Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:04 PM GMT

PDB ID	:	1N5A
Title	:	Crystal structure of the Murine class I Major Histocompatibility Complex of H-2DB, B2-Microglobulin, and A 9-Residue immunodominant peptide epitope gp33 derived from LCMV
Authors	:	Achour, A.; Michaelsson, J.; Harris, R.A.; Odeberg, J.; Grufman, P.; Sandberg, J.K.; Levitsky, V.; Karre, K.; Sandalova, T.; Schneider, G.
Deposited on	:	2002-11-05
Resolution	:	2.85 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:

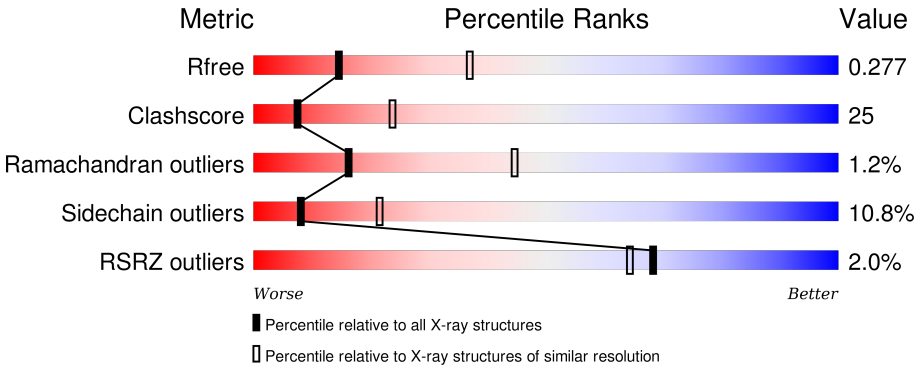
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	276	52% 39% 8%
1	D	276	53% 37% 7%
1	G	276	6% 53% 39% 6%
1	J	276	2% 58% 36%
2	B	99	54% 37% 6%

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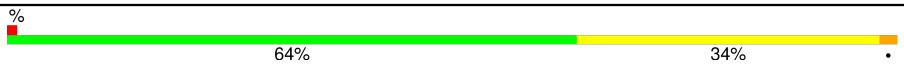
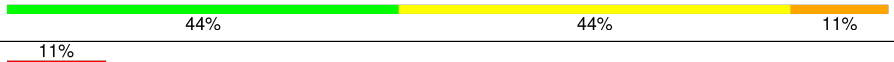
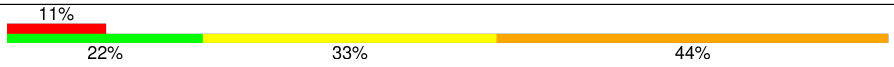
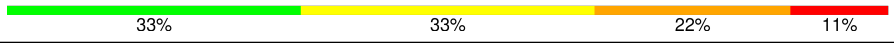
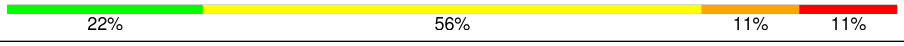
Mol	Chain	Length	Quality of chain
2	E	99	
2	H	99	
2	K	99	
3	C	9	
3	F	9	
3	I	9	
3	L	9	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12633 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2265	1430	400	426	9			
1	D	274	Total	C	N	O	S	0	0	0
			2248	1420	398	421	9			
1	G	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			
1	J	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			812	519	137	150	6			
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 nonameric peptide, gp33 derived from lymphocytic choriomeningitis virus.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			73	48	11	13	1			
3	F	9	Total	C	N	O	S	0	0	0
			73	48	11	13	1			
3	I	9	Total	C	N	O	S	0	0	0
			73	48	11	13	1			
3	L	9	Total	C	N	O	S	0	0	0
			73	48	11	13	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	9	MET	CYS	ENGINEERED	UNP Q9QDK7
F	9	MET	CYS	ENGINEERED	UNP Q9QDK7
I	9	MET	CYS	ENGINEERED	UNP Q9QDK7
L	9	MET	CYS	ENGINEERED	UNP Q9QDK7

- Molecule 4 is water.

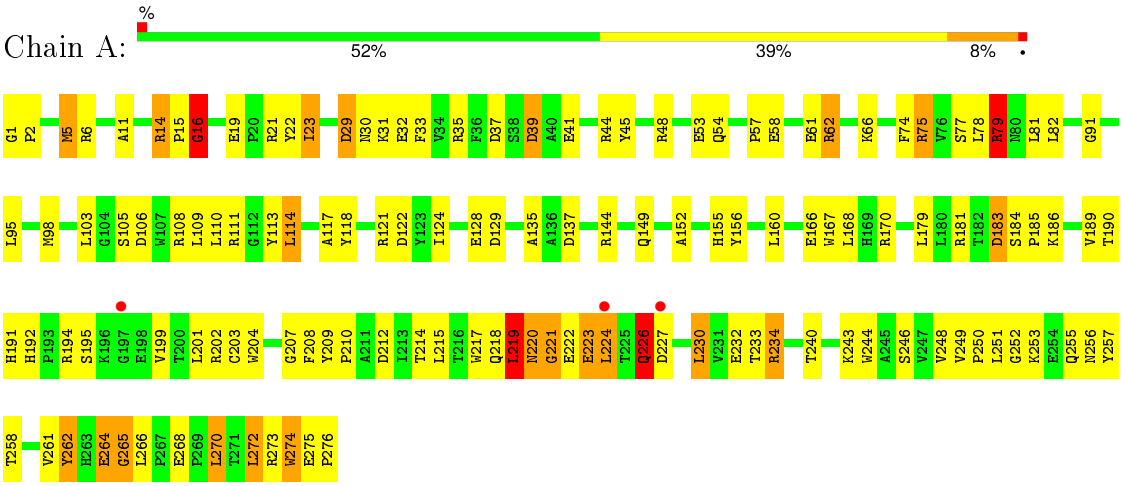
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	B	7	Total O 7 7	0	0
4	D	12	Total O 12 12	0	0
4	E	2	Total O 2 2	0	0
4	G	9	Total O 9 9	0	0
4	H	5	Total O 5 5	0	0
4	J	10	Total O 10 10	0	0
4	K	7	Total O 7 7	0	0
4	L	1	Total O 1 1	0	0

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.

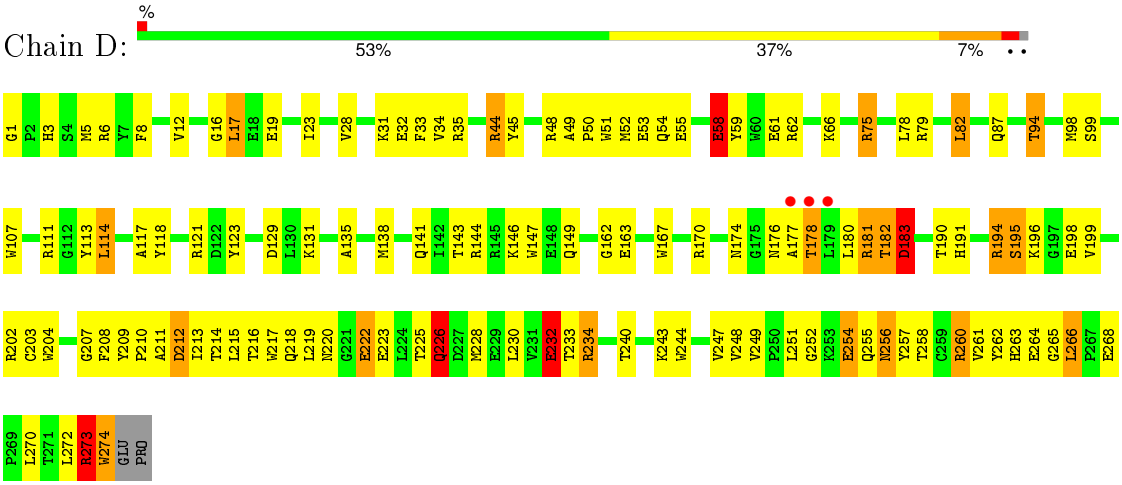
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain A:



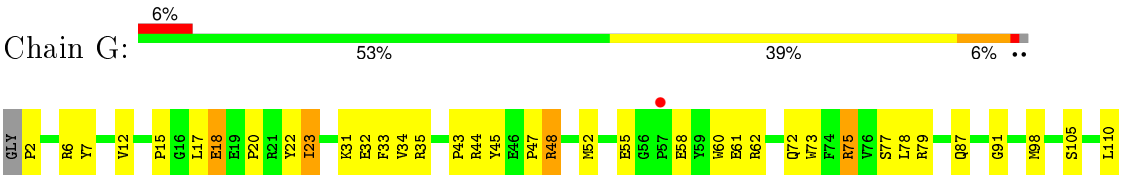
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

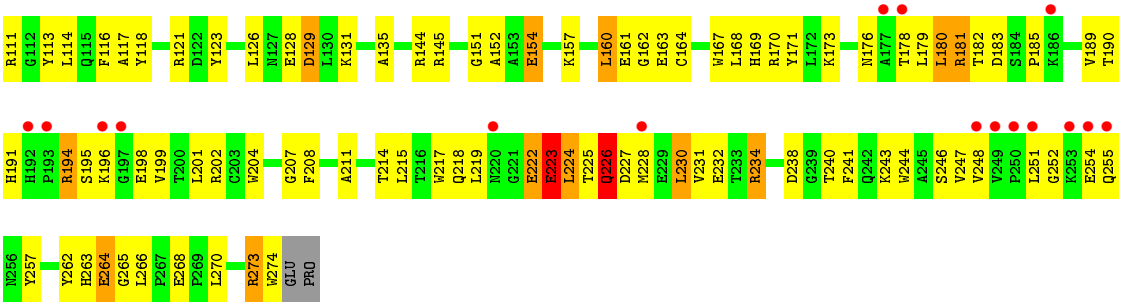
Chain D:



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

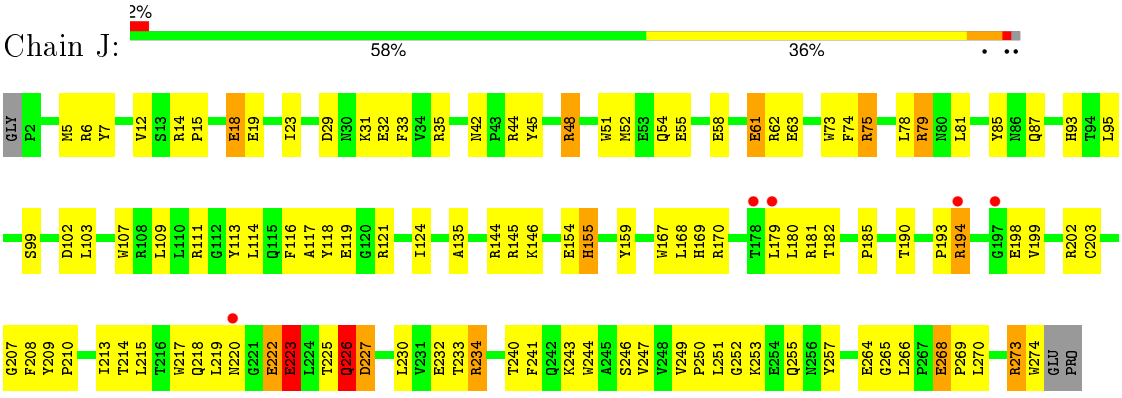
Chain G:





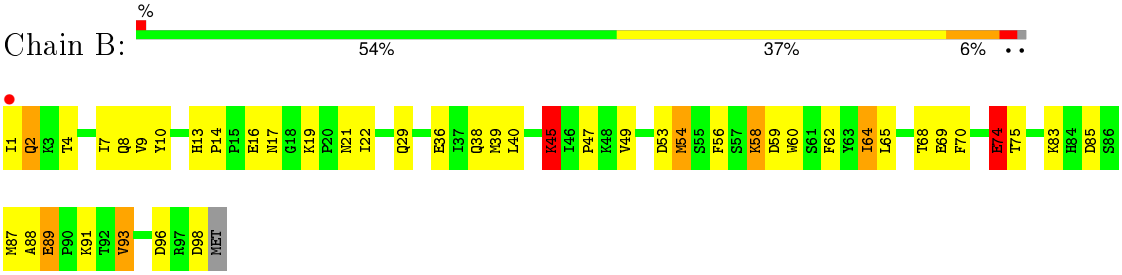
• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain J:



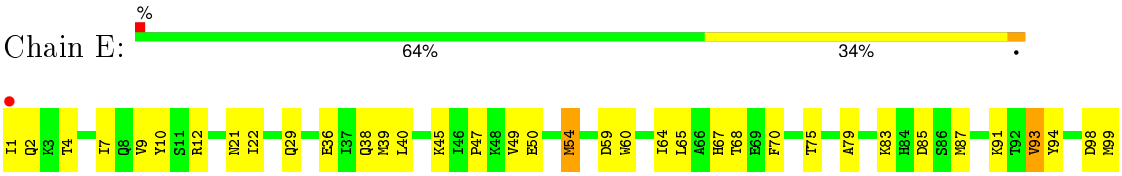
• Molecule 2: Beta-2-microglobulin

Chain B:



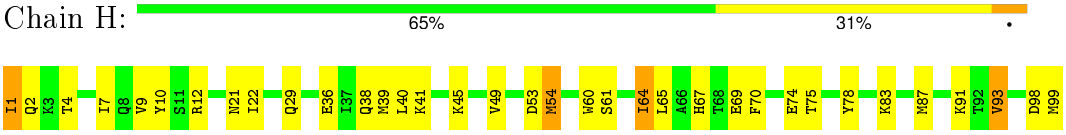
• Molecule 2: Beta-2-microglobulin

Chain E:



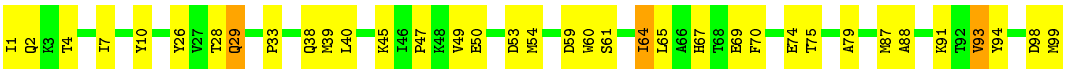
• Molecule 2: Beta-2-microglobulin

Chain H:



• Molecule 2: Beta-2-microglobulin

Chain K:

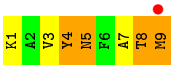


• Molecule 3: nonameric peptide, gp33 derived from lymphocytic choriomeningitis virus

Chain C:

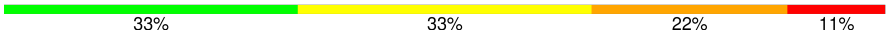
• Molecule 3: nonameric peptide, gp33 derived from lymphocytic choriomeningitis virus

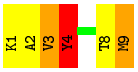
Chain F:



• Molecule 3: nonameric peptide, gp33 derived from lymphocytic choriomeningitis virus

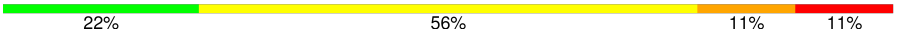
Chain I:

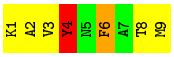




• Molecule 3: nonameric peptide, gp33 derived from lymphocytic choriomeningitis virus

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	92.00Å 122.66Å 99.18Å 90.00° 103.34° 90.00°	Depositor
Resolution (Å)	19.92 – 2.85 19.93 – 2.84	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.92-2.85) 90.8 (19.93-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.95 (at 2.83Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.251 , 0.279 0.252 , 0.277	Depositor DCC
R_{free} test set	2280 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 15.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 45779 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	12633	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.47% 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	1.00	8/2332 (0.3%)	1.16	21/3166 (0.7%)
1	D	1.08	14/2314 (0.6%)	1.16	17/3142 (0.5%)
1	G	1.04	11/2310 (0.5%)	1.05	8/3136 (0.3%)
1	J	1.03	9/2310 (0.4%)	1.03	6/3136 (0.2%)
2	B	0.94	1/838 (0.1%)	1.22	10/1138 (0.9%)
2	E	0.91	0/847	1.02	1/1148 (0.1%)
2	H	0.86	0/847	0.99	1/1148 (0.1%)
2	K	0.89	0/847	1.00	1/1148 (0.1%)
3	C	1.63	1/74 (1.4%)	1.30	1/97 (1.0%)
3	F	2.99	8/74 (10.8%)	1.16	0/97
3	I	2.02	3/74 (4.1%)	2.20	4/97 (4.1%)
3	L	1.58	1/74 (1.4%)	2.36	6/97 (6.2%)
All	All	1.04	56/12941 (0.4%)	1.11	76/17550 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	J	0	1
All	All	0	2

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	9	MET	C-OXT	-17.64	0.89	1.23
1	D	58	GLU	CD-OE1	-10.75	1.13	1.25
3	I	4	TYR	CB-CG	-10.09	1.36	1.51
1	J	58	GLU	CD-OE2	-9.89	1.14	1.25
1	A	58	GLU	CD-OE2	-9.75	1.15	1.25
1	G	58	GLU	CD-OE2	-9.68	1.15	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	ARG	NE-CZ	-9.28	1.21	1.33
1	D	58	GLU	CD-OE2	-9.15	1.15	1.25
1	A	111	ARG	CZ-NH1	-8.51	1.22	1.33
1	J	154	GLU	CG-CD	-8.45	1.39	1.51
1	G	58	GLU	CD-OE1	-8.07	1.16	1.25
1	G	61	GLU	CD-OE2	-7.63	1.17	1.25
1	D	58	GLU	CG-CD	-7.47	1.40	1.51
3	F	4	TYR	CE2-CZ	-7.47	1.28	1.38
1	J	232	GLU	CD-OE2	-7.23	1.17	1.25
3	L	4	TYR	CB-CG	-7.16	1.41	1.51
3	F	4	TYR	CE1-CZ	-7.06	1.29	1.38
1	G	223	GLU	CB-CG	-7.03	1.38	1.52
1	J	61	GLU	CD-OE2	-7.02	1.18	1.25
1	J	61	GLU	CG-CD	-6.97	1.41	1.51
1	D	62	ARG	CZ-NH1	-6.92	1.24	1.33
3	F	4	TYR	CB-CG	-6.82	1.41	1.51
1	D	62	ARG	CZ-NH2	-6.82	1.24	1.33
1	G	61	GLU	CG-CD	-6.76	1.41	1.51
1	G	79	ARG	NE-CZ	-6.73	1.24	1.33
1	A	58	GLU	CD-OE1	-6.67	1.18	1.25
1	D	61	GLU	CD-OE1	-6.57	1.18	1.25
3	F	4	TYR	CG-CD1	-6.46	1.30	1.39
1	G	232	GLU	CD-OE2	-6.40	1.18	1.25
3	F	4	TYR	CD1-CE1	-6.25	1.29	1.39
1	G	182	THR	CB-OG1	6.24	1.55	1.43
1	J	58	GLU	CD-OE1	-6.21	1.18	1.25
1	D	247	VAL	CB-CG2	-6.01	1.40	1.52
1	J	61	GLU	CD-OE1	-5.91	1.19	1.25
1	A	41	GLU	CD-OE1	-5.81	1.19	1.25
1	D	58	GLU	CB-CG	-5.73	1.41	1.52
1	D	61	GLU	CD-OE2	-5.62	1.19	1.25
1	J	62	ARG	CZ-NH2	-5.59	1.25	1.33
1	A	79	ARG	NE-CZ	-5.54	1.25	1.33
3	I	4	TYR	CA-CB	-5.51	1.41	1.53
1	A	53	GLU	CG-CD	-5.42	1.43	1.51
1	G	79	ARG	CG-CD	-5.38	1.38	1.51
1	A	144	ARG	CZ-NH1	-5.31	1.26	1.33
1	D	61	GLU	CG-CD	-5.27	1.44	1.51
3	F	4	TYR	CD2-CE2	-5.21	1.31	1.39
1	G	77	SER	CB-OG	-5.16	1.35	1.42
1	D	232	GLU	CD-OE2	-5.16	1.20	1.25
2	B	74	GLU	CB-CG	-5.12	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	247	VAL	CB-CG1	-5.11	1.42	1.52
3	C	4	TYR	CE2-CZ	-5.07	1.31	1.38
1	J	62	ARG	CZ-NH1	-5.06	1.26	1.33
3	I	3	VAL	C-N	-5.05	1.22	1.34
1	D	232	GLU	CG-CD	-5.02	1.44	1.51
3	F	4	TYR	CG-CD2	-5.02	1.32	1.39
1	D	274	TRP	CB-CG	5.01	1.59	1.50
1	G	247	VAL	CB-CG1	-5.01	1.42	1.52

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	75	ARG	NE-CZ-NH1	-14.72	112.94	120.30
3	I	4	TYR	CB-CG-CD2	-14.44	112.33	121.00
3	L	4	TYR	CB-CG-CD1	-12.93	113.24	121.00
1	D	274	TRP	N-CA-C	-12.84	76.34	111.00
1	A	111	ARG	NE-CZ-NH2	11.43	126.02	120.30
1	J	155	HIS	CA-CB-CG	-11.38	94.25	113.60
1	D	273	ARG	C-N-CA	-11.35	93.34	121.70
1	A	221	GLY	N-CA-C	-10.83	86.02	113.10
1	A	265	GLY	N-CA-C	-10.27	87.41	113.10
2	B	45	LYS	CD-CE-NZ	9.70	134.01	111.70
1	D	273	ARG	N-CA-C	-9.63	85.01	111.00
1	D	58	GLU	CA-CB-CG	-8.67	94.32	113.40
1	D	79	ARG	NE-CZ-NH2	8.17	124.39	120.30
3	L	4	TYR	CB-CA-C	7.60	125.60	110.40
1	D	75	ARG	CD-NE-CZ	-7.52	113.07	123.60
3	L	4	TYR	CG-CD2-CE2	-7.48	115.32	121.30
1	G	223	GLU	CA-CB-CG	7.29	129.43	113.40
1	D	75	ARG	CB-CG-CD	-7.23	92.80	111.60
2	B	85	ASP	CB-CG-OD2	7.14	124.73	118.30
2	B	2	GLN	N-CA-CB	-7.10	97.81	110.60
1	A	129	ASP	CB-CG-OD1	6.97	124.58	118.30
1	A	186	LYS	N-CA-C	-6.91	92.35	111.00
1	D	178	THR	N-CA-CB	-6.91	97.18	110.30
1	A	144	ARG	NE-CZ-NH2	6.85	123.72	120.30
3	I	4	TYR	CD1-CG-CD2	6.77	125.35	117.90
3	I	4	TYR	N-CA-CB	-6.71	98.52	110.60
1	A	186	LYS	N-CA-CB	-6.65	98.64	110.60
1	J	75	ARG	CD-NE-CZ	-6.57	114.40	123.60
2	B	74	GLU	CB-CA-C	-6.56	97.27	110.40
2	B	53	ASP	CB-CG-OD2	6.50	124.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	6	PHE	CB-CG-CD2	-6.50	116.25	120.80
1	A	58	GLU	OE1-CD-OE2	-6.42	115.59	123.30
2	H	53	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	137	ASP	CB-CG-OD1	6.29	123.97	118.30
1	A	111	ARG	NH1-CZ-NH2	-6.25	112.53	119.40
2	E	85	ASP	CB-CG-OD2	6.22	123.89	118.30
3	C	1	LYS	CD-CE-NZ	6.11	125.76	111.70
1	D	183	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	212	ASP	CB-CG-OD1	6.08	123.77	118.30
2	K	53	ASP	CB-CG-OD2	6.08	123.77	118.30
3	L	4	TYR	N-CA-CB	-6.01	99.78	110.60
2	B	1	ILE	CA-C-N	-6.00	104.00	117.20
1	D	62	ARG	NE-CZ-NH1	5.98	123.29	120.30
3	L	4	TYR	CD1-CG-CD2	5.98	124.48	117.90
3	I	4	TYR	CG-CD2-CE2	-5.91	116.57	121.30
1	D	17	LEU	CA-CB-CG	5.77	128.56	115.30
2	B	45	LYS	CG-CD-CE	5.76	129.17	111.90
1	D	16	GLY	N-CA-C	-5.74	98.76	113.10
1	A	66	LYS	CG-CD-CE	-5.69	94.82	111.90
1	J	154	GLU	OE1-CD-OE2	5.68	130.12	123.30
1	D	82	LEU	CB-CG-CD2	-5.65	101.40	111.00
1	D	62	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	A	5	MET	CG-SD-CE	5.55	109.08	100.20
1	G	182	THR	OG1-CB-CG2	-5.50	97.36	110.00
1	J	227	ASP	CB-CG-OD2	5.45	123.20	118.30
2	B	89	GLU	CA-CB-CG	-5.39	101.53	113.40
1	G	79	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	J	29	ASP	CB-CG-OD2	5.33	123.10	118.30
1	G	265	GLY	N-CA-C	-5.29	99.87	113.10
1	A	122	ASP	CB-CG-OD2	5.28	123.05	118.30
1	G	129	ASP	CB-CG-OD1	5.27	123.05	118.30
1	D	274	TRP	CA-CB-CG	5.27	123.72	113.70
1	A	272	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	D	62	ARG	NH1-CZ-NH2	-5.25	113.62	119.40
1	A	232	GLU	CB-CA-C	-5.25	99.90	110.40
2	B	96	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	82	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	A	185	PRO	CB-CA-C	-5.17	99.09	112.00
1	G	183	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	29	ASP	CB-CG-OD2	5.12	122.91	118.30
2	B	74	GLU	CB-CG-CD	-5.10	100.44	114.20
1	D	182	THR	N-CA-CB	-5.08	100.64	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	160	LEU	CA-CB-CG	-5.06	103.66	115.30
1	A	16	GLY	N-CA-C	5.04	125.71	113.10
1	J	102	ASP	CB-CG-OD2	5.02	122.82	118.30
1	G	264	GLU	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	223	GLU	Mainchain
1	J	223	GLU	Mainchain

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	2265	0	2136	144	0
1	D	2248	0	2123	133	0
1	G	2244	0	2118	119	0
1	J	2244	0	2118	132	0
2	B	812	0	787	34	0
2	E	821	0	796	38	0
2	H	821	0	796	25	0
2	K	821	0	796	30	0
3	C	73	0	74	6	0
3	F	73	0	74	13	0
3	I	73	0	73	9	0
3	L	73	0	74	17	0
4	A	12	0	0	1	0
4	B	7	0	0	0	0
4	D	12	0	0	0	0
4	E	2	0	0	0	0
4	G	9	0	0	2	0
4	H	5	0	0	0	0
4	J	10	0	0	0	0
4	K	7	0	0	0	0
4	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12633	0	11965	625	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 25.

All (625) 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:A:194:ARG:CG	1:A:195:SER:H	1.42	1.30
1:D:273:ARG:CG	1:D:274:TRP:O	1.77	1.30
1:A:1:GLY:O	1:A:105:SER:HA	1.38	1.21
1:G:181:ARG:HB2	1:G:181:ARG:HH11	1.07	1.18
1:J:155:HIS:HB3	3:L:6:PHE:CE1	1.79	1.16
1:D:146:LYS:HD3	3:F:9:MET:O	1.42	1.16
1:D:19:GLU:HB3	1:D:75:ARG:HH21	1.01	1.16
1:A:219:LEU:O	1:A:219:LEU:HD12	1.46	1.16
1:A:194:ARG:HG2	1:A:195:SER:N	1.54	1.15
1:A:264:GLU:O	1:A:264:GLU:CG	1.92	1.15
1:G:15:PRO:HD3	1:G:91:GLY:O	1.49	1.12
1:A:194:ARG:CG	1:A:195:SER:N	2.07	1.10
1:G:31:LYS:NZ	1:G:181:ARG:HH22	1.49	1.10
1:D:121:ARG:CZ	2:E:1:ILE:HD11	1.80	1.10
1:G:273:ARG:HD3	1:G:273:ARG:H	1.18	1.09
1:D:182:THR:HG21	1:D:265:GLY:HA3	1.16	1.09
1:G:255:GLN:HE22	1:G:274:TRP:HB3	1.14	1.06
1:A:14:ARG:HG2	1:A:16:GLY:H	1.20	1.05
1:D:19:GLU:HB3	1:D:75:ARG:NH2	1.72	1.05
1:A:218:GLN:C	1:A:220:ASN:H	1.46	1.05
1:A:194:ARG:HG3	1:A:195:SER:H	1.19	1.04
1:J:219:LEU:HG	1:J:219:LEU:O	1.55	1.04
1:G:181:ARG:NH1	1:G:181:ARG:HB2	1.73	1.04
2:B:39:MET:HE1	2:B:68:THR:HG22	1.39	1.03
1:J:155:HIS:CG	3:L:6:PHE:CZ	2.46	1.03
1:A:218:GLN:C	1:A:220:ASN:N	2.09	1.02
1:D:19:GLU:CB	1:D:75:ARG:HH21	1.73	1.02
1:A:218:GLN:O	1:A:220:ASN:N	1.95	0.99
1:D:258:THR:HA	1:D:273:ARG:HA	1.43	0.97
1:J:155:HIS:CB	3:L:6:PHE:CE1	2.47	0.97
1:D:273:ARG:HG2	1:D:274:TRP:C	1.73	0.97
1:D:273:ARG:HG2	1:D:274:TRP:O	0.81	0.97
1:A:62:ARG:NH2	3:C:1:LYS:HE3	1.78	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:HH11	1:A:14:ARG:HG3	1.25	0.96
1:D:121:ARG:CZ	2:E:1:ILE:CD1	2.44	0.94
1:G:181:ARG:CB	1:G:181:ARG:HH11	1.80	0.94
1:G:32:GLU:OE2	1:G:48:ARG:HD2	1.67	0.94
1:D:182:THR:HG21	1:D:265:GLY:CA	1.98	0.92
1:D:58:GLU:HG3	1:D:59:TYR:H	1.33	0.92
1:A:220:ASN:C	1:A:221:GLY:O	1.97	0.92
1:A:219:LEU:HD12	1:A:256:ASN:O	1.68	0.91
1:D:182:THR:CG2	1:D:265:GLY:HA3	2.01	0.91
1:J:234:ARG:NH2	2:K:99:MET:OXT	2.03	0.89
1:A:220:ASN:HD21	1:A:258:THR:HB	1.33	0.89
1:J:155:HIS:CB	3:L:6:PHE:CZ	2.58	0.87
1:A:14:ARG:HH11	1:A:14:ARG:CG	1.87	0.87
1:J:194:ARG:HG3	1:J:199:VAL:HG12	1.57	0.87
1:J:220:ASN:O	1:J:220:ASN:OD1	1.92	0.86
1:A:194:ARG:HG2	1:A:195:SER:H	1.16	0.85
1:G:31:LYS:NZ	1:G:181:ARG:NH2	2.25	0.84
1:D:146:LYS:CD	3:F:9:MET:O	2.25	0.84
1:D:82:LEU:HD12	1:D:87:GLN:HB2	1.60	0.83
1:G:31:LYS:HZ3	1:G:181:ARG:HH22	1.22	0.83
1:D:58:GLU:HG3	1:D:59:TYR:N	1.92	0.83
1:A:255:GLN:HE22	1:A:274:TRP:HB3	1.44	0.82
1:G:273:ARG:N	1:G:273:ARG:HD3	1.90	0.81
1:D:202:ARG:HG2	1:D:204:TRP:NE1	1.95	0.81
1:D:226:GLN:OE1	1:D:226:GLN:O	1.99	0.81
1:J:155:HIS:HB3	3:L:6:PHE:CZ	2.14	0.80
1:G:23:ILE:N	1:G:23:ILE:HD12	1.96	0.80
1:J:194:ARG:HA	1:J:198:GLU:O	1.81	0.79
1:G:20:PRO:HG3	1:G:75:ARG:HD2	1.62	0.79
1:A:23:ILE:N	1:A:23:ILE:HD12	1.97	0.79
1:D:143:THR:OG1	3:F:9:MET:HB3	1.83	0.79
1:J:273:ARG:HD3	1:J:273:ARG:H	1.48	0.79
1:A:220:ASN:ND2	1:A:258:THR:HB	1.98	0.78
1:A:264:GLU:O	1:A:264:GLU:HG2	1.04	0.78
1:J:61:GLU:OE1	1:J:61:GLU:HA	1.82	0.78
1:J:194:ARG:HB3	1:J:198:GLU:C	2.04	0.78
1:G:226:GLN:OE1	1:G:226:GLN:O	2.01	0.78
2:B:39:MET:HE1	2:B:68:THR:CG2	2.14	0.77
1:A:21:ARG:HG2	1:A:23:ILE:HD11	1.64	0.77
1:G:20:PRO:HG3	1:G:75:ARG:HH11	1.48	0.77
1:D:208:PHE:CE2	1:D:213:ILE:HD12	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:THR:O	1:D:225:THR:HG22	1.83	0.77
2:B:74:GLU:OE1	2:B:74:GLU:CA	2.24	0.76
1:A:14:ARG:HG2	1:A:16:GLY:N	1.97	0.76
1:J:222:GLU:H	1:J:222:GLU:CD	1.88	0.76
1:J:23:ILE:HD12	1:J:23:ILE:N	2.01	0.76
1:G:273:ARG:HG2	1:G:274:TRP:O	1.86	0.76
1:J:87:GLN:OE1	1:J:93:HIS:CE1	2.38	0.76
1:J:219:LEU:CG	1:J:219:LEU:O	2.34	0.76
1:D:218:GLN:OE1	1:D:260:ARG:CZ	2.33	0.76
1:D:32:GLU:OE2	1:D:48:ARG:HD2	1.86	0.75
1:D:1:GLY:O	1:D:3:HIS:CD2	2.38	0.75
1:G:6:ARG:NH2	1:G:113:TYR:CE2	2.54	0.75
1:J:14:ARG:HB3	1:J:15:PRO:HD2	1.68	0.75
1:D:208:PHE:CE2	1:D:213:ILE:CD1	2.69	0.75
1:G:20:PRO:CG	1:G:75:ARG:HD2	2.17	0.74
1:D:170:ARG:HH11	1:D:170:ARG:HG3	1.50	0.74
1:J:194:ARG:HB3	1:J:198:GLU:O	1.87	0.74
2:B:39:MET:CE	2:B:68:THR:HG22	2.18	0.74
1:A:219:LEU:CD1	1:A:219:LEU:O	2.33	0.74
1:G:31:LYS:HZ3	1:G:181:ARG:NH2	1.82	0.74
1:J:202:ARG:HD2	1:J:244:TRP:CD2	2.23	0.73
2:B:74:GLU:HA	2:B:74:GLU:OE1	1.88	0.73
1:A:219:LEU:CD1	1:A:256:ASN:O	2.37	0.73
1:J:32:GLU:OE2	1:J:35:ARG:HD2	1.87	0.73
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.23	0.73
1:A:194:ARG:HH12	1:A:248:VAL:HG11	1.54	0.72
1:G:18:GLU:N	1:G:18:GLU:OE1	2.21	0.72
1:A:219:LEU:HD11	1:A:256:ASN:ND2	2.05	0.72
1:J:202:ARG:HD2	1:J:244:TRP:CE3	2.23	0.72
1:A:275:GLU:O	1:A:275:GLU:HG3	1.89	0.71
1:D:66:LYS:HZ1	3:F:1:LYS:HG2	1.55	0.71
1:G:194:ARG:CB	1:G:198:GLU:O	2.39	0.71
2:E:1:ILE:HG23	2:E:1:ILE:O	1.89	0.71
1:G:190:THR:OG1	1:G:202:ARG:HB3	1.91	0.71
2:E:39:MET:HE1	2:E:68:THR:HG22	1.71	0.71
1:J:81:LEU:HD13	1:J:118:TYR:CD1	2.26	0.71
1:G:262:TYR:HA	4:G:277:HOH:O	1.88	0.71
1:G:194:ARG:NH2	1:G:198:GLU:OE1	2.24	0.71
1:J:214:THR:C	1:J:215:LEU:HD12	2.12	0.70
1:A:1:GLY:C	1:A:105:SER:HA	2.10	0.69
1:A:218:GLN:O	1:A:220:ASN:ND2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ARG:NH2	1:D:113:TYR:CE1	2.61	0.69
1:A:250:PRO:HB2	1:A:253:LYS:HB2	1.75	0.69
1:A:62:ARG:CZ	3:C:1:LYS:HE3	2.23	0.69
1:A:103:LEU:HD11	1:A:168:LEU:HD23	1.73	0.69
1:J:155:HIS:CD2	3:L:6:PHE:CE2	2.81	0.68
1:D:191:HIS:HB2	1:D:274:TRP:CH2	2.28	0.68
1:G:178:THR:HG22	1:G:179:LEU:HD23	1.76	0.68
1:J:208:PHE:CE1	1:J:241:PHE:HB2	2.29	0.68
1:D:35:ARG:NH2	2:E:54:MET:O	2.24	0.68
1:A:183:ASP:O	1:A:208:PHE:HA	1.93	0.68
1:J:194:ARG:CA	1:J:198:GLU:O	2.42	0.68
2:B:87:MET:HE2	2:B:91:LYS:HB2	1.76	0.68
1:D:19:GLU:CG	1:D:75:ARG:HH21	2.07	0.68
1:A:32:GLU:OE2	1:A:35:ARG:HD2	1.94	0.68
1:J:190:THR:OG1	1:J:202:ARG:HB3	1.94	0.67
1:D:263:HIS:O	1:D:266:LEU:HB2	1.96	0.66
1:G:31:LYS:HZ1	1:G:181:ARG:HH22	1.40	0.66
1:J:255:GLN:HE22	1:J:274:TRP:HB3	1.60	0.66
1:J:35:ARG:NH2	2:K:54:MET:O	2.23	0.66
1:J:226:GLN:O	1:J:226:GLN:OE1	2.13	0.66
1:D:19:GLU:CD	1:D:75:ARG:NH2	2.49	0.66
1:J:202:ARG:NH1	1:J:244:TRP:CH2	2.64	0.66
1:J:121:ARG:CZ	2:K:1:ILE:HD11	2.25	0.66
1:J:170:ARG:HG3	1:J:170:ARG:HH11	1.61	0.66
1:A:194:ARG:NH1	1:A:248:VAL:HG11	2.10	0.66
1:J:215:LEU:N	1:J:215:LEU:HD12	2.11	0.65
1:A:226:GLN:OE1	1:A:226:GLN:O	2.14	0.65
1:D:19:GLU:CD	1:D:75:ARG:HH21	1.99	0.65
1:D:121:ARG:NE	2:E:1:ILE:HD11	2.11	0.65
1:A:14:ARG:NH1	1:A:14:ARG:HG3	2.02	0.65
1:D:147:TRP:CZ2	3:F:9:MET:HG2	2.32	0.65
1:D:31:LYS:HG3	1:D:209:TYR:OH	1.96	0.65
1:D:135:ALA:H	1:D:144:ARG:HH21	1.45	0.65
1:G:20:PRO:CD	1:G:75:ARG:HD2	2.27	0.65
1:J:116:PHE:CD2	3:L:9:MET:CE	2.80	0.65
1:J:103:LEU:HD11	1:J:168:LEU:HD23	1.78	0.65
1:D:87:GLN:NE2	1:D:118:TYR:OH	2.26	0.64
1:G:191:HIS:NE2	1:G:199:VAL:HG21	2.11	0.64
1:G:273:ARG:N	1:G:273:ARG:CD	2.61	0.64
2:B:16:GLU:HG3	2:K:88:ALA:HB3	1.78	0.64
1:A:1:GLY:N	1:A:2:PRO:CD	2.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:VAL:HG22	1:D:94:THR:HG23	1.80	0.63
1:J:87:GLN:OE1	1:J:93:HIS:HE1	1.81	0.63
1:D:252:GLY:N	1:D:254:GLU:OE1	2.30	0.63
1:D:121:ARG:NH1	2:E:1:ILE:CD1	2.61	0.63
1:A:251:LEU:HD23	1:A:252:GLY:N	2.14	0.63
1:A:219:LEU:O	1:A:256:ASN:O	2.17	0.63
1:J:116:PHE:CD2	3:L:9:MET:HE3	2.34	0.62
1:D:211:ALA:O	1:D:212:ASP:C	2.36	0.62
1:A:194:ARG:NH1	1:A:248:VAL:CG1	2.63	0.62
1:D:273:ARG:CG	1:D:274:TRP:C	2.50	0.62
1:G:231:VAL:O	1:G:243:LYS:NZ	2.32	0.62
1:D:217:TRP:H	1:D:228:MET:HE2	1.65	0.62
1:A:218:GLN:O	1:A:219:LEU:C	2.39	0.61
1:J:32:GLU:OE2	1:J:48:ARG:HD2	2.00	0.61
1:A:29:ASP:O	1:A:30:ASN:HB2	1.98	0.61
1:G:218:GLN:HG2	1:G:223:GLU:HA	1.82	0.61
1:D:208:PHE:CD2	1:D:213:ILE:HD12	2.36	0.61
1:D:203:CYS:HB2	1:D:217:TRP:CZ2	2.36	0.61
1:A:44:ARG:HH22	1:A:61:GLU:HG2	1.65	0.61
1:A:31:LYS:NZ	1:A:181:ARG:HH22	1.98	0.61
1:J:167:TRP:CE3	1:J:170:ARG:HD3	2.36	0.60
1:D:51:TRP:O	1:D:54:GLN:HG3	2.00	0.60
1:J:202:ARG:CD	1:J:244:TRP:CE3	2.84	0.60
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.35	0.60
1:J:194:ARG:CB	1:J:198:GLU:O	2.49	0.60
1:J:7:TYR:CE2	3:L:2:ALA:HB2	2.37	0.60
1:A:22:TYR:C	1:A:23:ILE:HD12	2.22	0.60
3:F:5:ASN:N	3:F:5:ASN:HD22	2.00	0.60
1:J:103:LEU:CD1	1:J:168:LEU:HD23	2.32	0.59
1:J:222:GLU:N	1:J:222:GLU:CD	2.56	0.59
1:A:32:GLU:OE2	1:A:48:ARG:HD2	2.01	0.59
1:J:121:ARG:CZ	2:K:1:ILE:CD1	2.81	0.59
1:G:23:ILE:N	1:G:23:ILE:CD1	2.65	0.59
1:G:194:ARG:NH1	1:G:248:VAL:HG11	2.18	0.59
2:H:64:ILE:HG22	2:H:65:LEU:N	2.16	0.59
1:J:234:ARG:HD3	2:K:10:TYR:CE2	2.37	0.59
1:A:191:HIS:O	1:A:192:HIS:HD2	1.85	0.59
1:A:262:TYR:N	1:A:262:TYR:CD1	2.70	0.59
1:J:51:TRP:CZ3	1:J:52:MET:SD	2.96	0.59
1:A:202:ARG:HD2	1:A:244:TRP:CE3	2.37	0.59
1:A:79:ARG:HH11	1:A:79:ARG:HG2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:PRO:CG	1:G:75:ARG:HH11	2.15	0.58
2:E:64:ILE:HG22	2:E:65:LEU:N	2.17	0.58
1:J:111:ARG:HD2	1:J:113:TYR:CZ	2.37	0.58
1:G:251:LEU:HD23	1:G:252:GLY:N	2.18	0.58
1:A:194:ARG:O	1:A:195:SER:C	2.41	0.58
2:H:12:ARG:CZ	2:H:22:ILE:HD12	2.33	0.58
2:H:40:LEU:HD23	2:H:45:LYS:HA	1.84	0.58
1:D:234:ARG:HD3	2:E:10:TYR:CE2	2.39	0.58
1:A:114:LEU:HD22	1:A:114:LEU:C	2.24	0.58
1:G:178:THR:HG22	1:G:179:LEU:CD2	2.33	0.58
3:I:3:VAL:HG22	3:I:4:TYR:N	2.19	0.58
1:A:156:TYR:O	1:A:160:LEU:HG	2.03	0.58
2:H:21:ASN:OD1	2:H:22:ILE:N	2.33	0.58
1:G:230:LEU:HD12	1:G:230:LEU:C	2.24	0.58
1:A:1:GLY:H3	1:A:2:PRO:HD3	1.69	0.58
1:A:1:GLY:N	1:A:2:PRO:HD3	2.18	0.57
1:J:155:HIS:CG	3:L:6:PHE:CE2	2.91	0.57
1:A:14:ARG:CG	1:A:14:ARG:NH1	2.57	0.57
1:J:233:THR:OG1	1:J:243:LYS:HD2	2.04	0.57
1:D:121:ARG:CZ	2:E:1:ILE:HD12	2.33	0.57
1:J:63:GLU:OE2	3:L:1:LYS:HG2	2.05	0.57
1:D:225:THR:CG2	1:D:225:THR:O	2.52	0.57
1:D:19:GLU:CB	1:D:75:ARG:NH2	2.48	0.57
1:A:44:ARG:NH2	4:A:288:HOH:O	2.35	0.57
1:A:31:LYS:HD3	1:A:179:LEU:HD22	1.86	0.57
1:G:145:ARG:NH1	4:G:283:HOH:O	2.36	0.57
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.40	0.57
1:G:33:PHE:CD2	1:G:34:VAL:HG13	2.39	0.57
2:E:39:MET:HE2	2:E:49:VAL:HG13	1.85	0.57
2:B:87:MET:HE1	2:B:91:LYS:HD2	1.87	0.57
1:A:219:LEU:HD11	1:A:256:ASN:HD22	1.69	0.57
1:J:250:PRO:HG2	1:J:253:LYS:HB2	1.87	0.57
1:D:28:VAL:O	1:D:28:VAL:HG12	2.05	0.57
1:D:208:PHE:CE2	1:D:213:ILE:HD13	2.40	0.56
1:D:44:ARG:CG	1:D:44:ARG:HH11	2.16	0.56
2:E:40:LEU:HD23	2:E:45:LYS:HA	1.87	0.56
1:G:111:ARG:HD2	1:G:113:TYR:CZ	2.39	0.56
1:D:170:ARG:NH1	1:D:174:ASN:HD21	2.03	0.56
1:A:31:LYS:HZ1	1:A:181:ARG:HH22	1.54	0.56
1:D:23:ILE:HD12	1:D:23:ILE:N	2.20	0.56
1:G:266:LEU:HG	1:G:268:GLU:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:217:TRP:H	1:G:228:MET:HE2	1.69	0.56
1:G:255:GLN:HE22	1:G:274:TRP:CB	2.04	0.56
1:G:55:GLU:CD	1:G:170:ARG:HH21	2.09	0.56
3:F:7:ALA:C	3:F:8:THR:O	2.40	0.56
1:D:176:ASN:O	1:D:180:LEU:HD22	2.05	0.56
1:J:42:ASN:HD21	1:J:44:ARG:HD2	1.71	0.56
1:D:121:ARG:NH2	2:E:1:ILE:CD1	2.68	0.56
1:G:6:ARG:NH2	1:G:113:TYR:CD2	2.74	0.56
1:J:207:GLY:HA2	1:J:240:THR:HB	1.88	0.56
2:K:40:LEU:HD23	2:K:45:LYS:HA	1.88	0.56
1:D:208:PHE:CZ	1:D:213:ILE:HG21	2.40	0.56
1:G:35:ARG:NH2	2:H:54:MET:O	2.33	0.56
2:E:21:ASN:OD1	2:E:22:ILE:N	2.34	0.56
1:A:1:GLY:HA3	1:A:105:SER:CB	2.35	0.56
1:G:194:ARG:HB3	1:G:198:GLU:O	2.04	0.56
1:J:5:MET:O	1:J:6:ARG:HG2	2.06	0.56
2:B:17:ASN:ND2	2:B:74:GLU:OE1	2.39	0.56
1:J:14:ARG:HB3	1:J:15:PRO:CD	2.33	0.56
1:D:226:GLN:CD	1:D:226:GLN:O	2.44	0.55
1:A:23:ILE:CD1	1:A:23:ILE:N	2.67	0.55
2:H:64:ILE:CG2	2:H:65:LEU:N	2.70	0.55
1:D:6:ARG:NH2	1:D:113:TYR:CD1	2.74	0.55
1:D:176:ASN:CG	1:D:177:ALA:H	2.10	0.55
2:K:39:MET:HE1	2:K:67:HIS:C	2.27	0.55
1:D:207:GLY:HA2	1:D:240:THR:HB	1.89	0.55
2:K:87:MET:CE	2:K:91:LYS:HB2	2.37	0.55
1:J:31:LYS:HD3	1:J:179:LEU:HD21	1.88	0.55
1:D:167:TRP:CE3	1:D:170:ARG:HD3	2.41	0.55
1:D:191:HIS:HB2	1:D:274:TRP:CZ2	2.41	0.55
1:J:194:ARG:HG3	1:J:199:VAL:CG1	2.33	0.55
1:J:273:ARG:N	1:J:273:ARG:HD3	2.20	0.55
1:D:183:ASP:O	1:D:208:PHE:HA	2.06	0.55
1:J:6:ARG:NH2	1:J:113:TYR:CE1	2.74	0.55
1:D:191:HIS:NE2	1:D:199:VAL:HG21	2.22	0.55
2:B:39:MET:HE2	2:B:49:VAL:HG13	1.88	0.55
1:A:103:LEU:CD1	1:A:168:LEU:HD23	2.37	0.55
2:E:59:ASP:O	2:E:60:TRP:HB2	2.07	0.55
1:D:248:VAL:O	1:D:248:VAL:HG23	2.07	0.55
2:B:87:MET:CE	2:B:91:LYS:HB2	2.37	0.54
1:A:14:ARG:C	1:A:16:GLY:H	2.10	0.54
1:A:275:GLU:O	1:A:275:GLU:CG	2.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:GLY:HA2	1:D:240:THR:CB	2.38	0.54
1:A:202:ARG:HG2	1:A:204:TRP:NE1	2.23	0.54
2:H:12:ARG:NH1	2:H:22:ILE:HD12	2.23	0.54
1:J:155:HIS:HB3	3:L:6:PHE:HE1	1.58	0.54
1:D:218:GLN:HG2	1:D:222:GLU:C	2.28	0.54
1:J:107:TRP:HB3	1:J:169:HIS:HE2	1.73	0.54
1:A:219:LEU:HB2	1:A:224:LEU:HD22	1.90	0.54
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.42	0.54
1:A:219:LEU:HD12	1:A:219:LEU:C	2.12	0.54
1:J:194:ARG:HB3	1:J:198:GLU:N	2.23	0.54
1:D:218:GLN:OE1	1:D:260:ARG:NE	2.41	0.54
2:B:40:LEU:HD23	2:B:45:LYS:HA	1.89	0.54
1:A:31:LYS:HZ1	1:A:181:ARG:NH2	2.07	0.53
2:K:64:ILE:HG22	2:K:65:LEU:N	2.22	0.53
1:D:219:LEU:HD11	1:D:256:ASN:HD22	1.73	0.53
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.44	0.53
1:D:194:ARG:HB2	1:D:198:GLU:O	2.08	0.53
1:G:255:GLN:NE2	1:G:274:TRP:HB3	2.00	0.53
1:J:107:TRP:CE3	1:J:169:HIS:CD2	2.97	0.53
1:J:194:ARG:HE	1:J:251:LEU:HD12	1.74	0.53
2:K:39:MET:HE3	2:K:49:VAL:HG13	1.91	0.53
1:J:167:TRP:CZ3	1:J:170:ARG:HD3	2.44	0.53
1:A:74:PHE:CD2	1:A:95:LEU:HD23	2.44	0.52
1:G:194:ARG:NH1	1:G:248:VAL:CG1	2.71	0.52
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.43	0.52
1:D:261:VAL:HB	1:D:270:LEU:HB2	1.90	0.52
1:D:249:VAL:HG22	1:D:257:TYR:CZ	2.44	0.52
1:G:263:HIS:O	1:G:266:LEU:HB3	2.09	0.52
2:B:21:ASN:OD1	2:B:22:ILE:N	2.40	0.52
3:C:6:PHE:CD2	3:C:7:ALA:N	2.77	0.52
2:K:87:MET:HE1	2:K:91:LYS:HB2	1.91	0.52
1:G:222:GLU:CD	1:G:222:GLU:H	2.13	0.52
1:J:218:GLN:HG2	1:J:223:GLU:HA	1.92	0.52
1:D:233:THR:OG1	1:D:243:LYS:HD2	2.09	0.52
2:B:64:ILE:HG22	2:B:65:LEU:N	2.23	0.52
1:A:98:MET:SD	2:B:58:LYS:HA	2.49	0.52
1:D:33:PHE:CD2	1:D:34:VAL:HG13	2.45	0.52
1:J:209:TYR:CD1	1:J:210:PRO:HA	2.45	0.52
2:E:9:VAL:CG2	2:E:93:VAL:HG22	2.40	0.52
1:J:225:THR:O	1:J:227:ASP:N	2.43	0.52
2:B:16:GLU:HG3	2:K:88:ALA:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:LEU:HD23	1:D:252:GLY:N	2.24	0.52
1:G:73:TRP:CE2	3:I:8:THR:HA	2.45	0.52
1:J:251:LEU:HD23	1:J:252:GLY:N	2.26	0.52
1:G:33:PHE:C	1:G:48:ARG:HB2	2.30	0.51
2:K:39:MET:CE	2:K:49:VAL:HG13	2.40	0.51
1:A:191:HIS:O	1:A:192:HIS:CD2	2.63	0.51
1:D:121:ARG:NH1	2:E:1:ILE:HD12	2.25	0.51
1:D:208:PHE:CZ	1:D:213:ILE:HD12	2.44	0.51
1:A:255:GLN:C	1:A:257:TYR:H	2.14	0.51
1:G:194:ARG:HB2	1:G:198:GLU:O	2.11	0.51
1:J:33:PHE:C	1:J:48:ARG:HB2	2.31	0.51
2:B:7:ILE:HB	2:B:93:VAL:HG11	1.93	0.51
1:D:147:TRP:HZ2	3:F:9:MET:HG2	1.73	0.51
1:A:233:THR:OG1	1:A:243:LYS:HD2	2.11	0.51
3:F:7:ALA:O	3:F:8:THR:O	2.29	0.51
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.46	0.51
2:H:39:MET:HE1	2:H:67:HIS:C	2.31	0.51
1:A:219:LEU:HD22	1:A:257:TYR:CZ	2.47	0.50
1:D:121:ARG:NH1	2:E:1:ILE:HD11	2.20	0.50
1:A:251:LEU:C	1:A:251:LEU:HD23	2.30	0.50
1:J:185:PRO:CA	1:J:208:PHE:HB3	2.41	0.50
1:D:176:ASN:CG	1:D:177:ALA:N	2.65	0.50
1:A:194:ARG:HH11	1:A:248:VAL:HG12	1.77	0.50
1:A:255:GLN:NE2	1:A:274:TRP:HB3	2.20	0.50
1:G:33:PHE:HD2	1:G:52:MET:HG3	1.76	0.50
1:J:85:TYR:CB	1:J:87:GLN:HE21	2.24	0.50
2:E:87:MET:HE1	2:E:91:LYS:HE2	1.93	0.50
2:B:88:ALA:C	2:B:89:GLU:HG2	2.31	0.50
2:E:39:MET:CE	2:E:68:THR:HG22	2.39	0.50
1:J:226:GLN:O	1:J:227:ASP:C	2.49	0.50
1:J:180:LEU:O	1:J:180:LEU:HG	2.12	0.50
1:G:121:ARG:CZ	2:H:1:ILE:HD11	2.41	0.50
1:G:234:ARG:NH2	2:H:99:MET:OXT	2.43	0.50
1:J:194:ARG:CD	1:J:194:ARG:H	2.21	0.50
1:D:217:TRP:H	1:D:228:MET:CE	2.24	0.50
1:A:37:ASP:OD1	1:A:39:ASP:HB2	2.12	0.50
2:K:59:ASP:O	2:K:60:TRP:HB2	2.12	0.50
2:B:13:HIS:HB3	2:B:14:PRO:HD2	1.94	0.50
2:H:10:TYR:CD1	2:H:10:TYR:N	2.80	0.50
1:D:19:GLU:CG	1:D:75:ARG:NH2	2.74	0.49
1:D:190:THR:OG1	1:D:202:ARG:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:PHE:HD2	3:C:7:ALA:H	1.59	0.49
1:J:182:THR:OG1	1:J:265:GLY:HA3	2.12	0.49
1:J:234:ARG:HB2	2:K:10:TYR:CZ	2.47	0.49
1:G:202:ARG:HD3	1:G:246:SER:HB3	1.94	0.49
1:J:107:TRP:HB3	1:J:169:HIS:NE2	2.27	0.49
2:B:39:MET:CE	2:B:68:THR:CG2	2.84	0.49
2:B:36:GLU:HB2	2:B:83:LYS:HB3	1.95	0.49
1:J:266:LEU:HG	1:J:268:GLU:O	2.12	0.49
1:G:47:PRO:HG3	1:G:60:TRP:CZ2	2.47	0.49
1:J:73:TRP:CE2	3:L:8:THR:HA	2.47	0.49
2:E:39:MET:HE1	2:E:68:THR:CG2	2.42	0.49
1:J:23:ILE:CD1	1:J:23:ILE:N	2.74	0.49
1:A:77:SER:OG	3:C:9:MET:HG3	2.13	0.49
2:E:10:TYR:N	2:E:10:TYR:CD1	2.79	0.49
1:A:15:PRO:HD3	1:A:91:GLY:O	2.12	0.49
2:E:64:ILE:CG2	2:E:65:LEU:N	2.75	0.49
1:J:74:PHE:CD2	1:J:95:LEU:HD23	2.48	0.49
1:A:191:HIS:NE2	1:A:199:VAL:HG21	2.28	0.49
1:A:207:GLY:HA2	1:A:240:THR:HB	1.94	0.49
2:H:41:LYS:HG3	2:H:78:TYR:CE2	2.47	0.48
1:G:135:ALA:H	1:G:144:ARG:HH21	1.61	0.48
1:G:226:GLN:CD	1:G:226:GLN:O	2.50	0.48
1:D:55:GLU:CD	1:D:170:ARG:HH21	2.16	0.48
1:G:201:LEU:HD11	1:G:254:GLU:HB2	1.94	0.48
1:G:157:LYS:NZ	1:G:161:GLU:OE1	2.45	0.48
1:D:44:ARG:CG	1:D:44:ARG:NH1	2.75	0.48
1:A:33:PHE:C	1:A:48:ARG:HB2	2.33	0.48
1:A:31:LYS:HG3	1:A:209:TYR:OH	2.13	0.48
2:E:7:ILE:HB	2:E:93:VAL:HG11	1.96	0.48
1:D:262:TYR:CD1	1:D:262:TYR:N	2.82	0.48
1:J:207:GLY:HA2	1:J:240:THR:CB	2.42	0.48
1:J:213:ILE:HG12	1:J:214:THR:N	2.29	0.47
1:G:22:TYR:C	1:G:23:ILE:HD12	2.34	0.47
1:D:234:ARG:NH2	2:E:99:MET:OXT	2.45	0.47
1:G:98:MET:HE2	2:H:60:TRP:CH2	2.49	0.47
2:H:29:GLN:HA	2:H:61:SER:HB2	1.95	0.47
1:D:202:ARG:HG2	1:D:204:TRP:HE1	1.73	0.47
1:D:208:PHE:CZ	1:D:213:ILE:CD1	2.97	0.47
1:J:63:GLU:OE2	3:L:1:LYS:HE2	2.15	0.47
1:G:31:LYS:HZ1	1:G:181:ARG:NH2	2.02	0.47
2:E:39:MET:HE1	2:E:67:HIS:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:VAL:HG23	1:D:33:PHE:CE1	2.49	0.47
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.49	0.47
1:G:2:PRO:N	1:G:105:SER:HA	2.29	0.47
1:G:87:GLN:NE2	1:G:118:TYR:OH	2.39	0.47
1:A:194:ARG:HG3	1:A:195:SER:N	2.00	0.47
1:G:273:ARG:H	1:G:273:ARG:CD	2.05	0.47
1:J:202:ARG:HD3	1:J:246:SER:HB3	1.97	0.47
1:A:202:ARG:CD	1:A:244:TRP:CE3	2.97	0.47
1:G:190:THR:HG1	1:G:202:ARG:HB3	1.80	0.47
1:D:249:VAL:HG22	1:D:257:TYR:CE2	2.50	0.47
1:J:218:GLN:HG2	1:J:223:GLU:CA	2.44	0.47
2:B:59:ASP:O	2:B:60:TRP:HB2	2.15	0.47
1:D:258:THR:HG22	1:D:273:ARG:HB3	1.97	0.47
1:J:85:TYR:HB2	1:J:87:GLN:HE21	1.80	0.47
1:J:167:TRP:CE2	3:L:1:LYS:HD2	2.50	0.47
1:J:170:ARG:HH11	1:J:170:ARG:CG	2.26	0.47
1:G:252:GLY:N	1:G:254:GLU:OE1	2.48	0.47
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.50	0.47
1:J:249:VAL:HG22	1:J:257:TYR:CZ	2.50	0.47
2:H:74:GLU:OE1	2:H:74:GLU:N	2.47	0.47
1:G:211:ALA:HB2	1:G:241:PHE:CE2	2.50	0.47
1:G:20:PRO:CD	1:G:75:ARG:CD	2.92	0.46
1:D:129:ASP:O	1:D:131:LYS:HG3	2.15	0.46
1:G:225:THR:O	1:G:225:THR:HG22	2.15	0.46
1:G:207:GLY:HA2	1:G:240:THR:CB	2.45	0.46
1:J:234:ARG:HB2	2:K:10:TYR:OH	2.15	0.46
1:J:185:PRO:HA	1:J:208:PHE:HB3	1.96	0.46
1:G:123:TYR:HE2	3:I:9:MET:HG2	1.80	0.46
2:K:87:MET:HE1	2:K:91:LYS:HE2	1.96	0.46
1:G:43:PRO:O	1:G:44:ARG:HG3	2.15	0.46
1:G:154:GLU:H	1:G:154:GLU:CD	2.18	0.46
1:A:1:GLY:H2	1:A:2:PRO:CD	2.27	0.46
2:E:39:MET:CE	2:E:49:VAL:HG13	2.45	0.46
1:J:203:CYS:HB2	1:J:217:TRP:CZ2	2.49	0.46
1:G:185:PRO:HB3	1:G:208:PHE:HB3	1.97	0.46
1:J:273:ARG:CD	1:J:273:ARG:H	2.24	0.46
2:K:79:ALA:HB2	2:K:94:TYR:CD1	2.50	0.46
2:E:36:GLU:HB2	2:E:83:LYS:HB3	1.96	0.46
1:D:177:ALA:HA	1:D:180:LEU:HB2	1.98	0.46
1:G:116:PHE:CG	3:I:9:MET:HE3	2.50	0.46
1:A:207:GLY:HA2	1:A:240:THR:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:O	1:A:195:SER:O	2.33	0.46
1:A:167:TRP:CE3	1:A:170:ARG:HD3	2.51	0.46
1:D:1:GLY:O	1:D:3:HIS:NE2	2.48	0.46
1:G:202:ARG:HG2	1:G:204:TRP:NE1	2.31	0.46
1:A:230:LEU:C	1:A:230:LEU:HD12	2.35	0.46
1:D:49:ALA:HB1	1:D:50:PRO:HD2	1.97	0.46
1:G:251:LEU:HD23	1:G:251:LEU:C	2.37	0.46
2:H:39:MET:HE1	2:H:67:HIS:CA	2.46	0.46
1:A:275:GLU:O	1:A:276:PRO:OXT	2.34	0.46
1:D:232:GLU:O	1:D:232:GLU:HG2	2.11	0.46
1:D:181:ARG:HG3	1:D:182:THR:N	2.31	0.45
1:J:51:TRP:O	1:J:54:GLN:HG3	2.16	0.45
1:G:230:LEU:CD1	1:G:230:LEU:C	2.84	0.45
2:B:9:VAL:HG23	2:B:93:VAL:HG22	1.98	0.45
1:J:135:ALA:H	1:J:144:ARG:HH21	1.65	0.45
2:K:7:ILE:HB	2:K:93:VAL:HG11	1.98	0.45
1:D:99:SER:HA	1:D:113:TYR:O	2.17	0.45
2:H:87:MET:CE	2:H:91:LYS:HB2	2.46	0.45
1:G:224:LEU:HG	1:G:226:GLN:HB3	1.98	0.45
2:B:9:VAL:CG2	2:B:93:VAL:HG22	2.47	0.45
1:J:145:ARG:O	1:J:146:LYS:C	2.54	0.45
1:G:270:LEU:HD23	1:G:270:LEU:HA	1.75	0.45
1:A:214:THR:O	1:A:215:LEU:HD12	2.17	0.45
1:J:51:TRP:CZ3	1:J:52:MET:HG2	2.51	0.45
1:D:167:TRP:CZ3	1:D:170:ARG:HD3	2.52	0.45
1:D:66:LYS:NZ	3:F:1:LYS:HG2	2.30	0.45
2:B:16:GLU:CG	2:K:88:ALA:HB3	2.47	0.45
1:G:121:ARG:CZ	2:H:1:ILE:CD1	2.94	0.45
1:A:106:ASP:OD1	1:A:108:ARG:HB2	2.17	0.45
1:G:214:THR:C	1:G:215:LEU:HD12	2.37	0.45
1:J:31:LYS:HZ1	1:J:181:ARG:HH22	1.65	0.45
2:H:39:MET:HE3	2:H:49:VAL:HG13	1.99	0.45
1:G:160:LEU:HD23	1:G:160:LEU:HA	1.73	0.45
2:K:26:TYR:CE2	2:K:28:THR:HG21	2.52	0.45
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.99	0.45
1:G:154:GLU:N	1:G:154:GLU:CD	2.69	0.45
1:J:12:VAL:HG11	2:K:33:PRO:HG2	1.99	0.45
1:A:11:ALA:HA	1:A:21:ARG:O	2.17	0.45
1:J:213:ILE:HG12	1:J:214:THR:H	1.81	0.45
1:A:223:GLU:O	1:A:224:LEU:HD13	2.17	0.44
1:D:58:GLU:CG	1:D:59:TYR:N	2.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:TYR:CD1	1:A:210:PRO:HA	2.53	0.44
1:J:42:ASN:ND2	1:J:44:ARG:CD	2.80	0.44
2:B:7:ILE:HG22	2:B:8:GLN:N	2.33	0.44
1:A:1:GLY:HA3	1:A:105:SER:HB3	1.99	0.44
1:J:234:ARG:HD3	2:K:10:TYR:CZ	2.52	0.44
1:A:21:ARG:HG2	1:A:23:ILE:CD1	2.39	0.44
1:D:209:TYR:CD1	1:D:210:PRO:HA	2.53	0.44
1:J:31:LYS:NZ	1:J:181:ARG:HH22	2.14	0.44
3:L:3:VAL:HG22	3:L:4:TYR:N	2.31	0.44
1:A:57:PRO:O	1:A:61:GLU:HG3	2.17	0.44
2:B:64:ILE:CG2	2:B:65:LEU:N	2.76	0.44
1:A:202:ARG:HD3	1:A:246:SER:HB3	2.00	0.44
1:G:7:TYR:CE2	3:I:2:ALA:HB2	2.52	0.44
1:A:6:ARG:NH2	1:A:113:TYR:CD1	2.86	0.44
1:G:181:ARG:CB	1:G:181:ARG:NH1	2.56	0.44
1:A:62:ARG:HB3	1:A:62:ARG:HE	1.68	0.44
1:A:220:ASN:CA	1:A:221:GLY:O	2.64	0.44
1:A:250:PRO:O	1:A:251:LEU:C	2.56	0.44
3:F:5:ASN:ND2	3:F:5:ASN:N	2.66	0.44
1:D:180:LEU:HA	1:D:180:LEU:HD12	1.74	0.44
2:E:9:VAL:HG21	2:E:93:VAL:HG22	1.99	0.44
1:A:124:ILE:HG13	1:A:135:ALA:HB2	1.99	0.44
1:D:8:PHE:CE1	1:D:98:MET:HG2	2.53	0.44
1:D:114:LEU:HA	1:D:114:LEU:HD23	1.78	0.44
3:F:3:VAL:HG22	3:F:4:TYR:N	2.32	0.44
1:D:220:ASN:O	1:D:220:ASN:OD1	2.36	0.44
2:H:9:VAL:HG23	2:H:93:VAL:HG22	2.00	0.43
1:D:226:GLN:C	1:D:226:GLN:OE1	2.57	0.43
1:A:114:LEU:CD2	1:A:114:LEU:C	2.86	0.43
1:J:12:VAL:HG11	2:K:33:PRO:CG	2.48	0.43
2:H:7:ILE:HB	2:H:93:VAL:HG11	2.00	0.43
1:J:55:GLU:CD	1:J:170:ARG:HH21	2.22	0.43
1:G:73:TRP:CD1	3:I:8:THR:HG22	2.52	0.43
1:G:121:ARG:NE	2:H:1:ILE:HD11	2.34	0.43
1:A:14:ARG:C	1:A:16:GLY:N	2.70	0.43
1:A:31:LYS:HZ2	1:A:181:ARG:HH12	1.66	0.43
2:K:50:GLU:HG3	2:K:67:HIS:NE2	2.34	0.43
1:J:266:LEU:HD21	1:J:270:LEU:HG	2.00	0.43
1:A:121:ARG:HD2	1:A:121:ARG:HH11	1.70	0.43
1:G:202:ARG:HD2	1:G:244:TRP:CE3	2.53	0.43
1:G:189:VAL:HA	1:G:202:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:GLN:H	2:B:2:GLN:HG2	0.96	0.43
1:A:152:ALA:O	1:A:155:HIS:HB3	2.18	0.43
2:B:10:TYR:N	2:B:10:TYR:CD1	2.86	0.43
1:A:261:VAL:HB	1:A:270:LEU:HB2	1.99	0.43
1:A:272:LEU:HA	1:A:272:LEU:HD23	1.83	0.43
1:A:190:THR:OG1	1:A:202:ARG:HB3	2.18	0.43
1:D:216:THR:HA	1:D:228:MET:HE1	2.00	0.43
1:A:6:ARG:NH2	1:A:113:TYR:CE1	2.87	0.43
1:A:149:GLN:NE2	1:A:149:GLN:HA	2.34	0.43
2:K:10:TYR:CD1	2:K:10:TYR:N	2.87	0.43
1:J:215:LEU:N	1:J:215:LEU:CD1	2.80	0.42
2:E:59:ASP:O	2:E:60:TRP:CB	2.67	0.42
1:J:107:TRP:HE3	1:J:169:HIS:CD2	2.37	0.42
1:G:234:ARG:HD3	2:H:10:TYR:CE2	2.54	0.42
1:D:214:THR:O	1:D:215:LEU:HD12	2.19	0.42
2:E:79:ALA:HB2	2:E:94:TYR:CD1	2.54	0.42
1:A:54:GLN:HB3	1:A:54:GLN:HE21	1.64	0.42
1:D:58:GLU:HG2	1:D:58:GLU:H	1.25	0.42
1:J:31:LYS:HZ1	1:J:181:ARG:NH2	2.17	0.42
2:E:87:MET:CE	2:E:91:LYS:HB2	2.49	0.42
1:G:207:GLY:HA2	1:G:240:THR:OG1	2.19	0.42
1:A:219:LEU:O	1:A:220:ASN:HB2	2.18	0.42
1:J:118:TYR:CD2	1:J:119:GLU:HG2	2.55	0.42
1:G:18:GLU:CD	1:G:18:GLU:H	2.03	0.42
2:E:12:ARG:CZ	2:E:22:ILE:HD12	2.49	0.42
1:G:15:PRO:HD3	1:G:91:GLY:C	2.30	0.42
3:I:3:VAL:CG2	3:I:4:TYR:N	2.82	0.42
1:J:31:LYS:NZ	1:J:181:ARG:NH2	2.68	0.42
1:G:73:TRP:CZ2	3:I:8:THR:HA	2.54	0.42
1:G:163:GLU:O	1:G:164:CYS:C	2.57	0.42
2:E:9:VAL:HG23	2:E:93:VAL:HG22	2.01	0.42
1:G:17:LEU:O	1:G:18:GLU:C	2.58	0.42
1:J:99:SER:HA	1:J:113:TYR:O	2.19	0.42
1:D:28:VAL:HG23	1:D:33:PHE:CD1	2.55	0.42
1:J:79:ARG:HH11	1:J:79:ARG:HD2	1.57	0.42
1:J:273:ARG:N	1:J:273:ARG:CD	2.82	0.42
1:G:162:GLY:O	1:G:163:GLU:C	2.57	0.42
1:A:194:ARG:NH1	1:A:248:VAL:HG12	2.33	0.42
2:E:12:ARG:NH1	2:E:22:ILE:HD12	2.35	0.42
1:A:167:TRP:CZ3	1:A:170:ARG:HD3	2.55	0.42
1:G:151:GLY:O	1:G:152:ALA:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:VAL:O	1:A:248:VAL:HG23	2.20	0.41
1:D:182:THR:CB	1:D:265:GLY:HA3	2.50	0.41
1:J:19:GLU:OE1	1:J:75:ARG:HD2	2.19	0.41
1:D:107:TRP:CE3	1:J:269:PRO:HD3	2.54	0.41
1:G:169:HIS:O	1:G:173:LYS:HG3	2.20	0.41
1:J:251:LEU:HD23	1:J:251:LEU:C	2.39	0.41
2:K:50:GLU:HB2	2:K:67:HIS:CE1	2.55	0.41
1:G:176:ASN:O	1:G:180:LEU:HB3	2.20	0.41
1:A:110:LEU:HD12	1:A:110:LEU:HA	1.92	0.41
1:A:31:LYS:NZ	1:A:181:ARG:NH2	2.65	0.41
1:A:79:ARG:NH1	1:A:79:ARG:HG2	2.36	0.41
1:G:170:ARG:O	1:G:171:TYR:C	2.57	0.41
1:D:138:MET:O	1:D:141:GLN:HG2	2.21	0.41
1:A:1:GLY:HA3	1:A:105:SER:HB2	2.01	0.41
1:A:226:GLN:O	1:A:227:ASP:C	2.59	0.41
1:D:123:TYR:HE2	3:F:9:MET:SD	2.43	0.41
1:J:5:MET:C	1:J:6:ARG:HG2	2.40	0.41
1:G:238:ASP:C	1:G:238:ASP:OD1	2.58	0.41
1:G:129:ASP:O	1:G:131:LYS:HG3	2.21	0.41
1:G:217:TRP:H	1:G:228:MET:CE	2.32	0.41
1:J:159:TYR:CE2	3:L:3:VAL:HB	2.56	0.41
1:J:18:GLU:HG2	1:J:19:GLU:HG2	2.03	0.41
1:A:75:ARG:HH11	1:A:75:ARG:HD3	1.23	0.41
1:J:179:LEU:HA	1:J:179:LEU:HD23	1.62	0.41
1:A:234:ARG:HB2	2:B:10:TYR:CZ	2.56	0.41
1:G:126:LEU:HA	1:G:126:LEU:HD12	1.76	0.41
1:J:87:GLN:HE22	1:J:118:TYR:HE2	1.69	0.41
1:A:35:ARG:NH2	2:B:54:MET:O	2.54	0.41
1:J:103:LEU:HD23	1:J:109:LEU:HA	2.03	0.41
1:J:124:ILE:HG13	1:J:135:ALA:HB2	2.03	0.41
1:A:201:LEU:HD12	1:A:249:VAL:HG21	2.02	0.41
2:H:36:GLU:HB2	2:H:83:LYS:HB3	2.03	0.41
1:A:167:TRP:CE2	3:C:1:LYS:HD2	2.55	0.41
1:J:226:GLN:O	1:J:226:GLN:CD	2.58	0.41
1:J:121:ARG:HD2	1:J:121:ARG:HH11	1.71	0.41
1:G:55:GLU:OE2	1:G:170:ARG:NH2	2.54	0.41
1:D:162:GLY:O	1:D:163:GLU:C	2.59	0.41
1:G:167:TRP:CE2	3:I:1:LYS:HD2	2.56	0.41
1:D:202:ARG:HD3	1:D:244:TRP:CE3	2.56	0.40
2:E:50:GLU:HG3	2:E:67:HIS:NE2	2.36	0.40
1:D:214:THR:C	1:D:215:LEU:HD12	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.56	0.40
1:D:255:GLN:NE2	1:D:274:TRP:HD1	2.19	0.40
2:E:39:MET:CE	2:E:68:THR:CG2	2.99	0.40
1:D:5:MET:O	1:D:6:ARG:HG2	2.20	0.40
1:D:263:HIS:O	1:D:266:LEU:CB	2.67	0.40
2:K:29:GLN:HA	2:K:61:SER:HB2	2.03	0.40
2:B:56:PHE:HB3	2:B:62:PHE:CD1	2.55	0.40
1:G:168:LEU:HD12	1:G:168:LEU:O	2.22	0.40
1:G:219:LEU:HD13	1:G:257:TYR:CZ	2.56	0.40
1:G:75:ARG:O	1:G:75:ARG:HG3	2.20	0.40
1:D:266:LEU:HD21	1:D:270:LEU:HG	2.03	0.40
1:D:191:HIS:HD1	1:D:274:TRP:HZ2	1.69	0.40
1:G:218:GLN:HG2	1:G:223:GLU:CA	2.51	0.40
1:D:52:MET:O	1:D:54:GLN:N	2.53	0.40
1:D:32:GLU:OE2	1:D:35:ARG:HD2	2.22	0.40
1:A:189:VAL:HG12	1:A:190:THR:N	2.36	0.40
1:A:103:LEU:HD23	1:A:109:LEU:HA	2.04	0.40
1:A:266:LEU:HD21	1:A:270:LEU:HD23	2.03	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	274/276 (99%)	250 (91%)	20 (7%)	4 (2%)	13	38
1	D	272/276 (99%)	252 (93%)	15 (6%)	5 (2%)	11	33
1	G	271/276 (98%)	249 (92%)	19 (7%)	3 (1%)	17	47
1	J	271/276 (98%)	249 (92%)	20 (7%)	2 (1%)	26	59
2	B	96/99 (97%)	95 (99%)	0	1 (1%)	19	49
2	E	97/99 (98%)	94 (97%)	2 (2%)	1 (1%)	19	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	97/99 (98%)	95 (98%)	2 (2%)	0	100 100
2	K	97/99 (98%)	95 (98%)	1 (1%)	1 (1%)	19 49
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100 100
3	F	7/9 (78%)	5 (71%)	1 (14%)	1 (14%)	0 0
3	I	7/9 (78%)	5 (71%)	2 (29%)	0	100 100
3	L	7/9 (78%)	6 (86%)	1 (14%)	0	100 100
All	All	1503/1536 (98%)	1401 (93%)	84 (6%)	18 (1%)	16 44

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	226	GLN
1	G	180	LEU
1	J	226	GLN
1	A	16	GLY
1	A	219	LEU
1	A	226	GLN
3	F	8	THR
1	G	226	GLN
1	A	265	GLY
1	D	17	LEU
1	D	195	SER
1	D	53	GLU
1	D	212	ASP
1	G	18	GLU
2	B	47	PRO
2	E	47	PRO
2	K	47	PRO
1	J	193	PRO

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	234/234 (100%)	207 (88%)	27 (12%)	7 19
1	D	232/234 (99%)	205 (88%)	27 (12%)	7 18
1	G	232/234 (99%)	207 (89%)	25 (11%)	8 21
1	J	232/234 (99%)	216 (93%)	16 (7%)	19 45
2	B	93/94 (99%)	79 (85%)	14 (15%)	3 9
2	E	94/94 (100%)	85 (90%)	9 (10%)	10 28
2	H	94/94 (100%)	83 (88%)	11 (12%)	7 17
2	K	94/94 (100%)	83 (88%)	11 (12%)	7 17
3	C	7/7 (100%)	7 (100%)	0	100 100
3	F	7/7 (100%)	6 (86%)	1 (14%)	4 10
3	I	7/7 (100%)	5 (71%)	2 (29%)	0 1
3	L	7/7 (100%)	6 (86%)	1 (14%)	4 10
All	All	1333/1340 (100%)	1189 (89%)	144 (11%)	8 21

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	19	GLU
1	A	23	ILE
1	A	39	ASP
1	A	45	TYR
1	A	62	ARG
1	A	78	LEU
1	A	79	ARG
1	A	114	LEU
1	A	128	GLU
1	A	166	GLU
1	A	183	ASP
1	A	184	SER
1	A	219	LEU
1	A	220	ASN
1	A	222	GLU
1	A	223	GLU
1	A	224	LEU
1	A	226	GLN
1	A	230	LEU
1	A	234	ARG
1	A	262	TYR

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Mol	Chain	Res	Type
1	A	264	GLU
1	A	268	GLU
1	A	270	LEU
1	A	273	ARG
1	A	274	TRP
2	B	4	THR
2	B	19	LYS
2	B	29	GLN
2	B	38	GLN
2	B	45	LYS
2	B	54	MET
2	B	58	LYS
2	B	64	ILE
2	B	69	GLU
2	B	70	PHE
2	B	74	GLU
2	B	75	THR
2	B	93	VAL
2	B	98	ASP
1	D	44	ARG
1	D	45	TYR
1	D	58	GLU
1	D	78	LEU
1	D	94	THR
1	D	111	ARG
1	D	114	LEU
1	D	149	GLN
1	D	178	THR
1	D	181	ARG
1	D	183	ASP
1	D	194	ARG
1	D	195	SER
1	D	196	LYS
1	D	222	GLU
1	D	226	GLN
1	D	230	LEU
1	D	232	GLU
1	D	234	ARG
1	D	254	GLU
1	D	256	ASN
1	D	260	ARG
1	D	264	GLU

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Mol	Chain	Res	Type
1	D	266	LEU
1	D	268	GLU
1	D	272	LEU
1	D	273	ARG
2	E	2	GLN
2	E	4	THR
2	E	29	GLN
2	E	38	GLN
2	E	54	MET
2	E	70	PHE
2	E	75	THR
2	E	93	VAL
2	E	98	ASP
3	F	5	ASN
1	G	12	VAL
1	G	23	ILE
1	G	45	TYR
1	G	48	ARG
1	G	62	ARG
1	G	72	GLN
1	G	75	ARG
1	G	78	LEU
1	G	110	LEU
1	G	114	LEU
1	G	128	GLU
1	G	154	GLU
1	G	181	ARG
1	G	194	ARG
1	G	195	SER
1	G	196	LYS
1	G	222	GLU
1	G	223	GLU
1	G	224	LEU
1	G	226	GLN
1	G	227	ASP
1	G	230	LEU
1	G	234	ARG
1	G	264	GLU
1	G	273	ARG
2	H	1	ILE
2	H	2	GLN
2	H	4	THR

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Mol	Chain	Res	Type
2	H	38	GLN
2	H	54	MET
2	H	64	ILE
2	H	69	GLU
2	H	70	PHE
2	H	75	THR
2	H	93	VAL
2	H	98	ASP
3	I	4	TYR
3	I	9	MET
1	J	18	GLU
1	J	45	TYR
1	J	48	ARG
1	J	78	LEU
1	J	79	ARG
1	J	114	LEU
1	J	194	ARG
1	J	222	GLU
1	J	223	GLU
1	J	226	GLN
1	J	230	LEU
1	J	234	ARG
1	J	247	VAL
1	J	264	GLU
1	J	268	GLU
1	J	273	ARG
2	K	2	GLN
2	K	4	THR
2	K	29	GLN
2	K	38	GLN
2	K	64	ILE
2	K	69	GLU
2	K	70	PHE
2	K	74	GLU
2	K	75	THR
2	K	93	VAL
2	K	98	ASP
3	L	4	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	97	GLN
1	A	149	GLN
1	A	192	HIS
1	A	255	GLN
2	B	6	GLN
2	B	31	HIS
3	C	5	ASN
1	D	42	ASN
1	D	54	GLN
1	D	87	GLN
1	D	97	GLN
1	D	174	ASN
1	D	192	HIS
1	D	220	ASN
1	D	255	GLN
1	D	256	ASN
2	E	31	HIS
3	F	5	ASN
1	G	54	GLN
1	G	97	GLN
1	G	220	ASN
1	G	255	GLN
2	H	2	GLN
2	H	34	HIS
2	H	38	GLN
3	I	5	ASN
1	J	42	ASN
1	J	54	GLN
1	J	93	HIS
1	J	97	GLN
1	J	155	HIS
1	J	220	ASN
1	J	255	GLN
2	K	2	GLN
2	K	29	GLN
2	K	34	HIS
3	L	5	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 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	276/276 (100%)	-0.17	3 (1%) 82 80	2, 10, 24, 76	0
1	D	274/276 (99%)	-0.24	3 (1%) 82 80	2, 9, 24, 61	0
1	G	273/276 (98%)	0.14	17 (6%) 24 17	2, 9, 22, 65	0
1	J	273/276 (98%)	-0.16	5 (1%) 71 68	2, 9, 22, 64	0
2	B	98/99 (98%)	-0.31	1 (1%) 84 81	5, 8, 13, 17	0
2	E	99/99 (100%)	-0.23	1 (1%) 84 81	5, 8, 13, 34	0
2	H	99/99 (100%)	-0.19	0 100 100	5, 8, 13, 40	0
2	K	99/99 (100%)	-0.34	0 100 100	5, 8, 13, 36	0
3	C	9/9 (100%)	0.18	0 100 100	7, 9, 10, 11	0
3	F	9/9 (100%)	0.16	1 (11%) 7 4	7, 9, 10, 11	0
3	I	9/9 (100%)	0.32	0 100 100	7, 9, 10, 11	0
3	L	9/9 (100%)	0.17	0 100 100	7, 9, 10, 11	0
All	All	1527/1536 (99%)	-0.14	31 (2%) 68 64	2, 9, 22, 76	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	196	LYS	5.2
1	G	220	ASN	4.5
1	J	178	THR	4.4
1	D	177	ALA	4.2
1	G	251	LEU	4.1
1	D	178	THR	4.0
1	J	220	ASN	4.0
1	G	253	LYS	3.7
1	G	177	ALA	3.2
1	G	228	MET	3.2
1	A	197	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	178	THR	2.7
1	G	248	VAL	2.7
1	G	186	LYS	2.7
1	J	194	ARG	2.6
1	G	254	GLU	2.5
1	G	192	HIS	2.4
2	E	1	ILE	2.4
1	G	255	GLN	2.4
1	A	227	ASP	2.4
1	G	57	PRO	2.4
1	G	249	VAL	2.3
1	J	179	LEU	2.3
1	G	193	PRO	2.3
3	F	9	MET	2.2
1	G	250	PRO	2.1
1	A	224	LEU	2.1
2	B	1	ILE	2.1
1	D	179	LEU	2.0
1	G	197	GLY	2.0
1	J	197	GLY	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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.