Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:26 PM GMT

PDB ID	:	1AQD
Title	:	HLA-DR1 (DRA, DRB1 0101) HUMAN CLASS II HISTOCOMPATIBILITY PROTEIN (EXTRACELLULAR DOMAIN) COMPLEXED WITH ENDOGENOUS PEPTIDE
Authors	:	Murthy, V.L.; Stern, L.J.
Deposited on	:	1997-07-28
Resolution	:	2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

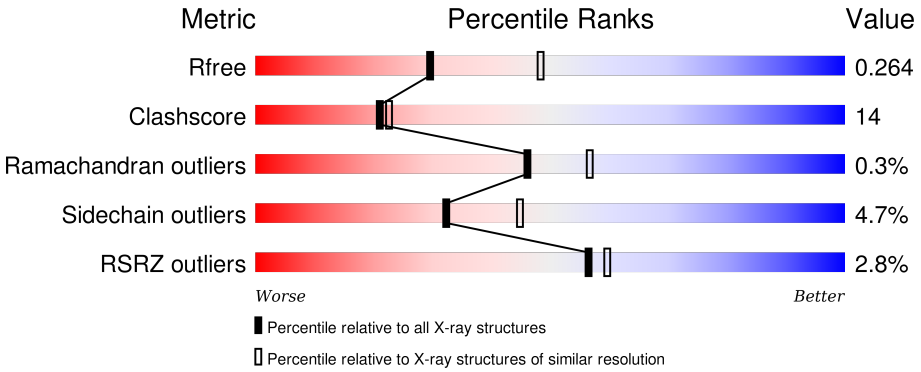
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	192	4% 63% 28% • 7%
1	D	192	2% 66% 26% • 8%
1	G	192	3% 57% 34% • 8%
1	J	192	2% 62% 29% • 8%
2	B	198	2% 65% 28% • 6%

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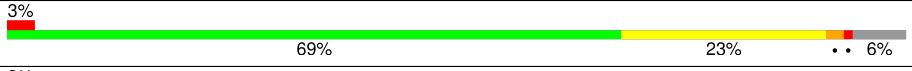
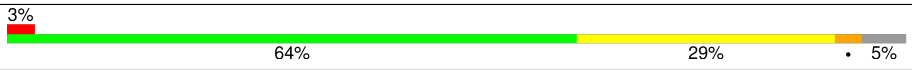
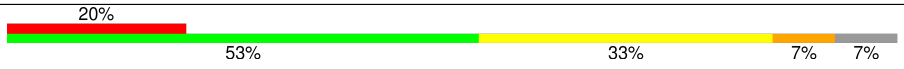
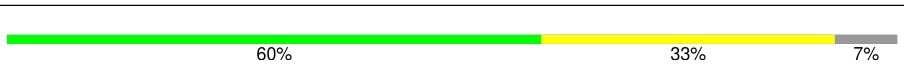
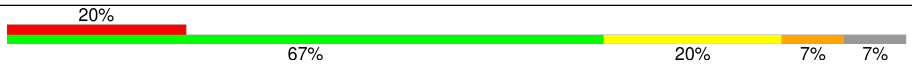
Mol	Chain	Length	Quality of chain
2	E	198	
2	H	198	
2	K	198	
3	C	15	
3	F	15	
3	I	15	
3	L	15	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12638 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-DR1 CLASS II HISTOCOMPATIBILITY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	61	0	0
			1473	954	239	275	5			
1	D	177	Total	C	N	O	S	56	0	0
			1454	941	237	271	5			
1	G	177	Total	C	N	O	S	45	0	0
			1454	941	237	271	5			
1	J	177	Total	C	N	O	S	41	0	0
			1454	941	237	271	5			

- Molecule 2 is a protein called HLA-DR1 CLASS II HISTOCOMPATIBILITY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	187	Total	C	N	O	S	85	0	0
			1537	969	276	286	6			
2	E	187	Total	C	N	O	S	82	0	0
			1537	969	276	286	6			
2	H	187	Total	C	N	O	S	69	0	0
			1537	969	276	286	6			
2	K	188	Total	C	N	O	S	136	0	0
			1548	975	280	287	6			

- Molecule 3 is a protein called HLA-A2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	14	Total	C	N	O	8	0	0
			124	81	24	19			
3	F	13	Total	C	N	O	16	0	0
			120	79	23	18			
3	I	14	Total	C	N	O	8	0	0
			124	81	24	19			
3	L	14	Total	C	N	O	16	0	0
			124	81	24	19			

- Molecule 4 is water.

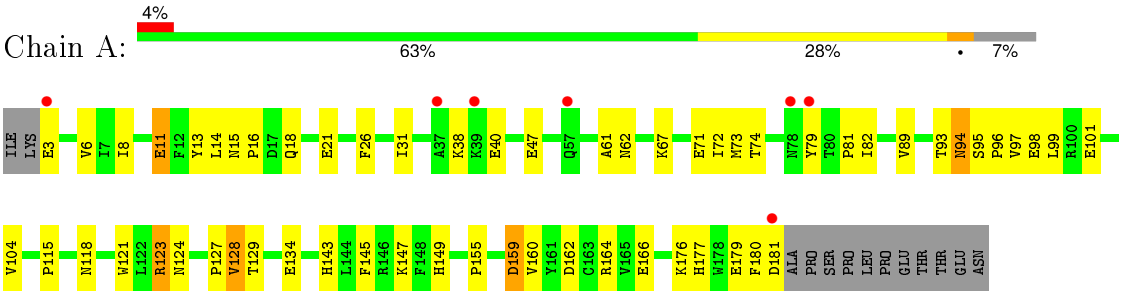
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	17	Total O 17 17	0	0
4	B	13	Total O 13 13	0	0
4	D	18	Total O 18 18	0	0
4	E	25	Total O 25 25	0	0
4	F	1	Total O 1 1	0	0
4	G	21	Total O 21 21	0	0
4	H	18	Total O 18 18	0	0
4	I	3	Total O 3 3	0	0
4	J	14	Total O 14 14	0	0
4	K	21	Total O 21 21	0	0
4	L	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

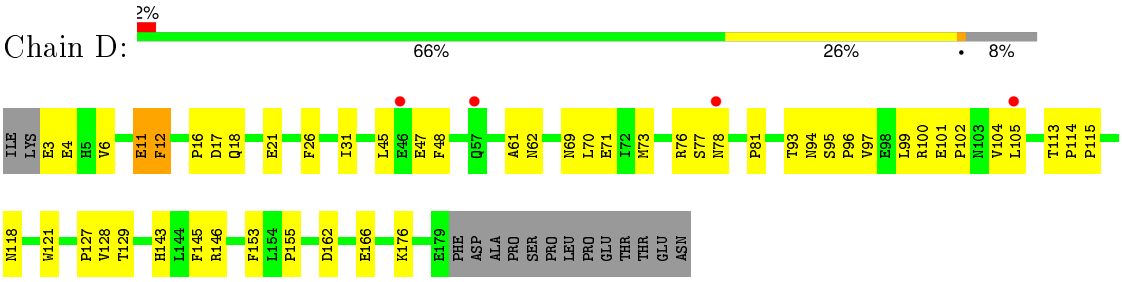
- Molecule 1: HLA-DR1 CLASS II HISTOCOMPATIBILITY PROTEIN

Chain A:



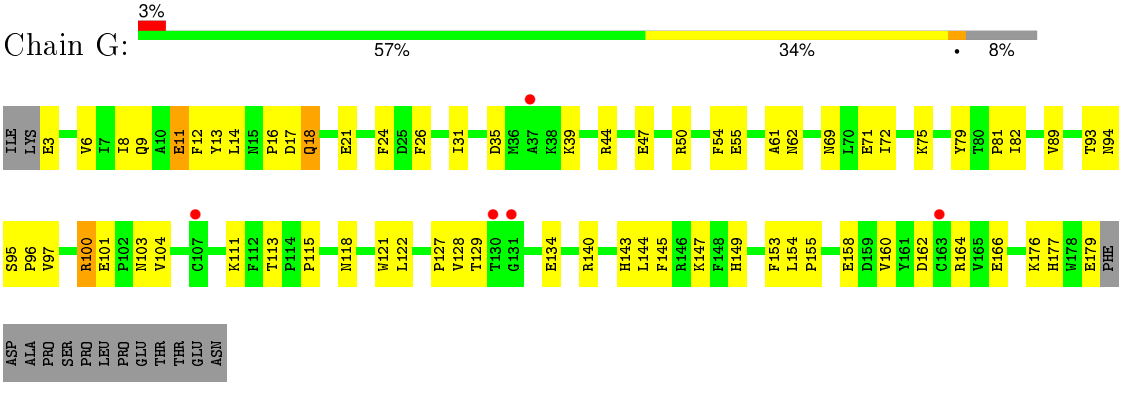
- Molecule 1: HLA-DR1 CLASS II HISTOCOMPATIBILITY PROTEIN

Chain D:



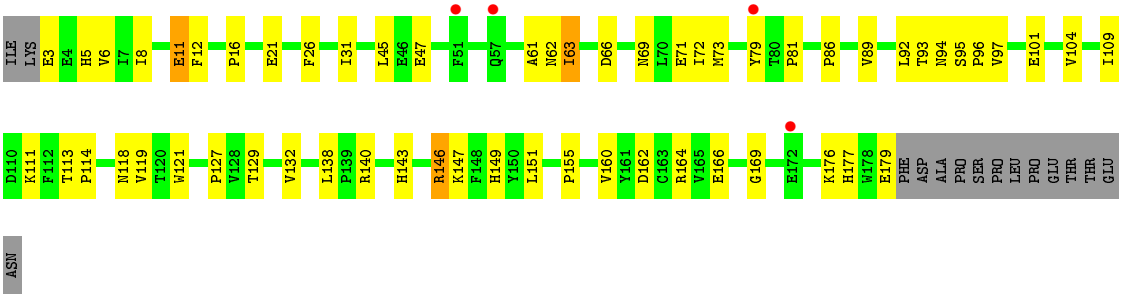
- Molecule 1: HLA-DR1 CLASS II HISTOCOMPATIBILITY PROTEIN

Chain G:



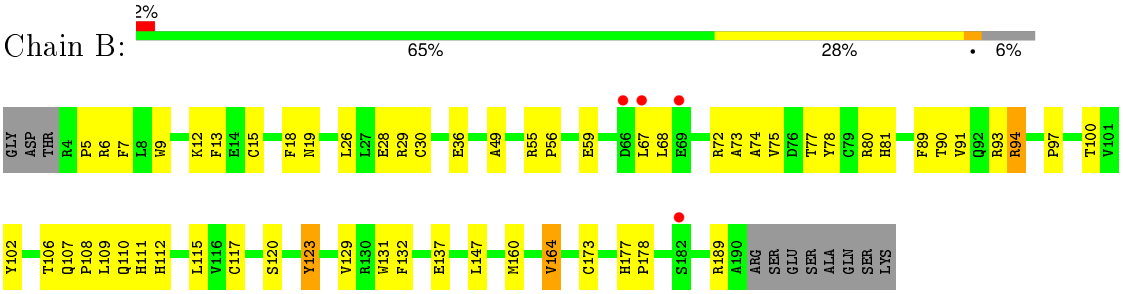
- Molecule 1: HLA-DR1 CLASS II HISTOCOMPATIBILITY PROTEIN

Chain J:



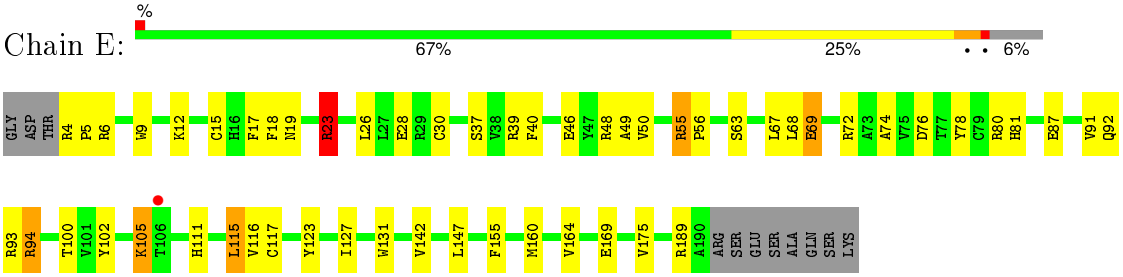
• Molecule 2: HLA-DR1 CLASS II HISTOCOMPATIBILITY PROTEIN

Chain B:



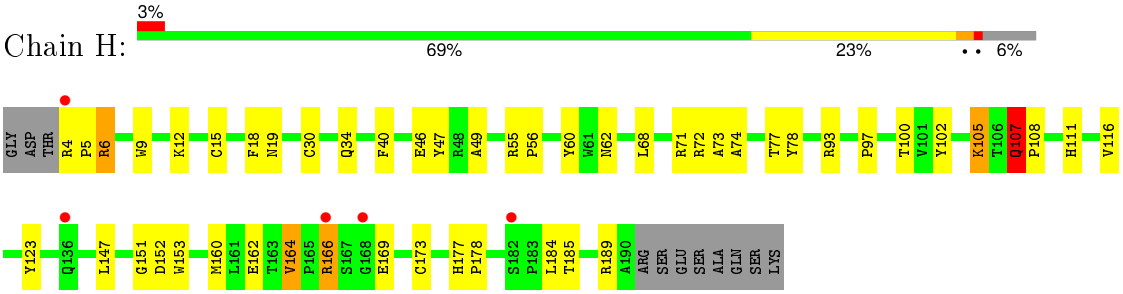
• Molecule 2: HLA-DR1 CLASS II HISTOCOMPATIBILITY PROTEIN

Chain E:



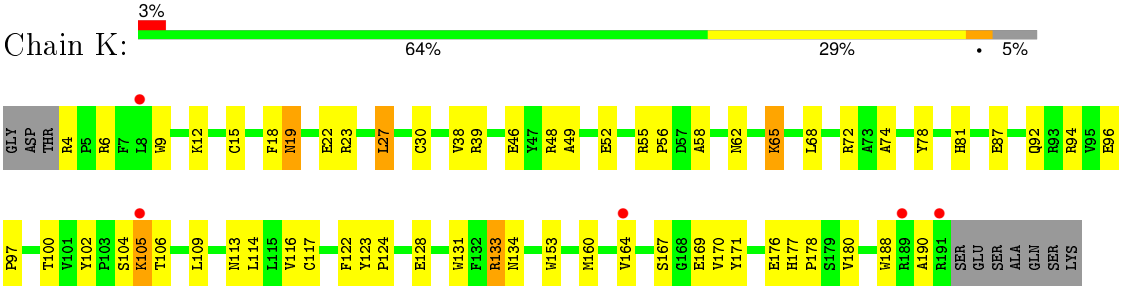
• Molecule 2: HLA-DR1 CLASS II HISTOCOMPATIBILITY PROTEIN

Chain H:



• Molecule 2: HLA-DR1 CLASS II HISTOCOMPATIBILITY PROTEIN

Chain K:



- Molecule 3: HLA-A2

Chain C:

- Molecule 3: HLA-A2

Chain F:

- Molecule 3: HLA-A2

Chain I:

- Molecule 3: HLA-A2

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	134.51Å 134.32Å 131.23Å 90.00° 104.82° 90.00°	Depositor
Resolution (Å)	6.00 – 2.45 19.75 – 2.45	Depositor EDS
% Data completeness (in resolution range)	89.0 (6.00-2.45) 89.1 (19.75-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.44Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.216 , 0.279 0.206 , 0.264	Depositor DCC
R_{free} test set	6967 reflections (10.12%)	DCC
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 87.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 73533 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12638	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.86	0/1518	0.97	2/2070 (0.1%)
1	D	0.86	0/1498	0.93	1/2043 (0.0%)
1	G	0.82	0/1498	0.94	1/2043 (0.0%)
1	J	0.87	0/1498	0.95	2/2043 (0.1%)
2	B	0.82	0/1577	0.99	2/2142 (0.1%)
2	E	0.88	1/1577 (0.1%)	1.01	5/2142 (0.2%)
2	H	0.82	0/1577	0.96	5/2142 (0.2%)
2	K	0.85	0/1588	0.97	4/2156 (0.2%)
3	C	0.85	0/129	1.25	1/173 (0.6%)
3	F	0.77	0/125	0.96	1/168 (0.6%)
3	I	0.66	0/129	0.88	1/173 (0.6%)
3	L	0.71	0/129	1.17	2/173 (1.2%)
All	All	0.85	1/12843 (0.0%)	0.97	27/17468 (0.2%)

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
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	69	GLU	CG-CD	5.15	1.59	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	146	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	123	ARG	NE-CZ-NH1	-7.55	116.53	120.30
2	E	23	ARG	NE-CZ-NH1	7.24	123.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	6	ARG	NE-CZ-NH2	-7.15	116.72	120.30
2	E	39	ARG	NE-CZ-NH2	-7.08	116.76	120.30
3	L	6	ARG	NE-CZ-NH1	7.00	123.80	120.30
2	K	133	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	E	94	ARG	NE-CZ-NH1	6.43	123.52	120.30
2	B	147	LEU	CB-CG-CD2	-6.37	100.17	111.00
2	H	71	ARG	NE-CZ-NH2	-6.19	117.21	120.30
2	H	6	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	K	164	VAL	N-CA-C	-5.89	95.09	111.00
3	F	6	ARG	NE-CZ-NH2	-5.80	117.40	120.30
2	H	164	VAL	N-CA-C	-5.63	95.79	111.00
1	A	123	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	J	92	LEU	CA-CB-CG	5.59	128.16	115.30
1	G	164	ARG	NE-CZ-NH2	-5.55	117.52	120.30
2	K	65	LYS	N-CA-C	5.55	125.98	111.00
2	E	55	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	K	133	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	H	71	ARG	NE-CZ-NH1	5.38	122.99	120.30
3	C	3	SER	N-CA-C	5.27	125.23	111.00
2	B	164	VAL	N-CA-C	-5.25	96.82	111.00
2	H	147	LEU	CB-CG-CD2	-5.17	102.21	111.00
1	D	146	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	E	164	VAL	N-CA-C	-5.07	97.31	111.00
3	I	6	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	123	TYR	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	1473	0	1407	54	0
1	D	1454	0	1394	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1454	0	1394	53	0
1	J	1454	0	1394	47	0
2	B	1537	0	1471	46	0
2	E	1537	0	1471	46	0
2	H	1537	0	1471	38	0
2	K	1548	0	1484	49	0
3	C	124	0	108	7	0
3	F	120	0	105	11	0
3	I	124	0	108	6	0
3	L	124	0	108	10	0
4	A	17	0	0	1	0
4	B	13	0	0	0	0
4	D	18	0	0	0	0
4	E	25	0	0	1	0
4	F	1	0	0	0	0
4	G	21	0	0	0	0
4	H	18	0	0	4	0
4	I	3	0	0	1	0
4	J	14	0	0	2	0
4	K	21	0	0	1	0
4	L	1	0	0	0	0
All	All	12638	0	11915	328	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 14.

All (328) 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:G:160:VAL:HG12	1:G:179:GLU:HG3	1.16	1.09
1:G:16:PRO:HD2	2:H:6:ARG:HD3	1.44	0.98
2:B:94:ARG:HG3	2:B:94:ARG:HH11	1.26	0.96
1:A:16:PRO:HD2	2:B:6:ARG:HD3	1.47	0.94
1:D:16:PRO:HD2	2:E:6:ARG:HD3	1.49	0.94
1:G:61:ALA:HB3	3:I:9:ARG:HH21	1.37	0.90
1:J:16:PRO:HD2	2:K:6:ARG:HD3	1.51	0.88
2:K:133:ARG:HD3	2:K:171:TYR:CE1	2.09	0.86
1:A:124:ASN:HD21	1:A:159:ASP:HB3	1.44	0.81
2:K:18:PHE:HB2	2:K:23:ARG:HB3	1.63	0.80
1:J:61:ALA:HB3	3:L:9:ARG:HH21	1.47	0.80
1:A:61:ALA:HB3	3:C:9:ARG:HH21	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:143:HIS:HD2	2:K:12:LYS:NZ	1.86	0.74
1:G:160:VAL:HG12	1:G:179:GLU:CG	2.10	0.73
1:A:124:ASN:ND2	1:A:159:ASP:HB3	2.04	0.72
1:D:3:GLU:HB2	2:E:18:PHE:CE2	2.24	0.72
1:D:61:ALA:HB3	3:F:9:ARG:HH21	1.53	0.71
1:J:3:GLU:HB2	2:K:18:PHE:CE2	2.25	0.71
2:K:133:ARG:HD3	2:K:171:TYR:CZ	2.25	0.71
1:G:81:PRO:HB3	2:H:5:PRO:HB2	1.74	0.70
2:K:81:HIS:CD2	3:L:6:ARG:HD2	2.27	0.69
2:B:94:ARG:NH1	2:B:94:ARG:HG3	1.96	0.69
2:E:23:ARG:HG2	2:E:23:ARG:HH11	1.57	0.68
1:A:99:LEU:HG	1:A:180:PHE:CE2	2.27	0.68
2:H:116:VAL:HG22	2:H:160:MET:HG2	1.75	0.68
2:E:18:PHE:HB2	2:E:23:ARG:HB3	1.75	0.68
1:A:61:ALA:CB	3:C:9:ARG:HH21	2.07	0.68
1:A:147:LYS:NZ	1:A:149:HIS:CE1	2.62	0.67
1:J:89:VAL:O	1:J:176:LYS:HE2	1.94	0.67
1:J:5:HIS:HE1	4:J:202:HOH:O	1.76	0.66
1:D:61:ALA:CB	3:F:9:ARG:HH21	2.08	0.66
1:G:47:GLU:O	1:G:50:ARG:HG2	1.94	0.66
1:A:147:LYS:NZ	1:A:149:HIS:HE1	1.93	0.66
2:E:117:CYS:HB2	2:E:131:TRP:CZ2	2.31	0.66
2:B:106:THR:O	2:B:106:THR:HG22	1.96	0.66
1:A:73:MET:HG3	2:B:9:TRP:CZ3	2.30	0.66
1:J:61:ALA:CB	3:L:9:ARG:HH21	2.08	0.66
1:A:160:VAL:HB	1:A:177:HIS:CE1	2.30	0.66
2:H:177:HIS:CD2	2:H:178:PRO:HD2	2.32	0.65
1:D:95:SER:HB2	1:D:96:PRO:CD	2.26	0.65
2:B:68:LEU:O	2:B:72:ARG:HG3	1.96	0.65
2:K:68:LEU:O	2:K:72:ARG:HG3	1.97	0.65
1:G:61:ALA:CB	3:I:9:ARG:HH21	2.08	0.65
1:G:143:HIS:HD2	2:H:12:LYS:NZ	1.97	0.62
1:G:118:ASN:HB2	1:G:166:GLU:HB2	1.81	0.62
1:D:118:ASN:HB2	1:D:166:GLU:HB2	1.80	0.62
2:H:34:GLN:HG3	4:H:215:HOH:O	2.01	0.61
1:D:95:SER:HB2	1:D:96:PRO:HD2	1.83	0.61
1:G:11:GLU:HA	1:G:21:GLU:O	2.01	0.61
1:J:143:HIS:HD2	2:K:12:LYS:HZ1	1.49	0.60
2:K:9:TRP:CH2	2:K:30:CYS:HB3	2.36	0.60
1:A:160:VAL:HG12	1:A:179:GLU:OE1	2.01	0.60
2:H:164:VAL:HB	2:H:166:ARG:HH21	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:127:ILE:HD11	2:E:175:VAL:CG1	2.31	0.60
2:H:74:ALA:O	2:H:78:TYR:HB3	2.02	0.60
2:E:81:HIS:CD2	3:F:6:ARG:HD2	2.36	0.60
1:G:101:GLU:OE1	1:G:101:GLU:HA	2.02	0.59
2:K:39:ARG:HD2	4:K:211:HOH:O	2.00	0.59
1:G:147:LYS:NZ	1:G:149:HIS:CE1	2.70	0.59
2:K:177:HIS:CD2	2:K:178:PRO:HD2	2.38	0.58
1:J:118:ASN:HB2	1:J:166:GLU:HB2	1.84	0.58
2:H:9:TRP:CH2	2:H:30:CYS:HB3	2.39	0.58
1:A:98:GLU:O	1:A:101:GLU:HB2	2.02	0.58
1:G:147:LYS:NZ	1:G:149:HIS:HE1	2.01	0.58
1:D:162:ASP:HA	1:D:176:LYS:O	2.03	0.58
1:D:17:ASP:OD2	2:E:6:ARG:HD2	2.04	0.57
1:A:147:LYS:HZ2	1:A:149:HIS:CE1	2.23	0.57
2:E:100:THR:HG22	2:E:102:TYR:HD1	1.70	0.57
2:E:68:LEU:HB3	2:E:72:ARG:NH1	2.19	0.57
1:G:115:PRO:HD3	1:G:145:PHE:CE1	2.40	0.57
1:A:147:LYS:HZ3	1:A:149:HIS:CE1	2.23	0.56
2:B:112:HIS:HA	2:B:164:VAL:HG22	1.87	0.56
1:A:98:GLU:HB2	1:A:101:GLU:HG3	1.86	0.56
2:B:93:ARG:O	2:B:94:ARG:HG3	2.05	0.56
2:E:23:ARG:NH1	2:E:23:ARG:HG2	2.16	0.56
2:K:116:VAL:HG22	2:K:160:MET:HG2	1.86	0.56
1:J:95:SER:HB2	1:J:96:PRO:CD	2.36	0.55
1:G:75:LYS:HD2	1:G:79:TYR:OH	2.06	0.55
1:G:82:ILE:HG22	2:H:6:ARG:HB2	1.88	0.55
2:K:133:ARG:CD	2:K:171:TYR:CE1	2.86	0.55
1:J:143:HIS:CD2	2:K:12:LYS:NZ	2.73	0.55
2:E:93:ARG:HG2	2:E:123:TYR:CD1	2.42	0.55
1:A:115:PRO:HD3	1:A:145:PHE:CE1	2.41	0.55
1:A:147:LYS:HZ2	1:A:149:HIS:HE1	1.54	0.55
2:B:13:PHE:CE1	2:B:28:GLU:HG3	2.42	0.55
2:E:9:TRP:CH2	2:E:30:CYS:HB3	2.42	0.55
1:D:143:HIS:HD2	2:E:12:LYS:NZ	2.05	0.55
1:A:11:GLU:HA	1:A:21:GLU:O	2.07	0.54
2:H:177:HIS:CG	2:H:178:PRO:HD2	2.42	0.54
1:J:26:PHE:HB2	1:J:31:ILE:HD11	1.90	0.54
1:G:147:LYS:HZ3	1:G:149:HIS:CE1	2.26	0.54
2:K:49:ALA:HB2	2:K:55:ARG:HA	1.89	0.54
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.89	0.54
2:E:49:ALA:HB2	2:E:55:ARG:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:12:HIS:HB3	4:I:110:HOH:O	2.06	0.54
1:D:97:VAL:CG1	1:D:155:PRO:HB3	2.38	0.54
1:G:6:VAL:HA	2:H:15:CYS:O	2.08	0.54
1:D:62:ASN:OD1	3:F:9:ARG:HG3	2.08	0.54
2:H:34:GLN:CG	4:H:215:HOH:O	2.55	0.54
2:K:52:GLU:CD	2:K:55:ARG:HH21	2.11	0.53
1:J:162:ASP:HA	1:J:176:LYS:O	2.07	0.53
2:E:87:GLU:O	2:E:92:GLN:HG2	2.08	0.53
1:D:69:ASN:HB3	3:F:13:GLN:HG3	1.89	0.53
1:J:79:TYR:CD1	1:J:79:TYR:N	2.77	0.53
1:A:162:ASP:HA	1:A:176:LYS:O	2.07	0.53
2:K:38:VAL:HG23	2:K:48:ARG:O	2.07	0.53
1:A:79:TYR:O	2:B:7:PHE:HE1	1.92	0.52
2:K:100:THR:HG22	2:K:102:TYR:HD1	1.74	0.52
2:B:177:HIS:CD2	2:B:178:PRO:HD2	2.44	0.52
1:G:89:VAL:O	1:G:176:LYS:HE2	2.09	0.52
1:A:81:PRO:HB3	2:B:5:PRO:HB2	1.89	0.52
2:B:106:THR:CG2	2:B:106:THR:O	2.57	0.52
2:H:107:GLN:OE1	2:H:111:HIS:HB3	2.09	0.52
1:A:82:ILE:HG22	2:B:6:ARG:HB2	1.92	0.52
2:B:109:LEU:O	2:B:110:GLN:HB2	2.09	0.52
1:D:73:MET:HG3	2:E:9:TRP:CZ3	2.44	0.52
2:B:49:ALA:HB2	2:B:55:ARG:HA	1.90	0.52
2:H:49:ALA:HB2	2:H:55:ARG:HA	1.92	0.52
1:G:26:PHE:HB2	1:G:31:ILE:HD11	1.92	0.52
1:J:113:THR:OG1	1:J:114:PRO:HA	2.10	0.52
1:D:99:LEU:O	1:D:100:ARG:HB2	2.10	0.51
1:J:93:THR:HA	1:J:104:VAL:O	2.10	0.51
2:B:68:LEU:HB3	2:B:72:ARG:NH1	2.25	0.51
1:G:16:PRO:HD2	2:H:6:ARG:CD	2.29	0.51
1:J:11:GLU:HA	1:J:21:GLU:O	2.10	0.51
2:H:46:GLU:HB2	2:H:62:ASN:OD1	2.10	0.51
1:A:95:SER:HB2	1:A:96:PRO:CD	2.41	0.51
1:G:143:HIS:HD2	2:H:12:LYS:HZ1	1.59	0.51
1:A:89:VAL:HG12	1:A:176:LYS:HG3	1.92	0.51
2:H:152:ASP:O	2:H:153:TRP:HB2	2.09	0.51
1:G:144:LEU:HD23	4:H:215:HOH:O	2.11	0.50
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.93	0.50
2:E:142:VAL:HG11	4:E:219:HOH:O	2.10	0.50
1:J:111:LYS:HG2	1:J:140:ARG:CZ	2.41	0.50
2:K:134:ASN:OD1	2:K:170:VAL:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100:THR:HG22	2:H:102:TYR:HD1	1.76	0.50
1:D:11:GLU:HA	1:D:21:GLU:O	2.11	0.50
2:E:127:ILE:HD11	2:E:175:VAL:HG11	1.93	0.50
1:A:143:HIS:HD2	2:B:12:LYS:NZ	2.10	0.50
2:B:100:THR:HG22	2:B:102:TYR:HD1	1.77	0.50
1:J:95:SER:HB2	1:J:96:PRO:HD2	1.93	0.49
1:D:45:LEU:O	1:D:48:PHE:HB2	2.12	0.49
1:J:6:VAL:HG12	1:J:8:ILE:HG13	1.93	0.49
1:D:121:TRP:O	1:D:127:PRO:HA	2.12	0.49
2:K:78:TYR:HE1	3:L:7:PHE:HA	1.77	0.49
1:J:132:VAL:HG12	1:J:151:LEU:HD13	1.95	0.49
2:E:23:ARG:CG	2:E:23:ARG:HH11	2.25	0.49
1:A:62:ASN:OD1	3:C:7:PHE:HE2	1.96	0.49
1:G:113:THR:HG21	4:H:215:HOH:O	2.12	0.49
1:D:12:PHE:C	1:D:12:PHE:CD1	2.86	0.48
2:B:93:ARG:O	2:B:94:ARG:NH1	2.46	0.48
2:B:55:ARG:O	2:B:59:GLU:HG3	2.13	0.48
1:A:89:VAL:O	1:A:176:LYS:HE2	2.14	0.48
2:B:29:ARG:HG2	2:B:36:GLU:OE2	2.13	0.48
1:A:98:GLU:CB	1:A:101:GLU:HG3	2.44	0.48
2:H:93:ARG:HG2	2:H:123:TYR:CD1	2.49	0.48
1:D:77:SER:O	1:D:78:ASN:HB3	2.14	0.47
1:J:45:LEU:HD11	2:K:153:TRP:HB2	1.94	0.47
2:K:117:CYS:HB2	2:K:131:TRP:CZ2	2.50	0.47
2:K:188:TRP:CH2	2:K:190:ALA:HB2	2.49	0.47
1:G:103:ASN:HB3	1:G:153:PHE:CE1	2.49	0.47
1:G:121:TRP:O	1:G:127:PRO:HA	2.15	0.47
2:K:170:VAL:O	2:K:170:VAL:HG13	2.15	0.47
1:A:155:PRO:HA	4:A:197:HOH:O	2.14	0.47
2:E:68:LEU:HB3	2:E:72:ARG:HH12	1.80	0.47
1:A:13:TYR:CE2	1:A:67:LYS:HG3	2.50	0.47
2:K:177:HIS:CG	2:K:178:PRO:HD2	2.49	0.46
1:A:16:PRO:HD2	2:B:6:ARG:CD	2.34	0.46
2:B:78:TYR:HE1	3:C:7:PHE:HA	1.80	0.46
1:G:93:THR:HA	1:G:104:VAL:O	2.15	0.46
1:J:160:VAL:HG12	1:J:179:GLU:CB	2.46	0.46
1:D:6:VAL:HA	2:E:15:CYS:O	2.15	0.46
1:J:121:TRP:O	1:J:127:PRO:HA	2.16	0.46
1:G:134:GLU:HB3	1:G:149:HIS:CD2	2.51	0.46
1:D:70:LEU:HD13	2:E:9:TRP:HB2	1.98	0.46
1:D:16:PRO:HG3	2:E:4:ARG:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:5:HIS:CE1	4:J:202:HOH:O	2.59	0.46
2:K:52:GLU:OE1	2:K:55:ARG:NH2	2.48	0.46
1:G:162:ASP:HA	1:G:176:LYS:O	2.16	0.46
1:J:86:PRO:HB3	1:J:169:GLY:C	2.36	0.46
1:J:86:PRO:HB3	1:J:169:GLY:O	2.16	0.46
1:G:6:VAL:HG12	1:G:8:ILE:HG13	1.97	0.46
1:J:62:ASN:OD1	3:L:7:PHE:HE2	1.99	0.46
1:G:54:PHE:CE1	1:G:55:GLU:O	2.69	0.46
1:J:63:ILE:O	1:J:66:ASP:HB2	2.16	0.46
1:D:3:GLU:HA	2:E:18:PHE:CD2	2.51	0.45
2:H:166:ARG:O	2:H:169:GLU:HB2	2.16	0.45
2:E:116:VAL:HG22	2:E:160:MET:HG2	1.97	0.45
2:E:81:HIS:CD2	3:F:6:ARG:CD	2.99	0.45
1:A:95:SER:HB2	1:A:96:PRO:HD2	1.97	0.45
2:H:34:GLN:HG2	2:H:34:GLN:O	2.16	0.45
1:J:143:HIS:CD2	2:K:12:LYS:HZ1	2.32	0.45
1:J:143:HIS:CD2	2:K:12:LYS:HZ2	2.35	0.45
2:B:9:TRP:CH2	2:B:30:CYS:HB3	2.51	0.45
2:H:68:LEU:HB3	2:H:72:ARG:NH1	2.32	0.45
1:J:12:PHE:C	1:J:12:PHE:CD1	2.89	0.45
2:B:81:HIS:CD2	3:C:6:ARG:HD2	2.51	0.45
2:B:73:ALA:O	2:B:77:THR:HG23	2.16	0.45
1:A:121:TRP:O	1:A:127:PRO:HA	2.17	0.45
2:E:115:LEU:HA	2:E:115:LEU:HD23	1.88	0.45
1:G:100:ARG:HA	1:G:154:LEU:HD11	1.98	0.45
1:A:160:VAL:HB	1:A:177:HIS:HE1	1.77	0.45
2:K:74:ALA:O	2:K:78:TYR:HB3	2.17	0.45
1:A:123:ARG:HB3	1:A:128:VAL:HG22	1.98	0.45
2:E:74:ALA:O	2:E:78:TYR:HB3	2.17	0.45
1:G:62:ASN:OD1	3:I:7:PHE:HE2	2.00	0.45
1:A:97:VAL:CG1	1:A:155:PRO:HB3	2.47	0.45
2:K:105:LYS:HE2	2:K:113:ASN:HA	1.99	0.45
2:K:97:PRO:HB3	2:K:122:PHE:HB3	1.99	0.45
1:A:93:THR:HA	1:A:104:VAL:O	2.16	0.45
2:H:55:ARG:N	2:H:56:PRO:CD	2.80	0.45
1:D:26:PHE:HB2	1:D:31:ILE:HD11	2.00	0.45
1:D:16:PRO:HD2	2:E:6:ARG:CD	2.34	0.44
2:B:97:PRO:HA	2:B:120:SER:O	2.17	0.44
1:G:44:ARG:NH2	2:H:151:GLY:O	2.50	0.44
1:D:97:VAL:HG13	1:D:155:PRO:HG3	1.99	0.44
2:E:76:ASP:OD1	2:E:80:ARG:HD2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:9:TRP:CZ2	2:K:30:CYS:HB3	2.52	0.44
2:B:93:ARG:HG2	2:B:123:TYR:CD1	2.52	0.44
1:G:12:PHE:CD1	1:G:12:PHE:C	2.91	0.44
2:E:68:LEU:O	2:E:72:ARG:HG3	2.16	0.44
1:G:3:GLU:HB2	2:H:18:PHE:CE2	2.53	0.44
2:E:46:GLU:OE2	2:E:48:ARG:NH1	2.49	0.44
2:K:55:ARG:HG2	2:K:55:ARG:HH11	1.81	0.44
1:J:97:VAL:HG13	1:J:155:PRO:CG	2.48	0.44
1:A:3:GLU:HB2	2:B:18:PHE:CE2	2.52	0.44
2:E:87:GLU:HG3	2:E:91:VAL:HB	1.99	0.44
2:K:94:ARG:HA	2:K:123:TYR:O	2.18	0.44
1:D:113:THR:OG1	1:D:114:PRO:HA	2.18	0.44
1:A:6:VAL:HA	2:B:15:CYS:O	2.18	0.44
2:B:75:VAL:HG12	2:B:80:ARG:NH1	2.32	0.44
1:D:93:THR:HA	1:D:104:VAL:O	2.17	0.44
2:K:81:HIS:CD2	3:L:6:ARG:CD	2.98	0.43
1:G:9:GLN:HB2	1:G:24:PHE:CE2	2.53	0.43
2:B:132:PHE:CE2	2:B:137:GLU:HB2	2.53	0.43
1:J:109:ILE:HD11	1:J:119:VAL:HG21	2.00	0.43
2:E:28:GLU:HB3	2:E:40:PHE:HB3	2.00	0.43
1:G:35:ASP:O	1:G:39:LYS:N	2.52	0.43
1:A:14:LEU:O	1:A:18:GLN:N	2.49	0.43
1:G:95:SER:HB2	1:G:96:PRO:HD2	2.01	0.43
1:A:15:ASN:O	2:B:6:ARG:HA	2.18	0.43
1:G:97:VAL:CG1	1:G:155:PRO:HB3	2.49	0.43
2:B:107:GLN:HA	2:B:108:PRO:HD2	1.65	0.43
2:K:55:ARG:N	2:K:56:PRO:CD	2.82	0.43
1:A:123:ARG:HD2	1:A:123:ARG:HH11	1.64	0.43
2:E:147:LEU:HD11	2:E:155:PHE:CD2	2.54	0.43
1:D:69:ASN:CB	3:F:13:GLN:HG3	2.49	0.43
1:G:95:SER:HB2	1:G:96:PRO:CD	2.49	0.43
1:G:97:VAL:HG13	1:G:155:PRO:CG	2.49	0.43
2:E:105:LYS:HE2	2:E:105:LYS:HB2	1.44	0.43
2:K:128:GLU:HB2	2:K:176:GLU:HB2	2.00	0.43
2:E:37:SER:O	2:E:50:VAL:N	2.42	0.43
1:D:97:VAL:HG13	1:D:155:PRO:CG	2.49	0.43
2:H:68:LEU:O	2:H:72:ARG:HG3	2.18	0.43
2:E:26:LEU:HD22	2:E:74:ALA:HB3	2.01	0.43
1:J:138:LEU:HB2	1:J:146:ARG:HB2	2.00	0.43
1:G:17:ASP:O	1:G:18:GLN:HB2	2.18	0.43
2:E:4:ARG:HG3	2:E:5:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:18:PHE:N	2:K:18:PHE:CD1	2.86	0.42
1:D:69:ASN:HB3	3:F:13:GLN:CG	2.49	0.42
2:B:115:LEU:O	2:B:160:MET:HA	2.18	0.42
1:G:3:GLU:HA	2:H:18:PHE:CD2	2.54	0.42
1:J:69:ASN:HB3	3:L:13:GLN:HG3	2.00	0.42
2:H:173:CYS:O	2:H:185:THR:HA	2.19	0.42
1:J:16:PRO:HD2	2:K:6:ARG:CD	2.34	0.42
2:E:78:TYR:HE1	3:F:7:PHE:HA	1.85	0.42
1:G:72:ILE:HD12	3:I:13:GLN:HB2	2.02	0.42
1:A:124:ASN:HD21	1:A:159:ASP:CB	2.24	0.42
1:D:3:GLU:HG2	1:D:3:GLU:O	2.18	0.42
2:B:55:ARG:HH11	2:B:55:ARG:HG2	1.83	0.42
1:A:72:ILE:CD1	3:C:13:GLN:HB2	2.49	0.42
2:H:162:GLU:OE2	1:J:177:HIS:ND1	2.53	0.42
2:K:104:SER:OG	2:K:114:LEU:HB3	2.19	0.42
2:B:55:ARG:N	2:B:56:PRO:CD	2.82	0.42
2:H:73:ALA:O	2:H:77:THR:HG23	2.19	0.42
1:D:101:GLU:HA	1:D:102:PRO:HD3	1.79	0.42
2:K:46:GLU:HB2	2:K:62:ASN:OD1	2.19	0.42
1:J:69:ASN:HB3	3:L:13:GLN:CG	2.50	0.42
2:B:129:VAL:HG13	2:B:173:CYS:SG	2.60	0.42
1:D:4:GLU:N	2:E:17:PHE:O	2.53	0.42
2:B:108:PRO:O	2:B:111:HIS:ND1	2.46	0.42
2:H:97:PRO:HG2	2:H:184:LEU:HD12	2.02	0.42
2:K:96:GLU:HG3	2:K:180:VAL:CG1	2.50	0.42
2:E:87:GLU:HG2	2:E:92:GLN:HG2	2.02	0.42
2:E:147:LEU:HG	2:E:155:PHE:HD2	1.84	0.42
1:A:38:LYS:HB2	1:A:40:GLU:HG2	2.02	0.42
1:G:12:PHE:HA	2:H:9:TRP:O	2.20	0.41
1:J:6:VAL:HA	2:K:15:CYS:O	2.20	0.41
1:D:76:ARG:NH2	3:F:14:TYR:O	2.53	0.41
1:J:147:LYS:NZ	1:J:149:HIS:CE1	2.88	0.41
2:B:26:LEU:HD22	2:B:74:ALA:HB3	2.02	0.41
1:G:160:VAL:HB	1:G:177:HIS:CE1	2.55	0.41
1:G:147:LYS:HZ2	1:G:149:HIS:CE1	2.36	0.41
1:A:3:GLU:HA	2:B:18:PHE:CD2	2.55	0.41
1:A:94:ASN:HD22	1:A:104:VAL:HB	1.86	0.41
1:G:14:LEU:HD11	2:H:6:ARG:HB3	2.02	0.41
2:K:58:ALA:O	2:K:62:ASN:HB2	2.20	0.41
2:K:87:GLU:HG2	2:K:92:GLN:HG2	2.03	0.41
1:A:124:ASN:CG	1:A:159:ASP:HB3	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:97:VAL:CG1	1:J:155:PRO:HB3	2.51	0.41
2:E:55:ARG:N	2:E:56:PRO:CD	2.83	0.41
2:H:100:THR:HG22	2:H:102:TYR:CD1	2.55	0.41
1:G:13:TYR:OH	1:G:18:GLN:HG3	2.21	0.41
1:A:160:VAL:CG1	1:A:179:GLU:OE1	2.68	0.41
2:K:27:LEU:CD2	2:K:39:ARG:HD3	2.51	0.41
1:A:74:THR:HG23	2:B:7:PHE:CD1	2.56	0.41
1:D:100:ARG:HA	1:D:100:ARG:HD3	1.93	0.41
1:G:122:LEU:HD23	1:G:127:PRO:HA	2.03	0.41
1:A:6:VAL:HG12	1:A:8:ILE:HG13	2.03	0.41
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.56	0.41
2:B:90:THR:OG1	2:B:91:VAL:N	2.53	0.41
1:J:72:ILE:HD12	3:L:13:GLN:HB2	2.03	0.41
2:H:40:PHE:HB2	2:H:47:TYR:CE1	2.56	0.41
2:K:19:ASN:O	2:K:22:GLU:HB2	2.20	0.41
1:G:111:LYS:HG2	1:G:140:ARG:CZ	2.50	0.41
1:J:143:HIS:HD2	2:K:12:LYS:HZ2	1.62	0.40
1:J:69:ASN:CG	3:L:13:GLN:HG2	2.41	0.40
1:D:105:LEU:HG	1:D:153:PHE:CE1	2.56	0.40
1:D:115:PRO:HD3	1:D:145:PHE:CE1	2.56	0.40
1:J:160:VAL:HG12	1:J:179:GLU:HB2	2.03	0.40
1:G:69:ASN:CG	3:I:13:GLN:HG2	2.42	0.40
2:H:105:LYS:HE3	2:H:105:LYS:HB2	1.47	0.40
3:C:8:LEU:HD23	3:C:8:LEU:HA	1.82	0.40
1:D:73:MET:HG2	3:F:13:GLN:OE1	2.21	0.40
1:A:134:GLU:HB3	1:A:149:HIS:CD2	2.57	0.40
2:E:127:ILE:HD11	2:E:175:VAL:HG13	2.03	0.40
1:J:101:GLU:O	1:J:155:PRO:HD2	2.21	0.40
2:B:89:PHE:CD1	2:B:90:THR:HG23	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	177/192 (92%)	170 (96%)	7 (4%)	0	100	100
1	D	175/192 (91%)	170 (97%)	5 (3%)	0	100	100
1	G	175/192 (91%)	172 (98%)	3 (2%)	0	100	100
1	J	175/192 (91%)	166 (95%)	9 (5%)	0	100	100
2	B	185/198 (93%)	172 (93%)	13 (7%)	0	100	100
2	E	185/198 (93%)	177 (96%)	8 (4%)	0	100	100
2	H	185/198 (93%)	172 (93%)	10 (5%)	3 (2%)	12	11
2	K	186/198 (94%)	178 (96%)	6 (3%)	2 (1%)	17	19
3	C	12/15 (80%)	10 (83%)	2 (17%)	0	100	100
3	F	11/15 (73%)	10 (91%)	1 (9%)	0	100	100
3	I	12/15 (80%)	12 (100%)	0	0	100	100
3	L	12/15 (80%)	12 (100%)	0	0	100	100
All	All	1490/1620 (92%)	1421 (95%)	64 (4%)	5 (0%)	46	57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	65	LYS
2	H	108	PRO
2	K	167	SER
2	H	60	TYR
2	H	107	GLN

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	164/176 (93%)	155 (94%)	9 (6%)	27	37
1	D	162/176 (92%)	153 (94%)	9 (6%)	26	36
1	G	162/176 (92%)	154 (95%)	8 (5%)	31	43
1	J	162/176 (92%)	153 (94%)	9 (6%)	26	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	169/178 (95%)	165 (98%)	4 (2%)	57 73
2	E	169/178 (95%)	158 (94%)	11 (6%)	21 28
2	H	169/178 (95%)	163 (96%)	6 (4%)	42 58
2	K	170/178 (96%)	162 (95%)	8 (5%)	32 45
3	C	11/12 (92%)	10 (91%)	1 (9%)	12 13
3	F	11/12 (92%)	11 (100%)	0	100 100
3	I	11/12 (92%)	11 (100%)	0	100 100
3	L	11/12 (92%)	11 (100%)	0	100 100
All	All	1371/1464 (94%)	1306 (95%)	65 (5%)	32 45

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	47	GLU
1	A	71	GLU
1	A	94	ASN
1	A	128	VAL
1	A	129	THR
1	A	159	ASP
1	A	164	ARG
1	A	181	ASP
2	B	19	ASN
2	B	67	LEU
2	B	94	ARG
2	B	189	ARG
3	C	3	SER
1	D	11	GLU
1	D	12	PHE
1	D	18	GLN
1	D	47	GLU
1	D	71	GLU
1	D	81	PRO
1	D	94	ASN
1	D	128	VAL
1	D	129	THR
2	E	19	ASN
2	E	23	ARG
2	E	63	SER

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Mol	Chain	Res	Type
2	E	67	LEU
2	E	69	GLU
2	E	94	ARG
2	E	105	LYS
2	E	111	HIS
2	E	115	LEU
2	E	169	GLU
2	E	189	ARG
1	G	11	GLU
1	G	18	GLN
1	G	71	GLU
1	G	94	ASN
1	G	100	ARG
1	G	128	VAL
1	G	129	THR
1	G	158	GLU
2	H	4	ARG
2	H	19	ASN
2	H	105	LYS
2	H	107	GLN
2	H	166	ARG
2	H	189	ARG
1	J	11	GLU
1	J	47	GLU
1	J	63	ILE
1	J	71	GLU
1	J	73	MET
1	J	81	PRO
1	J	94	ASN
1	J	129	THR
1	J	164	ARG
2	K	4	ARG
2	K	19	ASN
2	K	27	LEU
2	K	105	LYS
2	K	106	THR
2	K	109	LEU
2	K	124	PRO
2	K	169	GLU

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

Mol	Chain	Res	Type
1	A	143	HIS
1	A	149	HIS
2	B	150	ASN
1	D	94	ASN
1	D	143	HIS
1	D	149	HIS
2	E	10	GLN
2	E	156	GLN
1	G	18	GLN
1	G	143	HIS
1	G	149	HIS
2	H	19	ASN
2	H	156	GLN
1	J	143	HIS
1	J	149	HIS
2	K	156	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	179/192 (93%)	0.03	7 (3%) 43 47	21, 34, 60, 80	18 (10%)
1	D	177/192 (92%)	-0.14	4 (2%) 64 66	17, 31, 56, 70	16 (9%)
1	G	177/192 (92%)	-0.03	5 (2%) 56 60	18, 33, 62, 70	13 (7%)
1	J	177/192 (92%)	-0.16	4 (2%) 64 66	16, 31, 57, 69	12 (6%)
2	B	186/198 (93%)	-0.02	4 (2%) 65 68	19, 36, 59, 76	20 (10%)
2	E	187/198 (94%)	-0.15	1 (0%) 91 92	19, 31, 55, 68	20 (10%)
2	H	187/198 (94%)	-0.04	5 (2%) 58 61	19, 34, 58, 81	18 (9%)
2	K	178/198 (89%)	-0.04	5 (2%) 56 60	19, 32, 60, 79	15 (8%)
3	C	14/15 (93%)	0.80	3 (21%) 1 1	27, 57, 74, 78	1 (7%)
3	F	13/15 (86%)	0.51	1 (7%) 16 17	25, 44, 69, 75	2 (15%)
3	I	14/15 (93%)	0.36	0 100 100	27, 42, 61, 70	1 (7%)
3	L	14/15 (93%)	1.00	3 (21%) 1 1	27, 45, 73, 79	2 (14%)
All	All	1503/1620 (92%)	-0.04	42 (2%) 56 60	16, 33, 61, 81	138 (9%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	2	GLY	5.3
2	H	4	ARG	4.0
1	A	181	ASP	3.7
3	L	3	SER	3.5
2	K	191	ARG	3.4
2	K	8	LEU	3.2
2	K	105	LYS	3.1
1	A	37	ALA	3.0
1	G	130	THR	2.9
3	F	15	ALA	2.9
2	H	136	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
3	L	15	ALA	2.8
3	C	2	GLY	2.7
1	A	39	LYS	2.7
1	J	79	TYR	2.7
3	C	3	SER	2.7
2	B	67	LEU	2.6
1	D	105	LEU	2.6
1	A	78	ASN	2.6
2	K	164	VAL	2.5
1	D	46	GLU	2.5
1	J	172	GLU	2.4
1	D	57	GLN	2.4
1	A	57	GLN	2.4
2	B	69	GLU	2.4
2	H	168	GLY	2.4
1	G	131	GLY	2.3
1	J	51	PHE	2.3
1	A	79	TYR	2.3
2	B	182	SER	2.2
1	A	3	GLU	2.2
2	H	166	ARG	2.2
1	G	37	ALA	2.2
1	G	107	CYS	2.1
3	C	14	TYR	2.1
1	J	57	GLN	2.1
1	D	78	ASN	2.0
2	K	189	ARG	2.0
2	E	106	THR	2.0
2	H	182	SER	2.0
1	G	163	CYS	2.0
2	B	66	ASP	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 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.