



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:41 PM UTC

PDB ID : 3GYR / pdb_00003gyr
Title : Structure of Phenoxazinone synthase from Streptomyces antibioticus reveals a new type 2 copper center.
Authors : Smith, A.W.; Camara-Artigas, A.; Wang, M.; Francisco, W.A.; Allen, J.P.
Deposited on : 2009-04-05
Resolution : 2.30 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

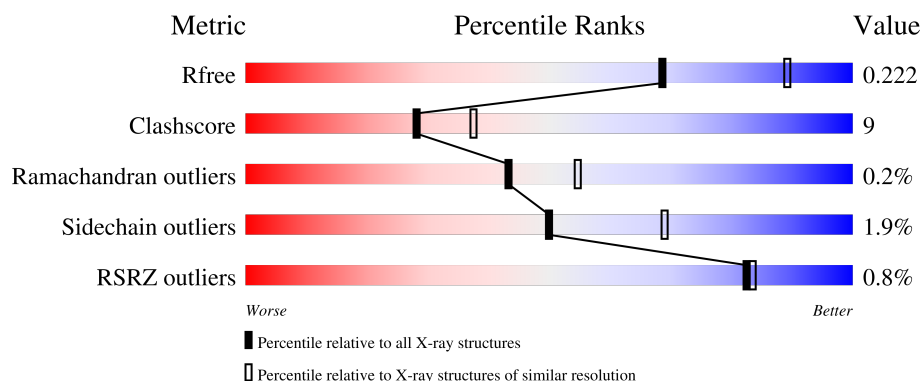
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	612	76% 19% • •
1	B	612	80% 16% •
1	C	612	84% 11% • •
1	D	612	81% 15% •
1	E	612	82% 13% • •

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Mol	Chain	Length	Quality of chain
1	F	612	% 79% 16%
1	G	612	% 79% 16%
1	H	612	77% 17%
1	I	612	% 75% 20%
1	J	612	% 79% 15%
1	K	612	77% 18%
1	L	612	78% 17%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 59241 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 Phenoxazinone synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	B	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	C	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	D	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	E	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	F	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	G	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	H	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	I	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	J	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	K	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			
1	L	587	Total	C	N	O	S	0	0	0
			4560	2886	812	847	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	496	ARG	ALA	engineered mutation	UNP Q53692
B	496	ARG	ALA	engineered mutation	UNP Q53692
C	496	ARG	ALA	engineered mutation	UNP Q53692
D	496	ARG	ALA	engineered mutation	UNP Q53692
E	496	ARG	ALA	engineered mutation	UNP Q53692

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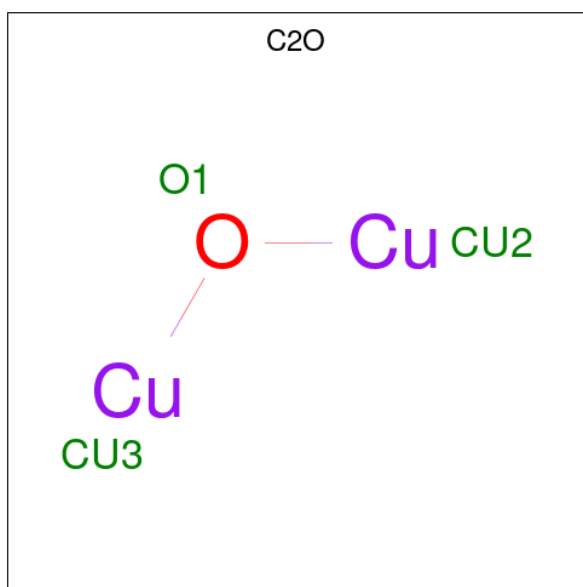
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Chain	Residue	Modelled	Actual	Comment	Reference
F	496	ARG	ALA	engineered mutation	UNP Q53692
G	496	ARG	ALA	engineered mutation	UNP Q53692
H	496	ARG	ALA	engineered mutation	UNP Q53692
I	496	ARG	ALA	engineered mutation	UNP Q53692
J	496	ARG	ALA	engineered mutation	UNP Q53692
K	496	ARG	ALA	engineered mutation	UNP Q53692
L	496	ARG	ALA	engineered mutation	UNP Q53692

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Cu 3 3	0	0
2	B	3	Total Cu 3 3	0	0
2	C	3	Total Cu 3 3	0	0
2	D	3	Total Cu 3 3	0	0
2	E	3	Total Cu 3 3	0	0
2	F	3	Total Cu 3 3	0	0
2	G	3	Total Cu 3 3	0	0
2	H	3	Total Cu 3 3	0	0
2	I	3	Total Cu 3 3	0	0
2	J	3	Total Cu 3 3	0	0
2	K	3	Total Cu 3 3	0	0
2	L	3	Total Cu 3 3	0	0

- Molecule 3 is CU-O-CU LINKAGE (CCD ID: C2O) (formula: Cu₂O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Cu	O	0	0
			3	2	1		
3	B	1	Total	Cu	O	0	0
			3	2	1		
3	C	1	Total	Cu	O	0	0
			3	2	1		
3	D	1	Total	Cu	O	0	0
			3	2	1		
3	E	1	Total	Cu	O	0	0
			3	2	1		
3	F	1	Total	Cu	O	0	0
			3	2	1		
3	G	1	Total	Cu	O	0	0
			3	2	1		
3	H	1	Total	Cu	O	0	0
			3	2	1		
3	I	1	Total	Cu	O	0	0
			3	2	1		
3	J	1	Total	Cu	O	0	0
			3	2	1		
3	K	1	Total	Cu	O	0	0
			3	2	1		
3	L	1	Total	Cu	O	0	0
			3	2	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

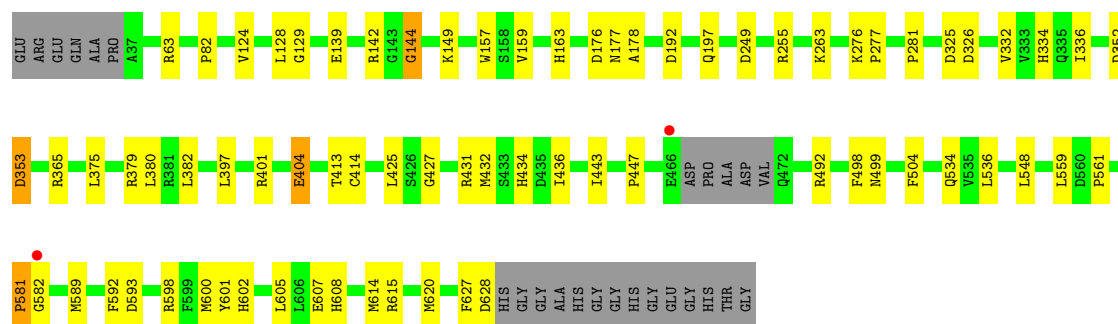


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		
4	K	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

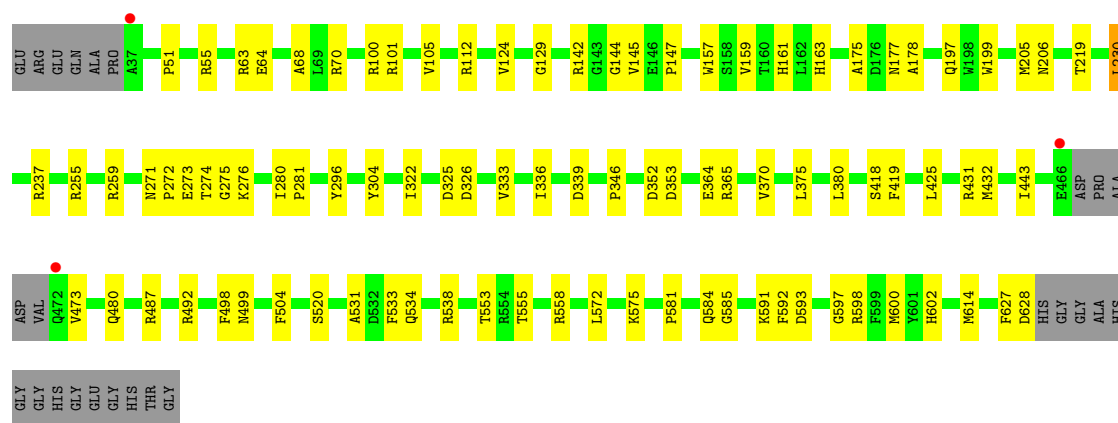
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	354	Total 354	O 354	0	0
5	B	362	Total 362	O 362	0	0
5	C	398	Total 398	O 398	0	0
5	D	386	Total 386	O 386	0	0
5	E	357	Total 357	O 357	0	0
5	F	361	Total 361	O 361	0	0
5	G	359	Total 359	O 359	0	0
5	H	376	Total 376	O 376	0	0
5	I	330	Total 330	O 330	0	0
5	J	388	Total 388	O 388	0	0
5	K	359	Total 359	O 359	0	0
5	L	347	Total 347	O 347	0	0

Chain C:  84% 11% . .



• Molecule 1: Phenoxazinone synthase

Chain D:  81% 15% .



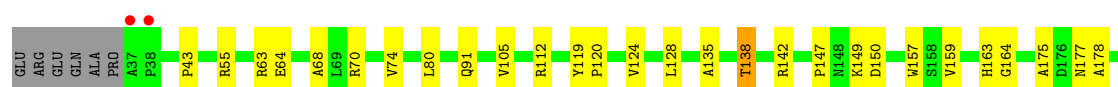
• Molecule 1: Phenoxazinone synthase

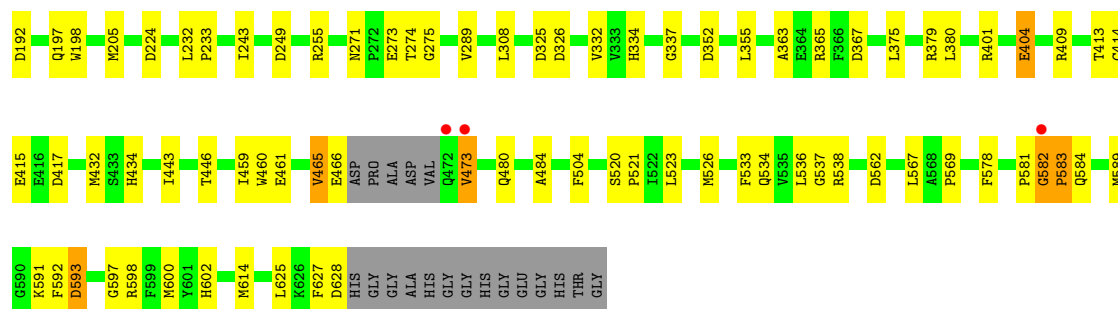
Chain E:  82% 13% . .

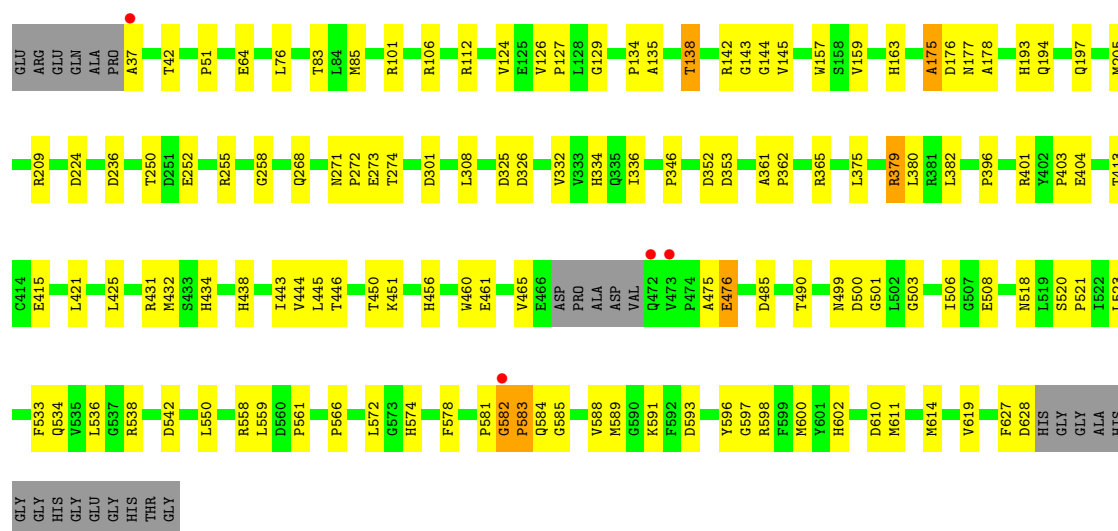


• Molecule 1: Phenoxazinone synthase

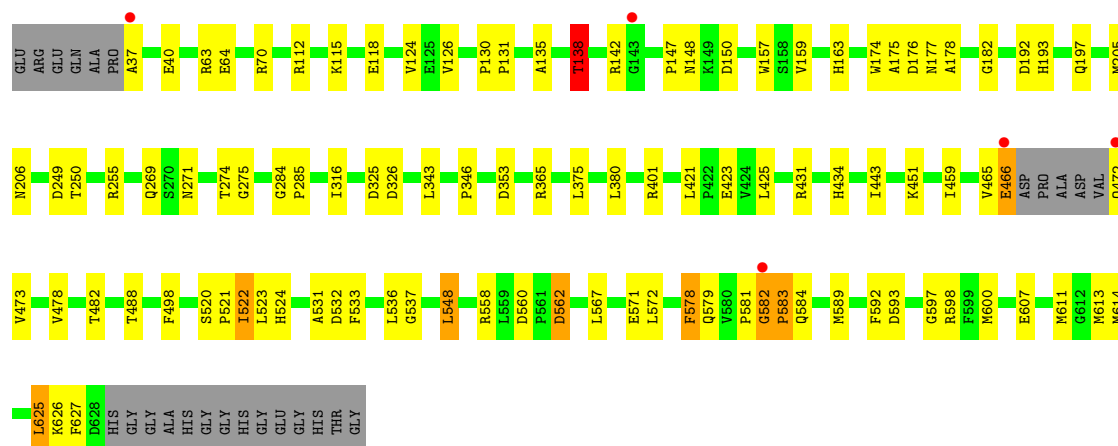
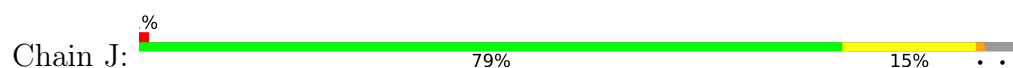
Chain F:  79% 16% . .



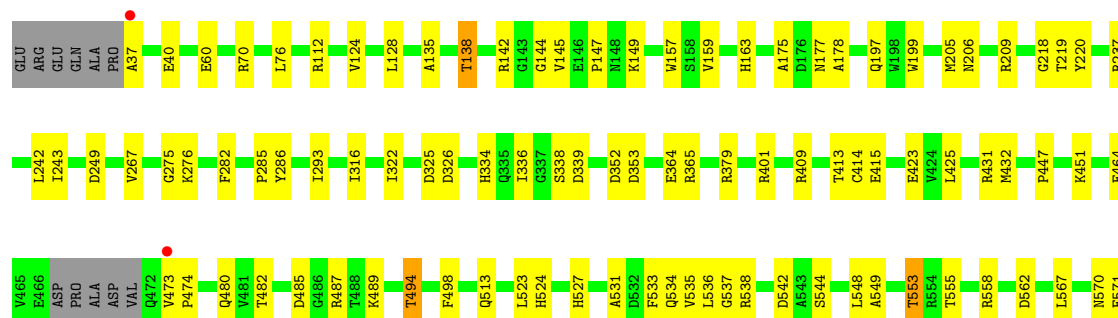
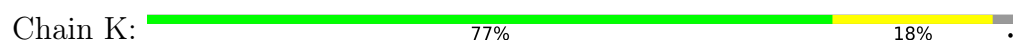


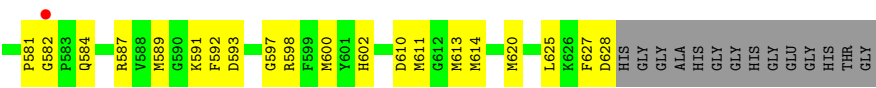


• Molecule 1: Phenoxazinone synthase

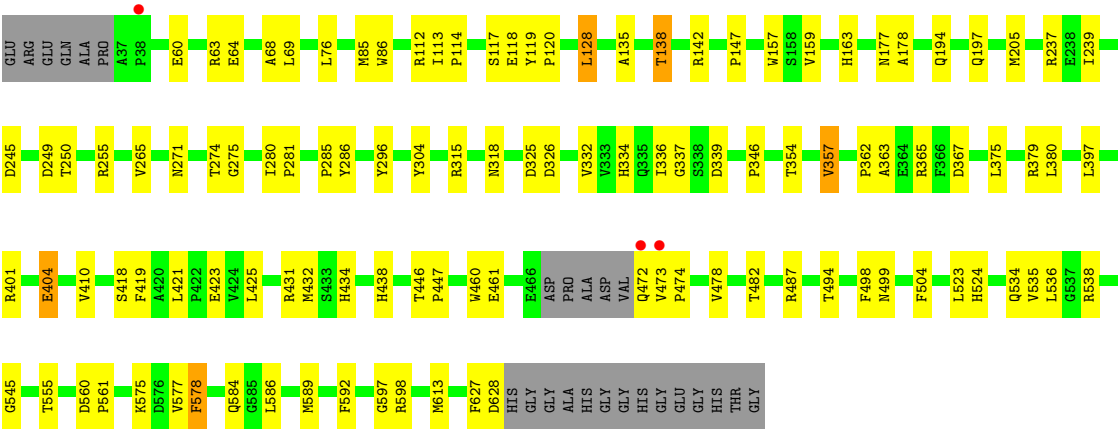
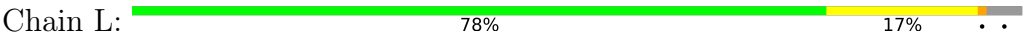


• Molecule 1: Phenoxazinone synthase





● Molecule 1: Phenoxazinone synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	109.49Å 163.46Å 164.35Å 117.04° 95.74° 107.23°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	86.3 (20.00-2.30) 86.2 (20.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.5.0072, CNS	Depositor
R, R_{free}	0.165 , 0.222 0.165 , 0.222	Depositor DCC
R_{free} test set	17920 reflections (4.33%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for -h,h+k+l,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	59241	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: C2O, GOL, CU

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	0.81	0/4697	0.97	6/6423 (0.1%)
1	B	0.83	0/4697	0.96	3/6423 (0.0%)
1	C	0.86	0/4697	0.97	4/6423 (0.1%)
1	D	0.86	1/4697 (0.0%)	0.95	5/6423 (0.1%)
1	E	0.83	0/4697	0.97	10/6423 (0.2%)
1	F	0.84	0/4697	0.96	4/6423 (0.1%)
1	G	0.84	0/4697	0.98	2/6423 (0.0%)
1	H	0.84	1/4697 (0.0%)	0.96	5/6423 (0.1%)
1	I	0.84	2/4697 (0.0%)	0.96	6/6423 (0.1%)
1	J	0.84	0/4697	0.97	9/6423 (0.1%)
1	K	0.82	0/4697	0.95	3/6423 (0.0%)
1	L	0.82	2/4697 (0.0%)	0.97	3/6423 (0.0%)
All	All	0.84	6/56364 (0.0%)	0.96	60/77076 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	5
1	D	0	5
1	E	0	2
1	F	0	4
1	G	0	2
1	H	0	2
1	I	0	1
1	J	0	3
1	K	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
All	All	0	37

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	421	LEU	C-O	-5.61	1.19	1.25
1	H	239	ILE	CA-CB	5.52	1.58	1.54
1	I	51	PRO	CA-C	5.52	1.54	1.51
1	D	51	PRO	CA-C	5.33	1.54	1.51
1	L	421	LEU	C-O	-5.11	1.20	1.25
1	L	239	ILE	CA-CB	5.03	1.58	1.54

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	LEU	N-CA-C	8.07	119.71	111.07
1	B	128	LEU	N-CA-C	7.70	120.34	111.11
1	E	284	GLY	CA-C-N	7.68	127.40	119.64
1	E	284	GLY	C-N-CA	7.68	127.40	119.64
1	K	128	LEU	N-CA-C	7.45	120.05	111.11
1	H	128	LEU	N-CA-C	7.29	120.15	111.33
1	A	446	THR	CA-C-N	7.18	124.83	119.66
1	A	446	THR	C-N-CA	7.18	124.83	119.66
1	F	128	LEU	N-CA-C	7.18	119.72	111.11
1	L	128	LEU	N-CA-C	7.16	119.99	111.33
1	G	70	ARG	CA-C-N	-6.75	113.35	120.03
1	G	70	ARG	C-N-CA	-6.75	113.35	120.03
1	E	128	LEU	N-CA-C	6.59	119.06	111.02
1	J	562	ASP	N-CA-C	-6.46	105.70	113.97
1	I	129	GLY	CA-C-N	6.42	124.35	119.66
1	I	129	GLY	C-N-CA	6.42	124.35	119.66
1	A	112	ARG	CA-C-N	-6.31	118.31	122.60
1	A	112	ARG	C-N-CA	-6.31	118.31	122.60
1	I	145	VAL	N-CA-C	6.03	117.35	109.58
1	D	145	VAL	N-CA-C	6.00	117.23	108.58
1	K	276	LYS	N-CA-C	5.92	118.30	110.36
1	A	499	ASN	N-CA-C	5.87	120.14	113.15
1	I	42	THR	CA-C-N	-5.81	113.98	119.85
1	I	42	THR	C-N-CA	-5.81	113.98	119.85
1	E	582	GLY	CA-C-N	5.75	127.03	119.84
1	E	582	GLY	C-N-CA	5.75	127.03	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	175	ALA	N-CA-C	5.68	118.20	111.33
1	F	80	LEU	CA-C-N	-5.66	114.55	120.38
1	F	80	LEU	C-N-CA	-5.66	114.55	120.38
1	K	145	VAL	N-CA-C	5.61	116.82	109.58
1	J	593	ASP	N-CA-CB	-5.50	101.58	110.71
1	E	51	PRO	O-C-N	5.49	123.73	121.15
1	D	520	SER	CA-C-N	-5.46	114.71	120.94
1	D	520	SER	C-N-CA	-5.46	114.71	120.94
1	J	182	GLY	N-CA-C	-5.43	108.22	114.69
1	H	499	ASN	N-CA-C	5.37	119.46	113.02
1	A	522	ILE	N-CA-C	5.31	116.96	108.89
1	J	138	THR	N-CA-C	-5.26	106.54	113.17
1	B	504	PHE	N-CA-C	5.25	116.87	108.41
1	E	524	HIS	CA-C-N	-5.22	113.31	119.84
1	E	524	HIS	C-N-CA	-5.22	113.31	119.84
1	J	343	LEU	CA-C-N	-5.20	113.67	119.19
1	J	343	LEU	C-N-CA	-5.20	113.67	119.19
1	H	421	LEU	CA-C-N	-5.15	115.26	120.31
1	H	421	LEU	C-N-CA	-5.15	115.26	120.31
1	J	522	ILE	N-CA-C	5.15	116.00	108.58
1	E	436	ILE	CB-CA-C	5.13	116.03	111.00
1	J	421	LEU	CA-C-N	-5.13	115.07	120.66
1	J	421	LEU	C-N-CA	-5.13	115.07	120.66
1	E	353	ASP	N-CA-C	5.12	117.99	111.69
1	C	620	MET	CA-C-N	-5.10	115.13	120.38
1	C	620	MET	C-N-CA	-5.10	115.13	120.38
1	L	447	PRO	CA-C-N	5.09	125.13	119.32
1	L	447	PRO	C-N-CA	5.09	125.13	119.32
1	H	593	ASP	N-CA-CB	-5.09	102.02	111.13
1	C	593	ASP	N-CA-CB	-5.08	102.28	110.71
1	B	447	PRO	O-C-N	5.06	123.53	121.15
1	F	593	ASP	N-CA-CB	-5.04	102.34	110.71
1	D	55	ARG	CA-C-N	5.01	124.70	119.64
1	D	55	ARG	C-N-CA	5.01	124.70	119.64

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	GLY	Peptide
1	A	592	PHE	Peptide
1	B	275	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	581	PRO	Peptide
1	B	592	PHE	Peptide
1	B	600	MET	Peptide
1	C	129	GLY	Peptide
1	C	144	GLY	Peptide
1	C	581	PRO	Peptide
1	C	592	PHE	Peptide
1	C	600	MET	Peptide
1	D	129	GLY	Peptide
1	D	144	GLY	Peptide
1	D	275	GLY	Peptide
1	D	592	PHE	Peptide
1	D	600	MET	Peptide
1	E	275	GLY	Peptide
1	E	592	PHE	Peptide
1	F	275	GLY	Peptide
1	F	562	ASP	Peptide
1	F	592	PHE	Peptide
1	F	600	MET	Peptide
1	G	275	GLY	Peptide
1	G	592	PHE	Peptide
1	H	275	GLY	Peptide
1	H	592	PHE	Peptide
1	I	144	GLY	Peptide
1	J	275	GLY	Peptide
1	J	592	PHE	Peptide
1	J	600	MET	Peptide
1	K	144	GLY	Peptide
1	K	275	GLY	Peptide
1	K	562	ASP	Peptide
1	K	581	PRO	Peptide
1	K	592	PHE	Peptide
1	L	275	GLY	Peptide
1	L	592	PHE	Peptide

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	4560	0	4408	99	0
1	B	4560	0	4408	76	0
1	C	4560	0	4408	63	0
1	D	4560	0	4408	89	0
1	E	4560	0	4408	73	0
1	F	4560	0	4408	79	0
1	G	4560	0	4408	89	0
1	H	4560	0	4408	87	0
1	I	4560	0	4408	107	0
1	J	4560	0	4408	76	0
1	K	4560	0	4408	92	0
1	L	4560	0	4408	100	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	3	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	3	0	0	0	0
3	J	3	0	0	0	0
3	K	3	0	0	0	0
3	L	3	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	1	0
4	E	6	0	8	0	0
4	F	6	0	8	0	0
4	G	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	6	0	8	1	0
4	I	6	0	8	0	0
4	J	6	0	8	0	0
4	K	6	0	8	2	0
4	L	6	0	8	0	0
5	A	354	0	0	10	0
5	B	362	0	0	11	0
5	C	398	0	0	11	0
5	D	386	0	0	8	0
5	E	357	0	0	10	0
5	F	361	0	0	9	0
5	G	359	0	0	10	0
5	H	376	0	0	12	0
5	I	330	0	0	15	0
5	J	388	0	0	12	0
5	K	359	0	0	10	0
5	L	347	0	0	10	0
All	All	59241	0	52992	957	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 9.

All (957) 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:L:138:THR:HG22	1:L:401:ARG:NH1	1.42	1.32
1:L:138:THR:CG2	1:L:401:ARG:NH1	2.04	1.20
1:L:555:THR:HG22	5:L:3298:HOH:O	1.49	1.12
1:K:494:THR:HG22	5:K:684:HOH:O	1.52	1.07
1:C:536:LEU:HD11	1:C:589:MET:HE3	1.26	1.07
1:K:197:GLN:HE21	1:K:219:THR:HG21	1.14	1.06
1:B:473:VAL:HG22	1:B:474:PRO:HD2	1.32	1.06
1:F:138:THR:CG2	1:F:401:ARG:NH1	2.21	1.03
1:F:138:THR:HG22	1:F:401:ARG:NH1	1.74	1.03
1:I:112:ARG:HD3	5:I:1455:HOH:O	1.59	1.01
1:L:536:LEU:HD11	1:L:589:MET:HE3	1.41	1.01
1:I:138:THR:CG2	1:I:401:ARG:HH11	1.76	0.99
1:B:473:VAL:HG22	1:B:474:PRO:CD	1.93	0.98
1:F:536:LEU:HD11	1:F:589:MET:HE3	1.43	0.98
1:G:556:PRO:HD2	5:G:4378:HOH:O	1.64	0.97
1:G:132:GLY:O	1:G:397:LEU:HD21	1.63	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:THR:HG22	1:F:401:ARG:HH11	1.26	0.96
1:J:138:THR:HG22	1:J:401:ARG:NH1	1.79	0.96
1:G:413:THR:HG21	1:G:415:GLU:HG3	1.48	0.95
1:J:138:THR:HG22	1:J:401:ARG:HH11	1.30	0.95
1:L:138:THR:HG22	1:L:401:ARG:HH11	1.00	0.95
1:G:112:ARG:HD3	5:G:2482:HOH:O	1.67	0.94
1:D:480:GLN:H	1:D:553:THR:HG21	1.31	0.93
1:A:209:ARG:NH1	1:A:610:ASP:HB3	1.84	0.93
1:I:627:PHE:O	1:I:628:ASP:HB2	1.65	0.92
1:A:209:ARG:NH1	1:A:610:ASP:CB	2.32	0.92
1:I:138:THR:HG22	1:I:401:ARG:HH11	1.35	0.91
1:C:427:GLY:HA2	5:C:4358:HOH:O	1.69	0.91
1:C:627:PHE:O	1:C:628:ASP:HB2	1.69	0.91
1:L:138:THR:CG2	1:L:401:ARG:HH11	1.76	0.89
1:A:209:ARG:HH12	1:A:610:ASP:HB3	1.35	0.89
1:B:112:ARG:HD3	5:B:1043:HOH:O	1.71	0.89
1:G:412:GLU:HG3	5:G:3026:HOH:O	1.71	0.88
1:C:432:MET:H	1:C:534:GLN:HE22	1.22	0.87
1:I:209:ARG:NH1	1:I:610:ASP:HB3	1.89	0.87
1:G:574:HIS:HD2	5:G:2039:HOH:O	1.55	0.87
1:C:536:LEU:CD1	1:C:589:MET:HE3	2.04	0.87
1:I:138:THR:CG2	1:I:401:ARG:NH1	2.37	0.87
1:L:473:VAL:HB	1:L:474:PRO:HA	1.57	0.87
1:I:413:THR:HG22	1:I:415:GLU:H	1.41	0.85
1:B:334:HIS:HD2	5:B:2420:HOH:O	1.60	0.85
1:G:209:ARG:NH1	1:G:610:ASP:HB3	1.92	0.85
1:C:144:GLY:HA3	5:C:4092:HOH:O	1.77	0.85
1:G:413:THR:HG22	1:G:414:CYS:H	1.42	0.85
1:K:138:THR:HG22	1:K:401:ARG:HH21	1.40	0.85
1:C:432:MET:H	1:C:534:GLN:NE2	1.75	0.84
1:K:432:MET:H	1:K:534:GLN:NE2	1.76	0.84
1:A:432:MET:H	1:A:534:GLN:NE2	1.76	0.84
1:K:138:THR:CG2	1:K:401:ARG:HH21	1.90	0.83
1:F:138:THR:CG2	1:F:401:ARG:HH11	1.88	0.83
1:E:480:GLN:H	1:E:553:THR:HG21	1.43	0.82
1:K:135:ALA:O	1:K:138:THR:HB	1.79	0.82
1:G:413:THR:CG2	1:G:415:GLU:HG3	2.08	0.82
1:G:255:ARG:HG3	1:G:255:ARG:HH11	1.42	0.81
1:F:434:HIS:HA	1:F:589:MET:HE1	1.61	0.81
1:A:432:MET:H	1:A:534:GLN:HE22	1.25	0.81
1:H:124:VAL:HG11	1:H:142:ARG:HG2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:ASP:HB2	5:C:1820:HOH:O	1.82	0.79
1:I:508:GLU:HG2	1:I:596:TYR:CE1	2.17	0.79
1:E:600:MET:HE2	5:E:1363:HOH:O	1.82	0.79
1:A:536:LEU:HD11	1:A:589:MET:HE3	1.65	0.79
1:J:138:THR:CG2	1:J:401:ARG:NH1	2.44	0.79
1:A:334:HIS:HD2	5:A:2857:HOH:O	1.64	0.79
1:I:536:LEU:HD11	1:I:589:MET:HE3	1.65	0.79
1:D:598:ARG:HH22	1:L:499:ASN:HD21	1.29	0.79
1:G:124:VAL:HG11	1:G:142:ARG:HG2	1.65	0.79
1:J:607:GLU:O	1:J:611:MET:HG3	1.82	0.79
1:E:581:PRO:O	1:E:582:GLY:O	2.01	0.79
1:H:466:GLU:HA	5:H:4158:HOH:O	1.83	0.78
1:F:112:ARG:HD3	5:F:2052:HOH:O	1.81	0.78
1:F:135:ALA:O	1:F:138:THR:HB	1.82	0.78
1:J:558:ARG:HB2	5:J:3620:HOH:O	1.82	0.78
1:G:432:MET:H	1:G:534:GLN:NE2	1.82	0.78
1:H:192:ASP:HB2	5:H:3435:HOH:O	1.83	0.77
1:B:538:ARG:HH11	1:B:584:GLN:HE22	1.32	0.77
1:L:536:LEU:CD1	1:L:589:MET:HE3	2.15	0.76
1:H:492:ARG:HD3	5:H:3084:HOH:O	1.84	0.76
1:H:431:ARG:HD2	1:H:534:GLN:NE2	2.01	0.76
1:J:192:ASP:HB2	5:J:3674:HOH:O	1.85	0.75
1:D:553:THR:HG23	5:D:1348:HOH:O	1.85	0.75
1:I:255:ARG:HH11	1:I:255:ARG:HG3	1.51	0.75
1:I:375:LEU:HD13	1:I:380:LEU:HD11	1.69	0.75
1:B:574:HIS:HD2	5:B:1279:HOH:O	1.70	0.75
1:D:353:ASP:HA	5:D:2019:HOH:O	1.87	0.75
1:A:147:PRO:O	1:A:149:LYS:HE2	1.86	0.74
1:L:555:THR:CG2	5:L:3298:HOH:O	2.18	0.74
1:B:209:ARG:NH1	1:B:610:ASP:HB3	2.03	0.74
1:K:432:MET:H	1:K:534:GLN:HE22	1.36	0.73
1:A:197:GLN:O	1:A:365:ARG:HD2	1.88	0.73
1:L:432:MET:H	1:L:534:GLN:HE22	1.36	0.73
1:A:473:VAL:HB	1:A:474:PRO:HD3	1.68	0.73
1:L:118:GLU:HG3	5:L:3413:HOH:O	1.88	0.73
1:G:413:THR:HG22	1:G:414:CYS:N	2.03	0.73
1:G:432:MET:H	1:G:534:GLN:HE22	1.37	0.72
1:A:375:LEU:HD13	1:A:380:LEU:HD11	1.70	0.72
1:K:205:MET:O	1:K:206:ASN:HB2	1.90	0.72
1:E:434:HIS:HA	1:E:589:MET:HE1	1.69	0.72
1:D:177:ASN:HD21	1:L:598:ARG:H	1.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:63:ARG:HD3	5:H:3738:HOH:O	1.88	0.72
1:F:124:VAL:HG11	1:F:142:ARG:HG2	1.72	0.72
1:F:536:LEU:CD1	1:F:589:MET:HE3	2.18	0.71
1:I:209:ARG:HD3	1:I:610:ASP:OD2	1.90	0.71
1:E:138:THR:HG22	1:E:401:ARG:HH21	1.54	0.71
1:I:508:GLU:HG2	1:I:596:TYR:HE1	1.56	0.71
1:L:432:MET:H	1:L:534:GLN:NE2	1.88	0.71
1:A:578:PHE:HB3	5:A:3150:HOH:O	1.89	0.71
1:E:205:MET:HE1	1:E:498:PHE:CE1	2.25	0.71
1:E:236:ASP:HB2	5:E:2752:HOH:O	1.91	0.71
1:B:536:LEU:HD11	1:B:589:MET:HE3	1.73	0.70
1:J:175:ALA:HB3	1:J:205:MET:HE2	1.73	0.70
1:L:473:VAL:HG11	1:L:478:VAL:HG11	1.73	0.70
1:D:142:ARG:HH21	1:D:147:PRO:HD3	1.56	0.70
1:G:132:GLY:O	1:G:397:LEU:CD2	2.37	0.70
1:D:598:ARG:H	1:L:177:ASN:HD21	1.39	0.70
1:K:591:LYS:HG2	1:K:593:ASP:HB2	1.73	0.70
1:J:560:ASP:OD1	1:J:562:ASP:HB3	1.91	0.70
1:D:602:HIS:HB3	1:D:614:MET:HG3	1.74	0.70
1:E:135:ALA:O	1:E:138:THR:HB	1.92	0.70
1:H:375:LEU:HD13	1:H:380:LEU:HD11	1.74	0.70
1:E:554:ARG:HG2	1:E:554:ARG:HH11	1.56	0.69
1:J:353:ASP:HA	5:J:1994:HOH:O	1.91	0.69
1:A:177:ASN:HD21	1:I:598:ARG:H	1.41	0.69
1:I:434:HIS:HA	1:I:589:MET:HE1	1.74	0.69
1:G:620:MET:SD	1:G:625:LEU:HD12	2.34	0.68
1:F:157:TRP:CE2	1:F:178:ALA:HB3	2.29	0.68
1:A:602:HIS:HB3	1:A:614:MET:HG3	1.75	0.68
1:A:527:HIS:HB2	1:A:577:VAL:HG22	1.76	0.67
1:D:63:ARG:HH12	1:L:63:ARG:NH1	1.92	0.67
1:A:157:TRP:CE2	1:A:178:ALA:HB3	2.28	0.67
1:K:197:GLN:NE2	1:K:219:THR:HG21	1.99	0.67
1:B:513:GLN:HE21	1:B:536:LEU:HD12	1.60	0.67
1:A:141:GLY:O	1:A:263:LYS:HE3	1.93	0.67
1:K:138:THR:CG2	1:K:401:ARG:NH2	2.58	0.67
1:J:451:LYS:HE3	5:J:3397:HOH:O	1.95	0.67
1:F:581:PRO:HG2	1:F:584:GLN:OE1	1.94	0.67
1:A:209:ARG:HH11	1:A:610:ASP:CB	2.06	0.67
1:D:364:GLU:OE2	4:D:5004:GOL:H12	1.95	0.66
1:J:375:LEU:HD13	1:J:380:LEU:HD11	1.77	0.66
1:H:157:TRP:CE2	1:H:178:ALA:HB3	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:513:GLN:HE21	1:K:536:LEU:HD12	1.60	0.66
1:C:63:ARG:HH22	1:G:63:ARG:NH2	1.94	0.66
1:H:536:LEU:HD11	1:H:589:MET:HE3	1.76	0.66
1:I:627:PHE:O	1:I:628:ASP:CB	2.43	0.66
1:E:138:THR:CG2	1:E:401:ARG:HH21	2.08	0.66
1:E:607:GLU:O	1:E:611:MET:HG3	1.94	0.66
1:G:627:PHE:O	1:G:628:ASP:HB2	1.96	0.66
1:L:494:THR:HG23	5:L:1773:HOH:O	1.96	0.66
1:C:413:THR:HG22	1:C:414:CYS:H	1.61	0.66
1:G:472:GLN:HA	1:G:472:GLN:OE1	1.94	0.66
1:B:63:ARG:HH11	1:H:63:ARG:NH2	1.94	0.66
1:J:581:PRO:O	1:J:582:GLY:O	2.14	0.65
1:K:600:MET:HE2	5:K:1557:HOH:O	1.96	0.65
1:L:461:GLU:O	1:L:494:THR:HG22	1.96	0.65
1:B:115:LYS:HE2	5:B:3104:HOH:O	1.95	0.65
1:F:446:THR:HG21	1:F:460:TRP:CE2	2.31	0.65
1:A:562:ASP:HB3	5:A:1583:HOH:O	1.96	0.65
1:B:607:GLU:O	1:B:611:MET:HG3	1.97	0.65
1:H:63:ARG:CD	5:H:3738:HOH:O	2.44	0.65
1:G:431:ARG:NH1	1:G:534:GLN:HE21	1.95	0.65
1:F:192:ASP:HB2	5:F:4347:HOH:O	1.95	0.65
1:H:209:ARG:NH1	1:H:610:ASP:HB3	2.12	0.65
1:J:157:TRP:CE2	1:J:178:ALA:HB3	2.31	0.65
1:J:175:ALA:CB	1:J:205:MET:HE2	2.27	0.65
1:L:112:ARG:HD3	5:L:2483:HOH:O	1.97	0.65
1:L:138:THR:HG21	1:L:401:ARG:NH1	2.10	0.65
1:C:602:HIS:HB3	1:C:614:MET:HG3	1.78	0.65
1:J:255:ARG:HG3	1:J:255:ARG:HH11	1.62	0.65
1:I:521:PRO:HA	1:I:582:GLY:HA3	1.79	0.65
1:I:209:ARG:HH11	1:I:610:ASP:CB	2.09	0.65
1:I:124:VAL:HG11	1:I:142:ARG:HG2	1.79	0.65
1:L:138:THR:HG22	1:L:401:ARG:HH12	1.54	0.65
1:G:209:ARG:HH11	1:G:610:ASP:HB3	1.62	0.64
1:D:333:VAL:HG22	1:D:370:VAL:HG12	1.77	0.64
1:E:70:ARG:NH2	5:E:2468:HOH:O	2.31	0.64
1:E:480:GLN:N	1:E:553:THR:HG21	2.12	0.64
1:G:209:ARG:HH11	1:G:610:ASP:CB	2.09	0.64
1:I:432:MET:H	1:I:534:GLN:NE2	1.96	0.64
1:A:101:ARG:HG3	1:A:193:HIS:O	1.98	0.64
1:I:138:THR:HG22	1:I:401:ARG:NH1	2.05	0.64
1:G:607:GLU:O	1:G:611:MET:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:135:ALA:O	1:I:138:THR:HB	1.98	0.64
1:B:209:ARG:HD3	1:B:610:ASP:OD2	1.98	0.64
1:H:175:ALA:HB3	1:H:205:MET:HE2	1.78	0.64
1:I:209:ARG:HH11	1:I:610:ASP:HB3	1.60	0.64
1:A:473:VAL:HB	1:A:474:PRO:CD	2.27	0.63
1:G:209:ARG:NH1	1:G:610:ASP:CB	2.61	0.63
1:K:197:GLN:HE21	1:K:219:THR:CG2	2.03	0.63
5:B:3404:HOH:O	1:H:620:MET:HE2	1.99	0.63
1:D:581:PRO:O	1:D:584:GLN:HB3	1.99	0.63
1:K:219:THR:HG22	1:K:220:TYR:H	1.62	0.63
1:K:553:THR:HG23	1:K:555:THR:O	1.99	0.63
1:L:627:PHE:O	1:L:628:ASP:HB2	1.99	0.63
1:H:322:ILE:HD12	1:H:326:ASP:HA	1.79	0.63
1:I:209:ARG:NH1	1:I:610:ASP:CB	2.62	0.63
1:H:336:ILE:HB	1:H:425:LEU:HD21	1.80	0.62
1:B:627:PHE:O	1:B:628:ASP:HB2	1.99	0.62
1:H:431:ARG:HA	1:H:534:GLN:HE22	1.64	0.62
1:I:456:HIS:CE1	1:I:611:MET:HE1	2.34	0.62
1:C:352:ASP:CG	1:C:353:ASP:H	2.06	0.62
1:I:456:HIS:CE1	1:I:611:MET:CE	2.82	0.62
1:H:523:LEU:C	1:H:523:LEU:HD23	2.23	0.62
1:E:538:ARG:HH11	1:E:584:GLN:HE22	1.47	0.62
1:J:431:ARG:NH1	1:J:572:LEU:O	2.33	0.62
1:F:55:ARG:CZ	5:F:3646:HOH:O	2.47	0.61
1:F:375:LEU:HD13	1:F:380:LEU:HD11	1.80	0.61
1:H:271:ASN:O	1:H:274:THR:O	2.18	0.61
1:J:582:GLY:O	1:J:584:GLN:N	2.32	0.61
1:F:413:THR:HG22	1:F:415:GLU:H	1.66	0.61
1:A:243:ILE:HD13	1:A:308:LEU:HD11	1.83	0.61
1:E:177:ASN:HD21	1:K:598:ARG:H	1.46	0.61
1:K:620:MET:SD	1:K:625:LEU:HD12	2.40	0.61
1:I:255:ARG:HG3	1:I:255:ARG:NH1	2.14	0.61
1:J:138:THR:CG2	1:J:401:ARG:HH11	2.07	0.61
1:D:271:ASN:HD22	1:D:274:THR:H	1.49	0.61
1:E:537:GLY:HA2	1:E:567:LEU:HD21	1.83	0.61
1:J:197:GLN:O	1:J:365:ARG:HD2	2.00	0.61
1:H:413:THR:HG22	1:H:414:CYS:H	1.66	0.61
1:L:375:LEU:HD13	1:L:380:LEU:HD11	1.81	0.61
1:B:325:ASP:O	1:B:326:ASP:HB2	2.01	0.61
1:A:413:THR:HG22	1:A:414:CYS:H	1.63	0.60
1:D:591:LYS:HG2	1:D:593:ASP:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:431:ARG:HD2	1:H:534:GLN:HE22	1.66	0.60
1:B:177:ASN:HD21	1:H:598:ARG:H	1.50	0.60
1:I:336:ILE:HB	1:I:425:LEU:HD21	1.83	0.60
1:G:255:ARG:HG3	1:G:255:ARG:NH1	2.15	0.60
1:I:76:LEU:HD21	1:I:85:MET:HE1	1.84	0.60
1:E:485:ASP:OD1	1:E:485:ASP:C	2.44	0.60
1:L:138:THR:CG2	1:L:401:ARG:HH12	2.09	0.60
1:B:434:HIS:HA	1:B:589:MET:HE1	1.83	0.60
1:D:271:ASN:HD21	1:D:273:GLU:HB2	1.66	0.60
1:L:157:TRP:CE2	1:L:178:ALA:HB3	2.37	0.60
1:L:346:PRO:HB2	5:L:2770:HOH:O	2.02	0.60
1:E:138:THR:HG22	1:E:401:ARG:HE	1.65	0.60
1:C:413:THR:HG22	1:C:414:CYS:N	2.17	0.60
1:I:134:PRO:HB3	1:I:138:THR:HG21	1.82	0.60
1:E:520:SER:O	1:E:582:GLY:HA2	2.01	0.59
1:C:334:HIS:HE1	5:C:1397:HOH:O	1.85	0.59
1:I:271:ASN:O	1:I:274:THR:O	2.19	0.59
1:C:139:GLU:HG2	5:C:3035:HOH:O	2.02	0.59
1:D:558:ARG:HD2	5:D:3558:HOH:O	2.01	0.59
1:G:375:LEU:HD13	1:G:380:LEU:HD11	1.83	0.59
1:F:142:ARG:HH21	1:F:147:PRO:HD3	1.67	0.59
1:K:364:GLU:OE2	4:K:5011:GOL:H12	2.02	0.59
1:C:157:TRP:CE2	1:C:178:ALA:HB3	2.37	0.59
1:G:205:MET:HE1	1:G:614:MET:HE3	1.84	0.59
1:I:581:PRO:O	1:I:582:GLY:O	2.21	0.59
1:K:571:GLU:O	1:K:571:GLU:HG2	2.03	0.59
1:G:397:LEU:HB2	5:G:1378:HOH:O	2.02	0.59
1:H:520:SER:HB2	1:H:521:PRO:HD2	1.84	0.59
1:B:322:ILE:HD12	1:B:326:ASP:HA	1.83	0.59
1:F:379:ARG:HG2	1:F:409:ARG:HG2	1.84	0.59
1:F:413:THR:HG22	1:F:414:CYS:N	2.18	0.59
1:D:346:PRO:HG3	1:D:425:LEU:HG	1.85	0.59
1:B:536:LEU:CD1	1:B:589:MET:HE3	2.32	0.58
1:K:602:HIS:HB3	1:K:614:MET:HG3	1.85	0.58
1:L:523:LEU:C	1:L:523:LEU:HD23	2.27	0.58
1:B:209:ARG:HH11	1:B:610:ASP:CB	2.17	0.58
1:D:538:ARG:HH11	1:D:584:GLN:HE22	1.51	0.58
1:E:205:MET:CE	1:E:498:PHE:CE1	2.86	0.58
1:G:431:ARG:NH1	1:G:534:GLN:NE2	2.51	0.58
1:B:465:VAL:HG12	1:B:490:THR:HG22	1.86	0.58
1:D:63:ARG:HH12	1:L:63:ARG:HH11	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:473:VAL:HG12	1:J:478:VAL:HG11	1.83	0.58
1:L:334:HIS:HD2	5:L:3995:HOH:O	1.85	0.58
1:C:177:ASN:HD21	1:G:598:ARG:H	1.51	0.58
1:E:245:ASP:O	1:E:246:ARG:HD3	2.04	0.58
1:A:577:VAL:HG12	1:A:577:VAL:O	2.02	0.58
1:C:197:GLN:O	1:C:365:ARG:HD2	2.02	0.58
1:A:334:HIS:HE1	5:A:1927:HOH:O	1.85	0.58
1:D:142:ARG:HE	1:D:147:PRO:HD3	1.67	0.58
1:D:432:MET:H	1:D:534:GLN:NE2	2.02	0.58
1:D:443:ILE:HD11	1:D:504:PHE:CE2	2.39	0.58
1:D:480:GLN:N	1:D:553:THR:HG21	2.12	0.58
1:D:443:ILE:HD11	1:D:504:PHE:CZ	2.38	0.58
1:E:432:MET:H	1:E:534:GLN:NE2	2.01	0.58
1:L:271:ASN:HD22	1:L:274:THR:H	1.52	0.58
1:H:607:GLU:O	1:H:611:MET:HG3	2.04	0.58
1:K:582:GLY:N	5:K:661:HOH:O	2.24	0.58
1:A:365:ARG:NH2	1:A:576:ASP:OD1	2.35	0.57
1:A:365:ARG:HH22	1:A:576:ASP:CG	2.12	0.57
1:A:434:HIS:HA	1:A:589:MET:HE1	1.85	0.57
1:C:276:LYS:HB2	1:C:277:PRO:HD2	1.85	0.57
1:C:582:GLY:N	5:C:869:HOH:O	2.37	0.57
1:E:138:THR:CG2	1:E:401:ARG:NH2	2.67	0.57
1:H:451:LYS:HE2	1:H:476:GLU:OE1	2.04	0.57
1:B:177:ASN:HD22	1:H:597:GLY:HA3	1.68	0.57
1:K:413:THR:HG22	1:K:415:GLU:H	1.68	0.57
1:B:473:VAL:CG2	1:B:474:PRO:HD2	2.22	0.57
1:H:627:PHE:O	1:H:628:ASP:HB3	2.04	0.57
1:A:523:LEU:HD21	1:A:579:GLN:HB3	1.86	0.57
1:E:536:LEU:HD11	1:E:589:MET:HE3	1.85	0.57
1:H:163:HIS:C	1:H:163:HIS:CD2	2.81	0.57
1:J:112:ARG:HD3	5:J:2162:HOH:O	2.05	0.57
1:L:404:GLU:CD	1:L:404:GLU:H	2.12	0.57
1:F:581:PRO:O	1:F:582:GLY:O	2.23	0.57
1:F:602:HIS:HB3	1:F:614:MET:HG3	1.87	0.57
1:J:135:ALA:O	1:J:138:THR:HB	2.04	0.57
1:A:598:ARG:H	1:I:177:ASN:HD21	1.51	0.57
1:D:255:ARG:HH11	1:E:345:ARG:NH1	2.01	0.57
1:G:157:TRP:CE2	1:G:178:ALA:HB3	2.40	0.57
1:K:413:THR:HG22	1:K:414:CYS:N	2.20	0.57
1:A:327:ARG:HD2	5:A:2261:HOH:O	2.04	0.57
1:C:598:ARG:H	1:G:177:ASN:HD21	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:194:GLN:NE2	5:E:1962:HOH:O	2.37	0.57
1:E:205:MET:O	1:E:206:ASN:HB2	2.02	0.57
1:F:197:GLN:O	1:F:365:ARG:HD2	2.03	0.57
1:H:431:ARG:HH11	1:H:534:GLN:HE21	1.51	0.57
1:F:68:ALA:HB1	1:F:112:ARG:HG3	1.87	0.57
1:G:197:GLN:O	1:G:365:ARG:HD2	2.05	0.56
5:I:669:HOH:O	1:J:423:GLU:HG3	2.05	0.56
1:G:209:ARG:HD3	1:G:610:ASP:OD2	2.05	0.56
1:H:402:TYR:HB3	1:H:404:GLU:OE2	2.05	0.56
1:D:177:ASN:ND2	1:L:597:GLY:HA3	2.21	0.56
1:I:334:HIS:HE1	5:I:692:HOH:O	1.87	0.56
1:J:537:GLY:HA2	1:J:567:LEU:HD21	1.87	0.56
1:K:159:VAL:HB	1:K:178:ALA:HA	1.88	0.56
1:L:271:ASN:O	1:L:274:THR:O	2.23	0.56
1:E:197:GLN:O	1:E:365:ARG:HD2	2.05	0.56
1:I:143:GLY:HA3	5:I:3277:HOH:O	2.05	0.56
1:K:209:ARG:NH1	1:K:610:ASP:HB3	2.18	0.56
1:B:115:LYS:CE	5:B:3104:HOH:O	2.53	0.56
1:B:177:ASN:ND2	1:H:597:GLY:HA3	2.21	0.56
1:E:325:ASP:O	1:E:326:ASP:HB2	2.05	0.56
1:I:197:GLN:O	1:I:365:ARG:HD2	2.05	0.56
1:C:432:MET:N	1:C:534:GLN:HE22	1.98	0.55
1:K:611:MET:HG2	5:K:2639:HOH:O	2.06	0.55
1:B:473:VAL:HG22	1:B:474:PRO:HD3	1.84	0.55
1:E:112:ARG:HD3	5:E:1825:HOH:O	2.05	0.55
1:H:276:LYS:HG3	1:H:277:PRO:HD2	1.88	0.55
1:C:336:ILE:HB	1:C:425:LEU:HD21	1.88	0.55
1:L:197:GLN:O	1:L:365:ARG:HD2	2.06	0.55
1:A:209:ARG:HH11	1:A:610:ASP:CG	2.15	0.55
1:E:138:THR:CG2	1:E:401:ARG:HE	2.20	0.55
1:C:63:ARG:HH22	1:G:63:ARG:HH21	1.54	0.55
1:E:255:ARG:HH11	1:E:255:ARG:HG2	1.71	0.55
1:G:555:THR:O	5:G:787:HOH:O	2.18	0.55
1:L:135:ALA:O	1:L:138:THR:HB	2.07	0.55
1:I:159:VAL:HB	1:I:178:ALA:HA	1.88	0.55
1:K:157:TRP:CE2	1:K:178:ALA:HB3	2.42	0.55
1:K:197:GLN:O	1:K:365:ARG:HD2	2.07	0.55
1:E:80:LEU:HB3	1:E:81:PRO:HD2	1.89	0.55
1:H:197:GLN:O	1:H:365:ARG:HD2	2.07	0.55
1:A:85:MET:HB3	1:A:214:ALA:O	2.07	0.55
1:B:413:THR:HG22	1:B:414:CYS:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:ARG:CD	5:E:1825:HOH:O	2.55	0.55
1:A:142:ARG:HD3	1:A:249:ASP:OD2	2.07	0.54
1:D:336:ILE:HB	1:D:425:LEU:HD11	1.90	0.54
1:A:333:VAL:HG22	1:A:370:VAL:HG12	1.89	0.54
1:F:159:VAL:HB	1:F:178:ALA:HA	1.89	0.54
1:D:627:PHE:O	1:D:628:ASP:HB2	2.07	0.54
1:E:138:THR:HG22	1:E:401:ARG:NH2	2.21	0.54
1:L:336:ILE:HB	1:L:425:LEU:HD21	1.89	0.54
1:L:473:VAL:HB	1:L:474:PRO:CA	2.32	0.54
1:A:115:LYS:HE2	5:A:3659:HOH:O	2.07	0.54
1:C:255:ARG:HG3	1:C:255:ARG:HH11	1.72	0.54
1:C:352:ASP:OD1	1:C:353:ASP:N	2.38	0.54
1:A:209:ARG:NH1	1:A:610:ASP:HB2	2.22	0.54
1:E:176:ASP:OD2	1:K:598:ARG:HD2	2.08	0.54
1:E:554:ARG:HG2	1:E:554:ARG:NH1	2.23	0.54
1:K:163:HIS:CE1	1:K:527:HIS:CE1	2.95	0.54
1:A:598:ARG:HH12	1:I:499:ASN:HD21	1.56	0.54
1:D:124:VAL:HG11	1:D:142:ARG:HG2	1.89	0.54
1:D:142:ARG:HH21	1:D:147:PRO:CD	2.21	0.54
1:F:598:ARG:H	1:J:177:ASN:HD21	1.56	0.54
1:I:520:SER:O	1:I:582:GLY:HA2	2.08	0.54
1:B:413:THR:HG22	1:B:414:CYS:H	1.70	0.54
1:H:413:THR:HG22	1:H:414:CYS:N	2.22	0.54
1:H:432:MET:H	1:H:534:GLN:NE2	2.06	0.54
1:E:433:SER:O	1:E:436:ILE:HG22	2.09	0.53
1:H:602:HIS:HB3	1:H:614:MET:HG3	1.89	0.53
1:K:142:ARG:HD3	1:K:249:ASP:OD2	2.07	0.53
1:A:146:GLU:HG2	5:A:1161:HOH:O	2.07	0.53
1:C:176:ASP:OD1	1:G:598:ARG:HD2	2.07	0.53
1:F:627:PHE:O	1:F:628:ASP:HB3	2.08	0.53
1:A:271:ASN:HD22	1:A:274:THR:H	1.55	0.53
1:F:521:PRO:HA	1:F:583:PRO:HD3	1.89	0.53
1:B:334:HIS:HE1	5:B:689:HOH:O	1.90	0.53
1:F:150:ASP:CG	1:J:626:LYS:HD2	2.34	0.53
1:I:157:TRP:CE2	1:I:178:ALA:HB3	2.43	0.53
1:C:325:ASP:O	1:C:326:ASP:HB2	2.09	0.53
1:J:193:HIS:NE2	1:J:532:ASP:OD2	2.28	0.53
1:H:237:ARG:HD3	5:H:970:HOH:O	2.09	0.53
1:H:523:LEU:HD23	1:H:524:HIS:N	2.24	0.53
1:A:547:ASP:HB3	1:A:550:LEU:HB3	1.90	0.53
1:D:322:ILE:HD12	1:D:326:ASP:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:473:VAL:HG23	1:E:474:PRO:HA	1.91	0.53
1:B:63:ARG:HD3	1:H:63:ARG:NH2	2.24	0.53
1:G:175:ALA:HB3	1:G:205:MET:HE2	1.90	0.53
1:A:255:ARG:HG3	1:A:255:ARG:HH11	1.73	0.53
1:B:176:ASP:O	1:H:597:GLY:HA2	2.09	0.52
1:F:63:ARG:NH2	1:J:63:ARG:HD3	2.25	0.52
1:E:432:MET:H	1:E:534:GLN:HE22	1.57	0.52
1:K:523:LEU:HD23	1:K:523:LEU:C	2.34	0.52
1:B:584:GLN:HB2	5:B:1416:HOH:O	2.09	0.52
1:H:356:PRO:HD2	5:H:2523:HOH:O	2.09	0.52
1:A:536:LEU:CD1	1:A:589:MET:HE3	2.38	0.52
1:D:352:ASP:OD2	1:D:353:ASP:N	2.42	0.52
1:F:521:PRO:HA	1:F:582:GLY:HA3	1.90	0.52
1:I:485:ASP:C	1:I:485:ASP:OD1	2.51	0.52
1:A:498:PHE:HA	1:A:614:MET:O	2.09	0.52
1:A:513:GLN:HE21	1:A:536:LEU:HD12	1.73	0.52
1:F:138:THR:HG21	1:F:401:ARG:NH1	2.21	0.52
1:A:442:LEU:C	1:A:443:ILE:HD13	2.35	0.52
1:D:177:ASN:HD22	1:L:597:GLY:CA	2.23	0.52
1:F:325:ASP:O	1:F:326:ASP:HB2	2.08	0.52
1:I:602:HIS:HB3	1:I:614:MET:HG3	1.91	0.52
1:L:472:GLN:C	1:L:473:VAL:HG13	2.34	0.52
1:C:124:VAL:HG11	1:C:142:ARG:HG2	1.90	0.52
1:K:336:ILE:HB	1:K:425:LEU:HD11	1.92	0.52
1:E:54:LEU:HD11	5:E:3984:HOH:O	2.10	0.52
1:L:472:GLN:HG3	1:L:473:VAL:HG13	1.92	0.52
1:K:112:ARG:HD3	5:K:1644:HOH:O	2.09	0.51
1:D:177:ASN:HD22	1:L:597:GLY:HA3	1.74	0.51
1:F:355:LEU:HD22	1:F:569:PRO:HG2	1.91	0.51
1:G:255:ARG:HH11	1:G:255:ARG:CG	2.15	0.51
1:G:336:ILE:HB	1:G:425:LEU:HD21	1.93	0.51
1:I:301:ASP:OD1	1:I:413:THR:HB	2.10	0.51
1:I:591:LYS:HE2	1:I:593:ASP:OD1	2.11	0.51
1:J:255:ARG:HG3	1:J:255:ARG:NH1	2.25	0.51
1:D:325:ASP:O	1:D:326:ASP:HB2	2.10	0.51
1:F:91:GLN:NE2	5:F:3521:HOH:O	2.42	0.51
1:F:523:LEU:HD23	1:F:523:LEU:C	2.36	0.51
1:A:591:LYS:HE3	5:A:4191:HOH:O	2.10	0.51
1:B:209:ARG:NH1	1:B:610:ASP:CB	2.71	0.51
1:G:68:ALA:HB1	1:G:112:ARG:HG3	1.93	0.51
1:E:431:ARG:NH2	1:E:572:LEU:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:620:MET:HE2	1:G:624:ALA:C	2.36	0.51
1:J:482:THR:HG1	1:J:488:THR:HG1	1.50	0.51
1:I:533:PHE:HB3	1:I:588:VAL:HG22	1.92	0.51
1:K:494:THR:CG2	5:K:684:HOH:O	2.30	0.51
1:L:68:ALA:HB1	1:L:112:ARG:HG3	1.93	0.51
1:C:581:PRO:O	1:C:582:GLY:O	2.28	0.51
1:D:531:ALA:HB3	1:D:533:PHE:CE1	2.46	0.51
1:D:581:PRO:HG2	1:D:584:GLN:OE1	2.10	0.51
1:H:209:ARG:NH1	1:H:610:ASP:CB	2.74	0.51
1:I:163:HIS:C	1:I:163:HIS:CD2	2.87	0.51
1:K:591:LYS:HE2	1:K:593:ASP:OD1	2.10	0.51
1:K:598:ARG:NH2	5:K:2199:HOH:O	2.44	0.51
1:B:531:ALA:HB3	1:B:533:PHE:CE1	2.46	0.51
1:G:472:GLN:OE1	1:G:472:GLN:CA	2.59	0.51
1:K:163:HIS:C	1:K:163:HIS:CD2	2.89	0.51
1:K:237:ARG:HD3	5:K:2479:HOH:O	2.11	0.51
1:A:163:HIS:CE1	1:A:363:ALA:HB1	2.45	0.50
1:B:598:ARG:H	1:H:177:ASN:HD21	1.57	0.50
1:G:538:ARG:HH11	1:G:584:GLN:HE22	1.58	0.50
1:B:584:GLN:HG2	1:B:585:GLY:N	2.25	0.50
1:C:176:ASP:O	1:G:597:GLY:HA2	2.11	0.50
1:D:274:THR:HB	1:D:276:LYS:HD2	1.94	0.50
1:I:432:MET:H	1:I:534:GLN:HE22	1.56	0.50
1:K:531:ALA:HB3	1:K:533:PHE:CE1	2.46	0.50
1:A:186:LEU:HD11	1:I:106:ARG:HG2	1.94	0.50
1:D:271:ASN:O	1:D:274:THR:O	2.30	0.50
1:I:346:PRO:HD3	1:I:425:LEU:HB2	1.93	0.50
1:A:337:GLY:N	1:A:367:ASP:HB3	2.27	0.50
1:B:375:LEU:HD13	1:B:380:LEU:HD11	1.93	0.50
1:J:269:GLN:O	5:J:3871:HOH:O	2.18	0.50
1:J:346:PRO:HD3	1:J:425:LEU:HB2	1.94	0.50
1:B:205:MET:O	1:B:206:ASN:HB2	2.12	0.50
1:B:446:THR:HG21	1:B:460:TRP:CE2	2.47	0.50
1:C:159:VAL:HB	1:C:178:ALA:HA	1.94	0.50
1:I:138:THR:HG21	1:I:401:ARG:NH1	2.24	0.50
1:J:205:MET:O	1:J:206:ASN:HB2	2.11	0.50
1:A:271:ASN:O	1:A:274:THR:O	2.29	0.50
1:C:499:ASN:ND2	1:G:598:ARG:HH22	2.09	0.50
1:G:511:HIS:NE2	5:G:2658:HOH:O	2.34	0.50
1:H:125:GLU:HG2	1:H:264:THR:OG1	2.12	0.50
1:I:451:LYS:NZ	1:I:476:GLU:OE1	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:ASN:HD22	1:J:597:GLY:HA3	1.77	0.50
1:D:627:PHE:O	1:D:628:ASP:CB	2.60	0.50
1:H:587:ARG:NH1	5:H:1191:HOH:O	2.37	0.50
1:A:484:ALA:C	1:A:486:GLY:H	2.20	0.50
1:F:177:ASN:HD21	1:J:598:ARG:H	1.60	0.50
1:G:255:ARG:NH1	1:G:255:ARG:CG	2.73	0.50
1:K:464:GLU:OE2	1:K:489:LYS:HD3	2.12	0.50
1:L:245:ASP:OD2	1:L:315:ARG:HD2	2.12	0.50
1:L:545:GLY:HA3	1:L:555:THR:O	2.11	0.50
1:F:70:ARG:NH2	5:F:2951:HOH:O	2.44	0.49
1:H:199:TRP:HA	1:H:219:THR:HA	1.94	0.49
1:J:124:VAL:HG11	1:J:142:ARG:HG2	1.94	0.49
1:K:537:GLY:HA2	1:K:567:LEU:HD21	1.93	0.49
1:B:554:ARG:HG2	1:B:554:ARG:HH11	1.77	0.49
1:D:197:GLN:O	1:D:365:ARG:HD2	2.12	0.49
1:F:443:ILE:HD12	1:F:443:ILE:N	2.27	0.49
1:G:598:ARG:NH2	5:G:1346:HOH:O	2.45	0.49
1:D:70:ARG:HD2	5:D:2882:HOH:O	2.12	0.49
1:D:271:ASN:ND2	1:D:273:GLU:HB2	2.27	0.49
1:F:432:MET:H	1:F:534:GLN:NE2	2.10	0.49
1:F:538:ARG:HH11	1:F:584:GLN:HE22	1.59	0.49
1:I:126:VAL:HG13	1:I:127:PRO:HD2	1.94	0.49
1:B:473:VAL:CG2	1:B:474:PRO:CD	2.78	0.49
1:G:620:MET:SD	1:G:625:LEU:CD1	3.01	0.49
1:I:431:ARG:NH1	1:I:572:LEU:O	2.45	0.49
1:L:362:PRO:O	1:L:363:ALA:HB3	2.13	0.49
1:E:598:ARG:H	1:K:177:ASN:HD21	1.58	0.49
1:F:520:SER:O	1:F:582:GLY:HA2	2.10	0.49
1:H:325:ASP:O	1:H:326:ASP:HB2	2.12	0.49
1:K:316:ILE:HD11	1:K:523:LEU:HD22	1.94	0.49
1:C:404:GLU:CD	1:C:404:GLU:H	2.21	0.49
1:D:538:ARG:HH11	1:D:584:GLN:NE2	2.11	0.49
1:G:86:TRP:CD2	1:G:113:ILE:HD13	2.48	0.49
1:I:83:THR:HG23	1:I:258:GLY:O	2.12	0.49
1:I:500:ASP:HB3	5:I:1771:HOH:O	2.11	0.49
1:K:431:ARG:NH2	1:K:535:VAL:O	2.45	0.49
1:L:128:LEU:HD23	1:L:265:VAL:HG11	1.93	0.49
1:A:197:GLN:O	1:A:365:ARG:CD	2.61	0.49
1:G:337:GLY:N	1:G:367:ASP:HB3	2.27	0.49
1:K:431:ARG:HD2	1:K:534:GLN:NE2	2.28	0.49
1:D:597:GLY:HA3	1:L:177:ASN:ND2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:ASP:OD2	1:J:626:LYS:HD2	2.13	0.49
1:J:70:ARG:HD2	5:J:1838:HOH:O	2.13	0.49
1:J:434:HIS:HA	1:J:589:MET:HE1	1.94	0.49
1:A:338:SER:O	1:A:339:ASP:C	2.56	0.48
1:D:161:HIS:NE2	1:D:163:HIS:HA	2.28	0.48
1:G:397:LEU:HD23	1:G:397:LEU:HA	1.67	0.48
1:L:86:TRP:CD2	1:L:113:ILE:HD13	2.48	0.48
1:D:597:GLY:HA3	1:L:177:ASN:HD22	1.77	0.48
1:J:142:ARG:HH21	1:J:147:PRO:HD3	1.77	0.48
1:L:434:HIS:CD2	1:L:438:HIS:CE1	3.01	0.48
1:A:159:VAL:HB	1:A:178:ALA:HA	1.95	0.48
1:B:194:GLN:NE2	5:B:4570:HOH:O	2.41	0.48
1:B:209:ARG:HH11	1:B:610:ASP:HB3	1.70	0.48
1:C:149:LYS:HG2	5:C:1112:HOH:O	2.13	0.48
1:C:443:ILE:HD11	1:C:504:PHE:CE2	2.48	0.48
1:L:114:PRO:O	1:L:117:SER:OG	2.28	0.48
1:A:336:ILE:HB	1:A:425:LEU:HD11	1.96	0.48
1:G:555:THR:HB	1:G:556:PRO:CD	2.43	0.48
1:H:147:PRO:O	1:H:149:LYS:NZ	2.47	0.48
1:A:148:ASN:OD1	1:A:148:ASN:C	2.56	0.48
1:B:532:ASP:HB3	5:B:1279:HOH:O	2.13	0.48
1:D:584:GLN:HB2	5:D:4134:HOH:O	2.14	0.48
1:H:446:THR:HG21	1:H:460:TRP:CE2	2.49	0.48
1:J:159:VAL:HB	1:J:178:ALA:HA	1.94	0.48
1:K:219:THR:OG1	1:K:242:LEU:HD21	2.14	0.48
1:K:542:ASP:OD1	1:K:544:SER:OG	2.21	0.48
1:F:175:ALA:HB3	1:F:205:MET:HE2	1.95	0.48
1:F:243:ILE:HG22	1:F:289:VAL:HG22	1.96	0.48
1:G:124:VAL:CG1	1:G:142:ARG:HG2	2.41	0.48
1:H:209:ARG:HH11	1:H:610:ASP:CB	2.26	0.48
1:C:163:HIS:C	1:C:163:HIS:CD2	2.91	0.48
1:F:598:ARG:HD2	1:J:176:ASP:OD1	2.13	0.48
1:G:355:LEU:HD11	5:G:1116:HOH:O	2.14	0.48
1:H:482:THR:HA	1:H:487:ARG:O	2.13	0.48
1:J:520:SER:HB2	1:J:521:PRO:HD2	1.95	0.48
1:L:205:MET:HE1	1:L:498:PHE:CE1	2.49	0.48
1:A:499:ASN:HD21	1:I:598:ARG:HH12	1.61	0.48
1:D:584:GLN:HG2	1:D:585:GLY:N	2.28	0.48
1:C:627:PHE:O	1:C:628:ASP:CB	2.53	0.48
1:E:63:ARG:NH1	1:K:60:GLU:OE1	2.47	0.48
1:E:177:ASN:HD22	1:K:597:GLY:HA3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:601:TYR:CE2	1:E:615:ARG:HB2	2.49	0.48
1:F:461:GLU:HG2	1:F:504:PHE:CZ	2.48	0.48
1:I:236:ASP:HB2	5:I:1012:HOH:O	2.14	0.48
1:J:465:VAL:HG12	1:J:466:GLU:N	2.28	0.48
1:L:69:LEU:N	1:L:69:LEU:HD12	2.29	0.48
1:G:334:HIS:HE1	5:G:1009:HOH:O	1.97	0.47
1:G:582:GLY:O	1:G:583:PRO:C	2.56	0.47
1:I:542:ASP:HA	5:I:4225:HOH:O	2.14	0.47
1:H:194:GLN:NE2	5:H:2938:HOH:O	2.34	0.47
1:J:37:ALA:HB3	1:J:40:GLU:OE1	2.14	0.47
1:J:578:PHE:HB3	5:J:1556:HOH:O	2.13	0.47
1:A:177:ASN:ND2	1:I:598:ARG:H	2.11	0.47
1:B:431:ARG:HA	1:B:534:GLN:HE22	1.79	0.47
1:D:418:SER:O	1:D:419:PHE:C	2.57	0.47
1:D:498:PHE:HA	1:D:614:MET:O	2.14	0.47
1:E:443:ILE:HD11	1:E:504:PHE:CZ	2.48	0.47
1:I:533:PHE:HB2	1:I:578:PHE:HZ	1.79	0.47
1:A:620:MET:HE3	1:I:157:TRP:CZ3	2.49	0.47
1:B:524:HIS:CE1	1:B:613:MET:HE1	2.49	0.47
1:D:280:ILE:HB	1:D:281:PRO:CD	2.44	0.47
1:E:554:ARG:NH1	1:E:554:ARG:CG	2.76	0.47
1:I:456:HIS:HE1	1:I:611:MET:HE1	1.76	0.47
1:A:413:THR:HG22	1:A:414:CYS:N	2.27	0.47
1:B:459:ILE:HG13	1:B:613:MET:HG3	1.96	0.47
1:B:492:ARG:HG3	1:B:492:ARG:HH11	1.80	0.47
1:E:68:ALA:HB1	1:E:112:ARG:HG3	1.97	0.47
1:G:536:LEU:HD11	1:G:589:MET:HE3	1.95	0.47
1:H:159:VAL:HB	1:H:178:ALA:HA	1.95	0.47
1:H:558:ARG:NH1	5:H:1505:HOH:O	2.45	0.47
1:J:148:ASN:OD1	1:J:150:ASP:HB2	2.13	0.47
1:C:498:PHE:HA	1:C:614:MET:O	2.15	0.47
1:D:142:ARG:NH2	1:D:147:PRO:HD3	2.27	0.47
1:J:560:ASP:C	1:J:562:ASP:H	2.21	0.47
1:K:413:THR:HG22	1:K:415:GLU:N	2.29	0.47
1:A:175:ALA:HB3	1:A:205:MET:HE2	1.96	0.47
1:D:499:ASN:ND2	1:L:598:ARG:HH22	2.12	0.47
1:D:597:GLY:CA	1:L:177:ASN:HD22	2.28	0.47
1:E:553:THR:HG23	5:E:1305:HOH:O	2.13	0.47
1:F:64:GLU:OE2	1:J:64:GLU:OE2	2.32	0.47
1:F:404:GLU:CD	1:F:404:GLU:H	2.23	0.47
1:H:498:PHE:HA	1:H:614:MET:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:568:ALA:HB3	1:H:571:GLU:HG2	1.96	0.47
1:J:115:LYS:NZ	5:J:3059:HOH:O	2.35	0.47
1:K:431:ARG:HD2	1:K:534:GLN:HE22	1.79	0.47
1:L:318:ASN:HB3	1:L:357:VAL:HG11	1.97	0.47
1:L:325:ASP:O	1:L:326:ASP:HB2	2.14	0.47
1:A:545:GLY:HA3	1:A:555:THR:O	2.13	0.47
1:C:598:ARG:HD2	1:G:176:ASP:OD2	2.15	0.47
1:E:159:VAL:HB	1:E:178:ALA:HA	1.96	0.47
1:I:325:ASP:O	1:I:326:ASP:HB2	2.15	0.47
1:J:498:PHE:HA	1:J:614:MET:O	2.15	0.47
1:D:280:ILE:HB	1:D:281:PRO:HD2	1.97	0.47
1:C:63:ARG:NH2	1:G:63:ARG:NH2	2.63	0.47
1:D:68:ALA:HB1	1:D:112:ARG:HG3	1.97	0.47
1:D:159:VAL:HB	1:D:178:ALA:HA	1.97	0.47
1:E:243:ILE:HD13	1:E:308:LEU:HD11	1.97	0.47
1:G:555:THR:HB	1:G:556:PRO:HD3	1.97	0.47
1:H:124:VAL:CG1	1:H:142:ARG:HG2	2.41	0.47
1:I:134:PRO:HG3	1:I:396:PRO:HB2	1.97	0.47
1:I:523:LEU:HD23	1:I:523:LEU:C	2.40	0.47
1:J:524:HIS:CE1	1:J:613:MET:HE1	2.49	0.47
1:C:492:ARG:NH1	5:C:2755:HOH:O	2.48	0.46
1:K:485:ASP:OD1	1:K:487:ARG:HB3	2.14	0.46
1:K:538:ARG:HH11	1:K:584:GLN:HE22	1.62	0.46
1:E:138:THR:CG2	1:E:401:ARG:NE	2.78	0.46
1:F:163:HIS:CE1	1:F:363:ALA:HB1	2.51	0.46
1:G:250:THR:HA	1:G:255:ARG:O	2.16	0.46
1:A:627:PHE:O	1:A:628:ASP:HB3	2.14	0.46
1:H:538:ARG:HH11	1:H:584:GLN:HE22	1.62	0.46
1:H:591:LYS:HG2	1:H:593:ASP:HB2	1.97	0.46
1:I:255:ARG:NH1	1:I:255:ARG:CG	2.78	0.46
1:K:197:GLN:O	1:K:365:ARG:CD	2.64	0.46
1:D:487:ARG:HB2	1:D:487:ARG:CZ	2.45	0.46
1:F:413:THR:HG22	1:F:414:CYS:H	1.79	0.46
1:G:562:ASP:O	1:G:564:PRO:HD3	2.15	0.46
1:K:482:THR:HA	1:K:487:ARG:O	2.15	0.46
1:L:285:PRO:HG2	1:L:286:TYR:CE1	2.50	0.46
1:A:482:THR:HG1	1:A:488:THR:HG1	1.64	0.46
1:D:499:ASN:HD21	1:L:598:ARG:HH22	1.62	0.46
1:E:538:ARG:HH11	1:E:584:GLN:NE2	2.12	0.46
1:F:473:VAL:HG11	1:F:480:GLN:HE22	1.81	0.46
1:A:431:ARG:NH2	1:A:535:VAL:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LEU:N	1:B:69:LEU:HD12	2.31	0.46
1:B:138:THR:OG1	1:B:401:ARG:NH1	2.49	0.46
1:C:447:PRO:HG3	5:C:4138:HOH:O	2.16	0.46
1:F:142:ARG:NH2	1:F:147:PRO:HD3	2.31	0.46
1:H:359:SER:HB3	4:H:5008:GOL:H31	1.97	0.46
1:K:485:ASP:OD1	1:K:487:ARG:CB	2.64	0.46
1:E:336:ILE:HB	1:E:425:LEU:HD21	1.96	0.46
1:G:119:TYR:HA	1:G:120:PRO:HD3	1.76	0.46
1:G:524:HIS:CE1	1:G:613:MET:HE1	2.50	0.46
1:H:163:HIS:CE1	1:H:363:ALA:HB1	2.51	0.46
1:H:433:SER:HB3	1:H:436:ILE:HG13	1.98	0.46
1:A:64:GLU:OE2	1:I:64:GLU:OE2	2.34	0.46
1:B:193:HIS:NE2	1:B:532:ASP:OD2	2.44	0.46
1:G:431:ARG:HA	1:G:534:GLN:HE22	1.81	0.46
1:I:600:MET:HE2	5:I:828:HOH:O	2.14	0.46
1:L:318:ASN:HB3	1:L:357:VAL:CG1	2.46	0.46
1:B:336:ILE:HB	1:B:425:LEU:HD21	1.97	0.46
1:D:602:HIS:HB3	1:D:614:MET:HA	1.97	0.46
1:E:157:TRP:CE2	1:E:178:ALA:HB3	2.51	0.46
1:C:601:TYR:CE2	1:C:615:ARG:HB2	2.51	0.46
1:F:582:GLY:O	1:F:583:PRO:C	2.58	0.46
1:J:271:ASN:O	1:J:274:THR:O	2.34	0.46
1:A:436:ILE:HG13	1:A:437:PRO:HD2	1.98	0.45
1:B:554:ARG:HG2	1:B:554:ARG:NH1	2.31	0.45
1:E:418:SER:O	1:E:419:PHE:C	2.58	0.45
1:F:255:ARG:HG3	1:F:255:ARG:HH11	1.81	0.45
1:F:465:VAL:O	1:F:466:GLU:HG3	2.16	0.45
1:K:473:VAL:HB	1:K:474:PRO:HA	1.98	0.45
1:L:434:HIS:HA	1:L:589:MET:HE1	1.98	0.45
1:C:139:GLU:O	1:C:263:LYS:NZ	2.48	0.45
1:G:487:ARG:HB2	1:G:487:ARG:CZ	2.46	0.45
1:H:382:LEU:HD12	1:H:382:LEU:HA	1.62	0.45
1:I:124:VAL:CG1	1:I:142:ARG:HG2	2.46	0.45
1:J:579:GLN:HG3	5:J:688:HOH:O	2.16	0.45
1:L:337:GLY:N	1:L:367:ASP:HB3	2.30	0.45
1:A:620:MET:HG2	1:I:157:TRP:CH2	2.52	0.45
1:E:379:ARG:NH2	5:E:1663:HOH:O	2.49	0.45
1:H:388:GLY:HA3	5:H:2013:HOH:O	2.15	0.45
1:L:578:PHE:HB3	5:L:1257:HOH:O	2.16	0.45
1:D:205:MET:O	1:D:206:ASN:HB2	2.17	0.45
1:F:334:HIS:HE1	5:F:1640:HOH:O	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:466:GLU:N	5:F:1806:HOH:O	2.49	0.45
1:H:85:MET:HB3	1:H:214:ALA:O	2.16	0.45
1:K:219:THR:HG22	1:K:220:TYR:N	2.29	0.45
1:L:339:ASP:HB2	1:L:575:LYS:HA	1.97	0.45
1:L:446:THR:HG21	1:L:460:TRP:CE2	2.51	0.45
1:A:620:MET:HE3	1:I:157:TRP:CH2	2.51	0.45
1:B:162:LEU:HG	1:B:165:ALA:HB2	1.98	0.45
1:B:523:LEU:C	1:B:523:LEU:HD23	2.42	0.45
1:D:64:GLU:OE2	1:L:64:GLU:OE2	2.35	0.45
1:D:237:ARG:HD3	5:D:2130:HOH:O	2.16	0.45
1:E:581:PRO:C	1:E:582:GLY:O	2.59	0.45
1:F:197:GLN:O	1:F:365:ARG:CD	2.65	0.45
1:K:352:ASP:CG	1:K:353:ASP:H	2.24	0.45
1:L:69:LEU:HD12	1:L:69:LEU:H	1.81	0.45
1:C:375:LEU:HD13	1:C:380:LEU:HD11	1.99	0.45
1:E:138:THR:HG22	1:E:401:ARG:NE	2.31	0.45
1:G:337:GLY:CA	1:G:367:ASP:HB3	2.46	0.45
1:K:334:HIS:HE1	5:K:672:HOH:O	2.00	0.45
1:A:138:THR:O	1:A:401:ARG:HD2	2.17	0.45
1:C:382:LEU:HD12	1:C:382:LEU:HA	1.80	0.45
1:J:582:GLY:O	1:J:583:PRO:C	2.60	0.45
1:D:259:ARG:HD2	5:D:1433:HOH:O	2.16	0.45
1:J:325:ASP:O	1:J:326:ASP:HB2	2.16	0.45
5:J:654:HOH:O	1:K:423:GLU:HG2	2.17	0.45
1:K:627:PHE:O	1:K:628:ASP:HB3	2.17	0.45
1:D:175:ALA:HB3	1:D:205:MET:HE2	2.00	0.44
1:B:535:VAL:HG13	1:B:586:LEU:HD11	1.99	0.44
1:H:611:MET:HE2	1:H:611:MET:HB3	1.84	0.44
1:I:379:ARG:HD2	5:I:4231:HOH:O	2.17	0.44
1:A:163:HIS:CD2	1:A:163:HIS:C	2.95	0.44
1:B:63:ARG:HH11	1:H:63:ARG:HH21	1.65	0.44
1:C:397:LEU:HB2	5:C:1942:HOH:O	2.16	0.44
1:I:250:THR:HA	1:I:255:ARG:O	2.17	0.44
1:J:536:LEU:HD11	1:J:589:MET:HE3	2.00	0.44
1:K:199:TRP:HB2	1:K:218:GLY:O	2.18	0.44
1:A:599:PHE:O	1:A:616:PRO:HA	2.18	0.44
1:E:70:ARG:HD2	5:E:2588:HOH:O	2.17	0.44
1:I:538:ARG:HH11	1:I:584:GLN:HE22	1.66	0.44
1:J:465:VAL:CG1	1:J:466:GLU:N	2.81	0.44
1:A:362:PRO:O	1:A:363:ALA:HB3	2.16	0.44
1:A:531:ALA:HB3	1:A:533:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:ASP:HB2	1:D:575:LYS:HA	1.98	0.44
1:D:432:MET:H	1:D:534:GLN:HE22	1.63	0.44
1:E:443:ILE:CD1	1:E:504:PHE:HZ	2.31	0.44
1:F:591:LYS:HE2	1:F:593:ASP:OD1	2.18	0.44
1:L:334:HIS:HE1	5:L:684:HOH:O	2.00	0.44
1:A:159:VAL:O	1:A:202:ASP:HA	2.18	0.44
1:L:545:GLY:CA	1:L:555:THR:HG23	2.47	0.44
1:A:504:PHE:N	1:A:504:PHE:CD1	2.85	0.44
1:B:431:ARG:NE	1:B:534:GLN:NE2	2.65	0.44
1:D:63:ARG:NH1	1:L:63:ARG:HH11	2.13	0.44
1:G:76:LEU:HD21	1:G:85:MET:HE1	2.00	0.44
1:H:370:VAL:HG11	1:H:372:PHE:CZ	2.53	0.44
1:I:271:ASN:ND2	1:I:273:GLU:H	2.15	0.44
1:I:566:PRO:HA	5:I:3613:HOH:O	2.18	0.44
1:J:316:ILE:HD11	1:J:523:LEU:HD22	1.99	0.44
1:A:545:GLY:HA2	1:A:555:THR:HG23	2.00	0.44
1:F:537:GLY:HA2	1:F:567:LEU:HD21	2.00	0.44
1:G:141:GLY:O	1:G:263:LYS:HE3	2.18	0.44
1:H:620:MET:SD	1:H:625:LEU:HD12	2.57	0.44
1:I:446:THR:HG21	1:I:460:TRP:CE2	2.52	0.44
1:I:533:PHE:HB2	1:I:578:PHE:CZ	2.53	0.44
1:J:548:LEU:N	1:J:548:LEU:HD23	2.33	0.44
1:H:271:ASN:HD22	1:H:274:THR:H	1.66	0.43
1:A:443:ILE:HD13	1:A:443:ILE:N	2.33	0.43
1:B:176:ASP:OD2	1:H:598:ARG:HD2	2.18	0.43
1:G:88:TYR:CD2	1:G:200:TYR:HE1	2.36	0.43
1:I:559:LEU:O	1:I:561:PRO:HD3	2.17	0.43
1:J:271:ASN:HD22	1:J:274:THR:H	1.66	0.43
1:K:322:ILE:HD12	1:K:326:ASP:HA	2.00	0.43
1:L:255:ARG:HG3	1:L:255:ARG:HH11	1.83	0.43
1:L:296:TYR:CD1	1:L:296:TYR:C	2.96	0.43
1:E:498:PHE:HA	1:E:614:MET:O	2.19	0.43
1:H:175:ALA:CB	1:H:205:MET:HE2	2.44	0.43
1:L:535:VAL:HG13	1:L:586:LEU:HD11	1.99	0.43
1:L:205:MET:CE	1:L:498:PHE:CE1	3.00	0.43
1:A:255:ARG:HG3	1:A:255:ARG:NH1	2.33	0.43
1:C:434:HIS:HA	1:C:589:MET:HE1	2.00	0.43
1:K:282:PHE:CD2	1:K:282:PHE:C	2.96	0.43
1:K:447:PRO:HG2	1:K:548:LEU:HD11	2.00	0.43
1:L:461:GLU:C	1:L:494:THR:HG22	2.43	0.43
1:A:323:ASP:OD1	1:A:323:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:175:ALA:HB3	1:I:205:MET:HE2	2.01	0.43
1:I:536:LEU:HD11	1:I:589:MET:HB2	2.01	0.43
1:I:536:LEU:CD1	1:I:589:MET:HE3	2.43	0.43
1:J:163:HIS:C	1:J:163:HIS:CD2	2.97	0.43
1:K:524:HIS:CE1	1:K:613:MET:HE1	2.54	0.43
1:A:54:LEU:HD11	5:A:4289:HOH:O	2.18	0.43
1:A:209:ARG:NH1	1:A:610:ASP:CG	2.76	0.43
1:B:177:ASN:HD22	1:H:597:GLY:CA	2.32	0.43
1:B:430:ARG:CZ	5:B:3569:HOH:O	2.67	0.43
1:D:431:ARG:HA	1:D:534:GLN:HE22	1.84	0.43
1:E:136:PRO:C	1:E:138:THR:H	2.25	0.43
1:E:523:LEU:C	1:E:523:LEU:HD23	2.44	0.43
1:E:582:GLY:O	1:E:584:GLN:N	2.52	0.43
1:H:338:SER:O	1:H:339:ASP:C	2.62	0.43
1:H:523:LEU:C	1:H:523:LEU:CD2	2.90	0.43
1:K:498:PHE:HA	1:K:614:MET:O	2.19	0.43
1:L:250:THR:HA	1:L:255:ARG:O	2.18	0.43
1:B:464:GLU:OE2	1:B:489:LYS:HE2	2.19	0.43
1:I:255:ARG:NE	1:J:423:GLU:OE1	2.51	0.43
1:I:450:THR:O	1:I:451:LYS:C	2.62	0.43
1:J:250:THR:HA	1:J:255:ARG:O	2.17	0.43
1:L:76:LEU:HD21	1:L:85:MET:HE1	2.01	0.43
1:L:142:ARG:HD2	1:L:249:ASP:OD2	2.19	0.43
1:L:194:GLN:NE2	5:L:1236:HOH:O	2.52	0.43
1:D:177:ASN:ND2	1:L:598:ARG:H	2.12	0.43
1:D:230:LEU:HD21	1:D:425:LEU:HD22	2.00	0.43
1:E:602:HIS:HB3	1:E:614:MET:HG3	2.01	0.43
1:F:177:ASN:HD22	1:J:597:GLY:CA	2.31	0.43
1:H:314:ALA:HA	1:H:605:LEU:HD22	2.01	0.43
1:H:404:GLU:CD	1:H:404:GLU:H	2.27	0.43
1:I:475:ALA:H	1:I:550:LEU:HD21	1.84	0.43
1:B:197:GLN:O	1:B:365:ARG:HD2	2.18	0.43
1:F:602:HIS:HB3	1:F:614:MET:HA	2.01	0.43
1:I:224:ASP:OD1	1:I:224:ASP:C	2.62	0.43
1:I:252:GLU:HG3	5:I:2806:HOH:O	2.18	0.43
1:A:147:PRO:O	1:A:149:LYS:CE	2.64	0.42
1:A:176:ASP:O	1:I:597:GLY:HA2	2.19	0.42
1:C:281:PRO:HA	1:C:607:GLU:HG2	2.00	0.42
1:D:199:TRP:HA	1:D:219:THR:HA	2.00	0.42
1:G:163:HIS:CD2	1:G:163:HIS:C	2.98	0.42
1:I:574:HIS:CD2	5:I:1319:HOH:O	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:142:ARG:HD3	1:J:249:ASP:OD1	2.19	0.42
1:J:531:ALA:HB3	1:J:533:PHE:CE1	2.54	0.42
1:A:379:ARG:HG2	1:A:409:ARG:HG2	2.01	0.42
1:A:485:ASP:OD2	1:A:487:ARG:HG2	2.19	0.42
1:D:112:ARG:HD3	5:D:984:HOH:O	2.18	0.42
1:F:232:LEU:O	1:F:233:PRO:C	2.59	0.42
1:F:581:PRO:C	1:F:582:GLY:O	2.60	0.42
1:H:591:LYS:HE3	1:H:593:ASP:OD1	2.19	0.42
1:I:101:ARG:HG3	1:I:193:HIS:O	2.18	0.42
1:I:268:GLN:NE2	1:I:272:PRO:HD3	2.33	0.42
1:D:271:ASN:ND2	1:D:273:GLU:H	2.17	0.42
1:F:119:TYR:HA	1:F:120:PRO:HD3	1.90	0.42
1:G:433:SER:OG	1:G:435:ASP:HB2	2.19	0.42
1:I:581:PRO:C	1:I:582:GLY:O	2.62	0.42
1:I:582:GLY:O	1:I:583:PRO:C	2.63	0.42
1:J:118:GLU:HB3	5:J:2503:HOH:O	2.19	0.42
1:K:175:ALA:HB3	1:K:205:MET:HE2	2.01	0.42
1:K:267:VAL:O	1:K:267:VAL:HG22	2.19	0.42
5:K:1301:HOH:O	1:L:423:GLU:HG2	2.18	0.42
1:B:64:GLU:OE2	1:H:64:GLU:OE2	2.37	0.42
1:B:68:ALA:HB1	1:B:112:ARG:HG3	2.02	0.42
1:E:255:ARG:HH11	1:E:255:ARG:CG	2.33	0.42
1:G:536:LEU:HD11	1:G:589:MET:HB2	2.01	0.42
1:K:338:SER:O	1:K:339:ASP:C	2.62	0.42
1:A:83:THR:HG23	1:A:258:GLY:O	2.18	0.42
1:C:431:ARG:HA	1:C:534:GLN:HE22	1.85	0.42
1:G:224:ASP:OD1	1:G:224:ASP:C	2.63	0.42
1:G:523:LEU:C	1:G:523:LEU:HD23	2.44	0.42
1:H:581:PRO:HG2	1:H:584:GLN:OE1	2.19	0.42
1:I:37:ALA:N	5:I:1486:HOH:O	2.52	0.42
1:L:159:VAL:HB	1:L:178:ALA:HA	2.01	0.42
1:L:560:ASP:HA	1:L:561:PRO:HD3	1.90	0.42
1:A:484:ALA:C	1:A:486:GLY:N	2.78	0.42
1:A:520:SER:O	1:A:582:GLY:HA3	2.19	0.42
1:D:177:ASN:ND2	1:L:597:GLY:CA	2.82	0.42
1:F:417:ASP:HB2	5:F:3791:HOH:O	2.19	0.42
1:G:492:ARG:NH1	1:G:492:ARG:HG3	2.34	0.42
1:I:403:PRO:HB3	5:I:2701:HOH:O	2.18	0.42
1:I:584:GLN:HG2	1:I:585:GLY:N	2.34	0.42
1:J:284:GLY:HA2	1:J:285:PRO:HD3	1.87	0.42
1:A:244:ALA:HA	1:A:312:SER:OG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ARG:NH2	5:A:2528:HOH:O	2.42	0.42
1:G:498:PHE:HA	1:G:614:MET:O	2.20	0.42
1:H:245:ASP:HA	1:H:286:TYR:O	2.19	0.42
1:I:382:LEU:HA	1:I:382:LEU:HD12	1.81	0.42
1:K:142:ARG:HE	1:K:147:PRO:HD3	1.84	0.42
1:B:559:LEU:C	1:B:559:LEU:HD23	2.45	0.42
1:G:205:MET:HE1	1:G:614:MET:CE	2.47	0.42
1:I:461:GLU:OE1	1:I:503:GLY:HA3	2.19	0.42
1:J:443:ILE:HG23	1:J:459:ILE:HG23	2.01	0.42
1:L:119:TYR:HA	1:L:120:PRO:HD3	1.81	0.42
1:B:148:ASN:C	1:B:148:ASN:OD1	2.62	0.42
1:B:157:TRP:CE2	1:B:178:ALA:HB3	2.54	0.42
1:G:401:ARG:HG3	1:G:401:ARG:HH11	1.85	0.42
1:I:506:ILE:O	1:I:619:VAL:HA	2.19	0.42
1:K:285:PRO:HG2	1:K:286:TYR:CE1	2.55	0.42
1:L:375:LEU:O	1:L:410:VAL:HB	2.20	0.42
1:B:159:VAL:HB	1:B:178:ALA:HA	2.01	0.42
1:C:276:LYS:HB2	1:C:277:PRO:CD	2.50	0.42
1:D:431:ARG:HH22	1:D:572:LEU:HB3	1.85	0.42
1:F:352:ASP:HB2	5:F:1612:HOH:O	2.20	0.42
1:F:459:ILE:HD11	1:F:526:MET:HE1	2.02	0.42
1:G:362:PRO:O	1:G:363:ALA:HB3	2.20	0.42
1:A:176:ASP:OD2	1:I:598:ARG:HD2	2.20	0.41
1:B:80:LEU:HB3	1:B:81:PRO:HD2	2.02	0.41
1:B:124:VAL:HG11	1:B:142:ARG:HG2	2.01	0.41
1:D:492:ARG:HE	1:D:492:ARG:HB2	1.50	0.41
1:I:434:HIS:CD2	1:I:438:HIS:CE1	3.08	0.41
1:K:451:LYS:HD3	1:K:549:ALA:O	2.19	0.41
1:L:280:ILE:HB	1:L:281:PRO:HD2	2.01	0.41
1:D:100:ARG:O	1:D:101:ARG:C	2.63	0.41
1:F:337:GLY:N	1:F:367:ASP:HB3	2.35	0.41
1:G:159:VAL:O	1:G:202:ASP:HA	2.20	0.41
1:K:379:ARG:HG2	1:K:409:ARG:HG2	2.02	0.41
1:A:382:LEU:HD12	1:A:382:LEU:HA	1.82	0.41
1:C:142:ARG:HD3	1:C:249:ASP:OD2	2.20	0.41
1:F:164:GLY:HA3	1:F:198:TRP:CD1	2.55	0.41
1:H:296:TYR:CD1	1:H:296:TYR:C	2.98	0.41
1:L:418:SER:O	1:L:419:PHE:C	2.62	0.41
1:C:82:PRO:HD3	1:D:230:LEU:HD13	2.03	0.41
1:D:598:ARG:H	1:L:177:ASN:ND2	2.14	0.41
1:C:352:ASP:CG	1:C:353:ASP:N	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:553:THR:OG1	1:D:555:THR:O	2.37	0.41
1:F:271:ASN:HD22	1:F:274:THR:H	1.68	0.41
1:G:602:HIS:HB3	1:G:614:MET:HG3	2.02	0.41
1:I:361:ALA:O	1:I:362:PRO:C	2.64	0.41
1:J:130:PRO:HA	1:J:131:PRO:HD3	1.96	0.41
1:J:571:GLU:O	1:J:571:GLU:HG3	2.20	0.41
1:L:482:THR:HA	1:L:487:ARG:O	2.21	0.41
1:A:149:LYS:HA	1:A:149:LYS:HD3	1.90	0.41
1:D:63:ARG:NH1	1:L:63:ARG:NH1	2.66	0.41
1:G:521:PRO:HA	1:G:583:PRO:HD3	2.03	0.41
1:H:209:ARG:NH2	5:H:4371:HOH:O	2.52	0.41
1:H:271:ASN:HD21	1:H:273:GLU:HB2	1.86	0.41
1:I:138:THR:O	1:I:401:ARG:HD2	2.20	0.41
1:K:37:ALA:HB3	1:K:40:GLU:OE1	2.21	0.41
1:A:230:LEU:HD23	1:A:230:LEU:HA	1.93	0.41
1:C:197:GLN:O	1:C:365:ARG:CD	2.67	0.41
1:F:597:GLY:HA3	1:J:177:ASN:ND2	2.35	0.41
1:H:237:ARG:HD2	1:H:304:TYR:CZ	2.55	0.41
1:K:536:LEU:HD11	1:K:589:MET:HE3	2.02	0.41
1:L:163:HIS:HE2	1:L:577:VAL:HG23	1.86	0.41
1:L:255:ARG:HG3	1:L:255:ARG:NH1	2.35	0.41
1:L:524:HIS:CE1	1:L:613:MET:HE1	2.56	0.41
1:C:177:ASN:HD22	1:G:597:GLY:HA3	1.85	0.41
1:E:177:ASN:ND2	1:K:598:ARG:H	2.16	0.41
1:J:174:TRP:CD1	1:J:176:ASP:HB2	2.55	0.41
1:J:625:LEU:C	1:J:627:PHE:N	2.78	0.41
1:K:587:ARG:HH11	1:K:587:ARG:HD2	1.75	0.41
1:L:142:ARG:HH21	1:L:147:PRO:HD3	1.86	0.41
1:A:303:TRP:CZ3	1:A:371:ASP:HB2	2.56	0.41
1:B:372:PHE:HE1	1:B:380:LEU:HD12	1.86	0.41
1:B:627:PHE:O	1:B:628:ASP:CB	2.67	0.41
1:C:142:ARG:HD3	1:C:249:ASP:CG	2.46	0.41
1:C:605:LEU:HD12	1:C:608:HIS:CE1	2.56	0.41
1:D:296:TYR:CD1	1:D:296:TYR:C	2.99	0.41
1:D:443:ILE:CD1	1:D:504:PHE:HZ	2.34	0.41
1:E:86:TRP:CD2	1:E:113:ILE:HD13	2.56	0.41
1:G:325:ASP:O	1:G:326:ASP:HB2	2.21	0.41
1:I:445:LEU:HB2	1:I:518:ASN:HA	2.02	0.41
1:K:76:LEU:HD23	1:K:76:LEU:HA	1.93	0.41
1:K:138:THR:HG21	1:K:401:ARG:NH2	2.35	0.41
1:K:413:THR:CG2	1:K:414:CYS:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:LEU:HD13	1:D:380:LEU:HD11	2.02	0.41
1:F:271:ASN:ND2	1:F:273:GLU:H	2.19	0.41
1:I:194:GLN:NE2	5:I:3156:HOH:O	2.52	0.41
1:J:142:ARG:HD2	1:J:249:ASP:OD2	2.21	0.41
1:E:520:SER:O	1:E:582:GLY:CA	2.66	0.40
1:F:142:ARG:HD3	1:F:249:ASP:OD2	2.21	0.40
1:H:520:SER:O	1:H:582:GLY:HA3	2.22	0.40
1:L:504:PHE:CD1	1:L:504:PHE:N	2.88	0.40
1:B:250:THR:HA	1:B:255:ARG:O	2.21	0.40
1:C:142:ARG:HD3	1:C:249:ASP:OD1	2.20	0.40
1:D:157:TRP:CE2	1:D:178:ALA:HB3	2.56	0.40
1:F:224:ASP:C	1:F:224:ASP:OD1	2.64	0.40
1:F:533:PHE:HB2	1:F:578:PHE:HZ	1.86	0.40
1:G:130:PRO:HA	1:G:131:PRO:HD3	1.79	0.40
1:I:352:ASP:OD2	1:I:353:ASP:N	2.55	0.40
1:K:124:VAL:HG11	1:K:142:ARG:HG2	2.02	0.40
1:L:237:ARG:HD2	1:L:304:TYR:CZ	2.56	0.40
1:L:538:ARG:HH11	1:L:584:GLN:HE22	1.69	0.40
1:C:443:ILE:HD11	1:C:504:PHE:HE2	1.84	0.40
1:C:559:LEU:O	1:C:561:PRO:HD3	2.20	0.40
1:E:597:GLY:CA	1:K:177:ASN:HD22	2.34	0.40
1:G:271:ASN:O	1:G:274:THR:O	2.39	0.40
1:K:209:ARG:NH1	1:K:610:ASP:CB	2.84	0.40
1:K:473:VAL:HG11	1:K:480:GLN:CD	2.45	0.40
1:D:304:TYR:HB2	1:D:370:VAL:HG23	2.03	0.40
1:E:285:PRO:HG2	1:E:286:TYR:CE1	2.56	0.40
1:F:43:PRO:HB3	1:F:404:GLU:HG3	2.03	0.40
1:H:575:LYS:HB2	1:H:578:PHE:HE1	1.86	0.40
1:K:325:ASP:O	1:K:326:ASP:HB2	2.21	0.40
1:K:513:GLN:NE2	1:K:536:LEU:HD12	2.32	0.40
1:K:570:ASN:OD1	4:K:5011:GOL:H32	2.21	0.40
1:L:163:HIS:CD2	1:L:163:HIS:C	3.00	0.40
1:A:395:ASP:C	1:A:397:LEU:H	2.29	0.40
1:A:598:ARG:HD2	1:I:176:ASP:OD2	2.22	0.40
1:B:86:TRP:CD2	1:B:113:ILE:HD13	2.56	0.40
1:B:224:ASP:OD1	1:B:224:ASP:C	2.65	0.40
1:C:401:ARG:HD3	5:C:2373:HOH:O	2.22	0.40
1:D:431:ARG:NH2	1:D:572:LEU:O	2.55	0.40
1:K:76:LEU:HB3	1:K:293:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	583/612 (95%)	558 (96%)	23 (4%)	2 (0%)	36	46
1	B	583/612 (95%)	560 (96%)	22 (4%)	1 (0%)	43	55
1	C	583/612 (95%)	557 (96%)	26 (4%)	0	100	100
1	D	583/612 (95%)	561 (96%)	22 (4%)	0	100	100
1	E	583/612 (95%)	558 (96%)	23 (4%)	2 (0%)	36	46
1	F	583/612 (95%)	556 (95%)	24 (4%)	3 (0%)	24	31
1	G	583/612 (95%)	556 (95%)	24 (4%)	3 (0%)	24	31
1	H	583/612 (95%)	564 (97%)	18 (3%)	1 (0%)	43	55
1	I	583/612 (95%)	546 (94%)	34 (6%)	3 (0%)	24	31
1	J	583/612 (95%)	552 (95%)	29 (5%)	2 (0%)	36	46
1	K	583/612 (95%)	560 (96%)	23 (4%)	0	100	100
1	L	583/612 (95%)	558 (96%)	25 (4%)	0	100	100
All	All	6996/7344 (95%)	6686 (96%)	293 (4%)	17 (0%)	43	55

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	582	GLY
1	G	555	THR
1	G	556	PRO
1	G	583	PRO
1	H	473	VAL
1	A	473	VAL
1	A	485	ASP
1	F	582	GLY
1	F	583	PRO
1	I	582	GLY
1	J	582	GLY
1	J	583	PRO

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Mol	Chain	Res	Type
1	E	583	PRO
1	B	473	VAL
1	F	484	ALA
1	I	583	PRO
1	I	501	GLY

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	484/499 (97%)	473 (98%)	11 (2%)	44	63
1	B	484/499 (97%)	471 (97%)	13 (3%)	39	58
1	C	484/499 (97%)	478 (99%)	6 (1%)	63	79
1	D	484/499 (97%)	480 (99%)	4 (1%)	73	86
1	E	484/499 (97%)	476 (98%)	8 (2%)	53	72
1	F	484/499 (97%)	474 (98%)	10 (2%)	47	66
1	G	484/499 (97%)	474 (98%)	10 (2%)	47	66
1	H	484/499 (97%)	471 (97%)	13 (3%)	39	58
1	I	484/499 (97%)	473 (98%)	11 (2%)	44	63
1	J	484/499 (97%)	476 (98%)	8 (2%)	53	72
1	K	484/499 (97%)	477 (99%)	7 (1%)	59	76
1	L	484/499 (97%)	474 (98%)	10 (2%)	47	66
All	All	5808/5988 (97%)	5697 (98%)	111 (2%)	50	69

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	105	VAL
1	A	128	LEU
1	A	243	ILE
1	A	332	VAL

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Mol	Chain	Res	Type
1	A	382	LEU
1	A	404	GLU
1	A	443	ILE
1	A	548	LEU
1	A	558	ARG
1	A	578	PHE
1	B	70	ARG
1	B	105	VAL
1	B	115	LYS
1	B	332	VAL
1	B	379	ARG
1	B	382	LEU
1	B	411	ARG
1	B	418	SER
1	B	473	VAL
1	B	548	LEU
1	B	563	THR
1	B	575	LYS
1	B	626	LYS
1	C	332	VAL
1	C	353	ASP
1	C	379	ARG
1	C	404	GLU
1	C	436	ILE
1	C	548	LEU
1	D	105	VAL
1	D	230	LEU
1	D	272	PRO
1	D	473	VAL
1	E	70	ARG
1	E	138	THR
1	E	353	ASP
1	E	418	SER
1	E	436	ILE
1	E	445	LEU
1	E	473	VAL
1	E	626	LYS
1	F	74	VAL
1	F	105	VAL
1	F	138	THR
1	F	149	LYS
1	F	308	LEU

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Mol	Chain	Res	Type
1	F	332	VAL
1	F	404	GLU
1	F	465	VAL
1	F	473	VAL
1	F	625	LEU
1	G	332	VAL
1	G	362	PRO
1	G	379	ARG
1	G	436	ILE
1	G	443	ILE
1	G	445	LEU
1	G	473	VAL
1	G	487	ARG
1	G	548	LEU
1	G	558	ARG
1	H	70	ARG
1	H	105	VAL
1	H	126	VAL
1	H	237	ARG
1	H	276	LYS
1	H	379	ARG
1	H	404	GLU
1	H	411	ARG
1	H	435	ASP
1	H	472	GLN
1	H	473	VAL
1	H	611	MET
1	H	625	LEU
1	I	138	THR
1	I	308	LEU
1	I	332	VAL
1	I	379	ARG
1	I	404	GLU
1	I	443	ILE
1	I	444	VAL
1	I	465	VAL
1	I	476	GLU
1	I	490	THR
1	I	558	ARG
1	J	126	VAL
1	J	138	THR
1	J	466	GLU

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Mol	Chain	Res	Type
1	J	472	GLN
1	J	522	ILE
1	J	548	LEU
1	J	578	PHE
1	J	625	LEU
1	K	70	ARG
1	K	138	THR
1	K	149	LYS
1	K	243	ILE
1	K	494	THR
1	K	553	THR
1	K	558	ARG
1	L	60	GLU
1	L	138	THR
1	L	332	VAL
1	L	354	THR
1	L	357	VAL
1	L	379	ARG
1	L	397	LEU
1	L	404	GLU
1	L	431	ARG
1	L	578	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	177	ASN
1	A	191	ASN
1	A	271	ASN
1	A	334	HIS
1	A	472	GLN
1	A	480	GLN
1	A	499	ASN
1	A	513	GLN
1	A	534	GLN
1	B	91	GLN
1	B	177	ASN
1	B	191	ASN
1	B	271	ASN
1	B	334	HIS
1	B	456	HIS

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Mol	Chain	Res	Type
1	B	499	ASN
1	B	513	GLN
1	B	534	GLN
1	B	574	HIS
1	B	584	GLN
1	C	91	GLN
1	C	177	ASN
1	C	191	ASN
1	C	194	GLN
1	C	271	ASN
1	C	318	ASN
1	C	334	HIS
1	C	480	GLN
1	C	499	ASN
1	C	534	GLN
1	D	91	GLN
1	D	177	ASN
1	D	191	ASN
1	D	269	GLN
1	D	271	ASN
1	D	334	HIS
1	D	499	ASN
1	D	534	GLN
1	D	584	GLN
1	E	177	ASN
1	E	191	ASN
1	E	194	GLN
1	E	269	GLN
1	E	271	ASN
1	E	456	HIS
1	E	472	GLN
1	E	513	GLN
1	E	534	GLN
1	E	574	HIS
1	E	584	GLN
1	E	608	HIS
1	F	177	ASN
1	F	191	ASN
1	F	271	ASN
1	F	334	HIS
1	F	513	GLN
1	F	534	GLN

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Mol	Chain	Res	Type
1	G	177	ASN
1	G	191	ASN
1	G	318	ASN
1	G	334	HIS
1	G	534	GLN
1	G	574	HIS
1	G	584	GLN
1	H	177	ASN
1	H	191	ASN
1	H	269	GLN
1	H	271	ASN
1	H	334	HIS
1	H	472	GLN
1	H	480	GLN
1	H	499	ASN
1	H	534	GLN
1	H	574	HIS
1	H	584	GLN
1	I	91	GLN
1	I	177	ASN
1	I	191	ASN
1	I	269	GLN
1	I	271	ASN
1	I	334	HIS
1	I	456	HIS
1	I	499	ASN
1	I	513	GLN
1	I	534	GLN
1	I	574	HIS
1	I	584	GLN
1	J	177	ASN
1	J	191	ASN
1	J	271	ASN
1	J	472	GLN
1	J	480	GLN
1	J	499	ASN
1	J	511	HIS
1	J	534	GLN
1	J	584	GLN
1	K	177	ASN
1	K	191	ASN
1	K	194	GLN

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Mol	Chain	Res	Type
1	K	197	GLN
1	K	269	GLN
1	K	271	ASN
1	K	334	HIS
1	K	480	GLN
1	K	513	GLN
1	K	534	GLN
1	K	584	GLN
1	L	91	GLN
1	L	177	ASN
1	L	191	ASN
1	L	194	GLN
1	L	271	ASN
1	L	318	ASN
1	L	334	HIS
1	L	472	GLN
1	L	480	GLN
1	L	499	ASN
1	L	513	GLN
1	L	534	GLN

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](#)

Of 60 ligands modelled in this entry, 36 are monoatomic - leaving 24 for Mogul analysis.

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	$\# Z > 2$
3	C2O	D	1002	1	0,2,2	-	-	-		
3	C2O	G	1002	1	0,2,2	-	-	-		
4	GOL	I	5009	-	5,5,5	0.27	0	5,5,5	0.95	0
3	C2O	H	1002	1	0,2,2	-	-	-		
4	GOL	L	5012	-	5,5,5	0.51	0	5,5,5	1.00	0
4	GOL	C	5003	-	5,5,5	0.50	0	5,5,5	1.11	0
4	GOL	D	5004	-	5,5,5	0.41	0	5,5,5	0.85	0
4	GOL	G	5007	-	5,5,5	0.21	0	5,5,5	0.64	0
3	C2O	J	1002	1	0,2,2	-	-	-		
4	GOL	K	5011	-	5,5,5	0.39	0	5,5,5	1.25	1 (20%)
4	GOL	B	5002	-	5,5,5	0.39	0	5,5,5	0.77	0
4	GOL	J	5010	-	5,5,5	0.28	0	5,5,5	0.58	0
3	C2O	C	1002	1	0,2,2	-	-	-		
4	GOL	A	5001	-	5,5,5	0.47	0	5,5,5	0.99	0
4	GOL	E	5005	-	5,5,5	0.39	0	5,5,5	0.75	0
3	C2O	F	1002	1	0,2,2	-	-	-		
4	GOL	H	5008	-	5,5,5	0.40	0	5,5,5	0.82	0
3	C2O	I	1002	1	0,2,2	-	-	-		
3	C2O	K	1002	1	0,2,2	-	-	-		
3	C2O	B	1002	1	0,2,2	-	-	-		
4	GOL	F	5006	-	5,5,5	0.25	0	5,5,5	0.84	0
3	C2O	A	1002	1	0,2,2	-	-	-		
3	C2O	L	1002	1	0,2,2	-	-	-		
3	C2O	E	1002	1	0,2,2	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	H	5008	-	-	3/4/4/4	-
4	GOL	K	5011	-	-	0/4/4/4	-
4	GOL	F	5006	-	-	4/4/4/4	-
4	GOL	B	5002	-	-	2/4/4/4	-
4	GOL	I	5009	-	-	2/4/4/4	-
4	GOL	J	5010	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	5001	-	-	4/4/4/4	-
4	GOL	L	5012	-	-	3/4/4/4	-
4	GOL	C	5003	-	-	2/4/4/4	-
4	GOL	D	5004	-	-	0/4/4/4	-
4	GOL	G	5007	-	-	3/4/4/4	-
4	GOL	E	5005	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	5011	GOL	O2-C2-C1	2.08	117.79	109.18

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	5002	GOL	O2-C2-C3-O3
4	C	5003	GOL	O1-C1-C2-C3
4	G	5007	GOL	O1-C1-C2-C3
4	E	5005	GOL	O1-C1-C2-O2
4	F	5006	GOL	O2-C2-C3-O3
4	A	5001	GOL	O1-C1-C2-C3
4	A	5001	GOL	C1-C2-C3-O3
4	B	5002	GOL	C1-C2-C3-O3
4	E	5005	GOL	O1-C1-C2-C3
4	E	5005	GOL	C1-C2-C3-O3
4	F	5006	GOL	O1-C1-C2-C3
4	F	5006	GOL	C1-C2-C3-O3
4	H	5008	GOL	O1-C1-C2-C3
4	H	5008	GOL	C1-C2-C3-O3
4	I	5009	GOL	O1-C1-C2-C3
4	J	5010	GOL	O1-C1-C2-C3
4	L	5012	GOL	O1-C1-C2-C3
4	A	5001	GOL	O1-C1-C2-O2
4	C	5003	GOL	O1-C1-C2-O2
4	G	5007	GOL	O1-C1-C2-O2
4	H	5008	GOL	O1-C1-C2-O2
4	J	5010	GOL	O1-C1-C2-O2
4	E	5005	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	5001	GOL	O2-C2-C3-O3
4	L	5012	GOL	O1-C1-C2-O2
4	F	5006	GOL	O1-C1-C2-O2
4	G	5007	GOL	C1-C2-C3-O3
4	I	5009	GOL	O1-C1-C2-O2
4	L	5012	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5004	GOL	1	0
4	K	5011	GOL	2	0
4	H	5008	GOL	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	587/612 (95%)	-0.62	7 (1%) 76 77	6, 26, 50, 68	2 (0%)
1	B	587/612 (95%)	-0.60	7 (1%) 76 77	5, 24, 46, 69	4 (0%)
1	C	587/612 (95%)	-0.78	2 (0%) 90 90	14, 22, 46, 67	0
1	D	587/612 (95%)	-0.81	3 (0%) 87 87	14, 22, 44, 66	0
1	E	587/612 (95%)	-0.71	5 (0%) 81 82	5, 23, 47, 71	1 (0%)
1	F	587/612 (95%)	-0.63	5 (0%) 81 82	5, 23, 47, 69	3 (0%)
1	G	587/612 (95%)	-0.70	6 (1%) 79 80	14, 24, 47, 70	1 (0%)
1	H	587/612 (95%)	-0.67	3 (0%) 87 87	5, 24, 45, 70	2 (0%)
1	I	587/612 (95%)	-0.59	4 (0%) 84 85	6, 25, 53, 74	2 (0%)
1	J	587/612 (95%)	-0.72	5 (0%) 81 82	4, 23, 45, 61	2 (0%)
1	K	587/612 (95%)	-0.65	3 (0%) 87 87	5, 24, 49, 68	1 (0%)
1	L	587/612 (95%)	-0.67	3 (0%) 87 87	5, 25, 49, 71	1 (0%)
All	All	7044/7344 (95%)	-0.68	53 (0%) 82 83	4, 24, 48, 74	19 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	473	VAL	31.0
1	F	473	VAL	29.4
1	L	472	GLN	29.4
1	H	473	VAL	29.3
1	F	472	GLN	28.3
1	E	472	GLN	28.3
1	K	473	VAL	28.3
1	H	472	GLN	27.5
1	A	472	GLN	27.3
1	B	472	GLN	26.9
1	I	473	VAL	26.4

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Mol	Chain	Res	Type	RSRZ
1	I	472	GLN	25.9
1	J	472	GLN	25.3
1	J	466	GLU	8.2
1	A	473	VAL	6.6
1	G	38	PRO	6.3
1	F	38	PRO	5.5
1	A	252	GLU	5.1
1	B	418	SER	5.1
1	F	582	GLY	5.1
1	G	132	GLY	4.4
1	B	38	PRO	4.3
1	E	466	GLU	3.9
1	E	582	GLY	3.8
1	G	582	GLY	3.8
1	K	582	GLY	3.7
1	L	473	VAL	3.6
1	J	582	GLY	3.5
1	G	466	GLU	3.5
1	J	37	ALA	3.4
1	L	38	PRO	3.1
1	C	582	GLY	2.8
1	C	466	GLU	2.8
1	I	582	GLY	2.8
1	K	37	ALA	2.6
1	G	37	ALA	2.6
1	D	37	ALA	2.5
1	D	466	GLU	2.5
1	B	466	GLU	2.4
1	A	474	PRO	2.3
1	A	57	ALA	2.3
1	B	57	ALA	2.3
1	A	414	CYS	2.3
1	I	37	ALA	2.3
1	B	582	GLY	2.2
1	A	37	ALA	2.2
1	H	129	GLY	2.2
1	E	414	CYS	2.1
1	D	472	GLN	2.1
1	J	143	GLY	2.1
1	E	473	VAL	2.1
1	G	413	THR	2.0
1	F	37	ALA	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($\text{\AA}^2$)	Q<0.9
4	GOL	B	5002	6/6	0.91	0.12	33,39,42,42	0
4	GOL	D	5004	6/6	0.92	0.10	34,36,38,38	0
4	GOL	K	5011	6/6	0.92	0.12	29,41,42,43	0
4	GOL	L	5012	6/6	0.92	0.09	34,37,39,39	0
4	GOL	C	5003	6/6	0.93	0.09	26,28,32,34	0
4	GOL	H	5008	6/6	0.93	0.09	26,33,35,36	0
4	GOL	I	5009	6/6	0.94	0.09	28,36,39,40	0
4	GOL	F	5006	6/6	0.94	0.08	38,39,41,43	0
4	GOL	E	5005	6/6	0.94	0.10	35,40,43,43	0
3	C2O	G	1002	3/3	0.95	0.06	41,41,42,49	0
3	C2O	K	1002	3/3	0.95	0.07	42,42,45,46	0
4	GOL	A	5001	6/6	0.95	0.09	25,32,38,39	0
3	C2O	A	1002	3/3	0.95	0.07	41,41,44,52	0
3	C2O	B	1002	3/3	0.95	0.06	40,40,41,48	0
3	C2O	F	1002	3/3	0.95	0.07	38,38,39,48	0
3	C2O	H	1002	3/3	0.96	0.06	38,38,40,45	0
3	C2O	I	1002	3/3	0.96	0.06	37,37,46,47	0
3	C2O	J	1002	3/3	0.96	0.06	29,29,38,43	0
4	GOL	J	5010	6/6	0.96	0.06	27,35,35,37	0
3	C2O	C	1002	3/3	0.96	0.06	29,29,39,41	0
3	C2O	L	1002	3/3	0.96	0.06	39,39,41,46	0
4	GOL	G	5007	6/6	0.97	0.07	30,39,41,42	0
3	C2O	E	1002	3/3	0.97	0.06	32,32,40,40	0
3	C2O	D	1002	3/3	0.97	0.06	30,30,39,41	0
2	CU	E	1005	1/1	0.98	0.06	42,42,42,42	0
2	CU	A	1005	1/1	0.99	0.05	43,43,43,43	0
2	CU	B	1000	1/1	0.99	0.02	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CU	B	1004	1/1	0.99	0.02	40,40,40,40	0
2	CU	B	1005	1/1	0.99	0.03	37,37,37,37	0
2	CU	C	1005	1/1	0.99	0.05	37,37,37,37	0
2	CU	D	1004	1/1	0.99	0.03	38,38,38,38	0
2	CU	D	1005	1/1	0.99	0.04	38,38,38,38	0
2	CU	E	1000	1/1	0.99	0.04	45,45,45,45	0
2	CU	E	1004	1/1	0.99	0.02	41,41,41,41	0
2	CU	A	1000	1/1	0.99	0.02	50,50,50,50	0
2	CU	F	1000	1/1	0.99	0.03	42,42,42,42	0
2	CU	F	1005	1/1	0.99	0.04	38,38,38,38	0
2	CU	G	1004	1/1	0.99	0.03	43,43,43,43	0
2	CU	G	1005	1/1	0.99	0.04	39,39,39,39	0
2	CU	H	1000	1/1	0.99	0.03	49,49,49,49	0
2	CU	I	1005	1/1	0.99	0.04	42,42,42,42	0
2	CU	J	1000	1/1	0.99	0.02	40,40,40,40	0
2	CU	J	1005	1/1	0.99	0.06	39,39,39,39	0
2	CU	K	1000	1/1	0.99	0.02	43,43,43,43	0
2	CU	K	1004	1/1	0.99	0.02	40,40,40,40	0
2	CU	K	1005	1/1	0.99	0.04	42,42,42,42	0
2	CU	L	1005	1/1	0.99	0.06	41,41,41,41	0
2	CU	A	1004	1/1	0.99	0.03	41,41,41,41	0
2	CU	I	1000	1/1	1.00	0.02	46,46,46,46	0
2	CU	I	1004	1/1	1.00	0.02	43,43,43,43	0
2	CU	C	1004	1/1	1.00	0.02	39,39,39,39	0
2	CU	G	1000	1/1	1.00	0.02	43,43,43,43	0
2	CU	J	1004	1/1	1.00	0.02	41,41,41,41	0
2	CU	C	1000	1/1	1.00	0.03	43,43,43,43	0
2	CU	D	1000	1/1	1.00	0.03	37,37,37,37	0
2	CU	F	1004	1/1	1.00	0.02	42,42,42,42	0
2	CU	H	1004	1/1	1.00	0.02	43,43,43,43	0
2	CU	L	1000	1/1	1.00	0.03	43,43,43,43	0
2	CU	L	1004	1/1	1.00	0.02	43,43,43,43	0
2	CU	H	1005	1/1	1.00	0.06	36,36,36,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.