



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 12:58 PM JST

PDB ID : 5HGB
Title : HLA*A2402 complexed with HIV nef138 8mer epitope
Authors : Shi, Y.; Qi, J.; Gao, G.F.
Deposited on : 2016-01-08
Resolution : 2.40 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
Xtrriage (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

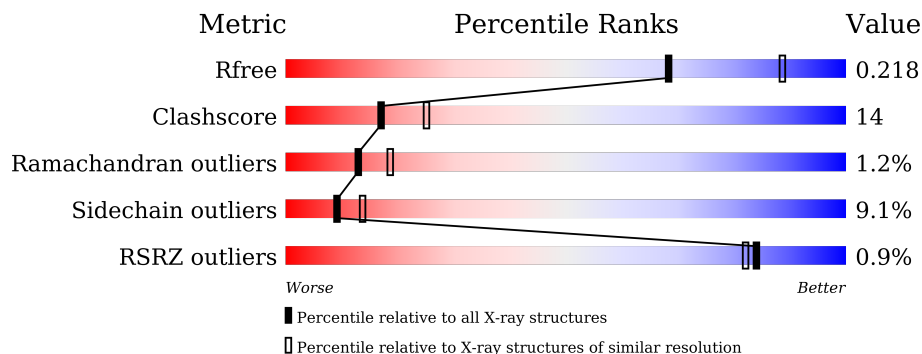
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	275	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 20px; position: relative;"> <div style="width: 69%; height: 100%; background-color: green;"></div> <div style="width: 27%; height: 100%; background-color: yellow;"></div> <div style="width: 4%; height: 100%; background-color: orange;"></div> <div style="width: 4%; height: 100%; background-color: red;"></div> </div> <div style="margin-left: 5px;">%</div> </div> <p style="text-align: center;">69% 27% •</p>
1	D	275	<div style="width: 100%; height: 20px; position: relative;"> <div style="width: 65%; height: 100%; background-color: green;"></div> <div style="width: 32%; height: 100%; background-color: yellow;"></div> <div style="width: 3%; height: 100%; background-color: orange;"></div> <div style="width: 0%; height: 100%; background-color: red;"></div> </div> <p style="text-align: center;">65% 32% •</p>
1	G	275	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 20px; position: relative;"> <div style="width: 69%; height: 100%; background-color: green;"></div> <div style="width: 28%; height: 100%; background-color: yellow;"></div> <div style="width: 3%; height: 100%; background-color: orange;"></div> <div style="width: 0%; height: 100%; background-color: red;"></div> </div> <div style="margin-left: 5px;">%</div> </div> <p style="text-align: center;">69% 28% •</p>
1	J	275	<div style="width: 100%; height: 20px; position: relative;"> <div style="width: 65%; height: 100%; background-color: green;"></div> <div style="width: 32%; height: 100%; background-color: yellow;"></div> <div style="width: 3%; height: 100%; background-color: orange;"></div> <div style="width: 0%; height: 100%; background-color: red;"></div> </div> <p style="text-align: center;">65% 32% •</p>
2	B	100	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 10px; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 100%; height: 20px; position: relative;"> <div style="width: 3%; height: 100%; background-color: red;"></div> <div style="width: 66%; height: 100%; background-color: green;"></div> <div style="width: 22%; height: 100%; background-color: yellow;"></div> <div style="width: 9%; height: 100%; background-color: orange;"></div> <div style="width: 0%; height: 100%; background-color: red;"></div> </div> <div style="margin-left: 5px;">%</div> </div> <p style="text-align: center;">69% 22% 8% •</p>
2	E	100	<div style="width: 100%; height: 20px; position: relative;"> <div style="width: 64%; height: 100%; background-color: green;"></div> <div style="width: 33%; height: 100%; background-color: yellow;"></div> <div style="width: 3%; height: 100%; background-color: orange;"></div> <div style="width: 0%; height: 100%; background-color: red;"></div> </div> <p style="text-align: center;">64% 33% ••</p>

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Mol	Chain	Length	Quality of chain
2	H	100	 % 65% 28% 5%
2	K	100	 2% 70% 24% 5%
3	C	8	 50% 50%
3	F	8	 38% 50% 12%
3	I	8	 62% 38%
3	L	8	 25% 75%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13137 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 class I histocompatibility antigen, A-24 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	274	2221	1382	403	426	10	0	0	0
1	D	274	2221	1382	403	426	10	0	0	0
1	G	274	2221	1382	403	426	10	0	0	0
1	J	274	2221	1382	403	426	10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P05534
D	0	MET	-	initiating methionine	UNP P05534
G	0	MET	-	initiating methionine	UNP P05534
J	0	MET	-	initiating methionine	UNP P05534

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	836	533	141	158	4	0	0	0
2	E	100	836	533	141	158	4	0	0	0
2	H	100	836	533	141	158	4	0	0	0
2	K	100	836	533	141	158	4	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
E	0	MET	-	initiating methionine	UNP P61769
H	0	MET	-	initiating methionine	UNP P61769
K	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Protein Nef.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			75	52	12	11			
3	F	8	Total	C	N	O	0	0	0
			75	52	12	11			
3	I	8	Total	C	N	O	0	0	0
			75	52	12	11			
3	L	8	Total	C	N	O	0	0	0
			75	52	12	11			

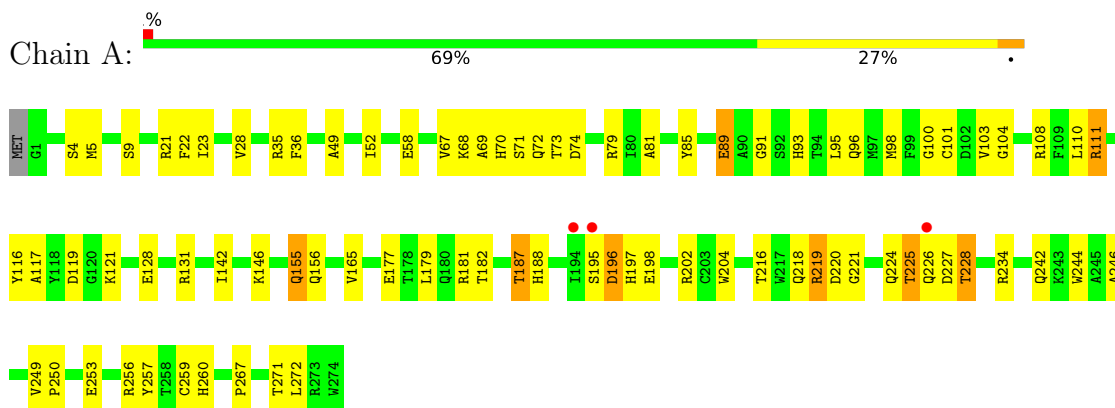
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total	O	0	0
			114	114		
4	B	35	Total	O	0	0
			35	35		
4	C	5	Total	O	0	0
			5	5		
4	D	102	Total	O	0	0
			102	102		
4	E	28	Total	O	0	0
			28	28		
4	F	4	Total	O	0	0
			4	4		
4	G	140	Total	O	0	0
			140	140		
4	H	46	Total	O	0	0
			46	46		
4	I	5	Total	O	0	0
			5	5		
4	J	99	Total	O	0	0
			99	99		
4	K	23	Total	O	0	0
			23	23		
4	L	8	Total	O	0	0
			8	8		

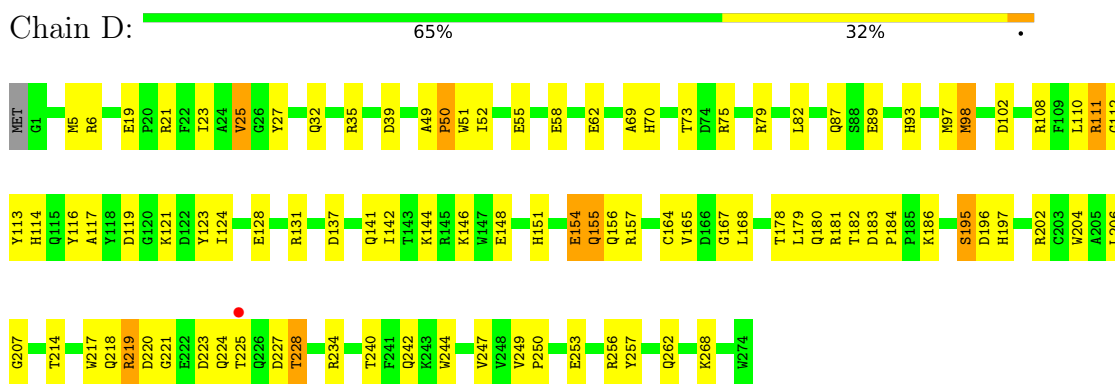
3 Residue-property plots

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

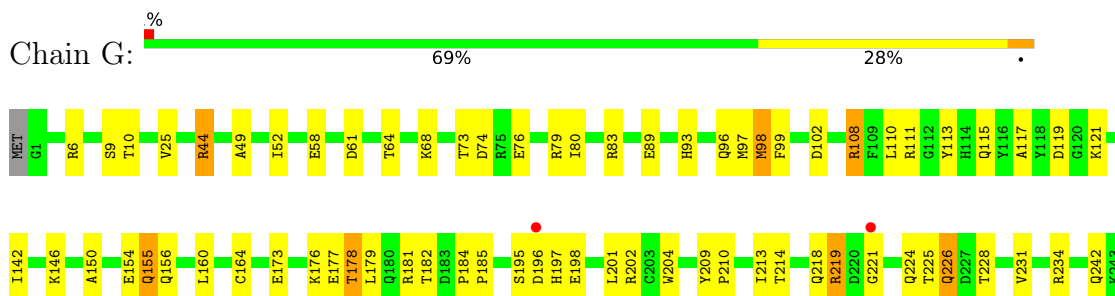
- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain



- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain



- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain





- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain

Chain J: 65% 32%



- Molecule 2: Beta-2-microglobulin

Chain B: 3% 69% 22% 8%



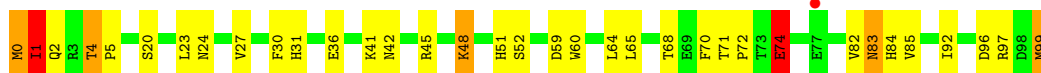
- Molecule 2: Beta-2-microglobulin

Chain E: 3% 64% 33% 2%



- Molecule 2: Beta-2-microglobulin

Chain H: 3% 65% 28% 5%



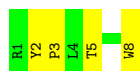
- Molecule 2: Beta-2-microglobulin

Chain K: 2% 70% 24% 5%

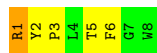


- Molecule 3: Protein Nef

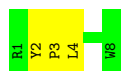
Chain C: 50% 50%



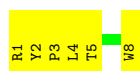
- Molecule 3: Protein Nef



- Molecule 3: Protein Nef



- Molecule 3: Protein Nef



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.95Å 152.51Å 90.17Å 90.00° 90.12° 90.00°	Depositor
Resolution (Å)	35.98 – 2.40 37.73 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.8 (35.98-2.40) 98.8 (37.73-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.195 , 0.218 0.202 , 0.218	Depositor DCC
R_{free} test set	3788 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtrriage
Anisotropy	0.553	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13137	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.70 % 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 1.4694e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.26	0/2281	0.45	0/3092
1	D	0.27	0/2281	0.45	0/3092
1	G	0.27	0/2281	0.46	0/3092
1	J	0.27	0/2281	0.45	0/3092
2	B	0.27	0/859	0.46	0/1162
2	E	0.28	0/859	0.45	0/1162
2	H	0.28	0/859	0.48	0/1162
2	K	0.25	0/859	0.43	0/1162
3	C	0.31	0/79	0.49	0/106
3	F	0.25	0/79	0.41	0/106
3	I	0.27	0/79	0.49	0/106
3	L	0.28	0/79	0.43	0/106
All	All	0.27	0/12876	0.45	0/17440

There are no bond length outliers.

There are no bond angle outliers.

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	2221	0	2082	57	0
1	D	2221	0	2082	65	0
1	G	2221	0	2082	61	0
1	J	2221	0	2082	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	836	0	803	24	0
2	E	836	0	803	27	0
2	H	836	0	803	37	0
2	K	836	0	803	29	0
3	C	75	0	71	4	0
3	F	75	0	71	4	0
3	I	75	0	71	2	0
3	L	75	0	71	6	0
4	A	114	0	0	5	0
4	B	35	0	0	5	0
4	C	5	0	0	0	0
4	D	102	0	0	2	0
4	E	28	0	0	7	0
4	F	4	0	0	0	0
4	G	140	0	0	4	0
4	H	46	0	0	11	0
4	I	5	0	0	0	0
4	J	99	0	0	4	0
4	K	23	0	0	3	0
4	L	8	0	0	0	0
All	All	13137	0	11824	340	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 (340) 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)
2:K:1:ILE:HG23	2:K:2:GLN:N	1.40	1.17
2:K:1:ILE:CG2	2:K:2:GLN:H	1.50	1.15
2:K:1:ILE:CG2	2:K:2:GLN:N	2.12	1.06
2:H:71:THR:HA	4:H:104:HOH:O	1.66	0.95
1:D:250:PRO:HB2	1:D:253:GLU:HG3	1.53	0.89
2:E:22:PHE:HA	4:E:101:HOH:O	1.73	0.88
3:I:4:LEU:HD11	1:J:150:ALA:HB1	1.59	0.83
1:G:224:GLN:HB3	4:G:304:HOH:O	1.80	0.82
1:J:234:ARG:HE	1:J:242:GLN:HE21	1.30	0.80
2:H:68:THR:HG22	4:H:101:HOH:O	1.84	0.78
1:D:214:THR:HB	1:D:262:GLN:HB2	1.66	0.77
2:B:68:THR:HG22	4:B:102:HOH:O	1.86	0.76
2:H:83:ASN:HD22	2:H:84:HIS:H	1.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1:ILE:HG23	2:K:2:GLN:H	0.63	0.73
1:J:248:VAL:HG22	4:J:301:HOH:O	1.88	0.73
2:H:20:SER:HA	4:H:104:HOH:O	1.88	0.72
1:A:89:GLU:HG3	1:A:89:GLU:O	1.89	0.72
2:E:68:THR:O	4:E:101:HOH:O	2.07	0.72
1:J:234:ARG:HH22	2:K:99:MET:HE1	1.55	0.71
1:J:28:VAL:HG11	1:J:179:LEU:HD13	1.73	0.70
1:J:224:GLN:O	1:J:225:THR:HG22	1.90	0.70
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.40	0.70
2:K:1:ILE:O	2:K:2:GLN:HG3	1.92	0.69
1:A:216:THR:HB	1:A:260:HIS:HB2	1.74	0.69
2:E:68:THR:C	4:E:101:HOH:O	2.30	0.68
2:H:23:LEU:HB3	4:H:101:HOH:O	1.92	0.68
1:D:225:THR:HG23	4:D:302:HOH:O	1.93	0.68
2:B:0:MET:O	2:B:1:ILE:HB	1.94	0.68
1:D:155:GLN:HG3	1:D:156:GLN:N	2.09	0.68
2:B:23:LEU:HB3	4:B:102:HOH:O	1.94	0.67
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.29	0.67
2:K:1:ILE:O	2:K:2:GLN:CB	2.42	0.67
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.30	0.67
1:D:142:ILE:O	1:D:146:LYS:HG3	1.95	0.66
1:D:49:ALA:O	1:D:52:ILE:HG22	1.94	0.66
2:E:0:MET:O	2:E:1:ILE:HB	1.96	0.65
1:G:204:TRP:HZ2	2:H:99:MET:O	1.79	0.65
2:K:1:ILE:O	2:K:2:GLN:CG	2.44	0.65
1:A:21:ARG:HE	1:A:23:ILE:HD11	1.60	0.65
1:D:111:ARG:HD2	1:D:128:GLU:HG3	1.79	0.65
1:D:234:ARG:HE	1:D:242:GLN:HE21	1.45	0.64
1:D:137:ASP:O	1:D:141:GLN:HG3	1.98	0.63
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.33	0.63
1:A:155:GLN:HG3	1:A:156:GLN:N	2.14	0.62
1:G:98:MET:HG3	1:G:115:GLN:HG3	1.81	0.62
2:H:85:VAL:HG13	4:H:105:HOH:O	2.00	0.62
1:D:111:ARG:HG3	1:D:112:GLY:N	2.15	0.62
1:D:69:ALA:O	1:D:73:THR:HG23	1.99	0.62
1:A:91:GLY:HA2	1:G:108:ARG:NH2	2.16	0.61
1:G:177:GLU:HG2	4:G:368:HOH:O	2.01	0.61
2:B:83:ASN:HD22	2:B:84:HIS:H	1.48	0.60
1:A:69:ALA:O	1:A:73:THR:HG23	2.01	0.60
1:G:79:ARG:HD2	4:G:346:HOH:O	2.01	0.60
2:K:18:GLY:N	4:K:101:HOH:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:SER:HB2	4:A:311:HOH:O	2.01	0.60
1:G:249:VAL:HG22	1:G:257:TYR:CZ	2.36	0.60
2:B:48:LYS:HE3	2:B:48:LYS:HA	1.83	0.60
1:J:93:HIS:HD2	1:J:119:ASP:OD2	1.85	0.60
1:A:224:GLN:O	1:A:225:THR:HG22	2.02	0.59
1:A:111:ARG:HD2	1:A:128:GLU:HG3	1.85	0.59
2:H:72:PRO:HD2	4:H:104:HOH:O	2.02	0.59
1:D:157:ARG:HD3	4:D:388:HOH:O	2.01	0.59
1:G:155:GLN:HE21	1:G:156:GLN:HE22	1.49	0.59
1:D:51:TRP:CZ2	1:D:179:LEU:HD11	2.38	0.59
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.38	0.59
1:J:234:ARG:HH22	2:K:99:MET:CE	2.16	0.58
1:D:111:ARG:HG2	1:D:113:TYR:CZ	2.39	0.58
1:A:182:THR:HG23	1:A:182:THR:O	2.03	0.58
1:G:225:THR:O	1:G:228:THR:HG22	2.04	0.57
1:A:197:HIS:CD2	1:A:198:GLU:HG3	2.40	0.57
1:D:220:ASP:OD1	1:D:256:ARG:HG2	2.05	0.57
1:J:249:VAL:HG22	1:J:257:TYR:CZ	2.39	0.57
1:J:266:LEU:HD13	1:J:270:LEU:HG	1.85	0.57
1:D:151:HIS:O	1:D:154:GLU:HG2	2.04	0.57
1:G:49:ALA:O	1:G:52:ILE:HG22	2.04	0.57
2:H:96:ASP:HB3	2:H:99:MET:HB3	1.87	0.57
2:K:40:LEU:HA	2:K:44:GLU:O	2.05	0.57
1:D:27:TYR:CZ	4:E:102:HOH:O	2.57	0.56
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.88	0.56
1:A:104:GLY:HA3	4:A:332:HOH:O	2.05	0.56
1:D:249:VAL:HG22	1:D:257:TYR:CZ	2.40	0.56
1:G:142:ILE:O	1:G:146:LYS:HG3	2.06	0.56
1:J:220:ASP:OD1	1:J:256:ARG:HG2	2.06	0.56
2:K:1:ILE:O	2:K:2:GLN:HB2	2.04	0.56
1:A:142:ILE:O	1:A:146:LYS:HG3	2.05	0.56
2:H:83:ASN:HD22	2:H:84:HIS:N	2.04	0.56
1:G:250:PRO:HG2	1:G:253:GLU:OE2	2.06	0.55
2:H:5:PRO:HD2	4:H:103:HOH:O	2.05	0.55
1:D:195:SER:O	1:D:197:HIS:N	2.30	0.55
1:G:76:GLU:HA	1:G:79:ARG:HD3	1.88	0.55
1:G:234:ARG:HE	1:G:242:GLN:HE21	1.54	0.55
1:J:64:THR:O	1:J:68:LYS:HB2	2.06	0.55
2:B:74:GLU:CD	2:B:74:GLU:H	2.09	0.55
1:D:123:TYR:HD2	1:D:124:ILE:HG22	1.71	0.55
1:J:202:ARG:HD3	1:J:244:TRP:CE3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:10:TYR:O	2:K:23:LEU:HD12	2.07	0.55
1:G:93:HIS:HD2	1:G:119:ASP:OD2	1.90	0.54
1:J:69:ALA:O	1:J:73:THR:HG23	2.07	0.54
1:J:9:SER:OG	1:J:97:MET:HB3	2.07	0.54
1:J:204:TRP:HE3	1:J:206:LEU:HD21	1.71	0.54
1:A:70:HIS:CD2	3:C:5:THR:HG21	2.42	0.54
2:H:51:HIS:HD2	2:H:52:SER:O	1.89	0.54
2:K:31:HIS:CD2	2:K:32:PRO:HA	2.42	0.54
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.42	0.54
1:G:195:SER:O	1:G:197:HIS:N	2.37	0.54
2:K:72:PRO:HD2	4:K:101:HOH:O	2.06	0.54
1:A:58:GLU:CD	1:A:58:GLU:H	2.11	0.54
2:E:69:GLU:HA	4:E:101:HOH:O	2.07	0.54
1:J:137:ASP:O	1:J:141:GLN:HG3	2.07	0.54
1:G:96:GLN:OE1	2:H:31:HIS:HE1	1.91	0.54
1:G:155:GLN:HE21	1:G:156:GLN:NE2	2.06	0.53
2:K:99:MET:HG2	4:K:104:HOH:O	2.07	0.53
1:D:225:THR:O	1:D:228:THR:HG22	2.08	0.53
2:E:59:ASP:O	2:E:60:TRP:HB2	2.08	0.53
2:H:31:HIS:HD2	4:H:117:HOH:O	1.91	0.53
1:G:228:THR:N	4:G:304:HOH:O	2.42	0.53
2:H:24:ASN:HB3	2:H:65:LEU:HD11	1.89	0.53
1:J:216:THR:HB	1:J:260:HIS:HB2	1.91	0.53
2:E:51:HIS:HA	2:E:65:LEU:O	2.08	0.53
1:D:234:ARG:HE	1:D:242:GLN:NE2	2.06	0.53
1:J:178:THR:HG22	1:J:179:LEU:N	2.24	0.53
1:J:151:HIS:O	1:J:154:GLU:HG2	2.08	0.52
2:B:83:ASN:ND2	2:B:84:HIS:H	2.07	0.52
1:G:150:ALA:HB1	3:L:4:LEU:HD11	1.91	0.52
2:H:97:ARG:NH1	2:H:97:ARG:HB3	2.24	0.52
1:J:202:ARG:HG2	1:J:204:TRP:NE1	2.24	0.52
1:D:58:GLU:O	1:D:62:GLU:HG3	2.10	0.52
2:K:63:TYR:O	2:K:64:LEU:HD13	2.10	0.52
1:D:27:TYR:CE1	4:E:102:HOH:O	2.55	0.52
1:G:259:CYS:O	1:G:271:THR:HA	2.10	0.52
1:J:195:SER:O	1:J:197:HIS:N	2.32	0.52
1:A:218:GLN:OE1	1:A:221:GLY:HA2	2.10	0.51
1:G:219:ARG:HB3	1:G:219:ARG:HH11	1.76	0.51
1:J:70:HIS:CD2	3:L:5:THR:HG21	2.45	0.51
1:D:204:TRP:HZ2	2:E:99:MET:O	1.93	0.51
2:B:70:PHE:HD2	2:B:78:TYR:CZ	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:155:GLN:HG3	1:J:156:GLN:N	2.26	0.51
1:A:116:TYR:HE1	4:A:301:HOH:O	1.94	0.51
1:D:27:TYR:CZ	1:D:32:GLN:HB2	2.46	0.51
2:H:74:GLU:N	2:H:74:GLU:CD	2.64	0.51
1:D:89:GLU:HG2	1:D:89:GLU:O	2.10	0.51
2:B:96:ASP:HB3	2:B:99:MET:HB3	1.93	0.51
1:G:224:GLN:O	1:G:225:THR:HG22	2.09	0.51
1:D:93:HIS:HD2	1:D:119:ASP:OD2	1.93	0.50
3:L:2:TYR:CD1	3:L:3:PRO:HD2	2.46	0.50
1:A:259:CYS:O	1:A:271:THR:HA	2.11	0.50
2:E:75:LYS:HG3	2:E:76:ASP:N	2.26	0.50
1:G:173:GLU:O	1:G:176:LYS:HB2	2.11	0.50
2:H:5:PRO:HB3	2:H:30:PHE:HB3	1.93	0.50
1:A:234:ARG:HE	1:A:242:GLN:NE2	2.07	0.50
2:E:96:ASP:HB3	2:E:99:MET:HB3	1.93	0.50
1:D:234:ARG:HH22	2:E:99:MET:CE	2.25	0.50
2:E:1:ILE:HG23	2:E:1:ILE:O	2.11	0.50
1:J:204:TRP:HZ2	2:K:99:MET:O	1.95	0.50
1:G:218:GLN:OE1	1:G:221:GLY:HA2	2.11	0.50
1:D:217:TRP:CD1	1:D:247:VAL:HG13	2.46	0.50
1:A:9:SER:OG	1:A:70:HIS:HE1	1.95	0.49
2:K:0:MET:O	2:K:1:ILE:O	2.30	0.49
1:D:202:ARG:HD3	1:D:244:TRP:CE3	2.47	0.49
1:A:91:GLY:HA2	1:G:108:ARG:HH22	1.76	0.49
1:A:204:TRP:HZ2	2:B:99:MET:O	1.95	0.49
1:A:250:PRO:HB2	1:A:253:GLU:HG3	1.93	0.49
2:H:1:ILE:HD13	2:H:2:GLN:N	2.26	0.49
1:G:184:PRO:HG3	1:G:265:GLY:O	2.12	0.49
1:A:187:THR:HB	1:A:272:LEU:HD11	1.94	0.49
2:H:1:ILE:HD13	2:H:2:GLN:H	1.78	0.49
2:H:83:ASN:ND2	2:H:84:HIS:H	2.07	0.49
1:D:97:MET:HG2	1:D:98:MET:N	2.28	0.49
1:A:188:HIS:HD2	4:A:345:HOH:O	1.95	0.48
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.48	0.48
2:H:48:LYS:HE3	2:H:48:LYS:HA	1.94	0.48
2:B:85:VAL:HG22	4:B:105:HOH:O	2.13	0.48
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.49	0.48
1:A:72:GLN:OE1	1:A:72:GLN:HA	2.13	0.48
1:G:99:PHE:CE1	1:G:160:LEU:HD21	2.49	0.47
1:J:234:ARG:HE	1:J:242:GLN:NE2	2.06	0.47
1:D:111:ARG:HG3	1:D:112:GLY:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:ARG:HD3	1:G:113:TYR:OH	2.14	0.47
3:I:2:TYR:CG	3:I:3:PRO:HD2	2.48	0.47
1:D:35:ARG:HD3	2:E:53:ASP:OD2	2.15	0.47
2:B:41:LYS:O	2:B:42:ASN:HB2	2.14	0.47
1:D:55:GLU:OE1	1:D:55:GLU:HA	2.14	0.47
1:G:201:LEU:HB2	1:G:247:VAL:HG23	1.97	0.47
1:G:209:TYR:CD1	1:G:210:PRO:HA	2.50	0.47
1:A:225:THR:HG23	1:A:226:GLN:N	2.29	0.47
1:J:89:GLU:O	1:J:89:GLU:HG2	2.15	0.47
1:A:70:HIS:HD1	3:C:2:TYR:HH	1.58	0.47
2:E:39:LEU:HD13	2:E:68:THR:HG22	1.97	0.46
1:G:119:ASP:CG	2:H:0:MET:HG2	2.36	0.46
1:G:155:GLN:OE1	1:J:150:ALA:O	2.32	0.46
1:A:81:ALA:O	1:A:85:TYR:HD2	1.97	0.46
1:A:271:THR:C	1:A:272:LEU:HD23	2.36	0.46
2:E:23:LEU:O	2:E:67:TYR:HA	2.15	0.46
2:B:5:PRO:HB3	2:B:30:PHE:HB3	1.96	0.46
2:H:51:HIS:HA	2:H:65:LEU:O	2.16	0.46
1:J:249:VAL:HG11	1:J:254:GLU:HA	1.98	0.46
1:A:234:ARG:HH12	2:B:99:MET:HE1	1.79	0.46
3:F:2:TYR:CG	3:F:3:PRO:HD2	2.51	0.46
1:D:21:ARG:HE	1:D:23:ILE:HD11	1.81	0.46
1:D:70:HIS:CD2	3:F:5:THR:HG21	2.51	0.46
1:G:9:SER:O	1:G:96:GLN:HA	2.16	0.46
1:J:204:TRP:CE3	1:J:206:LEU:HD21	2.51	0.46
2:K:23:LEU:O	2:K:67:TYR:HA	2.16	0.46
1:J:74:ASP:HA	1:J:77:ASN:HB2	1.98	0.46
1:D:25:VAL:HG11	1:D:27:TYR:HE1	1.81	0.45
1:D:224:GLN:O	1:D:225:THR:CG2	2.64	0.45
1:J:181:ARG:NH2	4:J:307:HOH:O	2.49	0.45
2:K:59:ASP:O	2:K:60:TRP:HB2	2.17	0.45
1:A:218:GLN:O	1:A:257:TYR:HA	2.17	0.45
1:G:219:ARG:HB2	1:G:224:GLN:HE21	1.81	0.45
1:G:271:THR:C	1:G:272:LEU:HD23	2.37	0.45
1:D:25:VAL:CG1	1:D:27:TYR:HE1	2.30	0.45
1:G:80:ILE:HA	1:G:83:ARG:HD3	1.99	0.45
1:G:155:GLN:HG3	1:G:156:GLN:HE21	1.80	0.45
2:H:51:HIS:CD2	2:H:52:SER:O	2.70	0.45
1:G:89:GLU:O	1:G:89:GLU:HG2	2.16	0.45
3:C:2:TYR:CG	3:C:3:PRO:HD2	2.52	0.45
1:A:195:SER:O	1:A:197:HIS:N	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:GLN:NE2	3:F:6:PHE:HE2	2.15	0.45
1:G:6:ARG:NH2	1:G:102:ASP:OD1	2.50	0.45
1:D:167:GLY:HA3	3:F:1:ARG:HG3	1.98	0.45
1:J:133:TRP:HB2	1:J:144:LYS:HG3	1.99	0.45
1:J:51:TRP:CZ2	1:J:179:LEU:HD11	2.52	0.44
1:J:181:ARG:CZ	4:J:311:HOH:O	2.64	0.44
1:A:36:PHE:HB3	1:A:67:VAL:HG21	1.99	0.44
1:A:225:THR:O	1:A:227:ASP:N	2.46	0.44
1:G:76:GLU:HA	1:G:79:ARG:HH11	1.82	0.44
1:A:220:ASP:OD2	1:A:256:ARG:NH2	2.51	0.44
1:D:51:TRP:CE2	1:D:179:LEU:HD11	2.53	0.44
1:G:97:MET:HG2	1:G:98:MET:N	2.33	0.44
1:G:98:MET:HG3	1:G:115:GLN:CG	2.48	0.44
1:J:219:ARG:HD3	1:J:256:ARG:NH2	2.33	0.44
1:J:194:ILE:O	1:J:195:SER:HB3	2.17	0.44
2:E:68:THR:O	2:E:68:THR:HG23	2.18	0.44
1:D:207:GLY:HA2	1:D:240:THR:HB	2.00	0.44
1:G:64:THR:HG22	1:G:68:LYS:HD2	1.98	0.44
1:G:213:ILE:HG12	1:G:214:THR:N	2.33	0.44
1:J:98:MET:HG3	1:J:115:GLN:HG2	1.99	0.44
1:J:201:LEU:O	1:J:246:ALA:HA	2.18	0.44
2:E:40:LEU:O	2:E:78:TYR:HA	2.17	0.43
1:J:123:TYR:CZ	1:J:140:ALA:HA	2.53	0.43
1:A:5:MET:O	1:A:100:GLY:HA3	2.18	0.43
1:G:178:THR:HG22	1:G:179:LEU:N	2.33	0.43
1:G:202:ARG:HD3	1:G:244:TRP:CE3	2.53	0.43
2:B:96:ASP:O	2:B:99:MET:HG3	2.19	0.43
1:D:182:THR:HG23	1:D:182:THR:O	2.17	0.43
2:K:1:ILE:HA	2:K:1:ILE:HD13	1.78	0.43
1:A:219:ARG:HB2	1:A:224:GLN:NE2	2.34	0.43
1:D:5:MET:HB2	1:D:168:LEU:HD13	1.99	0.43
1:D:25:VAL:CG1	1:D:27:TYR:CE1	3.02	0.43
1:D:82:LEU:HD22	1:D:87:GLN:HB2	2.01	0.43
1:J:259:CYS:O	1:J:271:THR:HA	2.17	0.43
1:A:188:HIS:CD2	4:A:345:HOH:O	2.70	0.43
2:K:2:GLN:HG2	2:K:32:PRO:HD3	1.99	0.43
2:K:40:LEU:O	2:K:78:TYR:HA	2.17	0.43
1:A:49:ALA:O	1:A:52:ILE:HG22	2.19	0.43
1:D:218:GLN:OE1	1:D:221:GLY:HA2	2.19	0.43
2:H:4:THR:CB	4:H:103:HOH:O	2.67	0.43
1:J:6:ARG:NH2	1:J:102:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:36:GLU:O	2:E:82:VAL:HA	2.19	0.43
1:A:95:LEU:HD21	3:C:8:TRP:CZ2	2.53	0.43
3:L:2:TYR:CG	3:L:3:PRO:HD2	2.54	0.43
2:H:0:MET:O	2:H:1:ILE:HB	2.19	0.43
2:H:41:LYS:O	2:H:42:ASN:HB2	2.19	0.43
1:J:44:ARG:HA	1:J:64:THR:HG23	2.01	0.43
1:J:108:ARG:NH1	4:J:313:HOH:O	2.52	0.43
2:B:64:LEU:HD12	2:B:64:LEU:HA	1.93	0.42
2:H:36:GLU:O	2:H:82:VAL:HA	2.19	0.42
1:D:131:ARG:HD2	1:D:157:ARG:NH1	2.34	0.42
1:G:231:VAL:HG22	1:G:244:TRP:O	2.18	0.42
1:J:5:MET:O	1:J:100:GLY:HA3	2.18	0.42
2:B:12:ARG:NH2	4:B:106:HOH:O	2.53	0.42
1:D:21:ARG:NH1	1:D:39:ASP:HB2	2.34	0.42
1:D:224:GLN:O	1:D:225:THR:HG22	2.19	0.42
1:A:197:HIS:HD2	1:A:198:GLU:HG3	1.83	0.42
2:E:63:TYR:O	2:E:64:LEU:HD13	2.19	0.42
1:G:197:HIS:HD2	1:G:198:GLU:HG3	1.85	0.42
2:E:10:TYR:HB3	2:E:99:MET:HE1	2.02	0.42
2:E:1:ILE:O	2:E:1:ILE:CG2	2.67	0.42
1:G:204:TRP:CZ2	2:H:99:MET:O	2.67	0.42
1:J:127:LYS:HE2	1:J:134:THR:OG1	2.20	0.42
2:B:51:HIS:HA	2:B:65:LEU:O	2.19	0.42
1:J:229:GLU:O	1:J:229:GLU:HG2	2.16	0.42
1:D:183:ASP:HA	1:D:184:PRO:HD3	1.93	0.42
1:G:10:THR:HG23	1:G:96:GLN:HG2	2.01	0.42
2:K:54:LEU:HA	2:K:64:LEU:HD11	2.01	0.42
1:G:234:ARG:HH22	2:H:99:MET:CE	2.33	0.42
1:J:250:PRO:HB2	1:J:253:GLU:HG3	2.02	0.42
1:D:6:ARG:NH2	1:D:102:ASP:OD1	2.53	0.41
2:K:70:PHE:HD2	2:K:78:TYR:CZ	2.37	0.41
1:A:28:VAL:HG11	1:A:179:LEU:HD13	2.01	0.41
1:D:204:TRP:CE3	1:D:206:LEU:HD21	2.55	0.41
2:H:59:ASP:O	2:H:60:TRP:HB2	2.19	0.41
1:J:95:LEU:HG	3:L:8:TRP:CH2	2.55	0.41
1:A:35:ARG:HD3	2:B:53:ASP:OD2	2.21	0.41
1:D:202:ARG:HG2	1:D:204:TRP:NE1	2.35	0.41
1:G:44:ARG:NH2	1:G:61:ASP:OD1	2.53	0.41
1:J:111:ARG:HG2	1:J:113:TYR:CE1	2.56	0.41
1:J:234:ARG:HD2	2:K:10:TYR:CE2	2.56	0.41
1:J:99:PHE:CE2	3:L:3:PRO:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:173:GLU:O	1:J:176:LYS:HB2	2.19	0.41
2:B:74:GLU:CD	2:B:74:GLU:N	2.73	0.41
1:G:249:VAL:HG22	1:G:257:TYR:CE1	2.56	0.41
2:H:4:THR:HB	4:H:103:HOH:O	2.19	0.41
1:J:106:ASP:OD2	1:J:108:ARG:HD3	2.20	0.41
2:B:39:LEU:O	2:B:46:ILE:HG13	2.21	0.41
1:D:144:LYS:O	1:D:148:GLU:HG3	2.20	0.41
2:E:51:HIS:HD2	2:E:52:SER:O	2.03	0.41
2:H:0:MET:N	4:H:108:HOH:O	2.53	0.41
1:J:49:ALA:O	1:J:52:ILE:HG22	2.20	0.41
1:A:228:THR:HA	1:A:246:ALA:O	2.21	0.41
1:A:103:VAL:C	1:A:110:LEU:HD22	2.41	0.41
4:B:113:HOH:O	1:D:186:LYS:HE2	2.20	0.41
1:D:114:HIS:HE1	1:D:116:TYR:OH	2.04	0.41
1:D:219:ARG:HG3	1:D:257:TYR:CZ	2.56	0.41
2:E:31:HIS:CD2	2:E:32:PRO:HA	2.56	0.41
2:E:85:VAL:HG13	4:E:107:HOH:O	2.21	0.41
1:J:33:PHE:CD1	1:J:34:VAL:HG13	2.56	0.41
1:J:266:LEU:HA	1:J:267:PRO:HD3	1.96	0.41
1:A:22:PHE:CD2	1:A:71:SER:HB3	2.56	0.41
1:A:249:VAL:HG22	1:A:257:TYR:CE1	2.56	0.41
1:A:271:THR:O	1:A:272:LEU:HD23	2.21	0.41
1:D:117:ALA:HB2	2:E:60:TRP:CD2	2.55	0.41
1:G:225:THR:HG23	1:G:226:GLN:N	2.36	0.41
1:J:175:GLY:O	1:J:176:LYS:C	2.60	0.41
2:H:74:GLU:N	2:H:74:GLU:OE1	2.53	0.40
1:J:111:ARG:HG2	1:J:113:TYR:CZ	2.56	0.40
2:K:13:HIS:HB3	2:K:14:PRO:HD2	2.03	0.40
1:G:64:THR:CG2	1:G:68:LYS:HD2	2.50	0.40
1:G:184:PRO:HA	1:G:185:PRO:HD3	1.93	0.40
1:D:49:ALA:HA	1:D:50:PRO:HD2	1.89	0.40
1:D:234:ARG:HD2	2:E:10:TYR:CE2	2.55	0.40
1:J:72:GLN:HE22	1:J:75:ARG:NH1	2.19	0.40
1:A:187:THR:HG22	1:A:204:TRP:O	2.22	0.40
2:B:45:ARG:HH11	2:B:45:ARG:HD3	1.77	0.40
1:A:67:VAL:HG13	1:A:68:LYS:N	2.37	0.40
1:A:96:GLN:NE2	2:B:56:PHE:CG	2.89	0.40
1:D:19:GLU:OE2	1:D:75:ARG:HD3	2.21	0.40
1:G:111:ARG:HG2	1:G:111:ARG:HH11	1.87	0.40
1:G:117:ALA:HB2	2:H:60:TRP:CD2	2.55	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	272/275 (99%)	257 (94%)	13 (5%)	2 (1%)	22	32
1	D	272/275 (99%)	252 (93%)	16 (6%)	4 (2%)	10	14
1	G	272/275 (99%)	252 (93%)	18 (7%)	2 (1%)	22	32
1	J	272/275 (99%)	257 (94%)	12 (4%)	3 (1%)	14	20
2	B	98/100 (98%)	91 (93%)	6 (6%)	1 (1%)	15	23
2	E	98/100 (98%)	92 (94%)	5 (5%)	1 (1%)	15	23
2	H	98/100 (98%)	93 (95%)	2 (2%)	3 (3%)	4	3
2	K	98/100 (98%)	91 (93%)	5 (5%)	2 (2%)	7	9
3	C	6/8 (75%)	6 (100%)	0	0	100	100
3	F	6/8 (75%)	6 (100%)	0	0	100	100
3	I	6/8 (75%)	6 (100%)	0	0	100	100
3	L	6/8 (75%)	6 (100%)	0	0	100	100
All	All	1504/1532 (98%)	1409 (94%)	77 (5%)	18 (1%)	13	19

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1	ILE
1	D	196	ASP
2	E	1	ILE
1	G	196	ASP
1	J	176	LYS
1	J	196	ASP
2	K	1	ILE
2	K	2	GLN
1	D	195	SER
2	H	1	ILE
2	H	45	ARG
2	H	74	GLU

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Mol	Chain	Res	Type
1	J	195	SER
1	A	196	ASP
1	D	223	ASP
1	D	50	PRO
1	G	267	PRO
1	A	267	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	230/231 (100%)	212 (92%)	18 (8%)	12	19
1	D	230/231 (100%)	212 (92%)	18 (8%)	12	19
1	G	230/231 (100%)	211 (92%)	19 (8%)	11	17
1	J	230/231 (100%)	214 (93%)	16 (7%)	15	24
2	B	95/95 (100%)	82 (86%)	13 (14%)	3	4
2	E	95/95 (100%)	84 (88%)	11 (12%)	5	7
2	H	95/95 (100%)	84 (88%)	11 (12%)	5	7
2	K	95/95 (100%)	82 (86%)	13 (14%)	3	4
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	6 (86%)	1 (14%)	3	4
3	I	7/7 (100%)	7 (100%)	0	100	100
3	L	7/7 (100%)	6 (86%)	1 (14%)	3	4
All	All	1328/1332 (100%)	1207 (91%)	121 (9%)	9	14

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ASP
1	A	79	ARG
1	A	89	GLU
1	A	98	MET

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Mol	Chain	Res	Type
1	A	101	CYS
1	A	108	ARG
1	A	111	ARG
1	A	121	LYS
1	A	131	ARG
1	A	155	GLN
1	A	165	VAL
1	A	177	GLU
1	A	181	ARG
1	A	187	THR
1	A	196	ASP
1	A	219	ARG
1	A	225	THR
1	A	228	THR
2	B	0	MET
2	B	1	ILE
2	B	4	THR
2	B	48	LYS
2	B	64	LEU
2	B	70	PHE
2	B	74	GLU
2	B	77	GLU
2	B	83	ASN
2	B	85	VAL
2	B	92	ILE
2	B	97	ARG
2	B	99	MET
1	D	25	VAL
1	D	79	ARG
1	D	98	MET
1	D	108	ARG
1	D	110	LEU
1	D	111	ARG
1	D	121	LYS
1	D	154	GLU
1	D	155	GLN
1	D	164	CYS
1	D	165	VAL
1	D	178	THR
1	D	180	GLN
1	D	181	ARG
1	D	219	ARG

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Mol	Chain	Res	Type
1	D	227	ASP
1	D	228	THR
1	D	268	LYS
2	E	1	ILE
2	E	6	LYS
2	E	19	LYS
2	E	64	LEU
2	E	70	PHE
2	E	74	GLU
2	E	83	ASN
2	E	92	ILE
2	E	97	ARG
2	E	98	ASP
2	E	99	MET
3	F	1	ARG
1	G	25	VAL
1	G	44	ARG
1	G	58	GLU
1	G	73	THR
1	G	74	ASP
1	G	98	MET
1	G	108	ARG
1	G	110	LEU
1	G	121	LYS
1	G	154	GLU
1	G	155	GLN
1	G	164	CYS
1	G	178	THR
1	G	181	ARG
1	G	182	THR
1	G	219	ARG
1	G	226	GLN
1	G	255	GLN
1	G	258	THR
2	H	0	MET
2	H	1	ILE
2	H	4	THR
2	H	27	VAL
2	H	48	LYS
2	H	64	LEU
2	H	70	PHE
2	H	74	GLU

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Mol	Chain	Res	Type
2	H	83	ASN
2	H	92	ILE
2	H	99	MET
1	J	38	SER
1	J	71	SER
1	J	73	THR
1	J	74	ASP
1	J	98	MET
1	J	101	CYS
1	J	105	SER
1	J	121	LYS
1	J	154	GLU
1	J	155	GLN
1	J	165	VAL
1	J	180	GLN
1	J	182	THR
1	J	227	ASP
1	J	228	THR
1	J	268	LYS
2	K	0	MET
2	K	1	ILE
2	K	9	VAL
2	K	19	LYS
2	K	48	LYS
2	K	64	LEU
2	K	70	PHE
2	K	83	ASN
2	K	88	SER
2	K	91	LYS
2	K	92	ILE
2	K	97	ARG
2	K	99	MET
3	L	1	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	54	GLN
1	A	93	HIS
1	A	141	GLN
1	A	156	GLN

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Mol	Chain	Res	Type
1	A	174	ASN
1	A	197	HIS
1	A	224	GLN
1	A	242	GLN
1	A	255	GLN
2	B	31	HIS
2	B	51	HIS
2	B	83	ASN
1	D	72	GLN
1	D	86	ASN
1	D	93	HIS
1	D	114	HIS
1	D	141	GLN
1	D	156	GLN
1	D	174	ASN
1	D	224	GLN
1	D	242	GLN
1	D	255	GLN
1	D	262	GLN
2	E	31	HIS
2	E	51	HIS
2	E	83	ASN
1	G	43	GLN
1	G	93	HIS
1	G	114	HIS
1	G	141	GLN
1	G	156	GLN
1	G	174	ASN
1	G	180	GLN
1	G	188	HIS
1	G	197	HIS
1	G	224	GLN
1	G	226	GLN
1	G	242	GLN
1	G	255	GLN
2	H	31	HIS
2	H	51	HIS
2	H	83	ASN
1	J	43	GLN
1	J	72	GLN
1	J	86	ASN
1	J	93	HIS

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Mol	Chain	Res	Type
1	J	115	GLN
1	J	141	GLN
1	J	155	GLN
1	J	174	ASN
1	J	242	GLN
1	J	255	GLN
1	J	262	GLN
2	K	31	HIS
2	K	51	HIS
2	K	83	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	274/275 (99%)	-0.31	3 (1%) 80 79	25, 40, 83, 130	0
1	D	274/275 (99%)	-0.38	1 (0%) 92 91	24, 42, 69, 136	0
1	G	274/275 (99%)	-0.37	2 (0%) 87 86	21, 39, 72, 142	0
1	J	274/275 (99%)	-0.36	1 (0%) 92 91	25, 42, 71, 154	0
2	B	100/100 (100%)	-0.23	3 (3%) 50 49	24, 45, 83, 129	0
2	E	100/100 (100%)	-0.16	1 (1%) 82 80	28, 54, 85, 115	0
2	H	100/100 (100%)	-0.15	1 (1%) 82 80	24, 47, 80, 107	0
2	K	100/100 (100%)	-0.23	2 (2%) 65 63	26, 49, 85, 144	0
3	C	8/8 (100%)	-0.41	0 100 100	25, 29, 34, 37	0
3	F	8/8 (100%)	-0.37	0 100 100	29, 34, 42, 43	0
3	I	8/8 (100%)	-0.40	0 100 100	30, 34, 36, 38	0
3	L	8/8 (100%)	-0.35	0 100 100	24, 35, 37, 43	0
All	All	1528/1532 (99%)	-0.31	14 (0%) 84 82	21, 42, 78, 154	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	226	GLN	5.0
1	A	226	GLN	4.9
1	A	194	ILE	4.3
2	H	77	GLU	3.9
1	G	221	GLY	3.5
2	B	75	LYS	3.3
2	B	74	GLU	3.3
2	K	75	LYS	3.0
2	K	77	GLU	2.9
1	G	196	ASP	2.8
2	B	98	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	195	SER	2.3
1	D	225	THR	2.0
2	E	99	MET	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.