A:258:THR:CG2	1:A:273:ARG:NH2	2.83	0.42
3:F:1:ARG:CG	3:F:1:ARG:O	2.68	0.41
3:F:1:ARG:O	3:F:1:ARG:HG2	2.20	0.41
1:G:185:PRO:HB3	1:G:208:PHE:CD2	2.55	0.41
2:K:29:VAL:O	2:K:64:TYR:HA	2.20	0.41
3:F:8:THR:O	3:F:8:THR:CG2	2.68	0.41
1:G:8:PHE:HB3	2:H:57:PHE:CE1	2.55	0.41
2:H:38:GLU:O	2:H:83:VAL:HA	2.20	0.41
2:E:21:LYS:HA	2:E:22:PRO:HD3	1.67	0.41
1:G:167:SER:CB	3:I:1:ARG:O	2.68	0.41
1:J:55:GLU:HG2	1:J:59:TYR:HB2	2.01	0.41
2:E:12:TYR:CB	2:E:100:HIS:HE1	2.31	0.41
1:G:150:ALA:CB	3:I:11:TYR:HE1	2.21	0.41
1:A:155:ARG:CZ	3:C:8:THR:HG23	2.51	0.41
1:J:171:TYR:CZ	3:L:2:VAL:CG2	2.92	0.41
1:D:196:ASP:OD1	1:D:196:ASP:N	2.52	0.41
1:D:234:ARG:HD3	2:E:12:TYR:CE1	2.56	0.41
1:G:64:THR:HG22	1:G:68:LYS:HE2	2.02	0.41
1:A:73:THR:HG23	3:C:10:GLU:HG3	2.03	0.41
2:K:5:ARG:HB3	2:K:31:GLY:O	2.21	0.41
2:H:31:GLY:N	2:H:62:SER:OG	2.53	0.41
2:H:93:ILE:HG22	2:H:93:ILE:O	2.21	0.41
1:G:147:TRP:N	1:G:147:TRP:HD1	2.17	0.40
1:G:211:LYS:HG3	1:G:241:PHE:CE2	2.56	0.40
2:K:88:LEU:HD22	2:K:92:LYS:HB2	2.03	0.40
1:G:152:VAL:CG1	1:G:156:ARG:NH1	2.79	0.40
2:E:34:PRO:HB2	2:E:36:GLN:OE1	2.20	0.40
2:B:26:ASN:HB3	2:B:66:LEU:HD11	2.03	0.40
1:G:58:ASP:N	1:G:58:ASP:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:57:PHE:HB3	2:H:63:PHE:CD1	2.56	0.40
1:J:73:THR:O	1:J:76:VAL:HG22	2.21	0.40
1:J:120:GLY:CA	2:K:5:ARG:HH22	2.34	0.40
1:G:170:ARG:O	1:G:174:MET:CG	2.68	0.40
1:J:89:GLU:O	1:J:90:ALA:C	2.57	0.40
1:A:103:LEU:HD11	1:A:107:GLY:HA2	2.03	0.40
1:G:98:MET:HB3	1:G:98:MET:HE2	1.84	0.40
1:J:73:THR:HG21	3:L:9:ALA:HB1	2.04	0.40
1:J:235:PRO:O	2:K:12:TYR:OH	2.28	0.40
3:L:8:THR:O	3:L:8:THR:HG22	2.22	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	271/273 (99%)	261 (96%)	10 (4%)	0	100 100
1	D	271/273 (99%)	259 (96%)	12 (4%)	0	100 100
1	G	271/273 (99%)	257 (95%)	11 (4%)	3 (1%)	14 26
1	J	271/273 (99%)	257 (95%)	14 (5%)	0	100 100
2	B	95/97 (98%)	94 (99%)	1 (1%)	0	100 100
2	E	95/97 (98%)	93 (98%)	2 (2%)	0	100 100
2	H	95/97 (98%)	95 (100%)	0	0	100 100
2	K	95/97 (98%)	93 (98%)	2 (2%)	0	100 100
3	C	10/12 (83%)	7 (70%)	3 (30%)	0	100 100
3	F	10/12 (83%)	6 (60%)	2 (20%)	2 (20%)	0 0
3	I	10/12 (83%)	6 (60%)	4 (40%)	0	100 100
3	L	10/12 (83%)	5 (50%)	4 (40%)	1 (10%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1504/1528 (98%)	1433 (95%)	65 (4%)	6 (0%)	34 54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	10	GLU
1	G	17	ARG
1	G	16	ASP
1	G	196	ASP
3	F	2	VAL
3	L	5	VAL

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	232/232 (100%)	222 (96%)	10 (4%)	29 53
1	D	232/232 (100%)	221 (95%)	11 (5%)	26 49
1	G	232/232 (100%)	211 (91%)	21 (9%)	9 18
1	J	232/232 (100%)	221 (95%)	11 (5%)	26 49
2	B	90/90 (100%)	89 (99%)	1 (1%)	73 89
2	E	90/90 (100%)	89 (99%)	1 (1%)	73 89
2	H	90/90 (100%)	85 (94%)	5 (6%)	21 40
2	K	90/90 (100%)	88 (98%)	2 (2%)	52 77
3	C	11/11 (100%)	8 (73%)	3 (27%)	0 0
3	F	11/11 (100%)	9 (82%)	2 (18%)	1 3
3	I	10/11 (91%)	7 (70%)	3 (30%)	0 0
3	L	11/11 (100%)	7 (64%)	4 (36%)	0 0
All	All	1331/1332 (100%)	1257 (94%)	74 (6%)	21 40

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

Mol	Chain	Res	Type
1	D	14	ARG
1	D	16	ASP
1	D	17	ARG
1	D	35	ARG
1	D	138	MET
1	D	170	ARG
1	D	181	ARG
1	D	195	SER
1	D	218	GLN
1	D	219	ARG
1	D	222	GLN
2	E	71	PHE
3	F	1	ARG
3	F	12	TRP
1	A	17	ARG
1	A	62	GLU
1	A	145	ARG
1	A	197	LEU
1	A	218	GLN
1	A	219	ARG
1	A	220	GLU
1	A	224	GLN
1	A	227	ASP
1	A	262	GLN
2	B	71	PHE
3	C	1	ARG
3	C	8	THR
3	C	11	TYR
1	G	17	ARG
1	G	19	ASP
1	G	21	ARG
1	G	55	GLU
1	G	138	MET
1	G	146	LYS
1	G	157	ARG
1	G	170	ARG
1	G	173	GLU
1	G	174	MET
1	G	176	LYS
1	G	177	ASP
1	G	181	ARG
1	G	195	SER
1	G	197	LEU

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Mol	Chain	Res	Type
1	G	218	GLN
1	G	220	GLU
1	G	222	GLN
1	G	224	GLN
1	G	226	GLN
1	G	247	LEU
2	H	60	ASP
2	H	62	SER
2	H	71	PHE
2	H	92	LYS
2	H	93	ILE
3	I	1	ARG
3	I	10	GLU
3	I	11	TYR
1	J	17	ARG
1	J	19	ASP
1	J	35	ARG
1	J	92	SER
1	J	144	LYS
1	J	145	ARG
1	J	170	ARG
1	J	176	LYS
1	J	195	SER
1	J	220	GLU
1	J	222	GLN
2	K	5	ARG
2	K	71	PHE
3	L	7	ASN
3	L	8	THR
3	L	10	GLU
3	L	11	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	218	GLN
1	A	218	GLN
2	B	100	HIS
1	G	96	GLN
1	G	141	GLN
1	G	255	GLN
2	H	36	GLN

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Mol	Chain	Res	Type
2	H	100	HIS
1	J	53	GLN
3	L	7	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 monosaccharides 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	273/273 (100%)	-0.53	1 (0%) 92 93	7, 20, 49, 77	0
1	D	273/273 (100%)	-0.47	1 (0%) 92 93	4, 19, 50, 70	0
1	G	273/273 (100%)	0.14	9 (3%) 46 50	17, 49, 72, 87	0
1	J	273/273 (100%)	0.06	8 (2%) 51 55	16, 46, 66, 90	0
2	B	97/97 (100%)	-0.67	0 100 100	10, 23, 39, 52	0
2	E	97/97 (100%)	-0.65	0 100 100	8, 21, 37, 45	0
2	H	97/97 (100%)	-0.07	1 (1%) 82 84	26, 46, 62, 74	0
2	K	97/97 (100%)	-0.28	0 100 100	20, 41, 56, 70	0
3	C	12/12 (100%)	0.26	0 100 100	17, 38, 53, 56	0
3	F	12/12 (100%)	0.33	0 100 100	13, 36, 60, 65	0
3	I	12/12 (100%)	2.19	4 (33%) 0 0	67, 73, 99, 100	0
3	L	12/12 (100%)	1.38	3 (25%) 0 0	55, 65, 81, 84	0
All	All	1528/1528 (100%)	-0.22	27 (1%) 68 71	4, 34, 64, 100	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	LEU	4.6
3	I	11	TYR	4.3
3	I	9	ALA	3.9
1	J	197	LEU	3.7
1	J	133	TRP	3.7
1	D	197	LEU	3.5
2	H	4	ALA	3.5
3	I	12	TRP	3.5
1	G	136	ALA	3.4
3	I	8	THR	3.4
1	J	17	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	123	TYR	2.7
3	L	12	TRP	2.7
3	L	8	THR	2.7
1	G	110	LEU	2.6
1	J	15	PRO	2.6
1	G	197	LEU	2.5
1	G	91	GLY	2.5
3	L	9	ALA	2.4
1	J	90	ALA	2.4
1	G	17	ARG	2.3
1	J	226	GLN	2.3
1	G	133	TRP	2.1
1	J	130	LEU	2.1
1	G	139	ALA	2.0
1	G	167	SER	2.0
1	J	176	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.