



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:27 PM UTC

PDB ID : 2GID / pdb_00002gid
Title : Crystal structures of trypanosoma brucei MRP1/MRP2
Authors : Schumacher, M.A.; Karamooz, E.; Zikova, A.; Trantirek, L.; Lukes, J.
Deposited on : 2006-03-28
Resolution : 3.35 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

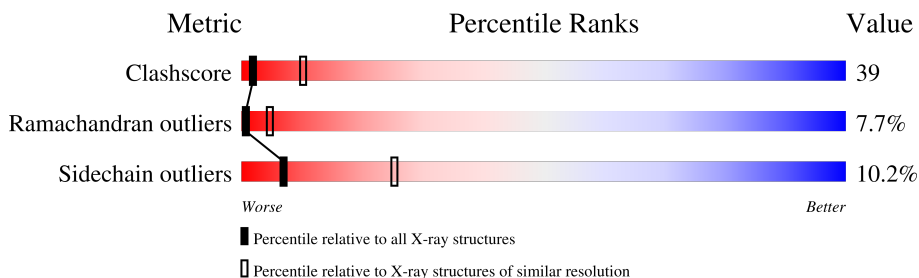
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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))
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	195	19% 45% 12% • 23%
1	G	195	30% 34% 12% • 23%
1	H	195	25% 37% 15% 23%
1	P	195	20% 48% 8% • 23%
2	B	187	24% 42% 10% • 22%
2	D	187	36% 35% 7% 22%
2	J	187	34% 36% 7% 22%
2	K	187	27% 38% 11% • 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9747 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 mitochondrial RNA-binding protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	Se	0	0	0
			1224	774	223	223	1	3			
1	G	151	Total	C	N	O	S	Se	0	0	0
			1228	778	224	222	1	3			
1	H	151	Total	C	N	O	S	Se	0	0	0
			1231	779	224	224	1	3			
1	P	151	Total	C	N	O	S	Se	0	0	0
			1228	778	224	222	1	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	MSE	MET	modified residue	UNP Q952G2
A	125	MSE	MET	modified residue	UNP Q952G2
A	204	MSE	MET	modified residue	UNP Q952G2
G	110	MSE	MET	modified residue	UNP Q952G2
G	125	MSE	MET	modified residue	UNP Q952G2
G	204	MSE	MET	modified residue	UNP Q952G2
H	110	MSE	MET	modified residue	UNP Q952G2
H	125	MSE	MET	modified residue	UNP Q952G2
H	204	MSE	MET	modified residue	UNP Q952G2
P	110	MSE	MET	modified residue	UNP Q952G2
P	125	MSE	MET	modified residue	UNP Q952G2
P	204	MSE	MET	modified residue	UNP Q952G2

- Molecule 2 is a protein called mitochondrial RNA-binding protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	Se	0	0	0
			1195	754	220	217	1	3			
2	D	146	Total	C	N	O	S	Se	0	0	0
			1195	754	220	217	1	3			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	K	146	Total	C	N	O	S	Se	0	0	0
			1195	754	220	217	1	3			
2	J	146	Total	C	N	O	S	Se	0	0	0
			1195	754	220	217	1	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	43	GLU	LEU	conflict	UNP P90629
B	46	MSE	MET	modified residue	UNP P90629
B	109	MSE	MET	modified residue	UNP P90629
B	139	MSE	MET	modified residue	UNP P90629
D	43	GLU	LEU	conflict	UNP P90629
D	46	MSE	MET	modified residue	UNP P90629
D	109	MSE	MET	modified residue	UNP P90629
D	139	MSE	MET	modified residue	UNP P90629
K	43	GLU	LEU	conflict	UNP P90629
K	46	MSE	MET	modified residue	UNP P90629
K	109	MSE	MET	modified residue	UNP P90629
K	139	MSE	MET	modified residue	UNP P90629
J	43	GLU	LEU	conflict	UNP P90629
J	46	MSE	MET	modified residue	UNP P90629
J	109	MSE	MET	modified residue	UNP P90629
J	139	MSE	MET	modified residue	UNP P90629

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	11	Total	O	0	0
			11	11		
3	D	6	Total	O	0	0
			6	6		
3	G	1	Total	O	0	0
			1	1		
3	H	4	Total	O	0	0
			4	4		
3	K	8	Total	O	0	0
			8	8		
3	J	7	Total	O	0	0
			7	7		

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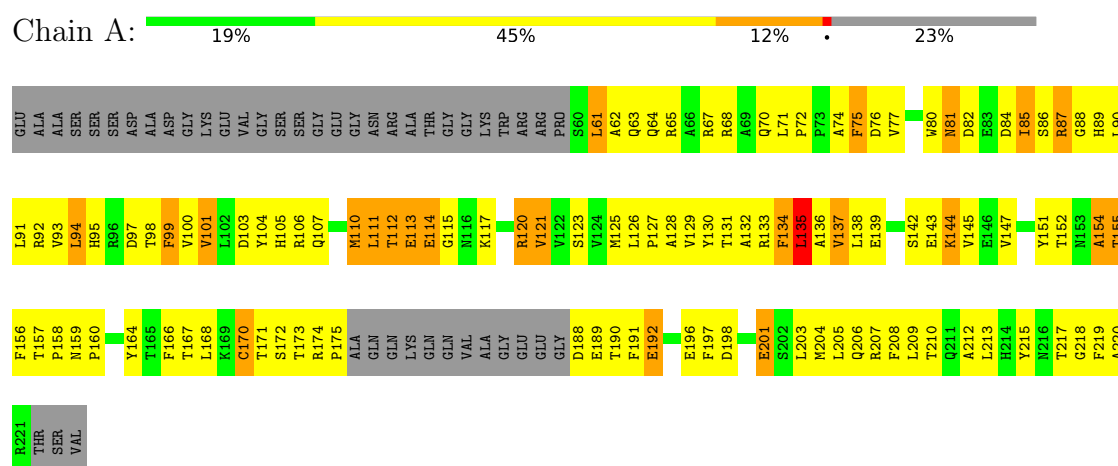
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	15	Total	O	0	0
			15	15		

3 Residue-property plots

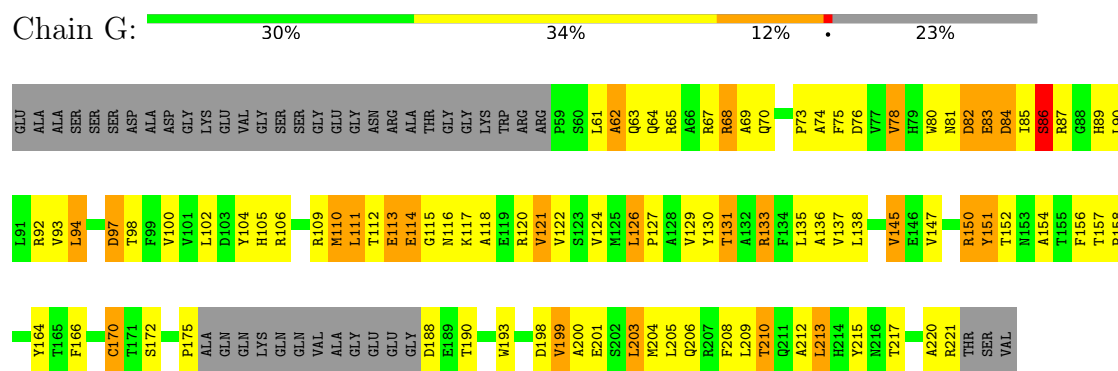
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

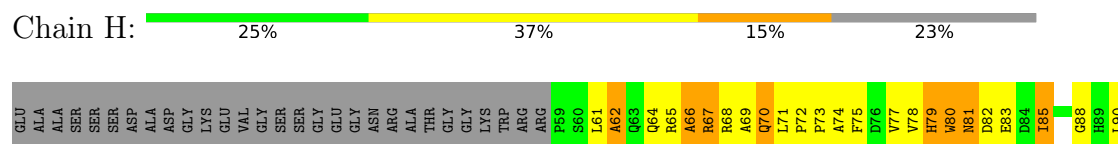
• Molecule 1: mitochondrial RNA-binding protein 2

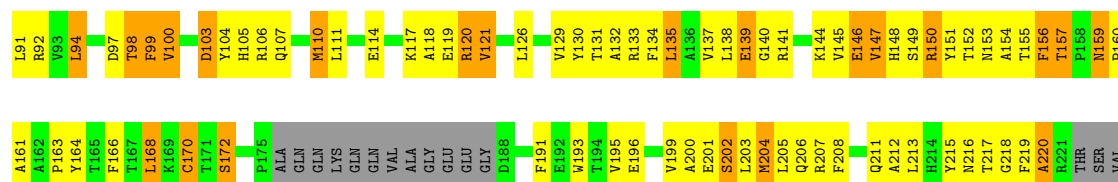


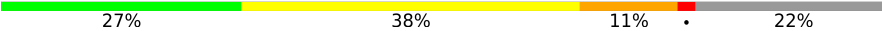
• Molecule 1: mitochondrial RNA-binding protein 2

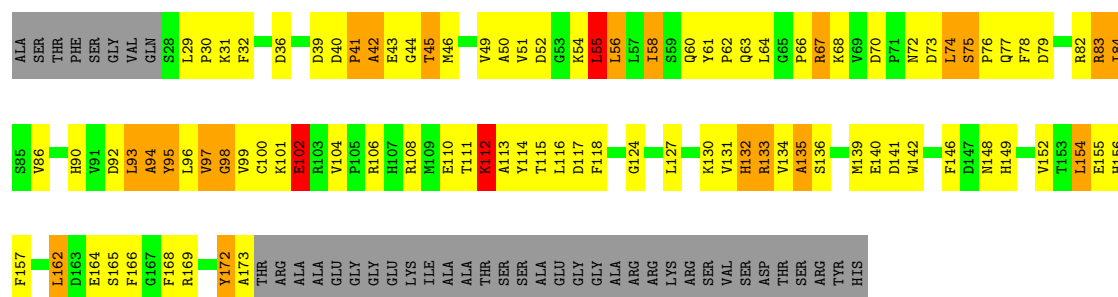


• Molecule 1: mitochondrial RNA-binding protein 2

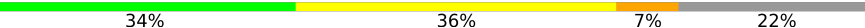


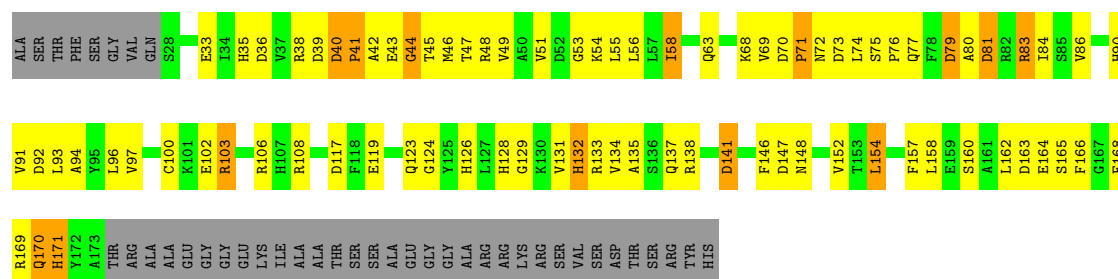


Chain K: 



• Molecule 2: mitochondrial RNA-binding protein 1

Chain J: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	235.99Å 235.99Å 85.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	78.84 – 3.35	Depositor
% Data completeness (in resolution range)	99.2 (78.84-3.35)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9747	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	0/1250	1.10	10/1693 (0.6%)
1	G	0.52	0/1255	1.05	9/1700 (0.5%)
1	H	0.54	0/1258	1.07	13/1704 (0.8%)
1	P	0.58	0/1255	1.03	8/1700 (0.5%)
2	B	0.57	0/1222	1.15	14/1645 (0.9%)
2	D	0.62	0/1222	1.06	6/1645 (0.4%)
2	J	0.60	0/1222	1.18	11/1645 (0.7%)
2	K	0.57	0/1222	1.15	13/1645 (0.8%)
All	All	0.57	0/9906	1.10	84/13377 (0.6%)

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	97	VAL	N-CA-C	-9.53	101.46	110.42
2	K	55	LEU	N-CA-C	8.29	122.01	108.99
1	P	95	HIS	N-CA-C	-7.87	99.50	110.35
1	H	150	ARG	N-CA-C	-7.83	104.67	112.97
2	K	83	ARG	N-CA-C	7.66	120.46	110.43
2	D	93	LEU	N-CA-C	-7.39	102.92	110.97
2	J	38	ARG	N-CA-C	7.30	119.16	108.86
1	A	137	VAL	N-CA-C	-7.21	103.43	110.72
1	G	87	ARG	N-CA-C	-7.17	103.55	111.36
1	A	94	LEU	N-CA-C	7.07	117.92	108.38
2	J	58	ILE	N-CA-C	-6.97	100.59	109.30
2	B	29	LEU	CA-C-N	6.96	126.93	119.76
2	B	29	LEU	C-N-CA	6.96	126.93	119.76
2	K	94	ALA	N-CA-C	-6.87	102.64	111.02
2	J	40	ASP	CA-C-N	6.81	128.36	119.84
2	J	40	ASP	C-N-CA	6.81	128.36	119.84
1	G	86	SER	N-CA-C	-6.74	96.45	110.80
1	P	217	THR	N-CA-C	-6.68	104.99	113.01
1	H	66	ALA	N-CA-C	-6.61	104.48	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	152	VAL	N-CA-C	-6.50	104.31	110.42
2	D	102	GLU	N-CA-C	6.38	120.40	112.24
1	P	70	GLN	N-CA-C	-6.35	106.75	114.75
2	B	87	ARG	N-CA-C	-6.35	100.17	110.20
2	K	154	LEU	N-CA-C	-6.33	104.47	111.82
2	J	70	ASP	CA-C-N	6.29	127.70	119.84
2	J	70	ASP	C-N-CA	6.29	127.70	119.84
2	D	166	PHE	N-CA-C	-6.24	106.63	114.56
2	J	44	GLY	N-CA-C	-6.22	104.58	112.54
1	H	208	PHE	N-CA-C	-6.21	104.14	111.03
1	P	202	SER	N-CA-C	-6.16	104.49	111.14
1	G	126	LEU	CA-C-N	6.14	126.05	119.85
1	G	126	LEU	C-N-CA	6.14	126.05	119.85
1	A	134	PHE	N-CA-C	-6.11	103.36	111.24
1	A	170	CYS	N-CA-C	6.09	118.33	109.07
1	A	154	ALA	N-CA-C	6.07	118.19	109.14
1	H	199	VAL	CB-CA-C	-6.05	103.95	111.70
2	K	84	ILE	N-CA-C	-5.98	99.87	108.48
2	D	103	ARG	N-CA-C	-5.96	105.87	113.02
2	J	103	ARG	N-CA-C	-5.96	98.11	110.80
1	A	123	SER	N-CA-C	5.94	117.15	107.23
1	H	135	LEU	N-CA-C	-5.93	104.89	111.36
2	K	95	TYR	N-CA-C	5.93	118.22	111.11
2	B	29	LEU	CA-CB-CG	5.87	136.84	116.30
2	B	77	GLN	N-CA-C	-5.87	105.31	112.88
1	H	220	ALA	N-CA-C	-5.83	106.20	113.38
2	B	153	THR	N-CA-C	5.81	118.36	111.33
2	B	29	LEU	N-CA-C	5.77	118.65	110.40
1	H	202	SER	N-CA-C	-5.73	104.03	111.02
1	G	170	CYS	N-CA-C	5.71	118.08	109.23
1	H	172	SER	N-CA-C	5.66	117.60	107.80
2	K	61	TYR	CA-C-N	5.66	126.91	119.84
2	K	61	TYR	C-N-CA	5.66	126.91	119.84
1	H	94	LEU	N-CA-C	5.64	118.44	109.81
1	H	110	MSE	N-CA-C	-5.64	102.91	110.24
2	D	56	LEU	N-CA-C	-5.58	100.20	109.46
2	B	79	ASP	N-CA-C	5.57	118.71	108.58
1	A	139	GLU	N-CA-C	5.56	118.53	111.69
1	G	154	ALA	N-CA-C	5.48	115.48	108.24
2	B	147	ASP	N-CA-C	5.48	118.51	109.85
1	G	65	ARG	N-CA-C	-5.44	107.00	113.97
2	K	116	LEU	N-CA-C	5.43	118.09	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	56	LEU	N-CA-C	5.42	118.45	109.46
1	H	170	CYS	N-CA-C	5.39	117.17	108.32
2	J	79	ASP	N-CA-C	5.38	118.09	107.98
2	D	118	PHE	N-CA-C	-5.36	100.17	108.90
1	P	158	PRO	N-CA-C	-5.32	103.44	111.41
1	P	166	PHE	N-CA-C	5.29	117.72	109.52
2	K	43	GLU	N-CA-C	5.29	119.60	113.20
2	J	92	ASP	N-CA-C	-5.21	105.66	112.23
1	P	122	VAL	N-CA-C	5.21	117.27	109.20
2	B	93	LEU	N-CA-C	-5.20	105.04	111.33
1	H	196	GLU	N-CA-C	5.16	117.35	107.75
1	H	62	ALA	N-CA-C	-5.16	106.25	112.54
1	P	194	THR	N-CA-C	5.16	116.82	108.26
2	B	47	THR	N-CA-C	5.15	118.43	107.67
1	G	210	THR	N-CA-C	-5.15	105.58	111.14
1	A	192	GLU	N-CA-C	5.11	117.44	109.52
2	B	55	LEU	N-CA-C	5.08	117.34	108.76
1	G	126	LEU	N-CA-C	5.07	116.07	109.64
1	A	101	VAL	N-CA-C	5.05	116.52	109.55
1	A	75	PHE	N-CA-C	-5.05	100.04	110.80
2	J	81	ASP	N-CA-C	-5.02	107.54	113.97
2	B	33	GLU	N-CA-C	5.02	117.04	109.41
2	K	45	THR	N-CA-C	5.02	121.48	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	1224	0	1195	130	0
1	G	1228	0	1201	91	0
1	H	1231	0	1203	114	0
1	P	1228	0	1201	123	0
2	B	1195	0	1164	105	0
2	D	1195	0	1164	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1195	0	1164	74	0
2	K	1195	0	1164	89	0
3	A	4	0	0	0	0
3	B	11	0	0	0	0
3	D	6	0	0	0	0
3	G	1	0	0	0	0
3	H	4	0	0	0	0
3	J	7	0	0	0	0
3	K	8	0	0	0	0
3	P	15	0	0	0	0
All	All	9747	0	9456	752	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 39.

All (752) 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:H:90:LEU:HD13	1:H:91:LEU:N	1.71	1.05
1:G:100:VAL:HB	1:G:126:LEU:HB2	1.44	0.99
1:G:113:GLU:HG3	1:G:114:GLU:H	1.27	0.99
1:A:82:ASP:HA	1:A:111:LEU:HD22	1.45	0.99
1:H:90:LEU:HD13	1:H:91:LEU:H	1.19	0.98
1:G:201:GLU:HA	1:G:204:MSE:HE3	1.44	0.98
1:P:201:GLU:HA	1:P:204:MSE:HE3	1.45	0.97
2:B:29:LEU:HB2	2:B:30:PRO:HD2	1.42	0.97
2:K:84:ILE:HG12	2:K:133:ARG:HG2	1.48	0.94
2:K:31:LYS:HB3	2:K:50:ALA:HB2	1.51	0.92
1:H:111:LEU:HD23	1:H:117:LYS:HG2	1.52	0.92
1:P:82:ASP:HB3	1:P:110:MSE:HE3	1.52	0.92
2:B:162:LEU:HD23	2:B:162:LEU:O	1.71	0.91
2:D:96:LEU:HD22	2:D:118:PHE:CD2	2.07	0.89
1:A:85:ILE:HD11	1:A:110:MSE:HG2	1.52	0.89
1:H:64:GLN:O	1:H:67:ARG:HB2	1.73	0.89
1:G:109:ARG:HD3	1:G:115:GLY:HA3	1.57	0.87
1:P:72:PRO:HG2	1:P:96:ARG:HH21	1.40	0.87
1:A:76:ASP:OD1	1:A:92:ARG:HG2	1.75	0.87
1:H:71:LEU:HG	1:H:72:PRO:HD2	1.58	0.86
2:D:67:ARG:H	2:D:67:ARG:HD3	1.41	0.85
1:A:138:LEU:HD11	1:A:205:LEU:HD23	1.59	0.85
1:A:171:THR:HG22	1:A:192:GLU:HG2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:HD23	1:A:111:LEU:H	1.42	0.84
1:H:159:ASN:C	1:H:159:ASN:HD22	1.84	0.84
1:A:94:LEU:HD11	1:A:101:VAL:HB	1.59	0.83
1:H:159:ASN:ND2	1:H:161:ALA:H	1.75	0.83
1:H:204:MSE:HE1	2:J:91:VAL:HG23	1.59	0.83
1:P:170:CYS:HB2	1:P:193:TRP:NE1	1.93	0.82
1:A:135:LEU:HD21	1:A:206:GLN:HE21	1.42	0.82
1:G:203:LEU:HD23	1:G:204:MSE:N	1.94	0.82
1:A:91:LEU:HD12	1:A:103:ASP:O	1.80	0.81
1:A:167:THR:HG22	1:A:196:GLU:OE2	1.80	0.81
1:P:85:ILE:HG23	1:P:107:GLN:HB3	1.64	0.80
1:G:64:GLN:O	1:G:68:ARG:HB2	1.80	0.80
2:K:74:LEU:HD22	2:K:74:LEU:H	1.43	0.80
1:P:174:ARG:HE	1:P:175:PRO:HD2	1.47	0.80
2:B:80:ALA:O	2:B:83:ARG:HG2	1.82	0.79
1:H:67:ARG:HH12	1:H:71:LEU:HD13	1.46	0.79
2:K:31:LYS:HB3	2:K:50:ALA:CB	2.12	0.79
2:B:96:LEU:HD13	2:B:118:PHE:CE1	2.17	0.79
1:A:82:ASP:HA	1:A:111:LEU:CD2	2.11	0.79
1:H:74:ALA:HB2	1:H:94:LEU:HB3	1.65	0.79
2:B:89:ARG:HB2	2:B:92:ASP:OD1	1.83	0.78
2:K:111:THR:C	2:K:112:LYS:HD3	2.08	0.78
2:J:83:ARG:HE	2:J:134:VAL:HG11	1.47	0.78
1:A:82:ASP:CG	1:A:111:LEU:HD13	2.09	0.78
1:H:218:GLY:O	1:H:220:ALA:N	2.18	0.77
1:A:94:LEU:CD1	1:A:101:VAL:HB	2.15	0.76
1:G:102:LEU:HD11	1:G:126:LEU:HD11	1.67	0.76
1:G:150:ARG:HA	1:G:150:ARG:NE	2.00	0.76
1:H:94:LEU:H	1:H:94:LEU:HD23	1.51	0.76
2:D:35:HIS:CD2	2:D:46:MSE:HG2	2.20	0.75
2:D:77:GLN:O	2:D:77:GLN:HG3	1.84	0.75
2:D:84:ILE:HD11	2:D:133:ARG:HG2	1.66	0.75
2:J:123:GLN:HB3	2:J:147:ASP:HB3	1.67	0.75
1:G:109:ARG:HB3	1:G:113:GLU:OE1	1.87	0.74
2:K:130:LYS:HG2	2:K:141:ASP:OD2	1.87	0.74
1:A:63:GLN:HE22	1:A:67:ARG:NH2	1.85	0.74
1:P:76:ASP:HB3	1:P:90:LEU:HD11	1.67	0.74
1:A:70:GLN:O	1:A:71:LEU:HD12	1.87	0.74
1:P:60:SER:O	1:P:64:GLN:HG2	1.88	0.74
2:K:49:VAL:HG22	2:K:58:ILE:HG23	1.70	0.73
1:H:62:ALA:HA	1:H:65:ARG:HH11	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:137:VAL:HG21	1:P:145:VAL:CG1	2.17	0.73
2:J:46:MSE:HE1	2:J:48:ARG:NH2	2.03	0.73
2:D:44:GLY:HA3	2:D:63:GLN:HB2	1.71	0.73
2:D:59:SER:HA	2:D:84:ILE:O	1.89	0.72
2:D:106:ARG:NH1	2:D:119:GLU:OE2	2.23	0.72
1:P:93:VAL:HG13	1:P:102:LEU:HD23	1.70	0.72
2:K:108:ARG:HG3	2:K:117:ASP:OD1	1.90	0.72
1:H:147:VAL:HG23	1:H:154:ALA:HB3	1.71	0.72
1:P:85:ILE:HD11	1:P:110:MSE:HG3	1.72	0.72
1:H:90:LEU:HB3	1:H:105:HIS:HB2	1.72	0.71
2:K:97:VAL:O	2:K:100:CYS:N	2.23	0.71
1:P:145:VAL:CG1	1:P:156:PHE:HB3	2.20	0.71
2:B:114:TYR:HB2	2:B:131:VAL:HG12	1.73	0.71
2:J:39:ASP:O	2:J:41:PRO:HD3	1.90	0.71
2:B:61:TYR:HB2	2:B:78:PHE:HB3	1.73	0.71
1:H:91:LEU:HD22	1:H:195:VAL:HG21	1.72	0.71
2:D:126:HIS:CE1	2:D:128:HIS:HD2	2.09	0.70
1:G:110:MSE:HG2	1:G:111:LEU:H	1.57	0.70
1:G:145:VAL:HG13	1:G:156:PHE:HB3	1.72	0.70
1:A:218:GLY:O	1:A:220:ALA:N	2.25	0.70
1:H:152:THR:HG22	1:H:172:SER:OG	1.91	0.70
2:D:114:TYR:CB	2:D:131:VAL:HG12	2.21	0.70
1:A:86:SER:O	1:A:88:GLY:N	2.25	0.69
1:G:158:PRO:HA	1:G:166:PHE:HD1	1.57	0.69
1:H:141:ARG:NH1	2:K:124:GLY:HA2	2.06	0.69
1:P:115:GLY:O	1:P:117:LYS:HD2	1.92	0.69
1:P:150:ARG:HE	1:P:150:ARG:HA	1.58	0.69
1:G:201:GLU:HA	1:G:204:MSE:CE	2.22	0.69
2:K:104:VAL:HG13	1:P:199:VAL:HG11	1.75	0.69
2:J:47:THR:HG22	2:J:48:ARG:N	2.08	0.69
1:H:168:LEU:O	1:H:168:LEU:HD13	1.94	0.68
2:B:39:ASP:O	2:B:41:PRO:HD3	1.92	0.68
2:D:84:ILE:CD1	2:D:133:ARG:HG2	2.23	0.68
1:P:94:LEU:CD1	1:P:101:VAL:HB	2.23	0.68
1:H:106:ARG:HG2	1:H:119:GLU:O	1.92	0.68
1:H:159:ASN:HD22	1:H:161:ALA:H	1.41	0.68
2:K:41:PRO:HG3	2:K:66:PRO:HA	1.76	0.68
2:J:54:LYS:HB3	2:J:90:HIS:ND1	2.08	0.68
1:H:100:VAL:HB	1:H:126:LEU:HB2	1.76	0.68
2:D:48:ARG:HG3	2:D:49:VAL:N	2.07	0.68
1:H:215:TYR:CE2	2:J:168:PHE:HB3	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:145:VAL:HG13	1:P:156:PHE:HB3	1.77	0.67
1:P:173:THR:HG22	1:P:189:GLU:O	1.94	0.67
2:B:106:ARG:HG2	2:B:107:HIS:N	2.10	0.67
2:B:106:ARG:HG3	2:B:119:GLU:HB3	1.77	0.67
2:K:41:PRO:HA	2:K:63:GLN:HG2	1.75	0.67
2:K:166:PHE:O	1:P:73:PRO:HB3	1.95	0.66
1:A:159:ASN:HD22	1:A:160:PRO:HD2	1.60	0.66
2:B:93:LEU:HD22	2:B:162:LEU:HB2	1.76	0.66
2:D:41:PRO:HA	2:D:63:GLN:NE2	2.10	0.66
1:P:77:VAL:HG23	1:P:91:LEU:O	1.96	0.66
1:A:173:THR:HA	1:A:189:GLU:O	1.95	0.66
2:B:116:LEU:HD13	2:B:127:LEU:HD21	1.77	0.66
1:H:168:LEU:HD11	1:H:195:VAL:HB	1.77	0.66
2:K:83:ARG:HG3	2:K:83:ARG:HH11	1.61	0.66
1:P:68:ARG:HA	1:P:71:LEU:HD23	1.77	0.66
2:B:41:PRO:HG3	2:B:63:GLN:HE21	1.60	0.66
1:G:127:PRO:HB2	1:G:129:VAL:HG12	1.77	0.66
1:H:159:ASN:C	1:H:159:ASN:ND2	2.54	0.66
1:P:60:SER:HB2	1:P:64:GLN:HE21	1.61	0.66
1:P:85:ILE:HG22	1:P:86:SER:H	1.60	0.66
1:P:122:VAL:HG22	1:P:123:SER:N	2.10	0.66
1:A:144:LYS:HG2	1:A:145:VAL:H	1.60	0.65
1:A:130:TYR:HA	1:A:133:ARG:HB2	1.78	0.65
2:B:31:LYS:HD2	2:B:48:ARG:HH11	1.60	0.65
1:H:66:ALA:O	1:H:69:ALA:HB3	1.96	0.65
1:P:126:LEU:HD11	1:P:147:VAL:HG21	1.77	0.65
1:H:90:LEU:CD1	1:H:91:LEU:N	2.56	0.65
1:A:68:ARG:O	1:A:71:LEU:HD13	1.96	0.65
1:G:145:VAL:CG1	1:G:156:PHE:HB3	2.27	0.65
2:D:103:ARG:HH11	2:D:103:ARG:HG2	1.61	0.64
2:D:96:LEU:HD22	2:D:118:PHE:HD2	1.62	0.64
2:D:116:LEU:HD13	2:D:127:LEU:HD11	1.77	0.64
1:H:146:GLU:HB3	1:H:155:THR:HG22	1.78	0.64
2:K:162:LEU:HD12	2:K:162:LEU:O	1.97	0.64
2:J:47:THR:HG22	2:J:48:ARG:H	1.61	0.64
1:H:204:MSE:HE2	2:J:94:ALA:CB	2.27	0.64
1:G:62:ALA:O	1:G:63:GLN:HG3	1.97	0.64
2:K:44:GLY:O	2:K:63:GLN:HB2	1.98	0.64
1:H:104:TYR:CD2	1:H:193:TRP:CE3	2.86	0.64
2:J:56:LEU:HG	2:J:93:LEU:HD13	1.78	0.64
1:A:154:ALA:HB2	1:A:170:CYS:SG	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:103:ASP:HB3	1:H:105:HIS:HE1	1.64	0.63
2:J:162:LEU:HD13	2:J:162:LEU:C	2.23	0.63
1:G:133:ARG:HH11	1:G:133:ARG:HB3	1.63	0.63
2:D:169:ARG:HH11	1:G:220:ALA:HA	1.62	0.63
2:K:168:PHE:HB3	1:P:215:TYR:CE2	2.34	0.63
2:J:40:ASP:O	2:J:42:ALA:N	2.32	0.63
1:P:78:VAL:HA	1:P:90:LEU:HD12	1.80	0.63
1:H:201:GLU:HA	1:H:204:MSE:HE3	1.81	0.63
2:K:31:LYS:CB	2:K:50:ALA:HB2	2.27	0.63
1:A:151:TYR:HB3	1:A:173:THR:O	1.99	0.62
1:A:167:THR:HG22	1:A:196:GLU:CD	2.24	0.62
2:D:147:ASP:O	2:D:150:PHE:HB2	1.99	0.62
2:B:111:THR:HG22	2:B:112:LYS:HE2	1.80	0.62
1:P:220:ALA:O	1:P:221:ARG:HB2	1.98	0.62
1:A:135:LEU:HD21	1:A:206:GLN:NE2	2.14	0.62
2:D:114:TYR:HB2	2:D:131:VAL:HG12	1.82	0.62
1:H:207:ARG:HH21	2:J:163:ASP:CG	2.08	0.62
2:J:154:LEU:CD2	2:J:158:LEU:HG	2.29	0.62
1:P:122:VAL:HG21	1:P:172:SER:OG	1.99	0.62
2:D:114:TYR:HB3	2:D:131:VAL:HG12	1.81	0.62
1:H:111:LEU:HA	1:H:117:LYS:HE2	1.82	0.62
2:B:106:ARG:HG2	2:B:107:HIS:H	1.65	0.62
2:K:32:PHE:CE1	2:K:49:VAL:HB	2.35	0.62
2:B:167:GLY:O	2:B:169:ARG:N	2.33	0.61
2:D:95:TYR:O	2:D:99:VAL:HG23	2.00	0.61
2:K:41:PRO:O	2:K:63:GLN:HB3	2.01	0.61
1:P:210:THR:HG22	1:P:211:GLN:N	2.14	0.61
1:A:130:TYR:O	1:A:133:ARG:N	2.33	0.61
1:A:77:VAL:O	1:A:90:LEU:HD22	2.00	0.61
1:A:135:LEU:HD22	2:B:156:HIS:HE2	1.64	0.61
1:G:76:ASP:HB3	1:G:90:LEU:HD11	1.82	0.61
2:J:44:GLY:HA3	2:J:63:GLN:HB2	1.82	0.61
1:P:198:ASP:OD1	1:P:201:GLU:HG3	2.01	0.61
2:B:68:LYS:HZ1	2:B:77:GLN:HB2	1.65	0.61
2:K:51:VAL:HB	2:K:56:LEU:CD2	2.31	0.61
1:P:100:VAL:HB	1:P:126:LEU:HD23	1.83	0.61
1:A:110:MSE:HE2	1:A:111:LEU:HD21	1.82	0.61
1:G:74:ALA:HB1	1:G:93:VAL:O	2.00	0.60
1:G:129:VAL:HG13	1:G:130:TYR:N	2.14	0.60
1:A:218:GLY:C	1:A:220:ALA:H	2.09	0.60
1:G:113:GLU:HG3	1:G:114:GLU:N	2.08	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:51:VAL:HB	2:K:56:LEU:HD23	1.83	0.60
2:J:162:LEU:O	2:J:162:LEU:HD22	2.01	0.60
1:A:164:TYR:CD2	2:D:103:ARG:HD3	2.37	0.60
2:B:91:VAL:O	2:B:94:ALA:HB3	2.01	0.60
2:D:55:LEU:HD11	2:D:87:ARG:NH1	2.16	0.60
2:J:84:ILE:HG13	2:J:133:ARG:NH1	2.17	0.60
1:A:127:PRO:O	1:A:129:VAL:N	2.35	0.60
2:K:152:VAL:O	2:K:155:GLU:HB2	2.02	0.60
2:J:108:ARG:HG3	2:J:117:ASP:OD2	2.01	0.60
1:H:137:VAL:HG21	1:H:145:VAL:HG12	1.84	0.59
1:A:64:GLN:O	1:A:65:ARG:HG3	2.01	0.59
2:K:95:TYR:O	2:K:99:VAL:HG23	2.02	0.59
1:A:111:LEU:H	1:A:111:LEU:CD2	2.06	0.59
1:G:198:ASP:O	1:G:199:VAL:C	2.45	0.59
2:J:100:CYS:C	2:J:102:GLU:H	2.10	0.59
1:H:74:ALA:HB2	1:H:94:LEU:CB	2.31	0.59
1:G:152:THR:HA	1:G:172:SER:HA	1.84	0.59
1:H:217:THR:O	2:K:30:PRO:HB3	2.02	0.59
2:K:46:MSE:HE3	2:K:46:MSE:O	2.03	0.59
1:A:152:THR:HA	1:A:172:SER:HA	1.84	0.59
1:A:159:ASN:HD22	1:A:160:PRO:CD	2.15	0.59
1:A:143:GLU:OE2	1:A:143:GLU:HA	2.01	0.59
2:D:28:SER:O	1:G:221:ARG:NH1	2.36	0.58
2:B:29:LEU:HB2	2:B:30:PRO:CD	2.27	0.58
2:K:164:GLU:OE1	2:K:164:GLU:HA	2.03	0.58
2:J:36:ASP:O	2:J:44:GLY:HA2	2.04	0.58
2:K:64:LEU:HD13	2:K:79:ASP:HB2	1.84	0.58
1:A:207:ARG:HG3	2:D:162:LEU:HD13	1.85	0.58
2:B:61:TYR:CB	2:B:78:PHE:HB3	2.33	0.58
2:K:94:ALA:CB	1:P:200:ALA:HB1	2.34	0.58
2:J:51:VAL:HA	2:J:55:LEU:O	2.03	0.58
2:B:79:ASP:CG	2:B:82:ARG:HD3	2.29	0.58
2:B:149:HIS:O	2:B:152:VAL:HB	2.03	0.58
1:A:126:LEU:HD22	1:A:147:VAL:HG11	1.84	0.58
1:A:198:ASP:CG	1:A:201:GLU:HG3	2.29	0.58
1:H:147:VAL:CG2	1:H:154:ALA:HB3	2.33	0.58
1:P:173:THR:HA	1:P:189:GLU:O	2.04	0.58
1:G:61:LEU:HB3	1:G:64:GLN:HE21	1.67	0.58
1:G:217:THR:HG22	1:G:217:THR:O	2.03	0.58
2:B:115:THR:O	2:B:129:GLY:HA3	2.04	0.57
2:D:93:LEU:HD21	2:D:162:LEU:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:VAL:HG23	1:G:204:MSE:HE2	1.86	0.57
1:A:82:ASP:CB	1:A:111:LEU:HD13	2.34	0.57
2:J:170:GLN:H	2:J:170:GLN:HE21	1.51	0.57
1:P:133:ARG:O	1:P:137:VAL:HG23	2.04	0.57
1:A:207:ARG:O	1:A:208:PHE:C	2.45	0.57
2:B:152:VAL:HG12	2:B:153:THR:N	2.19	0.57
2:K:68:LYS:HD3	2:K:73:ASP:OD2	2.04	0.57
1:A:74:ALA:HB2	1:A:94:LEU:HB3	1.85	0.57
1:P:173:THR:CA	1:P:189:GLU:HB3	2.35	0.57
1:P:82:ASP:HB3	1:P:110:MSE:CE	2.31	0.57
1:H:80:TRP:CH2	1:H:90:LEU:HB2	2.40	0.56
2:B:110:GLU:O	2:B:111:THR:HG23	2.05	0.56
2:D:48:ARG:HG3	2:D:49:VAL:H	1.70	0.56
2:D:142:TRP:O	2:D:143:SER:HB3	2.04	0.56
1:A:110:MSE:HB2	1:A:113:GLU:OE2	2.06	0.56
2:K:94:ALA:HB1	1:P:200:ALA:HB1	1.87	0.56
1:P:137:VAL:HG21	1:P:145:VAL:HG11	1.87	0.56
1:A:75:PHE:CE2	1:A:93:VAL:HB	2.40	0.56
2:D:115:THR:O	2:D:129:GLY:HA3	2.05	0.56
1:H:75:PHE:HE1	1:H:77:VAL:HG22	1.71	0.56
1:P:160:PRO:O	1:P:162:ALA:N	2.39	0.56
1:G:92:ARG:HH11	1:G:92:ARG:HB3	1.71	0.56
1:G:130:TYR:HD1	1:G:133:ARG:HD2	1.71	0.56
2:K:132:HIS:ND1	2:K:132:HIS:O	2.39	0.56
2:D:46:MSE:SE	2:D:46:MSE:C	2.99	0.55
1:A:62:ALA:HA	1:A:65:ARG:NH1	2.21	0.55
2:B:66:PRO:C	2:B:68:LYS:H	2.13	0.55
2:B:170:GLN:HE21	2:B:170:GLN:HA	1.69	0.55
2:J:164:GLU:O	2:J:166:PHE:N	2.40	0.55
1:P:167:THR:HG23	1:P:196:GLU:CD	2.32	0.55
1:G:203:LEU:HD23	1:G:203:LEU:C	2.30	0.55
1:P:59:PRO:O	1:P:63:GLN:HG3	2.07	0.55
1:P:85:ILE:CG2	1:P:107:GLN:HB3	2.35	0.55
1:P:173:THR:C	1:P:189:GLU:HB3	2.31	0.55
1:A:62:ALA:HA	1:A:65:ARG:CZ	2.36	0.55
1:G:105:HIS:ND1	1:G:120:ARG:HA	2.21	0.55
2:K:134:VAL:O	2:K:135:ALA:HB3	2.05	0.55
1:A:90:LEU:HD13	1:A:91:LEU:N	2.22	0.55
2:D:46:MSE:HB2	2:D:78:PHE:CD1	2.41	0.55
2:B:64:LEU:HB2	2:B:79:ASP:HB2	1.88	0.54
1:G:206:GLN:NE2	1:G:210:THR:OG1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:80:TRP:HH2	1:P:118:ALA:HB2	1.72	0.54
1:P:94:LEU:HD12	1:P:101:VAL:HB	1.89	0.54
1:G:82:ASP:C	1:G:84:ASP:H	2.15	0.54
2:K:74:LEU:HD22	2:K:74:LEU:N	2.20	0.54
2:K:83:ARG:HG3	2:K:83:ARG:NH1	2.22	0.54
2:B:31:LYS:HZ3	2:B:33:GLU:CD	2.15	0.54
1:G:133:ARG:HH11	1:G:133:ARG:CB	2.20	0.54
1:H:204:MSE:HE2	2:J:94:ALA:HB2	1.89	0.54
1:A:175:PRO:HA	1:A:188:ASP:N	2.23	0.54
1:H:131:THR:C	1:H:133:ARG:H	2.16	0.54
1:H:141:ARG:HH12	2:K:124:GLY:HA2	1.73	0.54
2:K:62:PRO:HG2	2:K:82:ARG:HB3	1.89	0.54
1:A:144:LYS:HG2	1:A:145:VAL:N	2.22	0.54
2:B:33:GLU:HG2	2:B:48:ARG:HA	1.88	0.54
2:B:127:LEU:HB3	2:B:144:VAL:CG1	2.38	0.54
1:H:145:VAL:CG1	1:H:156:PHE:HB3	2.38	0.54
1:A:107:GLN:HE22	1:A:111:LEU:HD23	1.72	0.54
2:D:51:VAL:HG12	2:D:157:PHE:CZ	2.43	0.54
2:D:156:HIS:CE1	1:G:210:THR:HG23	2.43	0.54
2:J:162:LEU:HD13	2:J:162:LEU:O	2.08	0.54
2:B:109:MSE:HE3	2:B:116:LEU:HB2	1.90	0.53
1:P:85:ILE:O	1:P:86:SER:CB	2.55	0.53
1:P:122:VAL:HG22	1:P:123:SER:H	1.72	0.53
2:J:41:PRO:O	2:J:63:GLN:HB3	2.08	0.53
1:A:145:VAL:CG1	1:A:156:PHE:HB3	2.39	0.53
1:A:215:TYR:HD1	1:A:220:ALA:HB2	1.72	0.53
2:K:110:GLU:HA	2:K:115:THR:HG22	1.90	0.53
2:B:41:PRO:HG3	2:B:66:PRO:HA	1.91	0.53
1:G:92:ARG:HB3	1:G:92:ARG:NH1	2.22	0.53
2:K:169:ARG:HG3	1:P:215:TYR:OH	2.09	0.53
1:P:220:ALA:O	1:P:221:ARG:CB	2.57	0.53
2:D:41:PRO:C	2:D:43:GLU:H	2.16	0.53
2:J:126:HIS:NE2	2:J:128:HIS:HB3	2.24	0.53
1:H:62:ALA:HA	1:H:65:ARG:NH1	2.21	0.53
1:P:163:PRO:O	1:P:164:TYR:HB2	2.07	0.53
1:A:90:LEU:HD13	1:A:90:LEU:C	2.33	0.53
1:A:171:THR:HG22	1:A:192:GLU:CG	2.37	0.53
1:H:206:GLN:HE21	1:H:207:ARG:HD2	1.73	0.53
2:J:83:ARG:NE	2:J:134:VAL:HG11	2.22	0.53
2:B:41:PRO:CG	2:B:66:PRO:HA	2.39	0.53
1:G:61:LEU:HD12	1:G:64:GLN:NE2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:103:ASP:HB3	1:H:105:HIS:CE1	2.44	0.53
2:K:132:HIS:HB3	2:K:139:MSE:SE	2.59	0.53
1:A:137:VAL:CG1	1:A:158:PRO:HD3	2.39	0.52
1:G:157:THR:O	1:G:166:PHE:HB3	2.09	0.52
1:G:133:ARG:O	1:G:136:ALA:HB3	2.09	0.52
2:D:127:LEU:HB3	2:D:144:VAL:HG23	1.91	0.52
1:P:174:ARG:HB2	1:P:189:GLU:OE2	2.08	0.52
1:A:201:GLU:HA	1:A:204:MSE:HE3	1.91	0.52
2:B:51:VAL:HG12	2:B:157:PHE:CZ	2.44	0.52
2:K:40:ASP:C	2:K:42:ALA:H	2.17	0.52
2:K:97:VAL:O	2:K:98:GLY:C	2.52	0.52
2:J:129:GLY:O	2:J:141:ASP:HA	2.10	0.52
1:P:159:ASN:OD1	1:P:161:ALA:HB3	2.10	0.52
2:B:99:VAL:HG22	2:B:104:VAL:HG23	1.92	0.52
1:P:106:ARG:HD2	1:P:121:VAL:HG13	1.91	0.52
2:J:46:MSE:HE1	2:J:48:ARG:HH21	1.75	0.52
1:P:204:MSE:O	1:P:205:LEU:C	2.53	0.52
1:H:94:LEU:HD23	1:H:94:LEU:N	2.24	0.52
1:A:120:ARG:HG2	1:A:121:VAL:H	1.75	0.52
1:G:105:HIS:HB3	1:G:118:ALA:HB1	1.92	0.52
1:A:89:HIS:HA	1:A:105:HIS:O	2.10	0.51
1:A:132:ALA:HB1	2:B:152:VAL:HG11	1.91	0.51
2:J:106:ARG:HB2	2:J:119:GLU:HB3	1.91	0.51
1:P:124:VAL:HG22	1:P:152:THR:HG21	1.91	0.51
2:K:29:LEU:O	2:K:31:LYS:HE3	2.10	0.51
1:A:86:SER:C	1:A:88:GLY:H	2.18	0.51
1:H:68:ARG:NH2	2:J:166:PHE:O	2.44	0.51
2:J:134:VAL:O	2:J:135:ALA:HB3	2.10	0.51
1:P:85:ILE:HG22	1:P:86:SER:N	2.25	0.51
2:B:147:ASP:O	2:B:150:PHE:HB2	2.10	0.51
1:H:159:ASN:HD21	1:H:161:ALA:CB	2.23	0.51
1:P:150:ARG:HA	1:P:150:ARG:NE	2.24	0.51
2:B:127:LEU:O	2:B:144:VAL:HG12	2.11	0.51
1:H:85:ILE:HD11	1:H:110:MSE:HG2	1.93	0.51
1:P:85:ILE:O	1:P:86:SER:OG	2.22	0.51
2:D:142:TRP:CG	2:D:143:SER:H	2.28	0.51
2:B:41:PRO:HG3	2:B:63:GLN:NE2	2.26	0.51
2:B:168:PHE:H	1:G:73:PRO:HB3	1.76	0.51
2:D:38:ARG:C	2:D:40:ASP:H	2.19	0.51
2:B:94:ALA:O	2:B:97:VAL:N	2.44	0.51
2:B:103:ARG:HG2	2:B:103:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:146:PHE:CD2	2:K:154:LEU:HD22	2.46	0.50
1:A:158:PRO:HB3	1:A:166:PHE:CE1	2.46	0.50
2:D:32:PHE:CE1	2:D:49:VAL:HB	2.46	0.50
2:D:88:LEU:HB3	2:D:92:ASP:HB3	1.93	0.50
1:H:159:ASN:HD21	1:H:161:ALA:HB3	1.76	0.50
1:P:77:VAL:CG2	1:P:91:LEU:HB3	2.41	0.50
1:P:126:LEU:HD21	1:P:134:PHE:HE2	1.76	0.50
1:P:173:THR:HA	1:P:189:GLU:HB3	1.93	0.50
2:B:121:SER:N	2:B:124:GLY:O	2.44	0.50
1:G:109:ARG:CD	1:G:115:GLY:HA3	2.37	0.50
1:A:198:ASP:OD1	1:A:198:ASP:C	2.54	0.50
2:B:54:LYS:HB3	2:B:90:HIS:ND1	2.26	0.50
1:G:61:LEU:O	1:G:64:GLN:HG2	2.12	0.50
2:J:75:SER:HB2	2:J:76:PRO:HD2	1.92	0.50
1:A:174:ARG:H	1:A:189:GLU:H	1.60	0.50
2:B:70:ASP:HB3	2:B:73:ASP:OD2	2.12	0.50
1:G:131:THR:C	1:G:133:ARG:H	2.19	0.50
1:H:61:LEU:O	1:H:65:ARG:HD2	2.12	0.50
1:P:85:ILE:HG12	1:P:107:GLN:NE2	2.26	0.50
1:A:72:PRO:HB3	1:A:95:HIS:O	2.12	0.50
1:H:68:ARG:HD3	1:H:71:LEU:HB3	1.93	0.50
2:B:96:LEU:HD13	2:B:118:PHE:CD1	2.47	0.50
1:H:94:LEU:H	1:H:94:LEU:CD2	2.22	0.50
1:H:131:THR:O	1:H:133:ARG:N	2.41	0.50
2:J:69:VAL:O	2:J:71:PRO:HD3	2.12	0.50
1:A:213:LEU:O	1:A:217:THR:HG23	2.11	0.49
2:D:41:PRO:HA	2:D:63:GLN:CD	2.36	0.49
1:H:74:ALA:CB	1:H:94:LEU:HB3	2.41	0.49
1:G:127:PRO:HD2	1:G:130:TYR:CD2	2.47	0.49
2:J:146:PHE:CG	2:J:154:LEU:HD12	2.46	0.49
1:A:147:VAL:CG2	1:A:154:ALA:HB3	2.42	0.49
1:H:67:ARG:HB3	1:H:67:ARG:NH1	2.27	0.49
1:P:198:ASP:CG	1:P:201:GLU:HG3	2.37	0.49
1:A:76:ASP:CG	1:A:92:ARG:HG2	2.35	0.49
1:H:135:LEU:O	1:H:139:GLU:HG3	2.12	0.49
2:K:132:HIS:ND1	2:K:132:HIS:C	2.70	0.49
1:P:80:TRP:CH2	1:P:118:ALA:HB2	2.47	0.49
1:A:86:SER:OG	1:A:87:ARG:N	2.45	0.49
2:B:107:HIS:O	2:B:117:ASP:HA	2.13	0.49
2:D:142:TRP:CG	2:D:143:SER:N	2.80	0.49
2:B:63:GLN:HA	2:B:78:PHE:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:VAL:HG23	1:G:147:VAL:O	2.11	0.49
1:G:157:THR:HB	1:G:158:PRO:CD	2.43	0.49
2:B:97:VAL:O	2:B:100:CYS:HB2	2.12	0.49
2:J:42:ALA:C	2:J:43:GLU:HG3	2.38	0.49
1:P:74:ALA:HB2	1:P:94:LEU:HA	1.94	0.49
1:A:85:ILE:HD11	1:A:110:MSE:HA	1.95	0.49
1:A:120:ARG:HG2	1:A:121:VAL:N	2.28	0.49
2:B:68:LYS:HD2	2:B:68:LYS:O	2.12	0.49
1:H:61:LEU:O	1:H:64:GLN:HB3	2.13	0.49
1:H:134:PHE:O	1:H:138:LEU:HG	2.13	0.49
1:P:106:ARG:HD2	1:P:121:VAL:CG1	2.42	0.49
2:B:51:VAL:HG12	2:B:157:PHE:HZ	1.77	0.49
1:P:165:THR:C	1:P:166:PHE:CD2	2.91	0.49
1:G:151:TYR:N	1:G:151:TYR:HD2	2.11	0.49
1:G:100:VAL:HG12	1:G:102:LEU:HD21	1.95	0.48
1:A:159:ASN:HD22	1:A:160:PRO:N	2.11	0.48
2:B:48:ARG:HG2	2:B:49:VAL:N	2.29	0.48
1:G:205:LEU:HG	1:G:209:LEU:HD12	1.96	0.48
2:K:162:LEU:HD12	2:K:162:LEU:C	2.38	0.48
1:P:137:VAL:HG21	1:P:145:VAL:HG12	1.93	0.48
1:H:212:ALA:O	1:H:213:LEU:C	2.56	0.48
1:G:131:THR:C	1:G:133:ARG:N	2.68	0.48
1:A:115:GLY:O	1:A:117:LYS:HD2	2.13	0.48
2:B:79:ASP:OD1	2:B:81:ASP:HB2	2.13	0.48
2:B:108:ARG:HD3	2:B:110:GLU:OE2	2.12	0.48
2:D:54:LYS:HB3	2:D:90:HIS:ND1	2.29	0.48
2:D:61:TYR:CD2	2:D:83:ARG:HB3	2.49	0.48
2:K:58:ILE:O	2:K:86:VAL:HG22	2.14	0.48
2:J:164:GLU:CD	2:J:169:ARG:HE	2.21	0.48
1:P:67:ARG:O	1:P:71:LEU:HD23	2.13	0.48
1:P:94:LEU:HD12	1:P:94:LEU:H	1.78	0.48
1:P:94:LEU:HD13	1:P:101:VAL:HB	1.95	0.48
1:P:212:ALA:O	1:P:216:ASN:HB2	2.12	0.48
2:K:68:LYS:H	2:K:77:GLN:NE2	2.12	0.48
1:A:197:PHE:HE1	1:A:205:LEU:HD13	1.78	0.48
1:H:80:TRP:CZ2	1:H:90:LEU:HD23	2.49	0.48
1:P:151:TYR:CD1	1:P:175:PRO:HG3	2.49	0.48
1:A:98:THR:OG1	1:A:99:PHE:N	2.47	0.48
1:A:159:ASN:ND2	1:A:160:PRO:HD2	2.27	0.48
1:G:80:TRP:CH2	1:G:118:ALA:HB2	2.49	0.48
1:G:82:ASP:O	1:G:84:ASP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:111:LEU:HA	1:H:117:LYS:CE	2.43	0.48
1:H:156:PHE:HD2	1:H:157:THR:N	2.12	0.48
1:P:174:ARG:NE	1:P:175:PRO:HD2	2.20	0.48
1:P:198:ASP:O	1:P:199:VAL:C	2.56	0.48
2:K:74:LEU:H	2:K:74:LEU:CD2	2.20	0.48
2:K:118:PHE:HE2	2:K:154:LEU:HD21	1.78	0.48
1:P:205:LEU:O	1:P:208:PHE:HB3	2.14	0.48
1:A:209:LEU:O	1:A:212:ALA:HB3	2.14	0.47
1:G:158:PRO:HA	1:G:166:PHE:CD1	2.44	0.47
2:K:36:ASP:HB3	2:K:45:THR:H	1.77	0.47
1:A:142:SER:OG	1:A:144:LYS:O	2.32	0.47
2:J:96:LEU:HB3	2:J:158:LEU:HD13	1.97	0.47
1:A:215:TYR:CD1	1:A:220:ALA:HB2	2.48	0.47
2:B:154:LEU:CD1	2:B:158:LEU:HG	2.44	0.47
1:G:151:TYR:N	1:G:151:TYR:CD2	2.82	0.47
2:J:58:ILE:HB	2:J:86:VAL:CG2	2.45	0.47
2:J:58:ILE:HB	2:J:86:VAL:HG22	1.97	0.47
2:K:67:ARG:O	2:K:68:LYS:C	2.56	0.47
1:G:131:THR:O	1:G:133:ARG:N	2.47	0.47
1:H:148:HIS:ND1	1:H:153:ASN:OD1	2.47	0.47
2:D:104:VAL:HG22	2:D:106:ARG:H	1.79	0.47
2:K:92:ASP:O	2:K:96:LEU:HG	2.15	0.47
1:P:170:CYS:HB2	1:P:193:TRP:CE2	2.49	0.47
1:A:68:ARG:HG3	1:A:68:ARG:HH11	1.80	0.47
1:A:86:SER:C	1:A:88:GLY:N	2.70	0.47
1:A:127:PRO:C	1:A:129:VAL:H	2.23	0.47
1:A:204:MSE:O	1:A:205:LEU:C	2.54	0.47
2:B:166:PHE:CE1	1:G:208:PHE:HB2	2.50	0.47
1:H:130:TYR:HA	1:H:133:ARG:HD2	1.97	0.47
2:K:50:ALA:HA	2:K:157:PHE:HZ	1.80	0.47
1:G:94:LEU:N	1:G:94:LEU:HD12	2.30	0.47
1:H:202:SER:OG	1:H:203:LEU:N	2.48	0.47
2:K:168:PHE:HB3	1:P:215:TYR:CD2	2.50	0.47
2:B:146:PHE:HD2	2:B:154:LEU:HB2	1.80	0.47
2:J:47:THR:CG2	2:J:48:ARG:N	2.78	0.47
1:P:74:ALA:HB2	1:P:94:LEU:HB3	1.95	0.47
1:P:106:ARG:HG2	1:P:119:GLU:O	2.14	0.47
1:A:70:GLN:C	1:A:71:LEU:HD12	2.39	0.47
2:J:40:ASP:C	2:J:42:ALA:H	2.23	0.47
2:D:169:ARG:NH1	1:G:220:ALA:HA	2.29	0.46
1:A:159:ASN:HD22	1:A:159:ASN:C	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:88:GLY:HA3	1:H:107:GLN:OE1	2.15	0.46
1:H:135:LEU:HA	1:H:138:LEU:HD12	1.97	0.46
1:P:65:ARG:C	1:P:67:ARG:H	2.23	0.46
1:A:84:ASP:OD1	1:A:86:SER:OG	2.25	0.46
2:B:112:LYS:CD	2:B:112:LYS:H	2.26	0.46
2:D:106:ARG:NH2	2:D:117:ASP:OD1	2.47	0.46
2:K:132:HIS:C	2:K:132:HIS:HD1	2.23	0.46
2:J:72:ASN:O	2:J:74:LEU:N	2.49	0.46
2:J:170:GLN:H	2:J:170:GLN:NE2	2.12	0.46
2:B:36:ASP:HB3	2:B:45:THR:HG23	1.98	0.46
2:D:55:LEU:HD11	2:D:87:ARG:HH11	1.80	0.46
2:D:87:ARG:O	2:D:114:TYR:OH	2.31	0.46
1:A:213:LEU:HD21	2:B:153:THR:HG22	1.96	0.46
2:B:96:LEU:HD22	2:B:118:PHE:CD1	2.51	0.46
2:B:157:PHE:O	2:B:160:SER:HB2	2.15	0.46
2:D:41:PRO:O	2:D:63:GLN:HB3	2.16	0.46
2:D:74:LEU:O	2:D:75:SER:C	2.58	0.46
1:G:138:LEU:HD21	1:G:205:LEU:HD23	1.97	0.46
2:J:56:LEU:HD23	2:J:56:LEU:HA	1.82	0.46
2:B:100:CYS:C	2:B:102:GLU:H	2.24	0.46
2:K:104:VAL:HG11	1:P:199:VAL:HG21	1.97	0.46
2:K:117:ASP:O	2:K:127:LEU:HD12	2.15	0.46
2:J:100:CYS:C	2:J:102:GLU:N	2.74	0.46
1:P:188:ASP:O	1:P:189:GLU:HB2	2.15	0.46
1:G:113:GLU:HB2	1:G:114:GLU:OE2	2.16	0.46
1:G:170:CYS:HB2	1:G:193:TRP:CE2	2.51	0.46
1:H:211:GLN:O	1:H:212:ALA:C	2.59	0.46
2:J:83:ARG:HD2	2:J:134:VAL:HG22	1.98	0.46
2:J:132:HIS:ND1	2:J:132:HIS:C	2.73	0.46
1:P:74:ALA:HB2	1:P:94:LEU:CB	2.45	0.46
2:B:91:VAL:HG13	2:B:92:ASP:N	2.30	0.46
2:J:133:ARG:NH1	2:J:133:ARG:HG2	2.30	0.46
1:G:89:HIS:HB2	1:G:104:TYR:HE2	1.81	0.46
2:K:41:PRO:CG	2:K:66:PRO:HA	2.45	0.46
2:K:73:ASP:C	2:K:75:SER:H	2.23	0.46
2:J:39:ASP:C	2:J:41:PRO:HD3	2.40	0.46
2:J:83:ARG:HD2	2:J:83:ARG:O	2.16	0.46
2:J:96:LEU:O	2:J:97:VAL:C	2.57	0.46
1:P:73:PRO:O	1:P:94:LEU:HA	2.16	0.46
1:P:145:VAL:HG13	1:P:145:VAL:O	2.16	0.46
1:A:127:PRO:HD2	1:A:130:TYR:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:ILE:O	2:B:46:MSE:HA	2.16	0.45
1:G:135:LEU:HD21	1:G:206:GLN:HE21	1.80	0.45
2:B:127:LEU:HB3	2:B:144:VAL:HG12	1.96	0.45
2:D:48:ARG:CG	2:D:49:VAL:N	2.78	0.45
1:P:77:VAL:HG23	1:P:91:LEU:HB3	1.98	0.45
1:P:124:VAL:HG12	1:P:125:MSE:O	2.16	0.45
1:P:209:LEU:O	1:P:212:ALA:HB3	2.16	0.45
1:A:134:PHE:O	1:A:136:ALA:N	2.49	0.45
2:J:68:LYS:HE2	2:J:77:GLN:HB2	1.97	0.45
1:A:90:LEU:HB3	1:A:105:HIS:HB2	1.98	0.45
2:B:69:VAL:O	2:B:70:ASP:CB	2.64	0.45
2:D:168:PHE:O	2:D:169:ARG:C	2.59	0.45
1:H:61:LEU:HA	1:H:64:GLN:HB3	1.99	0.45
2:B:160:SER:O	2:B:161:ALA:C	2.58	0.45
2:D:38:ARG:C	2:D:40:ASP:N	2.75	0.45
1:H:156:PHE:CD2	1:H:157:THR:N	2.85	0.45
1:H:159:ASN:HD22	1:H:160:PRO:N	2.13	0.45
2:K:97:VAL:O	2:K:99:VAL:N	2.49	0.45
2:B:94:ALA:O	2:B:95:TYR:C	2.58	0.45
1:G:109:ARG:CD	1:G:116:ASN:H	2.30	0.45
1:H:92:ARG:HG2	1:H:92:ARG:HH11	1.82	0.45
2:B:40:ASP:CG	2:B:42:ALA:HB3	2.41	0.45
1:G:198:ASP:OD1	1:G:200:ALA:HB3	2.17	0.45
2:J:152:VAL:HG21	1:P:136:ALA:HB2	1.98	0.45
2:K:46:MSE:HB2	2:K:78:PHE:CD1	2.51	0.45
1:P:122:VAL:CG2	1:P:123:SER:N	2.78	0.45
1:P:206:GLN:OE1	1:P:207:ARG:HD2	2.17	0.45
1:A:132:ALA:HB1	2:B:152:VAL:CG1	2.46	0.45
1:H:97:ASP:C	1:H:98:THR:HG23	2.42	0.45
1:H:130:TYR:O	1:H:133:ARG:HB2	2.17	0.45
1:H:168:LEU:O	1:H:168:LEU:HD22	2.17	0.45
2:K:93:LEU:O	2:K:97:VAL:HG23	2.17	0.45
2:K:104:VAL:CG1	1:P:199:VAL:HG11	2.46	0.45
2:J:148:ASN:O	2:J:152:VAL:HG23	2.16	0.45
1:A:106:ARG:NH1	1:A:106:ARG:HG3	2.31	0.45
1:A:126:LEU:CD2	1:A:147:VAL:HG11	2.47	0.45
2:B:108:ARG:HA	2:B:117:ASP:OD1	2.16	0.45
2:J:33:GLU:HG2	2:J:48:ARG:HB2	1.98	0.45
1:A:117:LYS:HD2	1:A:117:LYS:N	2.33	0.44
2:D:41:PRO:CA	2:D:63:GLN:NE2	2.80	0.44
1:G:175:PRO:HA	1:G:188:ASP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:164:TYR:O	1:H:166:PHE:CE2	2.70	0.44
2:K:112:LYS:HD3	2:K:112:LYS:N	2.31	0.44
2:J:46:MSE:SE	2:J:46:MSE:C	3.10	0.44
1:A:131:THR:O	1:A:135:LEU:HB2	2.18	0.44
1:G:102:LEU:HD12	1:G:124:VAL:HB	1.99	0.44
1:G:126:LEU:HA	1:G:127:PRO:HD3	1.73	0.44
1:G:129:VAL:HG13	1:G:130:TYR:H	1.82	0.44
1:G:150:ARG:HB3	1:G:151:TYR:HD2	1.83	0.44
1:P:111:LEU:HA	1:P:117:LYS:HG2	1.99	0.44
1:P:168:LEU:HD12	1:P:169:LYS:N	2.32	0.44
2:J:131:VAL:HG23	2:J:132:HIS:N	2.32	0.44
1:A:64:GLN:C	1:A:65:ARG:HG3	2.42	0.44
1:A:82:ASP:HB3	1:A:111:LEU:HD13	1.98	0.44
1:A:171:THR:HA	1:A:191:PHE:O	2.18	0.44
2:D:117:ASP:HB2	2:D:128:HIS:CE1	2.53	0.44
1:H:73:PRO:HG2	2:J:168:PHE:CD1	2.52	0.44
2:K:68:LYS:H	2:K:77:GLN:HE22	1.65	0.44
2:J:79:ASP:C	2:J:81:ASP:H	2.24	0.44
1:P:160:PRO:O	1:P:161:ALA:C	2.60	0.44
1:G:164:TYR:CD1	1:G:164:TYR:N	2.80	0.44
1:H:111:LEU:CD2	1:H:117:LYS:HG2	2.35	0.44
1:H:206:GLN:HE21	1:H:207:ARG:CD	2.31	0.44
1:H:207:ARG:NH2	2:J:163:ASP:OD2	2.51	0.44
1:P:158:PRO:HA	1:P:166:PHE:CD1	2.53	0.44
1:A:68:ARG:C	1:A:71:LEU:HD13	2.42	0.44
2:K:101:LYS:NZ	1:P:203:LEU:HD21	2.33	0.44
1:A:104:TYR:CD1	1:A:104:TYR:C	2.95	0.44
1:A:135:LEU:HD22	2:B:156:HIS:NE2	2.33	0.44
1:H:207:ARG:HG3	2:J:162:LEU:HD11	1.99	0.44
1:A:80:TRP:CH2	1:A:90:LEU:HB2	2.52	0.44
2:B:94:ALA:HA	2:B:162:LEU:CD1	2.48	0.44
1:G:67:ARG:HA	1:G:70:GLN:NE2	2.33	0.44
2:K:133:ARG:NH2	2:K:140:GLU:OE2	2.51	0.44
1:P:79:HIS:HB2	1:P:89:HIS:O	2.17	0.44
1:A:94:LEU:HD12	1:A:101:VAL:HB	1.96	0.44
2:B:166:PHE:CD1	1:G:208:PHE:HD2	2.36	0.44
2:D:107:HIS:NE2	2:D:109:MSE:HG2	2.33	0.44
1:G:135:LEU:HD23	1:G:135:LEU:HA	1.82	0.44
1:H:215:TYR:C	1:H:217:THR:H	2.25	0.44
2:K:118:PHE:CE2	2:K:154:LEU:HD21	2.53	0.44
1:P:70:GLN:CD	1:P:70:GLN:N	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:41:PRO:HB3	2:D:63:GLN:HE21	1.83	0.43
1:H:149:SER:C	1:H:151:TYR:H	2.25	0.43
1:G:129:VAL:CG1	1:G:130:TYR:N	2.80	0.43
2:J:160:SER:HB3	1:P:214:HIS:ND1	2.32	0.43
1:A:134:PHE:C	1:A:136:ALA:N	2.73	0.43
2:D:90:HIS:HE1	2:D:165:SER:OG	2.00	0.43
1:H:94:LEU:N	1:H:94:LEU:CD2	2.80	0.43
2:B:40:ASP:OD1	2:B:42:ALA:HB3	2.18	0.43
1:G:97:ASP:CG	1:G:98:THR:N	2.73	0.43
1:H:80:TRP:HH2	1:H:118:ALA:HB2	1.83	0.43
2:K:52:ASP:O	2:K:55:LEU:HD12	2.18	0.43
2:J:124:GLY:HA3	2:J:146:PHE:O	2.18	0.43
1:P:100:VAL:O	1:P:126:LEU:HB2	2.19	0.43
2:B:144:VAL:O	2:B:144:VAL:HG13	2.17	0.43
1:G:170:CYS:HB2	1:G:193:TRP:NE1	2.33	0.43
1:H:92:ARG:HG2	1:H:92:ARG:NH1	2.33	0.43
2:K:50:ALA:HA	2:K:157:PHE:CZ	2.52	0.43
1:A:61:LEU:N	1:A:61:LEU:HD22	2.34	0.43
1:A:105:HIS:N	1:A:105:HIS:ND1	2.65	0.43
2:B:41:PRO:HA	2:B:63:GLN:NE2	2.34	0.43
2:B:93:LEU:HD13	2:B:162:LEU:HA	2.01	0.43
2:D:105:PRO:C	2:D:106:ARG:HG2	2.43	0.43
1:G:106:ARG:HG2	1:G:121:VAL:HG21	1.99	0.43
1:H:129:VAL:HG23	1:H:130:TYR:N	2.34	0.43
1:P:84:ASP:OD1	1:P:85:ILE:O	2.37	0.43
2:B:134:VAL:O	2:B:135:ALA:C	2.60	0.43
1:H:61:LEU:HA	1:H:64:GLN:CB	2.49	0.43
1:H:201:GLU:O	1:H:202:SER:C	2.59	0.43
1:A:112:THR:HB	1:A:113:GLU:H	1.69	0.43
1:A:218:GLY:C	1:A:220:ALA:N	2.76	0.43
1:G:212:ALA:O	1:G:213:LEU:C	2.62	0.43
1:P:167:THR:HG23	1:P:196:GLU:OE2	2.18	0.43
1:A:209:LEU:O	1:A:210:THR:C	2.60	0.43
2:B:92:ASP:O	2:B:93:LEU:C	2.62	0.43
2:D:93:LEU:HD21	2:D:162:LEU:CA	2.49	0.43
1:P:155:THR:HG23	1:P:155:THR:O	2.18	0.43
1:H:135:LEU:HD13	2:K:156:HIS:CE1	2.54	0.42
1:H:154:ALA:CB	1:H:170:CYS:HB3	2.49	0.42
2:K:60:GLN:CD	2:K:142:TRP:HE1	2.27	0.42
1:P:209:LEU:O	1:P:210:THR:C	2.59	0.42
1:H:145:VAL:O	1:H:145:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:99:VAL:HG11	2:K:118:PHE:CD1	2.54	0.42
1:A:127:PRO:C	1:A:129:VAL:N	2.78	0.42
2:B:134:VAL:O	2:B:136:SER:N	2.52	0.42
1:H:91:LEU:HD23	1:H:195:VAL:HG11	2.00	0.42
1:H:99:PHE:C	1:H:100:VAL:HG23	2.44	0.42
1:P:85:ILE:C	1:P:87:ARG:H	2.26	0.42
1:P:95:HIS:O	1:P:96:ARG:HB2	2.19	0.42
1:A:107:GLN:NE2	1:A:111:LEU:HD23	2.33	0.42
1:A:144:LYS:CG	1:A:145:VAL:N	2.82	0.42
2:B:106:ARG:HG3	2:B:119:GLU:CB	2.46	0.42
2:B:162:LEU:HD23	2:B:162:LEU:C	2.42	0.42
1:H:106:ARG:HG3	1:H:119:GLU:HB3	2.01	0.42
2:K:100:CYS:C	2:K:102:GLU:H	2.26	0.42
1:A:100:VAL:HB	1:A:126:LEU:HB2	2.01	0.42
1:A:101:VAL:HG13	1:A:125:MSE:HG2	2.01	0.42
2:D:67:ARG:H	2:D:67:ARG:CD	2.18	0.42
2:D:156:HIS:NE2	1:G:135:LEU:HD13	2.34	0.42
1:P:211:GLN:O	1:P:215:TYR:HD2	2.02	0.42
2:B:40:ASP:OD2	2:B:42:ALA:HB3	2.18	0.42
1:H:91:LEU:HD12	1:H:92:ARG:N	2.35	0.42
2:K:93:LEU:HA	2:K:93:LEU:HD23	1.76	0.42
1:A:173:THR:C	1:A:174:ARG:HG3	2.44	0.42
1:A:203:LEU:HD23	1:A:203:LEU:O	2.20	0.42
2:B:107:HIS:CD2	2:B:109:MSE:HG3	2.54	0.42
2:B:128:HIS:ND1	2:B:128:HIS:N	2.67	0.42
2:D:88:LEU:HD22	2:D:109:MSE:SE	2.70	0.42
1:G:92:ARG:HD2	1:G:105:HIS:HE2	1.83	0.42
1:P:166:PHE:CD2	1:P:166:PHE:N	2.87	0.42
1:G:75:PHE:CE2	1:G:93:VAL:HB	2.54	0.42
1:H:170:CYS:SG	1:H:193:TRP:CE2	3.12	0.42
1:H:200:ALA:O	1:H:201:GLU:C	2.59	0.42
2:J:164:GLU:OE2	2:J:169:ARG:NH2	2.43	0.42
1:A:84:ASP:O	1:A:86:SER:N	2.52	0.42
2:B:93:LEU:HD13	2:B:162:LEU:CA	2.49	0.42
1:H:130:TYR:O	1:H:131:THR:C	2.62	0.42
2:J:49:VAL:HG12	2:J:157:PHE:CE1	2.54	0.42
2:J:51:VAL:HB	2:J:56:LEU:HD23	2.01	0.42
2:B:50:ALA:HB3	2:B:57:LEU:HD11	2.01	0.42
2:B:158:LEU:O	2:B:159:GLU:C	2.60	0.42
2:D:103:ARG:HG2	2:D:103:ARG:NH1	2.33	0.42
1:G:82:ASP:C	1:G:84:ASP:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:134:VAL:O	2:K:135:ALA:CB	2.68	0.42
2:J:44:GLY:CA	2:J:63:GLN:HB2	2.49	0.42
1:A:145:VAL:O	1:A:155:THR:HA	2.19	0.41
1:A:152:THR:HG22	1:A:172:SER:OG	2.19	0.41
1:H:163:PRO:O	1:H:164:TYR:HB2	2.20	0.41
1:P:170:CYS:HB2	1:P:193:TRP:HE1	1.79	0.41
2:B:69:VAL:O	2:B:70:ASP:HB2	2.20	0.41
1:H:106:ARG:HH11	1:H:119:GLU:CD	2.28	0.41
1:H:204:MSE:HE3	1:H:204:MSE:HB2	1.92	0.41
2:K:111:THR:HB	2:K:112:LYS:HE2	2.02	0.41
1:P:109:ARG:H	1:P:109:ARG:HG2	1.68	0.41
1:H:200:ALA:HB1	2:J:94:ALA:HB1	2.00	0.41
2:D:142:TRP:CZ2	2:D:144:VAL:HG13	2.55	0.41
1:H:78:VAL:HG12	1:H:79:HIS:N	2.34	0.41
1:H:81:ASN:C	1:H:83:GLU:H	2.28	0.41
2:K:146:PHE:CG	2:K:154:LEU:HD22	2.55	0.41
2:K:168:PHE:O	2:K:172:TYR:HB2	2.20	0.41
2:D:63:GLN:HG3	2:D:77:GLN:HE21	1.86	0.41
2:D:121:SER:N	2:D:124:GLY:O	2.44	0.41
1:H:159:ASN:ND2	1:H:161:ALA:HB3	2.35	0.41
1:H:207:ARG:HG3	2:J:162:LEU:CD1	2.50	0.41
2:K:29:LEU:HD22	2:K:52:ASP:HA	2.02	0.41
1:P:100:VAL:HB	1:P:126:LEU:HB3	2.03	0.41
2:B:32:PHE:CE1	2:B:49:VAL:HB	2.55	0.41
2:B:116:LEU:HB3	2:B:127:LEU:HD11	2.03	0.41
2:D:40:ASP:O	2:D:42:ALA:N	2.54	0.41
2:D:51:VAL:HG12	2:D:157:PHE:CE1	2.55	0.41
1:P:171:THR:HA	1:P:192:GLU:HA	2.02	0.41
1:G:175:PRO:HA	1:G:188:ASP:CB	2.50	0.41
1:P:68:ARG:HB3	1:P:68:ARG:NH1	2.36	0.41
1:P:85:ILE:HD11	1:P:110:MSE:CG	2.48	0.41
1:G:135:LEU:CD2	1:G:206:GLN:HE21	2.34	0.41
1:A:84:ASP:O	1:A:85:ILE:C	2.64	0.41
1:A:152:THR:HG22	1:A:172:SER:CB	2.51	0.41
1:A:152:THR:HG22	1:A:172:SER:HB3	2.02	0.41
1:A:198:ASP:OD1	1:A:201:GLU:HG3	2.20	0.41
2:B:94:ALA:O	2:B:97:VAL:HB	2.21	0.41
1:G:121:VAL:HB	1:G:122:VAL:H	1.63	0.41
1:H:130:TYR:CZ	1:H:147:VAL:HG12	2.56	0.41
2:K:90:HIS:O	2:K:93:LEU:HB2	2.21	0.41
2:K:169:ARG:O	2:K:173:ALA:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:PHE:O	1:A:135:LEU:C	2.63	0.41
1:A:158:PRO:HA	1:A:166:PHE:CD1	2.56	0.41
2:B:66:PRO:C	2:B:68:LYS:N	2.75	0.41
2:B:148:ASN:O	2:B:151:ALA:N	2.53	0.41
2:K:54:LYS:O	2:K:90:HIS:HA	2.21	0.41
2:K:130:LYS:C	2:K:131:VAL:HG13	2.46	0.41
1:P:110:MSE:O	1:P:117:LYS:HG2	2.21	0.41
1:A:85:ILE:CD1	1:A:110:MSE:HA	2.52	0.40
2:B:96:LEU:HD22	2:B:96:LEU:HA	1.82	0.40
1:G:85:ILE:O	1:G:86:SER:CB	2.68	0.40
1:G:215:TYR:CD1	1:G:220:ALA:HB2	2.57	0.40
2:K:31:LYS:HA	2:K:157:PHE:CE2	2.56	0.40
2:K:36:ASP:N	2:K:45:THR:O	2.51	0.40
1:A:81:ASN:HD22	1:A:81:ASN:HA	1.66	0.40
2:B:40:ASP:OD1	2:B:40:ASP:O	2.39	0.40
2:J:126:HIS:CE1	2:J:128:HIS:CD2	3.10	0.40
1:P:72:PRO:CG	1:P:96:ARG:HH21	2.20	0.40
1:H:119:GLU:C	1:H:120:ARG:O	2.62	0.40
2:J:35:HIS:HA	2:J:46:MSE:HA	2.04	0.40
1:A:113:GLU:O	1:A:115:GLY:N	2.54	0.40
2:B:94:ALA:HA	2:B:162:LEU:HD11	2.04	0.40
2:B:97:VAL:O	2:B:100:CYS:N	2.54	0.40
1:G:83:GLU:O	1:G:84:ASP:HB2	2.21	0.40
1:P:68:ARG:HB3	1:P:68:ARG:HH11	1.86	0.40
1:P:143:GLU:HA	1:P:143:GLU:OE1	2.22	0.40
1:A:126:LEU:HA	1:A:127:PRO:HD3	1.78	0.40
2:B:148:ASN:C	2:B:150:PHE:N	2.79	0.40
1:H:68:ARG:C	1:H:70:GLN:H	2.30	0.40
1:H:121:VAL:HG11	1:H:191:PHE:CE2	2.57	0.40
2:K:82:ARG:HH11	2:K:82:ARG:HG2	1.85	0.40
1:P:74:ALA:HB2	1:P:94:LEU:CA	2.51	0.40
1:P:127:PRO:HB2	1:P:130:TYR:HD2	1.86	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	146/195 (75%)	104 (71%)	32 (22%)	10 (7%)	1	6
1	G	147/195 (75%)	111 (76%)	19 (13%)	17 (12%)	0	1
1	H	147/195 (75%)	98 (67%)	32 (22%)	17 (12%)	0	1
1	P	147/195 (75%)	105 (71%)	33 (22%)	9 (6%)	1	7
2	B	144/187 (77%)	111 (77%)	24 (17%)	9 (6%)	1	7
2	D	144/187 (77%)	121 (84%)	18 (12%)	5 (4%)	3	16
2	J	144/187 (77%)	116 (81%)	20 (14%)	8 (6%)	1	9
2	K	144/187 (77%)	102 (71%)	28 (19%)	14 (10%)	0	3
All	All	1163/1528 (76%)	868 (75%)	206 (18%)	89 (8%)	1	5

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	ARG
1	A	113	GLU
1	A	128	ALA
1	A	219	PHE
2	B	70	ASP
2	B	135	ALA
2	B	168	PHE
1	H	70	GLN
1	H	99	PHE
1	H	219	PHE
2	J	41	PRO
2	J	171	HIS
1	P	189	GLU
1	A	85	ILE
1	A	121	VAL
2	B	172	TYR
1	G	83	GLU
1	G	84	ASP
1	G	86	SER
1	G	112	THR
1	G	113	GLU
1	G	121	VAL
1	H	82	ASP

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Mol	Chain	Res	Type
1	H	103	ASP
2	K	42	ALA
2	K	112	LYS
2	K	113	ALA
2	K	133	ARG
2	K	135	ALA
2	K	165	SER
2	J	103	ARG
2	J	165	SER
1	P	96	ARG
1	P	161	ALA
1	A	135	LEU
2	B	63	GLN
1	G	81	ASN
1	G	111	LEU
1	H	85	ILE
1	H	98	THR
1	H	100	VAL
1	H	120	ARG
1	H	132	ALA
1	H	216	ASN
2	K	136	SER
2	J	53	GLY
2	J	73	ASP
2	J	80	ALA
1	P	199	VAL
1	A	114	GLU
2	B	101	LYS
2	D	42	ALA
2	D	143	SER
1	G	62	ALA
1	G	110	MSE
1	G	117	LYS
1	G	199	VAL
1	H	79	HIS
1	H	121	VAL
2	K	148	ASN
1	P	86	SER
1	A	97	ASP
2	B	94	ALA
2	D	148	ASN
1	G	69	ALA

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Mol	Chain	Res	Type
1	G	97	ASP
1	G	131	THR
1	H	81	ASN
1	H	139	GLU
2	K	102	GLU
1	P	97	ASP
1	P	173	THR
1	P	193	TRP
1	A	120	ARG
2	D	41	PRO
1	G	137	VAL
1	H	80	TRP
2	K	41	PRO
2	K	67	ARG
2	K	72	ASN
2	B	134	VAL
1	P	121	VAL
1	G	78	VAL
2	J	71	PRO
2	B	66	PRO
2	D	49	VAL
1	H	140	GLY
2	K	98	GLY
2	K	76	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	131/159 (82%)	117 (89%)	14 (11%)	6	23
1	G	131/159 (82%)	119 (91%)	12 (9%)	8	30
1	H	132/159 (83%)	120 (91%)	12 (9%)	9	30
1	P	131/159 (82%)	119 (91%)	12 (9%)	8	30
2	B	129/155 (83%)	113 (88%)	16 (12%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	129/155 (83%)	113 (88%)	16 (12%)	4	18
2	J	129/155 (83%)	120 (93%)	9 (7%)	14	40
2	K	129/155 (83%)	114 (88%)	15 (12%)	5	20
All	All	1041/1256 (83%)	935 (90%)	106 (10%)	7	25

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	81	ASN
1	A	99	PHE
1	A	110	MSE
1	A	111	LEU
1	A	112	THR
1	A	114	GLU
1	A	135	LEU
1	A	144	LYS
1	A	155	THR
1	A	157	THR
1	A	168	LEU
1	A	190	THR
1	A	201	GLU
2	B	29	LEU
2	B	43	GLU
2	B	51	VAL
2	B	55	LEU
2	B	57	LEU
2	B	86	VAL
2	B	93	LEU
2	B	96	LEU
2	B	111	THR
2	B	112	LYS
2	B	119	GLU
2	B	152	VAL
2	B	153	THR
2	B	163	ASP
2	B	164	GLU
2	B	170	GLN
2	D	39	ASP
2	D	46	MSE
2	D	51	VAL

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Mol	Chain	Res	Type
2	D	67	ARG
2	D	69	VAL
2	D	81	ASP
2	D	85	SER
2	D	91	VAL
2	D	96	LEU
2	D	104	VAL
2	D	111	THR
2	D	123	GLN
2	D	153	THR
2	D	154	LEU
2	D	162	LEU
2	D	163	ASP
1	G	68	ARG
1	G	78	VAL
1	G	82	ASP
1	G	94	LEU
1	G	114	GLU
1	G	133	ARG
1	G	145	VAL
1	G	150	ARG
1	G	151	TYR
1	G	190	THR
1	G	203	LEU
1	G	213	LEU
1	H	67	ARG
1	H	114	GLU
1	H	144	LYS
1	H	146	GLU
1	H	147	VAL
1	H	150	ARG
1	H	156	PHE
1	H	157	THR
1	H	159	ASN
1	H	168	LEU
1	H	204	MSE
1	H	205	LEU
2	K	39	ASP
2	K	55	LEU
2	K	58	ILE
2	K	70	ASP
2	K	74	LEU

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Mol	Chain	Res	Type
2	K	75	SER
2	K	93	LEU
2	K	102	GLU
2	K	106	ARG
2	K	112	LYS
2	K	114	TYR
2	K	132	HIS
2	K	149	HIS
2	K	162	LEU
2	K	172	TYR
2	J	45	THR
2	J	83	ARG
2	J	132	HIS
2	J	137	GLN
2	J	138	ARG
2	J	141	ASP
2	J	154	LEU
2	J	170	GLN
2	J	171	HIS
1	P	70	GLN
1	P	77	VAL
1	P	94	LEU
1	P	109	ARG
1	P	112	THR
1	P	121	VAL
1	P	129	VAL
1	P	141	ARG
1	P	144	LYS
1	P	145	VAL
1	P	157	THR
1	P	210	THR

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

Mol	Chain	Res	Type
1	A	64	GLN
1	A	81	ASN
1	A	107	GLN
1	A	153	ASN
1	A	159	ASN
1	A	206	GLN
2	B	77	GLN

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Mol	Chain	Res	Type
2	B	107	HIS
2	B	126	HIS
2	B	148	ASN
2	B	170	GLN
2	B	171	HIS
2	D	77	GLN
2	D	90	HIS
2	D	128	HIS
2	D	137	GLN
2	D	171	HIS
1	G	64	GLN
1	G	70	GLN
1	G	153	ASN
1	G	206	GLN
1	H	79	HIS
1	H	81	ASN
1	H	159	ASN
1	H	206	GLN
2	K	72	ASN
2	K	77	GLN
2	K	123	GLN
2	K	137	GLN
2	K	148	ASN
2	J	128	HIS
2	J	137	GLN
2	J	149	HIS
2	J	170	GLN
1	P	64	GLN
1	P	116	ASN
1	P	211	GLN
1	P	216	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 [i](#)

There are no oligosaccharides 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.