



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:33 PM UTC

PDB ID : 1QK1 / pdb_00001qk1
Title : CRYSTAL STRUCTURE OF HUMAN UBIQUITOUS MITOCHONDRIAL CREATINE KINASE
Authors : Eder, M.; Schlattner, U.; Fritz-Wolf, K.; Wallimann, T.; Kabsch, W.
Deposited on : 1999-07-08
Resolution : 2.70 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

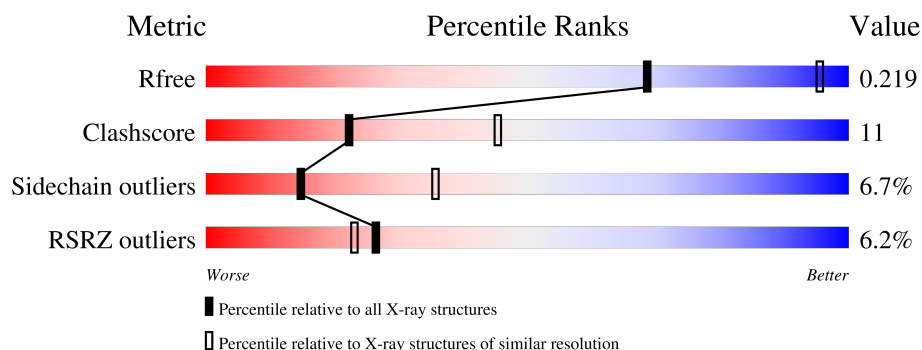
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	379	6% 76% 21% .
1	B	379	6% 74% 24% .
1	C	379	7% 76% 22% .
1	D	379	6% 77% 20% .
1	E	379	6% 72% 24% .
1	F	379	6% 74% 22% ..

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Mol	Chain	Length	Quality of chain
1	G	379	7% 74% 23% ••
1	H	379	6% 74% 22% •

2 Entry composition

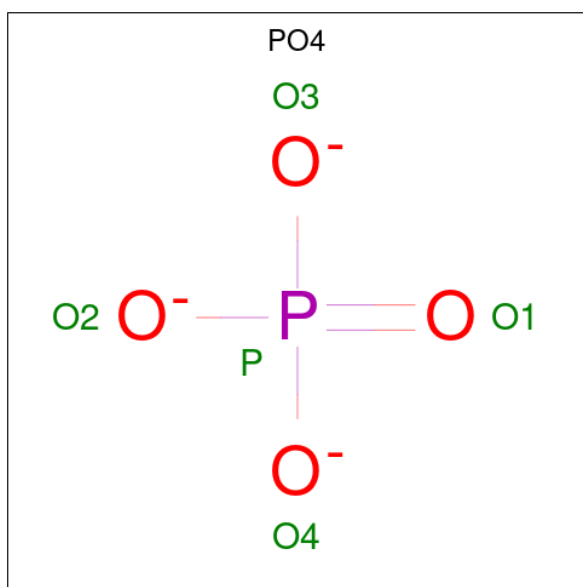
There are 3 unique types of molecules in this entry. The entry contains 24613 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CREATINE KINASE, UBIQUITOUS MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			3035	1898	558	564	15			
1	B	379	Total	C	N	O	S	0	0	0
			3035	1898	558	564	15			
1	C	379	Total	C	N	O	S	0	0	0
			3035	1898	558	564	15			
1	D	379	Total	C	N	O	S	0	0	0
			3035	1898	558	564	15			
1	E	379	Total	C	N	O	S	0	0	0
			3035	1898	558	564	15			
1	F	379	Total	C	N	O	S	0	0	0
			3035	1898	558	564	15			
1	G	379	Total	C	N	O	S	0	0	0
			3035	1898	558	564	15			
1	H	379	Total	C	N	O	S	0	0	0
			3035	1898	558	564	15			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		
3	B	36	Total	O	0	0
			36	36		
3	C	36	Total	O	0	0
			36	36		
3	D	40	Total	O	0	0
			40	40		

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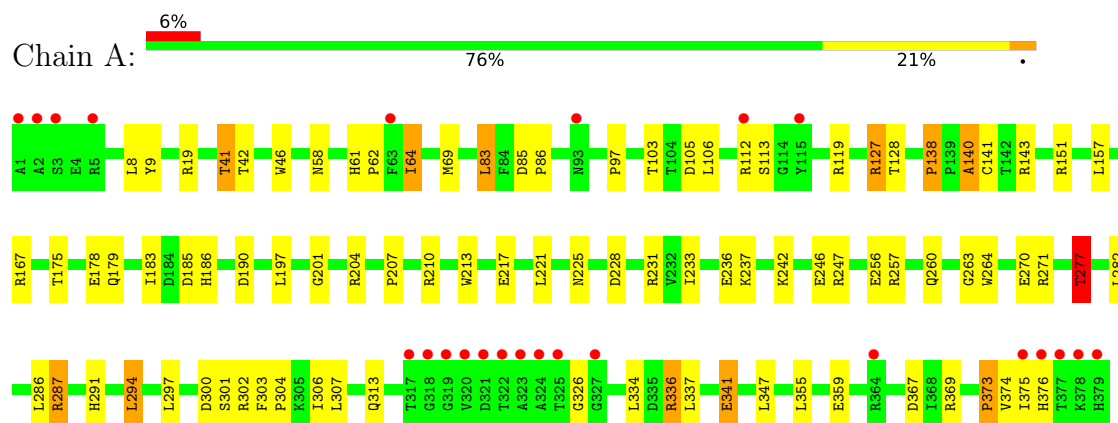
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	31	Total 31	O 31	0	0
3	F	34	Total 34	O 34	0	0
3	G	32	Total 32	O 32	0	0
3	H	38	Total 38	O 38	0	0

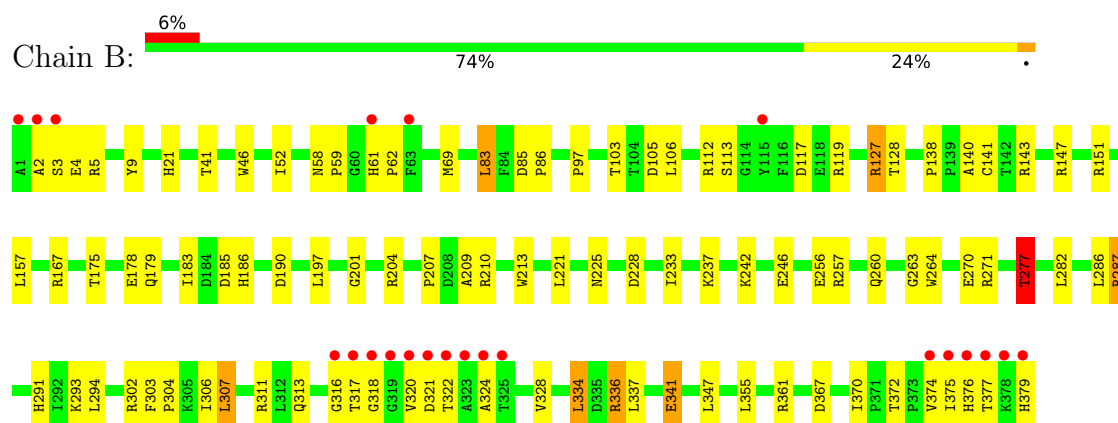
3 Residue-property plots [i](#)

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

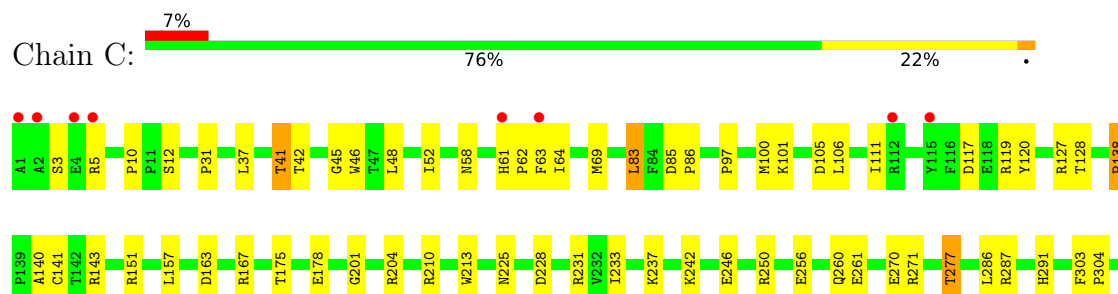
• Molecule 1: CREATINE KINASE, UBIQUITOUS MITOCHONDRIAL



• Molecule 1: CREATINE KINASE, UBIQUITOUS MITOCHONDRIAL

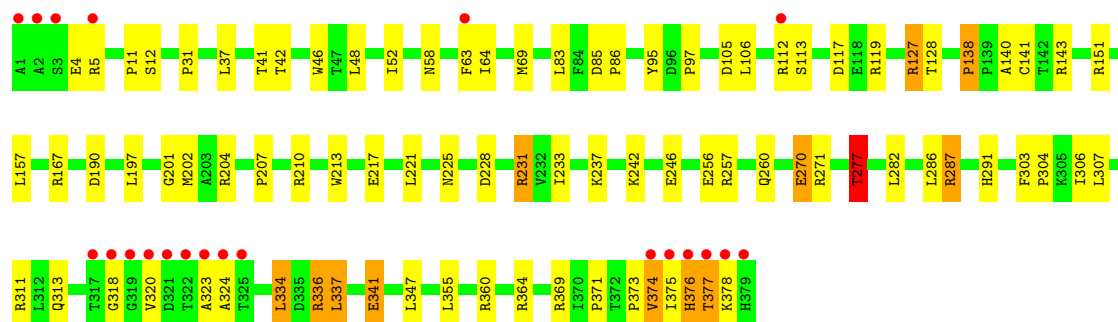
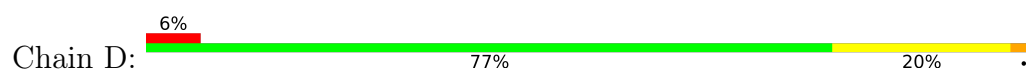


• Molecule 1: CREATINE KINASE, UBIQUITOUS MITOCHONDRIAL

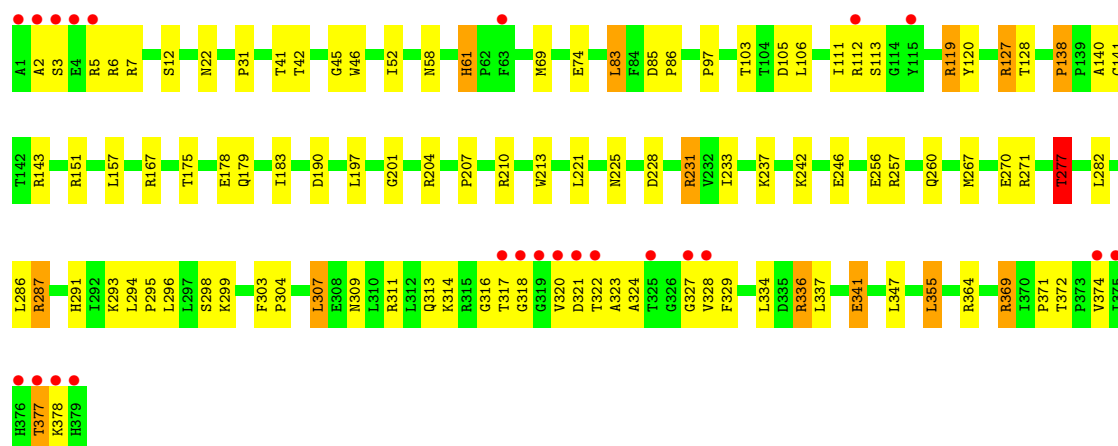
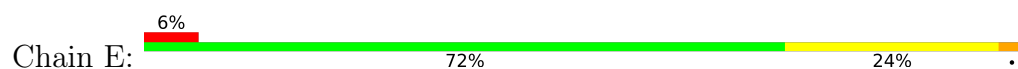




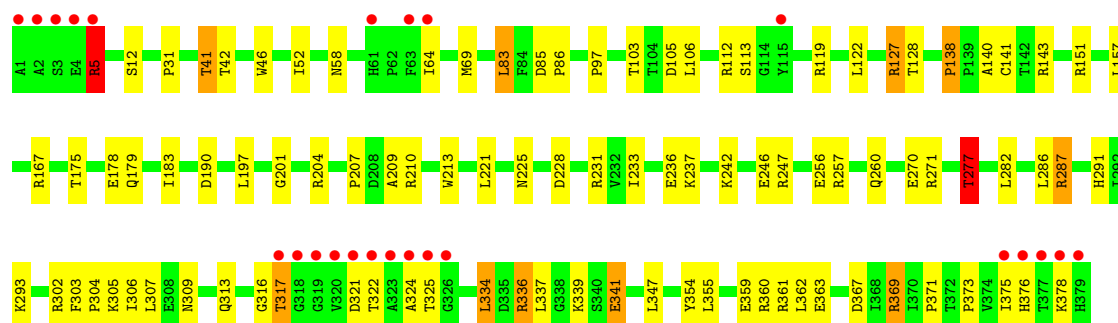
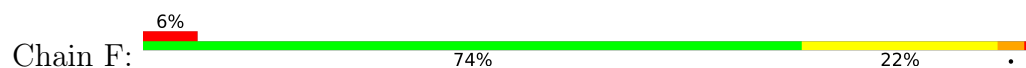
- Molecule 1: CREATINE KINASE, UBIQUITOUS MITOCHONDRIAL



- Molecule 1: CREATINE KINASE, UBIQUITOUS MITOCHONDRIAL



- Molecule 1: CREATINE KINASE, UBIQUITOUS MITOCHONDRIAL



- Molecule 1: CREATINE KINASE, UBIQUITOUS MITOCHONDRIAL

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.81Å 125.87Å 212.07Å 90.00° 96.71° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.70) 99.5 (50.00-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.69Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.195 , 0.219 0.195 , 0.219	Depositor DCC
R_{free} test set	6548 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24613	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.58	0/3099	0.98	15/4189 (0.4%)
1	B	0.57	0/3099	1.00	17/4189 (0.4%)
1	C	0.63	1/3099 (0.0%)	0.99	14/4189 (0.3%)
1	D	0.59	1/3099 (0.0%)	1.00	14/4189 (0.3%)
1	E	0.58	0/3099	0.98	13/4189 (0.3%)
1	F	0.59	0/3099	1.01	13/4189 (0.3%)
1	G	0.56	0/3099	1.00	15/4189 (0.4%)
1	H	0.58	0/3099	1.00	13/4189 (0.3%)
All	All	0.59	2/24792 (0.0%)	0.99	114/33512 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	10	PRO	CA-C	5.71	1.57	1.52
1	D	202	MET	SD-CE	-5.02	1.67	1.79

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	5	ARG	N-CA-C	-12.05	97.12	112.90
1	B	322	THR	N-CA-C	-8.31	102.30	111.36
1	G	5	ARG	N-CA-C	-7.81	103.89	113.50
1	C	375	ILE	N-CA-C	7.14	124.20	109.34
1	D	138	PRO	N-CA-C	7.02	119.27	110.70
1	C	291	HIS	N-CA-C	-6.86	97.33	108.52
1	H	138	PRO	N-CA-C	6.85	119.06	110.70
1	E	138	PRO	N-CA-C	6.80	118.99	110.70
1	C	138	PRO	N-CA-C	6.79	118.98	110.70
1	F	138	PRO	N-CA-C	6.78	118.97	110.70
1	D	286	LEU	N-CA-C	6.78	120.29	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	LEU	N-CA-C	6.74	120.65	109.46
1	E	286	LEU	N-CA-C	6.67	120.11	109.24
1	H	325	THR	N-CA-C	6.67	118.63	111.36
1	H	286	LEU	N-CA-C	6.65	120.51	109.46
1	G	138	PRO	N-CA-C	6.62	118.78	110.70
1	C	286	LEU	N-CA-C	6.61	120.43	109.46
1	G	286	LEU	N-CA-C	6.56	120.34	109.46
1	A	294	LEU	CA-C-N	6.55	125.78	118.97
1	A	294	LEU	C-N-CA	6.55	125.78	118.97
1	A	138	PRO	N-CA-C	6.50	118.63	110.70
1	E	291	HIS	N-CA-C	-6.44	98.02	108.52
1	F	286	LEU	N-CA-C	6.43	120.13	109.46
1	H	291	HIS	N-CA-C	-6.41	98.07	108.52
1	B	286	LEU	N-CA-C	6.37	120.04	109.46
1	A	291	HIS	N-CA-C	-6.35	98.17	108.52
1	F	291	HIS	N-CA-C	-6.34	98.19	108.52
1	D	58	ASN	CA-C-N	6.33	125.56	118.97
1	D	58	ASN	C-N-CA	6.33	125.56	118.97
1	F	277	THR	N-CA-C	6.33	119.16	111.82
1	E	277	THR	N-CA-C	6.29	119.12	111.82
1	F	58	ASN	CA-C-N	6.29	126.20	119.28
1	F	58	ASN	C-N-CA	6.29	126.20	119.28
1	D	291	HIS	N-CA-C	-6.26	98.32	108.52
1	H	233	ILE	N-CA-C	6.22	117.07	108.12
1	C	277	THR	N-CA-C	6.21	119.02	111.82
1	H	237	LYS	N-CA-C	-6.16	101.37	110.48
1	B	138	PRO	N-CA-C	6.11	118.15	110.70
1	D	233	ILE	N-CA-C	6.08	116.88	108.12
1	G	277	THR	N-CA-C	6.03	118.82	111.82
1	B	321	ASP	N-CA-C	-6.02	102.97	108.75
1	B	237	LYS	N-CA-C	-6.01	101.58	110.48
1	G	58	ASN	CA-C-N	6.01	125.72	119.05
1	G	58	ASN	C-N-CA	6.01	125.72	119.05
1	G	233	ILE	N-CA-C	6.01	116.77	108.12
1	G	270	GLU	N-CA-C	6.00	119.86	112.54
1	H	58	ASN	CA-C-N	5.97	125.85	119.28
1	H	58	ASN	C-N-CA	5.97	125.85	119.28
1	C	322	THR	N-CA-C	5.97	121.35	112.94
1	A	233	ILE	N-CA-C	5.96	116.69	108.12
1	B	233	ILE	N-CA-C	5.95	116.69	108.12
1	B	270	GLU	N-CA-C	5.94	119.79	112.54
1	G	325	THR	N-CA-C	5.93	118.87	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	THR	N-CA-C	5.89	118.65	111.82
1	F	317	THR	N-CA-C	-5.88	104.82	112.23
1	A	237	LYS	N-CA-C	-5.86	101.81	110.48
1	D	270	GLU	N-CA-C	5.86	119.68	112.54
1	D	277	THR	N-CA-C	5.81	118.56	111.82
1	E	233	ILE	N-CA-C	5.79	116.45	108.12
1	G	237	LYS	N-CA-C	-5.77	101.94	110.48
1	B	277	THR	N-CA-C	5.77	118.51	111.82
1	A	270	GLU	N-CA-C	5.73	119.53	112.54
1	E	7	ARG	N-CA-C	5.73	119.59	109.96
1	B	291	HIS	N-CA-C	-5.69	97.92	107.99
1	D	5	ARG	N-CA-C	-5.68	106.02	113.17
1	D	377	THR	N-CA-C	-5.67	105.67	112.59
1	C	233	ILE	N-CA-C	5.67	116.28	108.12
1	A	9	TYR	N-CA-C	-5.64	101.36	109.48
1	F	237	LYS	N-CA-C	-5.64	102.13	110.48
1	E	237	LYS	N-CA-C	-5.62	102.16	110.48
1	E	270	GLU	N-CA-C	5.60	119.37	112.54
1	H	270	GLU	N-CA-C	5.58	119.35	112.54
1	A	373	PRO	N-CA-C	5.53	119.55	111.03
1	G	291	HIS	N-CA-C	-5.52	98.22	107.99
1	F	270	GLU	N-CA-C	5.51	119.26	112.54
1	B	9	TYR	N-CA-C	-5.50	101.56	109.48
1	B	58	ASN	CA-C-N	5.47	125.55	119.32
1	B	58	ASN	C-N-CA	5.47	125.55	119.32
1	H	277	THR	N-CA-C	5.46	118.15	111.82
1	C	270	GLU	N-CA-C	5.45	119.19	112.54
1	C	376	HIS	N-CA-C	5.43	122.37	110.80
1	H	52	ILE	N-CA-C	5.43	119.04	112.80
1	D	237	LYS	N-CA-C	-5.42	102.46	110.48
1	B	209	ALA	N-CA-C	5.40	119.45	112.86
1	G	119	ARG	N-CA-C	-5.40	106.69	113.28
1	D	318	GLY	N-CA-C	-5.39	107.57	114.85
1	C	45	GLY	N-CA-C	5.37	123.01	115.43
1	C	237	LYS	N-CA-C	-5.34	102.58	110.48
1	E	58	ASN	CA-C-N	5.32	125.39	119.32
1	E	58	ASN	C-N-CA	5.32	125.39	119.32
1	H	9	TYR	N-CA-C	-5.27	101.89	109.48
1	F	233	ILE	N-CA-C	5.25	115.68	108.12
1	G	375	ILE	N-CA-C	5.25	115.87	108.36
1	F	52	ILE	N-CA-C	5.21	118.80	112.80
1	B	294	LEU	CA-C-N	5.20	124.82	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	294	LEU	C-N-CA	5.20	124.82	119.05
1	D	231	ARG	N-CA-C	-5.18	99.96	108.41
1	B	52	ILE	N-CA-C	5.17	118.75	112.80
1	C	52	ILE	N-CA-C	5.17	118.74	112.80
1	B	370	ILE	N-CA-C	-5.16	103.89	108.95
1	E	231	ARG	N-CA-C	-5.15	100.02	108.41
1	A	58	ASN	CA-C-N	5.15	125.19	119.32
1	A	58	ASN	C-N-CA	5.15	125.19	119.32
1	D	52	ILE	N-CA-C	5.14	118.71	112.80
1	F	209	ALA	N-CA-C	5.13	119.39	113.38
1	G	209	ALA	N-CA-C	5.12	119.10	112.86
1	A	326	GLY	N-CA-C	5.12	120.41	111.25
1	E	45	GLY	N-CA-C	5.10	122.62	115.43
1	C	58	ASN	CA-C-N	5.09	125.37	119.47
1	C	58	ASN	C-N-CA	5.09	125.37	119.47
1	E	52	ILE	N-CA-C	5.07	118.62	112.80
1	A	140	ALA	N-CA-C	5.04	120.82	114.31
1	G	118	GLU	N-CA-C	5.04	120.33	113.37
1	H	118	GLU	N-CA-C	5.00	119.14	113.19

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	3035	0	3010	64	0
1	B	3035	0	3010	60	0
1	C	3035	0	3010	87	0
1	D	3035	0	3010	55	0
1	E	3035	0	3010	69	0
1	F	3035	0	3010	66	0
1	G	3035	0	3010	71	0
1	H	3035	0	3010	74	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	1	0
2	H	5	0	0	0	0
3	A	46	0	0	2	0
3	B	36	0	0	2	0
3	C	36	0	0	2	0
3	D	40	0	0	3	0
3	E	31	0	0	1	0
3	F	34	0	0	1	0
3	G	32	0	0	2	0
3	H	38	0	0	1	0
All	All	24613	0	24080	512	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 11.

All (512) 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:C:151:ARG:HG2	1:E:151:ARG:HH11	1.15	1.10
1:F:5:ARG:HG3	1:F:5:ARG:HH11	1.31	0.95
1:C:318:GLY:HA2	1:C:323:ALA:HB2	1.54	0.90
1:B:151:ARG:HG2	1:B:151:ARG:HH11	1.41	0.86
1:G:302:ARG:HB3	1:G:370:ILE:HD11	1.56	0.85
1:G:117:ASP:OD1	1:G:119:ARG:HG3	1.75	0.85
1:C:361:ARG:HD3	1:C:368:ILE:HG22	1.61	0.82
1:C:303:PHE:HB3	1:C:304:PRO:HD3	1.62	0.80
1:C:151:ARG:HG2	1:E:151:ARG:NH1	1.94	0.80
1:D:360:ARG:O	1:D:364:ARG:HD2	1.83	0.79
1:F:303:PHE:HB3	1:F:304:PRO:HD3	1.65	0.78
1:E:293:LYS:HG2	1:E:328:VAL:HG22	1.65	0.78
1:G:6:ARG:HD2	3:G:2001:HOH:O	1.83	0.77
1:E:377:THR:HG23	1:E:378:LYS:H	1.49	0.77
1:E:303:PHE:HB3	1:E:304:PRO:HD3	1.66	0.76
1:B:303:PHE:HB3	1:B:304:PRO:HD3	1.66	0.76
1:F:339:LYS:HE2	1:F:376:HIS:HB2	1.67	0.75
1:A:373:PRO:HB2	1:A:375:ILE:HG12	1.67	0.74
1:G:303:PHE:HB3	1:G:304:PRO:HD3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:HIS:HD2	1:A:62:PRO:HD2	1.51	0.74
1:F:119:ARG:O	1:F:293:LYS:HE3	1.88	0.73
1:B:117:ASP:OD1	1:B:119:ARG:HG2	1.89	0.73
1:D:374:VAL:HG13	1:D:375:ILE:HG12	1.68	0.73
1:F:375:ILE:HD12	1:F:375:ILE:O	1.89	0.72
1:F:69:MET:HE1	1:F:83:LEU:HD13	1.71	0.71
1:C:318:GLY:CA	1:C:323:ALA:HB2	2.20	0.71
1:G:69:MET:HE1	1:G:83:LEU:HD13	1.71	0.71
1:B:3:SER:O	1:B:5:ARG:N	2.24	0.71
1:A:64:ILE:HD13	1:A:64:ILE:H	1.55	0.70
1:E:69:MET:HE1	1:E:83:LEU:HD13	1.74	0.70
1:B:69:MET:HE1	1:B:83:LEU:HD13	1.74	0.70
1:D:117:ASP:OD1	1:D:119:ARG:HG2	1.91	0.70
1:D:69:MET:HE1	1:D:83:LEU:HD13	1.73	0.69
1:B:106:LEU:HD23	1:B:341:GLU:HG3	1.74	0.69
1:H:61:HIS:CD2	1:H:63:PHE:HB2	2.27	0.69
1:E:106:LEU:HD23	1:E:341:GLU:HG3	1.75	0.69
1:B:2:ALA:HB1	1:B:4:GLU:HG3	1.74	0.69
1:F:339:LYS:HE2	1:F:376:HIS:CB	2.23	0.68
1:B:151:ARG:HG2	1:B:151:ARG:NH1	2.09	0.68
1:E:22:ASN:ND2	1:E:61:HIS:O	2.27	0.68
1:E:369:ARG:HB3	1:E:369:ARG:HH11	1.59	0.67
1:F:359:GLU:O	1:F:363:GLU:HG3	1.93	0.67
1:H:61:HIS:HB3	1:H:64:ILE:HD11	1.76	0.67
1:H:69:MET:HE1	1:H:83:LEU:HD13	1.74	0.67
1:A:151:ARG:HD2	1:H:151:ARG:HD3	1.76	0.67
1:C:69:MET:HE1	1:C:83:LEU:HD13	1.75	0.67
1:C:127:ARG:HG2	1:C:128:THR:N	2.10	0.67
1:C:339:LYS:HG2	1:C:377:THR:CB	2.23	0.67
1:C:375:ILE:HD12	1:C:375:ILE:H	1.60	0.67
1:H:61:HIS:HB3	1:H:64:ILE:CD1	2.25	0.66
1:C:61:HIS:HB3	1:C:64:ILE:HG13	1.78	0.66
1:D:127:ARG:HG2	1:D:128:THR:N	2.11	0.66
1:E:31:PRO:HG3	1:H:263:GLY:HA2	1.78	0.66
1:F:5:ARG:HH11	1:F:5:ARG:CG	2.06	0.66
1:G:61:HIS:HD2	1:G:62:PRO:HD2	1.59	0.66
1:G:369:ARG:HD3	1:G:369:ARG:N	2.10	0.66
1:E:311:ARG:HG3	1:E:374:VAL:CG2	2.24	0.65
1:C:151:ARG:CG	1:E:151:ARG:HH11	2.03	0.65
1:A:106:LEU:HD23	1:A:341:GLU:HG3	1.79	0.65
1:B:263:GLY:HA2	1:C:31:PRO:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:ARG:HG2	1:E:128:THR:N	2.11	0.65
1:A:127:ARG:HG2	1:A:128:THR:N	2.11	0.64
1:G:61:HIS:CD2	1:G:62:PRO:HD2	2.33	0.64
1:G:106:LEU:HD23	1:G:341:GLU:HG3	1.80	0.64
1:F:106:LEU:HD23	1:F:341:GLU:HG3	1.80	0.64
1:H:106:LEU:HD23	1:H:341:GLU:HG3	1.79	0.64
1:H:127:ARG:HG2	1:H:128:THR:N	2.13	0.64
1:A:8:LEU:HD23	1:G:8:LEU:HD23	1.79	0.63
1:D:4:GLU:OE1	1:D:4:GLU:HA	1.98	0.63
1:F:167:ARG:HG3	1:F:167:ARG:HH11	1.61	0.63
1:B:317:THR:O	1:B:317:THR:HG22	1.99	0.63
1:B:61:HIS:HD2	1:B:62:PRO:HD2	1.63	0.63
1:D:106:LEU:HD23	1:D:341:GLU:HG3	1.80	0.63
1:E:112:ARG:O	1:E:113:SER:HB3	1.98	0.62
1:H:64:ILE:O	1:H:64:ILE:HD12	1.98	0.62
1:H:167:ARG:HG3	1:H:167:ARG:HH11	1.64	0.62
1:H:61:HIS:ND1	1:H:62:PRO:HD2	2.14	0.62
1:F:31:PRO:HG3	1:G:263:GLY:HA2	1.82	0.62
1:D:311:ARG:HG3	1:D:374:VAL:CG1	2.29	0.62
1:B:106:LEU:CD2	1:B:341:GLU:HG3	2.29	0.62
1:A:263:GLY:HA2	1:D:31:PRO:HG3	1.82	0.61
1:C:106:LEU:HD23	1:C:341:GLU:HG3	1.81	0.61
1:D:167:ARG:HG3	1:D:167:ARG:HH11	1.65	0.61
1:C:167:ARG:HG3	1:C:167:ARG:HH11	1.65	0.61
1:B:127:ARG:HG2	1:B:128:THR:N	2.14	0.61
1:E:167:ARG:HG3	1:E:167:ARG:HH11	1.64	0.61
1:A:69:MET:HE1	1:A:83:LEU:HD13	1.81	0.61
1:C:143:ARG:NH2	3:C:2013:HOH:O	2.33	0.61
1:G:167:ARG:HG3	1:G:167:ARG:HH11	1.66	0.61
1:B:61:HIS:CD2	1:B:62:PRO:HD2	2.36	0.61
1:C:101:LYS:H	1:C:378:LYS:HE2	1.66	0.61
1:B:167:ARG:HH11	1:B:167:ARG:HG3	1.65	0.60
1:F:112:ARG:O	1:F:113:SER:HB3	2.01	0.60
1:F:256:GLU:O	1:F:260:GLN:HG3	2.01	0.60
1:A:167:ARG:HG3	1:A:167:ARG:HH11	1.66	0.60
1:C:317:THR:H	1:C:323:ALA:HA	1.65	0.60
1:D:303:PHE:HB3	1:D:304:PRO:HD3	1.83	0.60
1:F:127:ARG:HG2	1:F:128:THR:N	2.14	0.60
1:C:317:THR:HB	1:C:322:THR:C	2.26	0.60
1:E:106:LEU:CD2	1:E:341:GLU:HG3	2.31	0.60
1:E:143:ARG:NH2	3:E:2015:HOH:O	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:GLY:HA3	1:B:320:VAL:HG21	1.84	0.59
1:B:105:ASP:O	1:B:341:GLU:HG2	2.02	0.59
1:C:256:GLU:O	1:C:260:GLN:HG3	2.03	0.59
1:C:369:ARG:NH1	1:C:369:ARG:HG3	2.16	0.59
1:A:106:LEU:CD2	1:A:341:GLU:HG3	2.33	0.59
1:D:256:GLU:O	1:D:260:GLN:HG3	2.01	0.59
1:C:325:THR:HG22	1:C:328:VAL:HB	1.84	0.58
1:G:127:ARG:HG2	1:G:128:THR:N	2.16	0.58
1:C:141:CYS:O	1:C:204:ARG:NH2	2.30	0.58
1:G:369:ARG:HD3	1:G:369:ARG:H	1.68	0.58
1:A:141:CYS:O	1:A:204:ARG:NH2	2.30	0.58
1:C:376:HIS:O	1:C:377:THR:HG23	2.03	0.58
1:A:201:GLY:O	1:A:204:ARG:HD3	2.04	0.58
1:F:317:THR:HG22	1:F:324:ALA:O	2.04	0.58
1:H:112:ARG:O	1:H:113:SER:HB3	2.03	0.58
1:G:201:GLY:O	1:G:204:ARG:HD3	2.03	0.58
1:H:106:LEU:CD2	1:H:341:GLU:HG3	2.35	0.57
1:D:377:THR:O	1:D:378:LYS:HB2	2.03	0.57
1:F:106:LEU:CD2	1:F:341:GLU:HG3	2.34	0.57
1:E:256:GLU:O	1:E:260:GLN:HG3	2.04	0.57
1:C:364:ARG:NE	1:C:366:GLN:OE1	2.38	0.57
1:B:313:GLN:HB3	1:B:334:LEU:HD23	1.87	0.57
1:C:359:GLU:O	1:C:363:GLU:HG3	2.05	0.57
1:B:256:GLU:O	1:B:260:GLN:HG3	2.05	0.57
1:C:201:GLY:O	1:C:204:ARG:HD3	2.05	0.57
1:G:106:LEU:CD2	1:G:341:GLU:HG3	2.35	0.57
1:D:106:LEU:CD2	1:D:341:GLU:HG3	2.35	0.56
1:H:313:GLN:HB3	1:H:334:LEU:HD23	1.87	0.56
1:C:3:SER:C	1:C:5:ARG:H	2.12	0.56
1:D:201:GLY:O	1:D:204:ARG:HD3	2.05	0.56
1:G:105:ASP:O	1:G:341:GLU:HG2	2.06	0.56
1:B:320:VAL:HG13	1:B:324:ALA:HB2	1.86	0.56
1:A:302:ARG:O	1:A:306:ILE:HG13	2.06	0.56
1:C:5:ARG:HG3	1:C:5:ARG:HH11	1.71	0.56
1:F:313:GLN:HB3	1:F:334:LEU:HD23	1.88	0.56
1:F:325:THR:HG22	1:F:325:THR:O	2.06	0.56
1:D:374:VAL:HG13	1:D:375:ILE:N	2.20	0.56
1:C:117:ASP:OD1	1:C:119:ARG:HB3	2.06	0.56
1:E:141:CYS:O	1:E:204:ARG:NH2	2.31	0.56
1:B:201:GLY:O	1:B:204:ARG:HD3	2.05	0.56
1:C:320:VAL:HG23	1:C:321:ASP:OD1	2.07	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:CYS:O	1:F:204:ARG:NH2	2.29	0.55
1:G:5:ARG:HH11	1:G:5:ARG:HB3	1.71	0.55
1:H:141:CYS:O	1:H:204:ARG:NH2	2.28	0.55
1:C:106:LEU:CD2	1:C:341:GLU:HG3	2.36	0.55
1:F:12:SER:CB	1:G:264:TRP:CD2	2.89	0.55
1:H:201:GLY:O	1:H:204:ARG:HD3	2.06	0.55
1:H:256:GLU:O	1:H:260:GLN:HG3	2.06	0.55
1:F:324:ALA:O	1:F:325:THR:HB	2.06	0.55
1:H:303:PHE:HB3	1:H:304:PRO:HD3	1.86	0.55
1:G:309:ASN:O	1:G:374:VAL:HG23	2.06	0.55
1:E:201:GLY:O	1:E:204:ARG:HD3	2.07	0.55
1:E:313:GLN:HB3	1:E:334:LEU:HD23	1.88	0.55
1:F:228:ASP:OD1	1:F:277:THR:HG23	2.07	0.55
1:H:117:ASP:OD1	1:H:119:ARG:CD	2.55	0.55
1:C:313:GLN:HB3	1:C:334:LEU:HD23	1.88	0.55
1:C:339:LYS:HE2	1:C:377:THR:OG1	2.06	0.55
1:A:143:ARG:NH2	3:A:2023:HOH:O	2.40	0.54
1:C:339:LYS:HG2	1:C:377:THR:HB	1.88	0.54
1:H:105:ASP:O	1:H:341:GLU:HG2	2.07	0.54
1:F:143:ARG:NH2	3:F:2017:HOH:O	2.40	0.54
1:G:313:GLN:HB3	1:G:334:LEU:HD23	1.89	0.54
1:G:256:GLU:O	1:G:260:GLN:HG3	2.07	0.54
1:A:228:ASP:OD1	1:A:277:THR:HG23	2.08	0.54
1:A:151:ARG:NH1	1:H:151:ARG:CD	2.71	0.54
1:A:151:ARG:HH11	1:H:151:ARG:HD3	1.73	0.54
1:H:291:HIS:CE1	1:H:317:THR:HG23	2.43	0.54
1:A:313:GLN:HB3	1:A:334:LEU:HD23	1.89	0.54
1:E:311:ARG:HG3	1:E:374:VAL:HG21	1.87	0.54
1:D:228:ASP:OD1	1:D:277:THR:HG23	2.08	0.53
1:A:61:HIS:HD2	1:A:62:PRO:CD	2.21	0.53
1:C:85:ASP:HB2	1:C:86:PRO:HD3	1.90	0.53
1:F:105:ASP:O	1:F:341:GLU:HG2	2.08	0.53
1:F:201:GLY:O	1:F:204:ARG:HD3	2.08	0.53
1:F:302:ARG:O	1:F:306:ILE:HG13	2.08	0.53
1:G:141:CYS:O	1:G:204:ARG:NH2	2.30	0.53
1:G:242:LYS:O	1:G:246:GLU:HG3	2.08	0.53
1:G:302:ARG:HB3	1:G:370:ILE:CD1	2.31	0.53
1:A:151:ARG:NH1	1:H:151:ARG:HD2	2.23	0.53
1:C:318:GLY:N	1:C:323:ALA:HB2	2.23	0.53
1:D:313:GLN:HB3	1:D:334:LEU:HD23	1.90	0.53
1:F:242:LYS:O	1:F:246:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:ARG:HH11	1:C:369:ARG:CG	2.22	0.53
1:D:141:CYS:O	1:D:204:ARG:NH2	2.30	0.53
1:G:69:MET:CE	1:G:83:LEU:HD13	2.39	0.53
1:C:369:ARG:HG3	1:C:369:ARG:HH11	1.72	0.53
1:F:228:ASP:OD1	1:F:277:THR:CG2	2.57	0.53
1:B:228:ASP:OD1	1:B:277:THR:HG23	2.09	0.52
1:G:228:ASP:OD1	1:G:277:THR:HG23	2.08	0.52
1:B:112:ARG:O	1:B:113:SER:HB3	2.08	0.52
1:A:112:ARG:O	1:A:113:SER:HB3	2.09	0.52
1:A:264:TRP:CD2	1:D:12:SER:CB	2.93	0.52
1:E:69:MET:CE	1:E:83:LEU:HD13	2.39	0.52
1:C:228:ASP:OD1	1:C:277:THR:HG23	2.10	0.52
1:G:143:ARG:NH2	3:G:2014:HOH:O	2.43	0.52
1:H:143:ARG:NH2	3:H:2019:HOH:O	2.43	0.52
1:H:85:ASP:HB2	1:H:86:PRO:HD3	1.92	0.52
1:H:339:LYS:HE2	1:H:377:THR:OG1	2.10	0.52
1:B:311:ARG:NH1	1:B:376:HIS:ND1	2.57	0.52
1:D:112:ARG:O	1:D:113:SER:HB3	2.09	0.52
1:G:302:ARG:CB	1:G:370:ILE:HD11	2.34	0.52
1:B:179:GLN:O	1:B:183:ILE:HG13	2.11	0.52
1:G:5:ARG:HB3	1:G:5:ARG:NH1	2.25	0.52
1:A:303:PHE:N	1:A:304:PRO:HD2	2.25	0.51
1:D:97:PRO:HB2	1:D:271:ARG:NH1	2.26	0.51
1:F:316:GLY:HA2	1:F:324:ALA:CB	2.40	0.51
1:A:105:ASP:O	1:A:341:GLU:HG2	2.11	0.51
1:E:85:ASP:HB2	1:E:86:PRO:HD3	1.93	0.51
1:B:264:TRP:CD2	1:C:12:SER:CB	2.94	0.51
1:D:242:LYS:O	1:D:246:GLU:HG3	2.11	0.51
1:H:5:ARG:HH11	1:H:5:ARG:HG2	1.75	0.51
1:H:228:ASP:OD1	1:H:277:THR:HG23	2.11	0.51
1:D:323:ALA:O	1:D:324:ALA:HB3	2.11	0.51
1:H:311:ARG:HG3	1:H:374:VAL:CG2	2.41	0.51
1:A:97:PRO:HB2	1:A:271:ARG:NH1	2.26	0.51
1:A:375:ILE:O	1:A:375:ILE:HG13	2.10	0.51
1:D:69:MET:CE	1:D:83:LEU:HD13	2.40	0.51
1:D:311:ARG:HG3	1:D:374:VAL:HG11	1.92	0.51
1:F:5:ARG:CG	1:F:5:ARG:NH1	2.70	0.51
1:A:256:GLU:O	1:A:260:GLN:HG3	2.12	0.50
1:C:105:ASP:O	1:C:341:GLU:HG2	2.11	0.50
1:D:64:ILE:HD12	1:D:64:ILE:N	2.25	0.50
1:F:69:MET:CE	1:F:83:LEU:HD13	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:MET:CE	1:B:83:LEU:HD13	2.40	0.50
1:B:287:ARG:HG2	1:B:336:ARG:NH2	2.26	0.50
1:E:105:ASP:O	1:E:341:GLU:HG2	2.11	0.50
1:A:61:HIS:ND1	1:A:64:ILE:HD11	2.26	0.50
1:C:61:HIS:ND1	1:C:62:PRO:HD2	2.27	0.50
1:E:242:LYS:O	1:E:246:GLU:HG3	2.12	0.50
1:G:85:ASP:HB2	1:G:86:PRO:HD3	1.92	0.50
1:H:287:ARG:HG2	1:H:336:ARG:NH2	2.27	0.50
1:C:339:LYS:HG2	1:C:377:THR:HG21	1.94	0.50
1:E:309:ASN:ND2	1:E:371:PRO:O	2.31	0.50
1:C:242:LYS:O	1:C:246:GLU:HG3	2.11	0.50
1:D:228:ASP:OD1	1:D:277:THR:CG2	2.60	0.50
1:F:12:SER:HB2	1:G:264:TRP:CD2	2.47	0.50
1:G:97:PRO:HB2	1:G:271:ARG:NH1	2.27	0.50
1:G:204:ARG:O	1:G:210:ARG:NH2	2.41	0.50
1:H:61:HIS:NE2	1:H:63:PHE:HB2	2.27	0.50
1:D:105:ASP:O	1:D:341:GLU:HG2	2.12	0.50
1:E:320:VAL:HG23	1:E:321:ASP:H	1.77	0.50
1:B:143:ARG:NH2	3:B:2014:HOH:O	2.43	0.49
1:D:83:LEU:O	1:D:86:PRO:HD2	2.11	0.49
1:C:325:THR:HG23	1:C:326:GLY:N	2.27	0.49
1:E:294:LEU:N	1:E:327:GLY:O	2.41	0.49
1:B:85:ASP:HB2	1:B:86:PRO:HD3	1.95	0.49
1:C:100:MET:HA	1:C:378:LYS:HE2	1.94	0.49
1:E:2:ALA:O	1:E:3:SER:HB2	2.11	0.49
1:E:228:ASP:OD1	1:E:277:THR:HG23	2.13	0.49
1:E:287:ARG:HG2	1:E:336:ARG:NH2	2.28	0.49
1:G:287:ARG:HG2	1:G:336:ARG:NH2	2.26	0.49
1:D:85:ASP:HB2	1:D:86:PRO:HD3	1.94	0.49
1:B:97:PRO:HB2	1:B:271:ARG:NH1	2.28	0.49
1:D:270:GLU:HG2	3:D:2033:HOH:O	2.13	0.49
1:E:311:ARG:HG3	1:E:374:VAL:HG22	1.92	0.49
1:G:364:ARG:HB2	1:G:366:GLN:HG3	1.95	0.49
1:H:69:MET:CE	1:H:83:LEU:HD13	2.40	0.49
1:A:151:ARG:CD	1:H:151:ARG:HD3	2.41	0.49
1:E:3:SER:C	1:E:5:ARG:H	2.20	0.49
1:E:97:PRO:HB2	1:E:271:ARG:NH1	2.27	0.49
1:E:204:ARG:O	1:E:210:ARG:NH2	2.40	0.49
1:G:61:HIS:HB3	1:G:64:ILE:HG13	1.95	0.49
1:A:85:ASP:HB2	1:A:86:PRO:HD3	1.95	0.49
1:A:61:HIS:CD2	1:A:62:PRO:HD2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:CYS:O	1:B:204:ARG:NH2	2.29	0.48
1:H:97:PRO:HB2	1:H:271:ARG:NH1	2.28	0.48
1:F:97:PRO:HB2	1:F:271:ARG:NH1	2.28	0.48
1:H:138:PRO:HD2	1:H:277:THR:HG21	1.96	0.48
1:C:119:ARG:O	1:C:119:ARG:HG3	2.12	0.48
1:C:325:THR:CG2	1:C:328:VAL:HB	2.44	0.48
1:C:69:MET:CE	1:C:83:LEU:HD13	2.41	0.48
1:F:64:ILE:O	1:F:64:ILE:HG13	2.11	0.48
1:C:151:ARG:CZ	1:E:151:ARG:HD2	2.43	0.48
1:C:228:ASP:OD1	1:C:277:THR:CG2	2.61	0.48
1:C:287:ARG:HG2	1:C:336:ARG:NH2	2.28	0.48
1:A:264:TRP:CE3	1:D:12:SER:HB2	2.48	0.48
1:C:64:ILE:O	1:C:64:ILE:HD12	2.14	0.48
1:A:242:LYS:O	1:A:246:GLU:HG3	2.13	0.48
1:G:61:HIS:HD2	1:G:62:PRO:CD	2.27	0.48
1:H:204:ARG:O	1:H:210:ARG:NH2	2.41	0.48
1:A:228:ASP:OD1	1:A:277:THR:CG2	2.62	0.48
1:D:46:TRP:CZ3	1:D:140:ALA:HB2	2.49	0.48
1:C:97:PRO:HB2	1:C:271:ARG:NH1	2.28	0.47
1:C:317:THR:HG22	1:C:319:GLY:H	1.77	0.47
1:B:46:TRP:CE3	1:B:140:ALA:HB2	2.50	0.47
1:B:242:LYS:O	1:B:246:GLU:HG3	2.14	0.47
1:E:374:VAL:O	1:E:374:VAL:HG23	2.14	0.47
1:H:157:LEU:HD13	1:H:213:TRP:CG	2.50	0.47
1:G:293:LYS:O	1:G:294:LEU:HD23	2.14	0.47
1:D:347:LEU:HD23	1:D:347:LEU:C	2.39	0.47
1:F:339:LYS:HE2	1:F:376:HIS:CG	2.49	0.47
1:F:354:TYR:OH	1:F:369:ARG:O	2.31	0.47
1:G:112:ARG:O	1:G:113:SER:HB3	2.14	0.47
1:B:46:TRP:CZ3	1:B:140:ALA:HB2	2.50	0.47
1:D:11:PRO:HD3	1:E:6:ARG:HH12	1.79	0.47
1:F:85:ASP:HB2	1:F:86:PRO:HD3	1.96	0.47
1:H:242:LYS:O	1:H:246:GLU:HG3	2.14	0.47
1:A:264:TRP:CD2	1:D:12:SER:HB2	2.49	0.47
1:A:297:LEU:HG	1:A:303:PHE:CD1	2.50	0.47
1:C:119:ARG:HG2	1:C:120:TYR:CE2	2.49	0.47
1:F:321:ASP:OD2	1:F:325:THR:HA	2.15	0.47
1:G:125:ARG:NH2	2:G:400:PO4:O1	2.44	0.47
1:G:228:ASP:OD1	1:G:277:THR:CG2	2.63	0.47
1:E:83:LEU:O	1:E:86:PRO:HD2	2.15	0.47
1:B:316:GLY:C	1:B:318:GLY:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:293:LYS:HG2	1:G:328:VAL:HG22	1.97	0.47
1:C:3:SER:C	1:C:5:ARG:N	2.73	0.47
1:E:323:ALA:O	1:E:324:ALA:HB2	2.15	0.47
1:A:138:PRO:HD2	1:A:277:THR:HG21	1.96	0.46
1:A:287:ARG:HG2	1:A:336:ARG:NH2	2.31	0.46
1:B:246:GLU:HB3	3:B:2030:HOH:O	2.14	0.46
1:E:138:PRO:HD2	1:E:277:THR:HG21	1.98	0.46
1:H:378:LYS:O	1:H:379:HIS:HB3	2.14	0.46
1:A:179:GLN:O	1:A:183:ILE:HG13	2.15	0.46
1:C:339:LYS:HE2	1:C:377:THR:HG1	1.81	0.46
1:A:294:LEU:HD23	1:A:359:GLU:HG3	1.98	0.46
1:B:204:ARG:O	1:B:210:ARG:NH2	2.41	0.46
1:B:264:TRP:CD2	1:C:12:SER:HB2	2.51	0.46
1:C:339:LYS:HG2	1:C:377:THR:CG2	2.45	0.46
1:G:294:LEU:O	1:G:298:SER:HB3	2.15	0.46
1:A:217:GLU:HG2	3:A:2031:HOH:O	2.16	0.46
1:D:63:PHE:C	1:D:64:ILE:HG13	2.40	0.46
1:G:4:GLU:O	1:G:4:GLU:HG3	2.15	0.46
1:G:61:HIS:HB3	1:G:64:ILE:CG1	2.46	0.46
1:F:287:ARG:HG2	1:F:336:ARG:NH2	2.31	0.46
1:B:228:ASP:OD1	1:B:277:THR:CG2	2.64	0.46
1:G:157:LEU:HD13	1:G:213:TRP:CG	2.51	0.46
1:H:361:ARG:NH1	1:H:367:ASP:O	2.49	0.46
1:D:143:ARG:NH2	3:D:2019:HOH:O	2.49	0.45
1:D:204:ARG:O	1:D:210:ARG:NH2	2.44	0.45
1:E:119:ARG:CG	1:E:120:TYR:CE2	3.00	0.45
1:A:204:ARG:O	1:A:210:ARG:NH2	2.39	0.45
1:B:210:ARG:HD2	1:B:225:ASN:O	2.16	0.45
1:A:347:LEU:C	1:A:347:LEU:HD23	2.41	0.45
1:C:61:HIS:HB3	1:C:64:ILE:CG1	2.46	0.45
1:F:210:ARG:HD2	1:F:225:ASN:O	2.16	0.45
1:G:295:PRO:HD2	1:G:359:GLU:OE2	2.15	0.45
1:F:12:SER:HB3	1:G:264:TRP:CD2	2.52	0.45
1:F:41:THR:HG23	1:F:42:THR:O	2.16	0.45
1:H:117:ASP:OD1	1:H:119:ARG:HD3	2.16	0.45
1:B:151:ARG:NH1	1:B:151:ARG:CG	2.78	0.45
1:B:361:ARG:NH1	1:B:367:ASP:O	2.50	0.45
1:D:287:ARG:HG2	1:D:336:ARG:NH2	2.31	0.45
1:H:355:LEU:HD12	1:H:355:LEU:HA	1.78	0.45
1:C:210:ARG:HD2	1:C:225:ASN:O	2.15	0.45
1:H:357:ASP:O	1:H:361:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:ASP:OD2	1:C:231:ARG:NH1	2.49	0.45
1:F:157:LEU:HD13	1:F:213:TRP:CG	2.52	0.45
1:A:69:MET:CE	1:A:83:LEU:HD13	2.45	0.45
1:G:64:ILE:HG13	1:G:64:ILE:O	2.17	0.45
1:B:83:LEU:O	1:B:86:PRO:HD2	2.17	0.45
1:E:31:PRO:HB3	1:H:263:GLY:O	2.17	0.45
1:E:167:ARG:HG3	1:E:167:ARG:NH1	2.32	0.45
1:E:293:LYS:C	1:E:295:PRO:HD3	2.41	0.45
1:G:347:LEU:C	1:G:347:LEU:HD23	2.42	0.45
1:F:83:LEU:O	1:F:86:PRO:HD2	2.18	0.44
1:E:228:ASP:OD1	1:E:277:THR:CG2	2.65	0.44
1:H:83:LEU:O	1:H:86:PRO:HD2	2.18	0.44
1:H:347:LEU:C	1:H:347:LEU:HD23	2.43	0.44
1:B:61:HIS:HD2	1:B:62:PRO:CD	2.30	0.44
1:C:151:ARG:NE	1:E:151:ARG:HD2	2.33	0.44
1:C:157:LEU:HD13	1:C:213:TRP:CG	2.52	0.44
1:F:167:ARG:HG3	1:F:167:ARG:NH1	2.29	0.44
1:D:46:TRP:CE3	1:D:140:ALA:HB2	2.52	0.44
1:E:316:GLY:HA3	1:E:322:THR:HB	2.00	0.44
1:F:354:TYR:CE1	1:F:371:PRO:HD3	2.52	0.44
1:H:210:ARG:HD2	1:H:225:ASN:O	2.17	0.44
1:H:228:ASP:OD1	1:H:277:THR:CG2	2.65	0.44
1:D:167:ARG:HG3	1:D:167:ARG:NH1	2.31	0.44
1:F:12:SER:HB2	1:G:264:TRP:CE3	2.52	0.44
1:H:320:VAL:HG23	1:H:321:ASP:H	1.82	0.44
1:C:61:HIS:HB3	1:C:64:ILE:CD1	2.47	0.44
1:C:204:ARG:O	1:C:210:ARG:NH2	2.42	0.44
1:D:306:ILE:HG12	1:D:371:PRO:HD2	2.00	0.44
1:A:19:ARG:HD3	1:C:261:GLU:HG2	2.00	0.44
1:B:347:LEU:HD23	1:B:347:LEU:C	2.43	0.44
1:C:61:HIS:CE1	1:C:63:PHE:HB2	2.53	0.44
1:F:46:TRP:CZ3	1:F:140:ALA:HB2	2.53	0.44
1:H:175:THR:OG1	1:H:178:GLU:HG3	2.18	0.44
1:A:41:THR:HG23	1:A:42:THR:O	2.17	0.44
1:A:151:ARG:NH1	1:H:151:ARG:HD3	2.33	0.44
1:D:41:THR:HG23	1:D:42:THR:O	2.18	0.44
1:E:157:LEU:HD13	1:E:213:TRP:CG	2.52	0.44
1:G:360:ARG:HA	1:G:363:GLU:OE1	2.17	0.44
1:B:374:VAL:O	1:B:375:ILE:C	2.61	0.44
1:E:317:THR:HG23	1:E:318:GLY:N	2.33	0.44
1:H:46:TRP:CZ3	1:H:140:ALA:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:6:ARG:HG3	1:H:6:ARG:HH11	1.81	0.43
1:B:61:HIS:CD2	1:B:62:PRO:CD	3.01	0.43
1:B:167:ARG:HG3	1:B:167:ARG:NH1	2.32	0.43
1:C:347:LEU:C	1:C:347:LEU:HD23	2.44	0.43
1:F:347:LEU:C	1:F:347:LEU:HD23	2.43	0.43
1:D:376:HIS:ND1	1:D:376:HIS:N	2.66	0.43
1:A:167:ARG:HG3	1:A:167:ARG:NH1	2.32	0.43
1:B:375:ILE:HG22	1:B:376:HIS:N	2.33	0.43
1:D:157:LEU:HD13	1:D:213:TRP:CG	2.53	0.43
1:F:46:TRP:CE3	1:F:140:ALA:HB2	2.53	0.43
1:C:175:THR:OG1	1:C:178:GLU:HG3	2.19	0.43
1:B:175:THR:OG1	1:B:178:GLU:HG3	2.19	0.43
1:F:167:ARG:HH11	1:F:167:ARG:CG	2.31	0.43
1:F:360:ARG:HG2	1:F:360:ARG:HH11	1.83	0.43
1:G:46:TRP:CZ3	1:G:140:ALA:HB2	2.54	0.43
1:G:138:PRO:HD2	1:G:277:THR:HG21	2.00	0.43
1:B:263:GLY:O	1:C:31:PRO:HB3	2.18	0.43
1:B:302:ARG:O	1:B:306:ILE:HG13	2.19	0.43
1:C:111:ILE:HD13	1:C:111:ILE:HA	1.82	0.43
1:F:138:PRO:HD2	1:F:277:THR:HG21	2.01	0.43
1:G:210:ARG:HD2	1:G:225:ASN:O	2.18	0.43
1:G:302:ARG:O	1:G:303:PHE:C	2.62	0.43
1:G:309:ASN:ND2	1:G:373:PRO:HG3	2.33	0.43
1:H:376:HIS:CD2	1:H:378:LYS:HD3	2.54	0.43
1:D:228:ASP:OD2	1:D:231:ARG:NH1	2.52	0.43
1:E:179:GLN:O	1:E:183:ILE:HG13	2.19	0.43
1:A:112:ARG:O	1:A:113:SER:CB	2.67	0.42
1:E:293:LYS:HA	1:E:327:GLY:O	2.19	0.42
1:E:347:LEU:C	1:E:347:LEU:HD23	2.44	0.42
1:H:46:TRP:CE3	1:H:140:ALA:HB2	2.54	0.42
1:A:185:ASP:O	1:A:186:HIS:HB2	2.18	0.42
1:C:339:LYS:CE	1:C:377:THR:OG1	2.67	0.42
1:D:217:GLU:HG2	3:D:2026:HOH:O	2.19	0.42
1:E:298:SER:HB2	1:E:329:PHE:CE1	2.53	0.42
1:E:307:LEU:HD11	1:E:355:LEU:HD21	2.00	0.42
1:F:236:GLU:HG3	1:F:247:ARG:HH22	1.84	0.42
1:F:376:HIS:C	1:F:378:LYS:H	2.27	0.42
1:G:100:MET:HE2	1:G:379:HIS:CE1	2.54	0.42
1:C:138:PRO:HD2	1:C:277:THR:HG21	2.02	0.42
1:C:364:ARG:HG3	1:C:366:GLN:HG3	2.00	0.42
1:H:179:GLN:O	1:H:183:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:HD2	1:A:225:ASN:O	2.19	0.42
1:B:143:ARG:O	1:B:147:ARG:HG3	2.19	0.42
1:E:119:ARG:HG2	1:E:120:TYR:CE2	2.55	0.42
1:G:307:LEU:HD12	1:G:307:LEU:HA	1.89	0.42
1:H:112:ARG:O	1:H:113:SER:CB	2.67	0.42
1:A:151:ARG:HD2	1:H:151:ARG:CD	2.46	0.42
1:A:151:ARG:HH11	1:H:151:ARG:CD	2.31	0.42
1:B:185:ASP:O	1:B:186:HIS:HB2	2.20	0.42
1:D:210:ARG:HD2	1:D:225:ASN:O	2.19	0.42
1:E:303:PHE:CE2	1:E:314:LYS:HD3	2.54	0.42
1:F:175:THR:OG1	1:F:178:GLU:HG3	2.20	0.42
1:A:157:LEU:HD13	1:A:213:TRP:CG	2.55	0.42
1:H:228:ASP:OD2	1:H:231:ARG:NH1	2.52	0.42
1:D:138:PRO:HD2	1:D:277:THR:HG21	2.00	0.42
1:F:316:GLY:HA2	1:F:324:ALA:HB1	2.00	0.42
1:H:376:HIS:HD2	1:H:378:LYS:HD3	1.84	0.42
1:B:21:HIS:CD2	1:B:59:PRO:HA	2.55	0.42
1:G:61:HIS:CD2	1:G:62:PRO:CD	3.03	0.42
1:A:228:ASP:OD2	1:A:231:ARG:NH1	2.53	0.42
1:A:300:ASP:OD1	1:A:301:SER:N	2.53	0.42
1:E:41:THR:HG23	1:E:42:THR:O	2.20	0.42
1:H:61:HIS:HB3	1:H:64:ILE:HD12	2.02	0.42
1:H:117:ASP:OD1	1:H:119:ARG:HD2	2.20	0.42
1:A:374:VAL:O	1:A:376:HIS:N	2.45	0.42
1:C:100:MET:CA	1:C:378:LYS:HE2	2.50	0.42
1:E:111:ILE:O	1:E:242:LYS:HE2	2.20	0.42
1:F:361:ARG:NH2	1:F:367:ASP:O	2.50	0.42
1:A:236:GLU:HG3	1:A:247:ARG:HH22	1.85	0.41
1:B:316:GLY:O	1:B:318:GLY:N	2.51	0.41
1:C:317:THR:HB	1:C:323:ALA:N	2.34	0.41
1:E:3:SER:C	1:E:5:ARG:N	2.78	0.41
1:F:12:SER:HB3	1:G:264:TRP:CE2	2.55	0.41
1:F:228:ASP:OD2	1:F:231:ARG:NH1	2.53	0.41
1:A:175:THR:OG1	1:A:178:GLU:HG3	2.18	0.41
1:E:210:ARG:HD2	1:E:225:ASN:O	2.21	0.41
1:G:37:LEU:HB2	1:G:48:LEU:HD22	2.02	0.41
1:H:311:ARG:HG3	1:H:374:VAL:HG22	2.00	0.41
1:A:119:ARG:HG2	1:A:119:ARG:O	2.19	0.41
1:B:157:LEU:HD13	1:B:213:TRP:CG	2.56	0.41
1:G:41:THR:HG23	1:G:42:THR:O	2.19	0.41
1:G:167:ARG:HG3	1:G:167:ARG:NH1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:296:LEU:N	1:E:296:LEU:HD12	2.35	0.41
1:H:41:THR:HG23	1:H:42:THR:O	2.20	0.41
1:H:119:ARG:HG2	1:H:120:TYR:CD2	2.55	0.41
1:C:46:TRP:CZ3	1:C:140:ALA:HB2	2.55	0.41
1:C:210:ARG:NH1	3:C:2023:HOH:O	2.54	0.41
1:E:364:ARG:HH11	1:E:364:ARG:HG2	1.86	0.41
1:H:117:ASP:OD2	1:H:360:ARG:NH2	2.54	0.41
1:C:41:THR:HG23	1:C:42:THR:O	2.21	0.41
1:C:101:LYS:H	1:C:378:LYS:CE	2.33	0.41
1:D:374:VAL:CG1	1:D:375:ILE:N	2.79	0.41
1:G:297:LEU:HD22	1:G:358:CYS:HB3	2.02	0.41
1:A:46:TRP:CZ3	1:A:140:ALA:HB2	2.56	0.41
1:D:95:TYR:CD2	1:D:337:LEU:HD13	2.56	0.41
1:E:175:THR:OG1	1:E:178:GLU:HG3	2.20	0.41
1:H:37:LEU:HB2	1:H:48:LEU:HD22	2.03	0.41
1:C:61:HIS:HE1	1:C:63:PHE:CD2	2.38	0.41
1:C:167:ARG:HG3	1:C:167:ARG:NH1	2.32	0.41
1:F:179:GLN:O	1:F:183:ILE:HG13	2.21	0.41
1:G:46:TRP:CE3	1:G:140:ALA:HB2	2.56	0.41
1:G:83:LEU:O	1:G:86:PRO:HD2	2.21	0.41
1:H:339:LYS:HE2	1:H:377:THR:CG2	2.50	0.41
1:A:83:LEU:O	1:A:86:PRO:HD2	2.21	0.41
1:C:37:LEU:HB2	1:C:48:LEU:HD22	2.03	0.41
1:F:309:ASN:ND2	1:F:373:PRO:HG3	2.36	0.41
1:H:254:GLU:OE2	1:H:257:ARG:NH2	2.23	0.41
1:B:307:LEU:HD12	1:B:307:LEU:HA	1.88	0.40
1:D:83:LEU:C	1:D:86:PRO:HD2	2.46	0.40
1:E:228:ASP:OD2	1:E:231:ARG:NH1	2.53	0.40
1:H:21:HIS:CD2	1:H:59:PRO:HA	2.57	0.40
1:E:74:GLU:HB2	1:E:267:MET:SD	2.61	0.40
1:F:122:LEU:HD21	1:F:293:LYS:HE2	2.03	0.40
1:A:64:ILE:HD13	1:A:64:ILE:N	2.31	0.40
1:E:12:SER:HB3	1:H:264:TRP:CD2	2.56	0.40
1:G:175:THR:OG1	1:G:178:GLU:HG3	2.20	0.40
1:C:163:ASP:OD2	1:C:250:ARG:NH2	2.55	0.40
1:D:37:LEU:HB2	1:D:48:LEU:HD22	2.03	0.40
1:E:46:TRP:CE3	1:E:140:ALA:HB2	2.57	0.40
1:F:12:SER:CB	1:G:264:TRP:CE2	3.05	0.40
1:F:324:ALA:O	1:F:325:THR:CB	2.68	0.40
1:G:228:ASP:OD2	1:G:231:ARG:NH1	2.54	0.40
1:B:293:LYS:HG2	1:B:328:VAL:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:174:MET:HE3	1:H:179:GLN:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	328/328 (100%)	308 (94%)	20 (6%)	17	40
1	B	328/328 (100%)	307 (94%)	21 (6%)	16	38
1	C	87/328 (26%)	85 (98%)	2 (2%)	44	73
1	D	243/328 (74%)	222 (91%)	21 (9%)	10	25
1	E	311/328 (95%)	289 (93%)	22 (7%)	13	33
1	F	328/328 (100%)	304 (93%)	24 (7%)	13	32
1	G	328/328 (100%)	306 (93%)	22 (7%)	15	36
1	H	328/328 (100%)	307 (94%)	21 (6%)	16	38
All	All	2281/2624 (87%)	2128 (93%)	153 (7%)	15	36

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	64	ILE
1	A	83	LEU
1	A	103	THR

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Mol	Chain	Res	Type
1	A	127	ARG
1	A	190	ASP
1	A	197	LEU
1	A	207	PRO
1	A	221	LEU
1	A	257	ARG
1	A	277	THR
1	A	282	LEU
1	A	287	ARG
1	A	307	LEU
1	A	336	ARG
1	A	337	LEU
1	A	341	GLU
1	A	355	LEU
1	A	367	ASP
1	A	369	ARG
1	B	41	THR
1	B	83	LEU
1	B	103	THR
1	B	127	ARG
1	B	190	ASP
1	B	197	LEU
1	B	207	PRO
1	B	221	LEU
1	B	257	ARG
1	B	277	THR
1	B	282	LEU
1	B	287	ARG
1	B	307	LEU
1	B	334	LEU
1	B	336	ARG
1	B	337	LEU
1	B	341	GLU
1	B	355	LEU
1	B	372	THR
1	B	377	THR
1	B	379	HIS
1	C	41	THR
1	C	83	LEU
1	D	127	ARG
1	D	151	ARG
1	D	190	ASP

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Mol	Chain	Res	Type
1	D	197	LEU
1	D	207	PRO
1	D	221	LEU
1	D	257	ARG
1	D	277	THR
1	D	282	LEU
1	D	287	ARG
1	D	307	LEU
1	D	320	VAL
1	D	334	LEU
1	D	336	ARG
1	D	337	LEU
1	D	341	GLU
1	D	355	LEU
1	D	369	ARG
1	D	373	PRO
1	D	374	VAL
1	D	376	HIS
1	E	61	HIS
1	E	83	LEU
1	E	103	THR
1	E	119	ARG
1	E	127	ARG
1	E	190	ASP
1	E	197	LEU
1	E	207	PRO
1	E	221	LEU
1	E	257	ARG
1	E	277	THR
1	E	282	LEU
1	E	287	ARG
1	E	299	LYS
1	E	307	LEU
1	E	336	ARG
1	E	337	LEU
1	E	341	GLU
1	E	355	LEU
1	E	369	ARG
1	E	372	THR
1	E	377	THR
1	F	5	ARG
1	F	41	THR

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Mol	Chain	Res	Type
1	F	83	LEU
1	F	103	THR
1	F	127	ARG
1	F	151	ARG
1	F	190	ASP
1	F	197	LEU
1	F	207	PRO
1	F	221	LEU
1	F	257	ARG
1	F	277	THR
1	F	282	LEU
1	F	287	ARG
1	F	305	LYS
1	F	307	LEU
1	F	322	THR
1	F	334	LEU
1	F	336	ARG
1	F	337	LEU
1	F	341	GLU
1	F	355	LEU
1	F	362	LEU
1	F	369	ARG
1	G	5	ARG
1	G	41	THR
1	G	83	LEU
1	G	103	THR
1	G	119	ARG
1	G	127	ARG
1	G	190	ASP
1	G	197	LEU
1	G	207	PRO
1	G	221	LEU
1	G	257	ARG
1	G	277	THR
1	G	282	LEU
1	G	287	ARG
1	G	305	LYS
1	G	307	LEU
1	G	321	ASP
1	G	336	ARG
1	G	337	LEU
1	G	341	GLU

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Mol	Chain	Res	Type
1	G	369	ARG
1	G	378	LYS
1	H	41	THR
1	H	83	LEU
1	H	103	THR
1	H	119	ARG
1	H	127	ARG
1	H	190	ASP
1	H	197	LEU
1	H	207	PRO
1	H	221	LEU
1	H	257	ARG
1	H	277	THR
1	H	282	LEU
1	H	287	ARG
1	H	307	LEU
1	H	336	ARG
1	H	337	LEU
1	H	341	GLU
1	H	355	LEU
1	H	357	ASP
1	H	360	ARG
1	H	374	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	179	GLN
1	A	240	ASN
1	A	366	GLN
1	A	376	HIS
1	B	58	ASN
1	B	61	HIS
1	B	179	GLN
1	B	240	ASN
1	B	260	GLN
1	B	366	GLN
1	C	58	ASN
1	D	179	GLN
1	D	240	ASN
1	E	58	ASN

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Mol	Chain	Res	Type
1	E	61	HIS
1	E	179	GLN
1	E	240	ASN
1	E	366	GLN
1	E	379	HIS
1	F	179	GLN
1	F	240	ASN
1	F	291	HIS
1	G	50	GLN
1	G	179	GLN
1	G	240	ASN
1	G	309	ASN
1	G	366	GLN
1	G	379	HIS
1	H	58	ASN
1	H	179	GLN
1	H	240	ASN
1	H	260	GLN
1	H	291	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	D	400	-	4,4,4	1.78	1 (25%)	6,6,6	0.44	0
2	PO4	B	400	-	4,4,4	1.64	1 (25%)	6,6,6	0.42	0
2	PO4	H	400	-	4,4,4	1.62	1 (25%)	6,6,6	0.46	0
2	PO4	C	400	-	4,4,4	1.65	0	6,6,6	0.48	0
2	PO4	A	400	-	4,4,4	1.75	2 (50%)	6,6,6	0.44	0
2	PO4	F	400	-	4,4,4	1.71	1 (25%)	6,6,6	0.44	0
2	PO4	E	400	-	4,4,4	1.61	0	6,6,6	0.46	0
2	PO4	G	400	-	4,4,4	1.66	0	6,6,6	0.47	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	400	PO4	P-O4	-2.28	1.48	1.54
2	B	400	PO4	P-O4	-2.18	1.48	1.54
2	D	400	PO4	P-O4	-2.17	1.48	1.54
2	A	400	PO4	P-O2	-2.16	1.48	1.54
2	F	400	PO4	P-O4	-2.14	1.48	1.54
2	A	400	PO4	P-O3	-2.07	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	400	PO4	1	0

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	379/379 (100%)	0.07	24 (6%)	26	23	23, 41, 84, 100	0
1	B	379/379 (100%)	0.05	22 (5%)	29	25	23, 40, 87, 100	0
1	C	379/379 (100%)	0.11	26 (6%)	23	20	23, 40, 84, 100	0
1	D	379/379 (100%)	0.06	21 (5%)	30	27	22, 41, 89, 100	0
1	E	379/379 (100%)	0.14	23 (6%)	27	24	23, 41, 88, 100	0
1	F	379/379 (100%)	0.07	24 (6%)	26	23	23, 40, 90, 100	0
1	G	379/379 (100%)	0.20	27 (7%)	22	19	24, 44, 97, 100	0
1	H	379/379 (100%)	0.05	22 (5%)	29	25	23, 40, 85, 100	0
All	All	3032/3032 (100%)	0.09	189 (6%)	26	23	22, 41, 91, 100	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	375	ILE	10.8
1	D	320	VAL	9.1
1	B	2	ALA	8.4
1	H	320	VAL	7.8
1	D	377	THR	7.7
1	C	320	VAL	7.5
1	A	1	ALA	7.4
1	H	377	THR	7.4
1	F	320	VAL	7.2
1	C	379	HIS	7.1
1	E	377	THR	7.1
1	G	324	ALA	6.9
1	H	376	HIS	6.9
1	A	377	THR	6.7
1	C	378	LYS	6.3
1	B	321	ASP	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	320	VAL	6.3
1	B	377	THR	6.3
1	F	2	ALA	6.3
1	H	323	ALA	6.3
1	A	322	THR	6.2
1	C	376	HIS	6.2
1	F	323	ALA	6.2
1	H	319	GLY	6.1
1	E	320	VAL	6.1
1	G	2	ALA	6.1
1	B	323	ALA	6.0
1	D	323	ALA	6.0
1	E	376	HIS	6.0
1	B	320	VAL	6.0
1	B	322	THR	5.8
1	H	324	ALA	5.8
1	B	379	HIS	5.8
1	E	379	HIS	5.7
1	A	323	ALA	5.6
1	C	322	THR	5.6
1	H	379	HIS	5.6
1	D	322	THR	5.6
1	G	320	VAL	5.5
1	C	375	ILE	5.5
1	C	323	ALA	5.5
1	H	2	ALA	5.4
1	F	376	HIS	5.4
1	A	375	ILE	5.3
1	D	376	HIS	5.2
1	G	1	ALA	5.2
1	G	378	LYS	5.2
1	G	115	TYR	5.0
1	C	2	ALA	5.0
1	E	319	GLY	5.0
1	C	324	ALA	4.9
1	G	377	THR	4.9
1	A	324	ALA	4.9
1	B	376	HIS	4.9
1	E	378	LYS	4.9
1	D	321	ASP	4.9
1	B	324	ALA	4.8
1	E	375	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	F	1	ALA	4.8
1	G	375	ILE	4.7
1	D	378	LYS	4.7
1	C	377	THR	4.7
1	H	321	ASP	4.7
1	B	375	ILE	4.7
1	H	1	ALA	4.6
1	B	319	GLY	4.6
1	F	379	HIS	4.6
1	A	378	LYS	4.5
1	H	318	GLY	4.5
1	G	376	HIS	4.5
1	F	324	ALA	4.5
1	F	319	GLY	4.5
1	F	375	ILE	4.5
1	C	1	ALA	4.4
1	C	319	GLY	4.4
1	C	321	ASP	4.3
1	D	319	GLY	4.3
1	G	323	ALA	4.3
1	D	2	ALA	4.3
1	F	322	THR	4.2
1	H	325	THR	4.2
1	G	379	HIS	4.1
1	D	1	ALA	4.1
1	F	3	SER	4.1
1	B	378	LYS	4.1
1	B	3	SER	4.0
1	B	325	THR	4.0
1	H	378	LYS	4.0
1	F	377	THR	4.0
1	A	376	HIS	4.0
1	E	321	ASP	4.0
1	E	112	ARG	4.0
1	F	325	THR	3.9
1	A	319	GLY	3.9
1	G	319	GLY	3.9
1	D	3	SER	3.8
1	E	325	THR	3.7
1	G	321	ASP	3.7
1	A	379	HIS	3.6
1	D	317	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	1	ALA	3.5
1	G	322	THR	3.5
1	H	322	THR	3.5
1	D	324	ALA	3.5
1	G	3	SER	3.5
1	D	379	HIS	3.5
1	D	318	GLY	3.4
1	E	2	ALA	3.4
1	C	115	TYR	3.4
1	D	325	THR	3.4
1	B	318	GLY	3.4
1	F	318	GLY	3.3
1	C	326	GLY	3.3
1	B	317	THR	3.2
1	F	4	GLU	3.2
1	G	318	GLY	3.2
1	H	375	ILE	3.1
1	F	63	PHE	3.1
1	C	318	GLY	3.1
1	C	112	ARG	3.0
1	A	317	THR	2.9
1	A	325	THR	2.9
1	C	61	HIS	2.9
1	H	112	ARG	2.9
1	H	115	TYR	2.9
1	A	318	GLY	2.9
1	H	326	GLY	2.9
1	B	1	ALA	2.9
1	H	365	GLY	2.8
1	C	374	VAL	2.8
1	D	63	PHE	2.8
1	E	374	VAL	2.8
1	B	63	PHE	2.8
1	A	2	ALA	2.7
1	G	4	GLU	2.7
1	A	93	ASN	2.7
1	G	63	PHE	2.7
1	E	115	TYR	2.7
1	F	115	TYR	2.7
1	F	321	ASP	2.7
1	G	329	PHE	2.7
1	A	364	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	318	GLY	2.6
1	F	378	LYS	2.6
1	A	321	ASP	2.6
1	G	112	ARG	2.6
1	G	325	THR	2.6
1	A	115	TYR	2.6
1	H	317	THR	2.6
1	E	63	PHE	2.6
1	B	374	VAL	2.5
1	F	317	THR	2.5
1	A	5	ARG	2.5
1	H	5	ARG	2.5
1	C	317	THR	2.5
1	H	3	SER	2.5
1	D	374	VAL	2.5
1	F	5	ARG	2.4
1	A	112	ARG	2.4
1	B	316	GLY	2.4
1	A	63	PHE	2.4
1	G	61	HIS	2.3
1	C	4	GLU	2.3
1	D	112	ARG	2.3
1	B	115	TYR	2.3
1	E	322	THR	2.3
1	G	374	VAL	2.3
1	E	328	VAL	2.3
1	G	120	TYR	2.3
1	C	5	ARG	2.3
1	E	4	GLU	2.2
1	A	3	SER	2.2
1	B	61	HIS	2.2
1	C	369	ARG	2.2
1	C	325	THR	2.2
1	D	5	ARG	2.2
1	F	64	ILE	2.2
1	E	317	THR	2.1
1	G	296	LEU	2.1
1	E	3	SER	2.1
1	C	327	GLY	2.1
1	G	317	THR	2.1
1	E	327	GLY	2.1
1	F	326	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	63	PHE	2.1
1	E	5	ARG	2.0
1	A	327	GLY	2.0
1	G	326	GLY	2.0
1	F	61	HIS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PO4	B	400	5/5	0.93	0.08	49,50,53,53	0
2	PO4	G	400	5/5	0.93	0.10	76,77,77,78	0
2	PO4	H	400	5/5	0.93	0.10	60,62,62,63	0
2	PO4	C	400	5/5	0.95	0.10	67,68,69,69	0
2	PO4	D	400	5/5	0.95	0.10	58,59,60,61	0
2	PO4	A	400	5/5	0.96	0.08	52,54,54,56	0
2	PO4	F	400	5/5	0.96	0.10	56,58,58,59	0
2	PO4	E	400	5/5	0.97	0.09	52,52,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.