



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:45 AM UTC

PDB ID : 3DYM / pdb_00003dym
Title : E. coli (lacZ) beta-galactosidase (H418E)
Authors : Juers, D.H.; Huber, R.E.; Matthews, B.W.
Deposited on : 2008-07-28
Resolution : 2.05 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

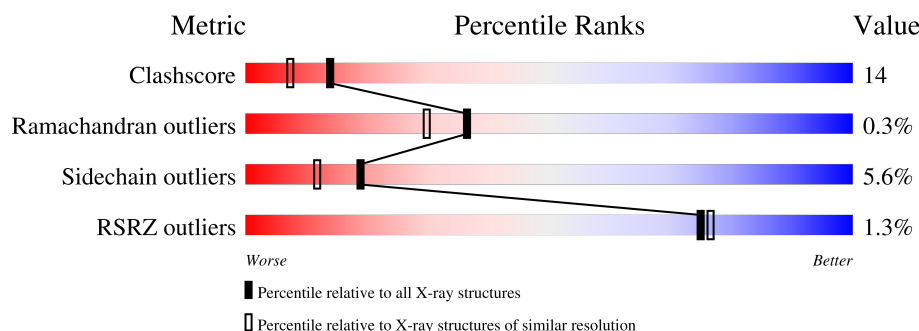
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	1023	% 64% 28% 6% ..
1	B	1023	% 62% 30% 6% ..
1	C	1023	% 62% 29% 7% .
1	D	1023	% 64% 30% 5% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DMS	C	8504	-	-	X	-
4	DMS	D	8412	-	-	X	-
4	DMS	D	8419	-	-	X	-
4	DMS	D	8703	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36314 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	0	0	0
			8124	5137	1438	1511	38			
1	B	1011	Total	C	N	O	S	0	0	0
			8124	5137	1438	1511	38			
1	C	1011	Total	C	N	O	S	0	0	0
			8124	5137	1438	1511	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8124	5137	1438	1511	38			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P00722
A	2	SER	-	expression tag	UNP P00722
A	3	HIS	-	expression tag	UNP P00722
A	4	MET	-	expression tag	UNP P00722
A	5	LEU	-	expression tag	UNP P00722
A	6	GLU	-	expression tag	UNP P00722
A	7	ASP	-	expression tag	UNP P00722
A	8	PRO	-	expression tag	UNP P00722
A	418	GLU	HIS	engineered mutation	UNP P00722
B	1	GLY	-	expression tag	UNP P00722
B	2	SER	-	expression tag	UNP P00722
B	3	HIS	-	expression tag	UNP P00722
B	4	MET	-	expression tag	UNP P00722
B	5	LEU	-	expression tag	UNP P00722
B	6	GLU	-	expression tag	UNP P00722
B	7	ASP	-	expression tag	UNP P00722
B	8	PRO	-	expression tag	UNP P00722
B	418	GLU	HIS	engineered mutation	UNP P00722
C	1	GLY	-	expression tag	UNP P00722
C	2	SER	-	expression tag	UNP P00722
C	3	HIS	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	-	expression tag	UNP P00722
C	5	LEU	-	expression tag	UNP P00722
C	6	GLU	-	expression tag	UNP P00722
C	7	ASP	-	expression tag	UNP P00722
C	8	PRO	-	expression tag	UNP P00722
C	418	GLU	HIS	engineered mutation	UNP P00722
D	1	GLY	-	expression tag	UNP P00722
D	2	SER	-	expression tag	UNP P00722
D	3	HIS	-	expression tag	UNP P00722
D	4	MET	-	expression tag	UNP P00722
D	5	LEU	-	expression tag	UNP P00722
D	6	GLU	-	expression tag	UNP P00722
D	7	ASP	-	expression tag	UNP P00722
D	8	PRO	-	expression tag	UNP P00722
D	418	GLU	HIS	engineered mutation	UNP P00722

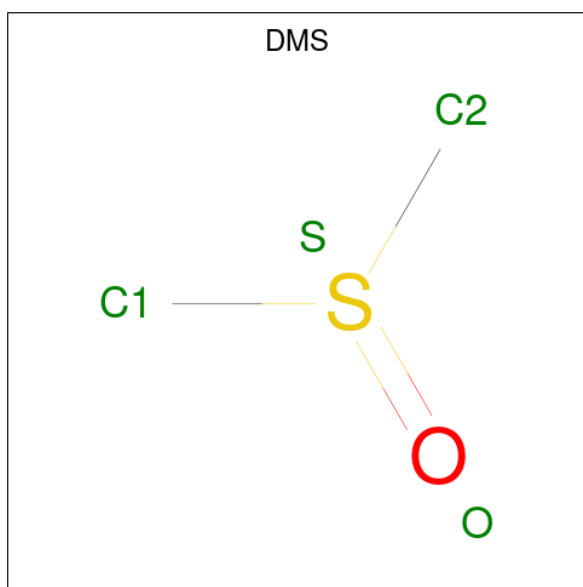
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Mg 4 4	0	0
2	B	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Na 4 4	0	0
3	B	4	Total Na 4 4	0	0
3	C	4	Total Na 4 4	0	0
3	D	4	Total Na 4 4	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	C	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0

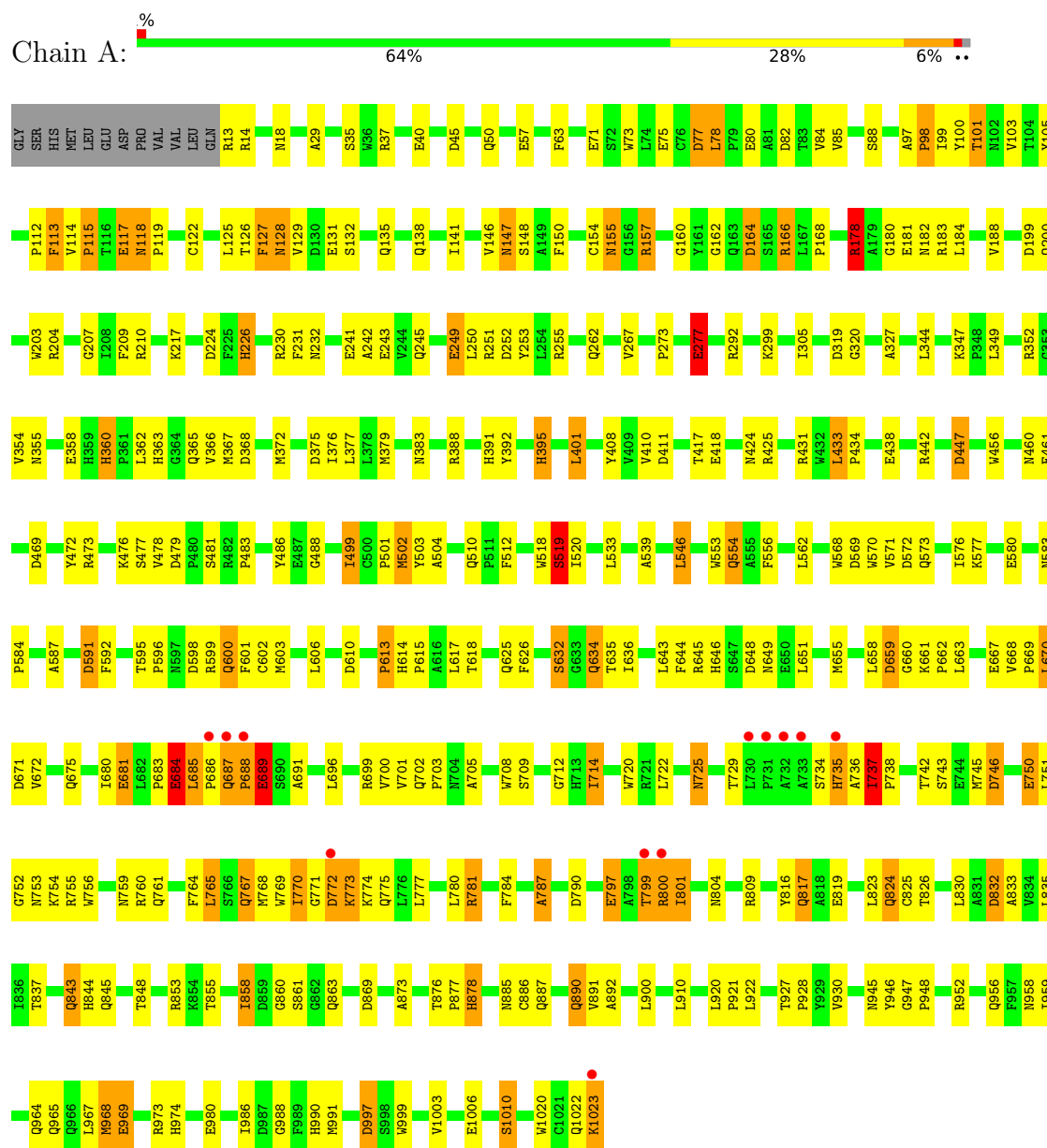
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	871	Total 871	O 871	0	0
5	B	864	Total 864	O 864	0	0
5	C	838	Total 838	O 838	0	0
5	D	891	Total 891	O 891	0	0

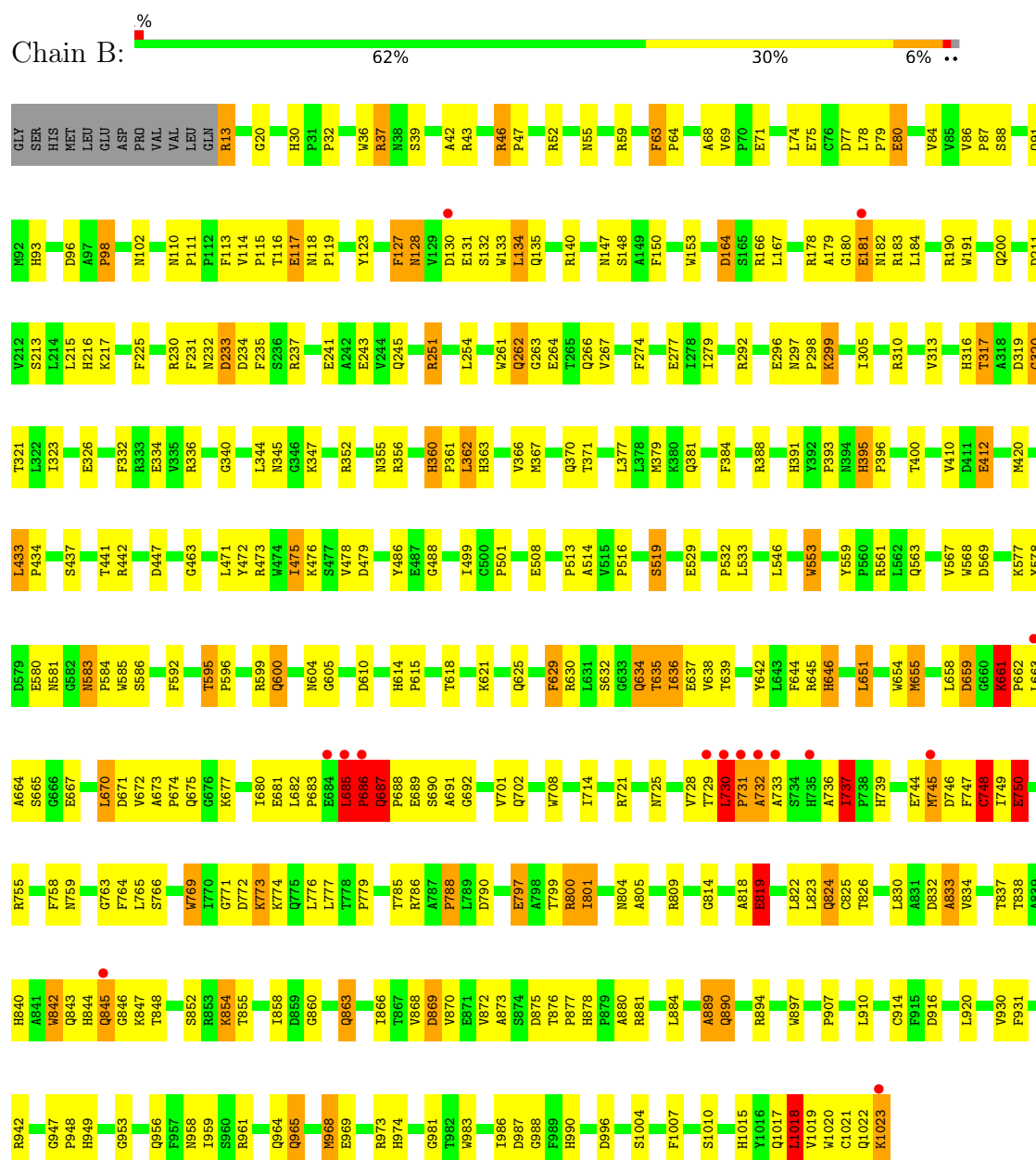
3 Residue-property plots

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

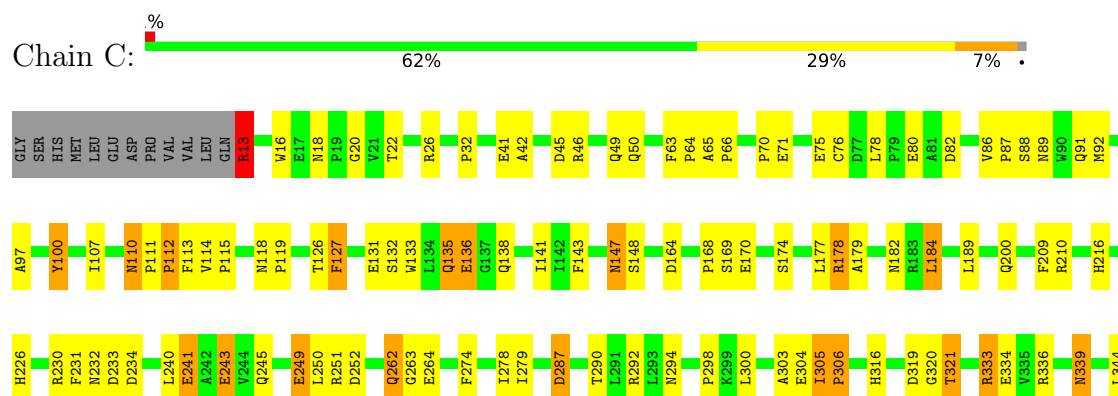
• Molecule 1: Beta-galactosidase

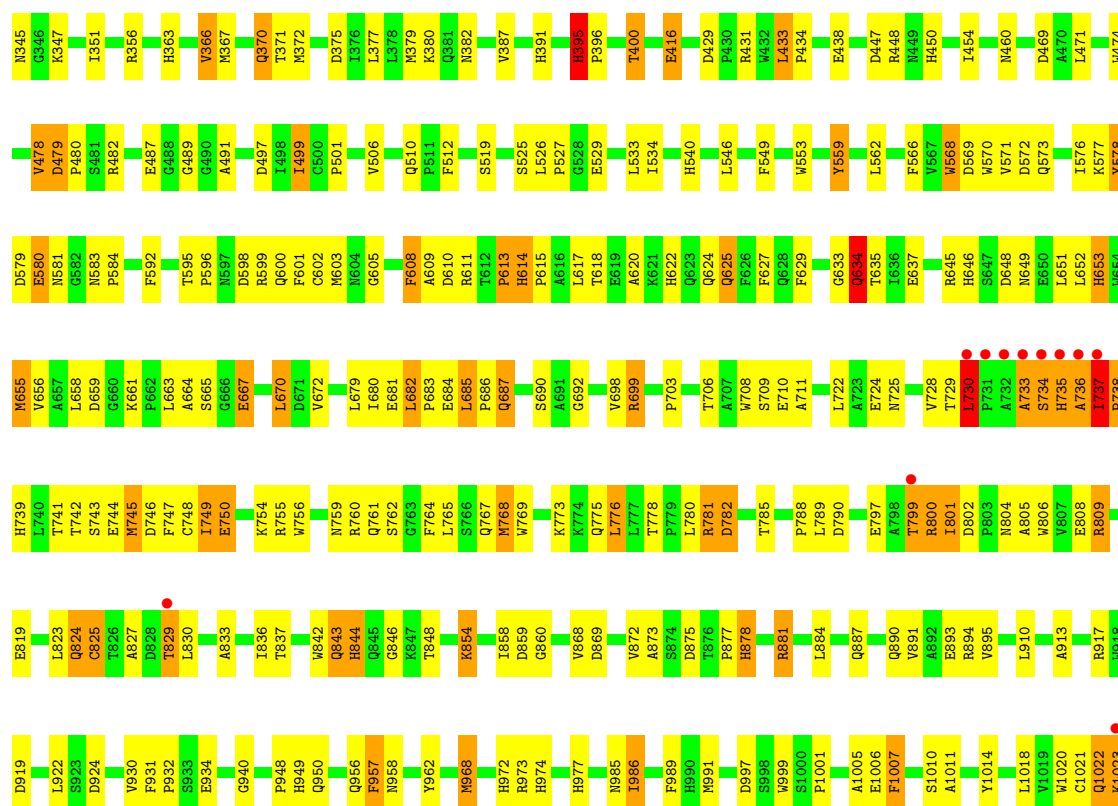


• Molecule 1: Beta-galactosidase

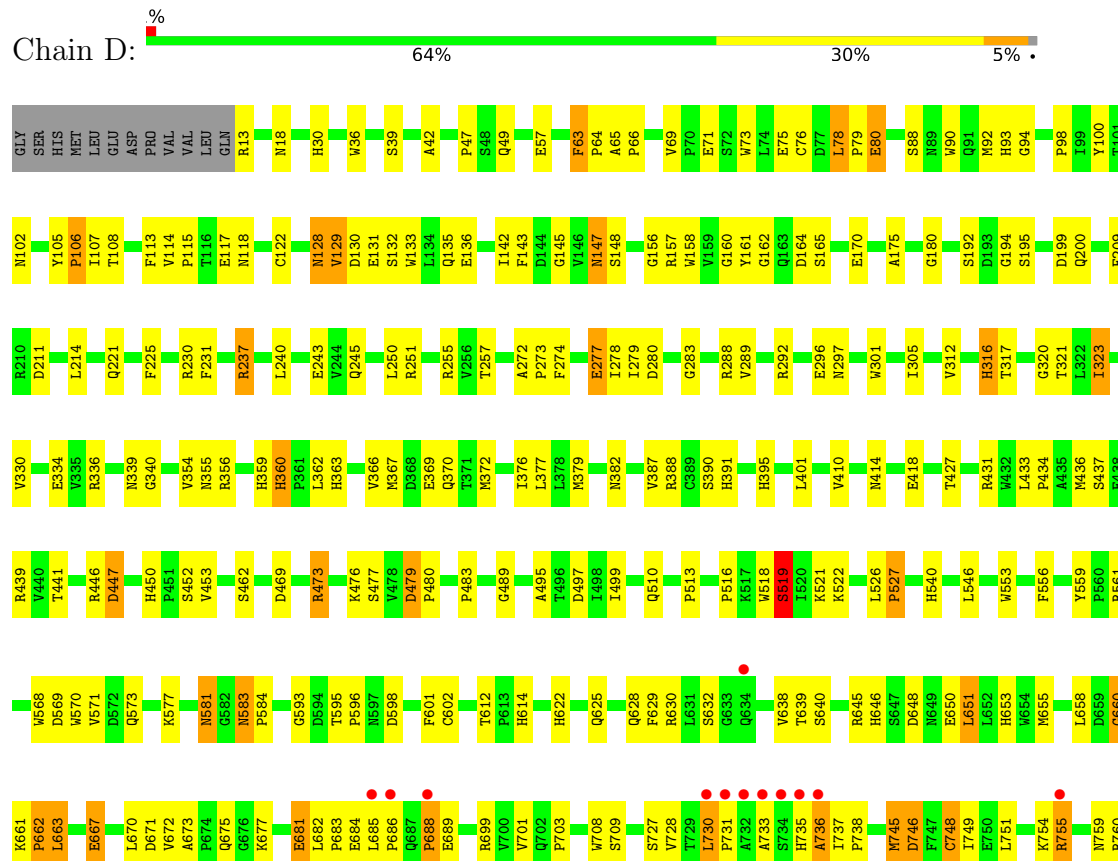


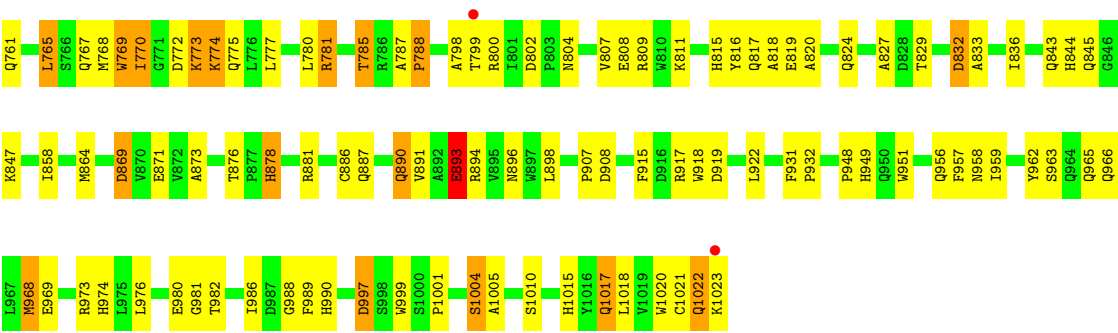
- Molecule 1: Beta-galactosidase





- Molecule 1: Beta-galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.34Å 167.16Å 200.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.50 – 2.05 34.50 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.50-2.05) 99.3 (34.50-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.05Å)	Xtrriage
Refinement program	TNT	Depositor
R, R_{free}	0.158 , 0.251 0.158 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtrriage
Anisotropy	0.484	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 109.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36314	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0670e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, DMS, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.25	9/8365 (0.1%)	1.89	175/11412 (1.5%)
1	B	1.25	0/8365	1.88	187/11412 (1.6%)
1	C	1.24	5/8365 (0.1%)	1.90	181/11412 (1.6%)
1	D	1.26	5/8365 (0.1%)	1.90	164/11412 (1.4%)
All	All	1.25	19/33460 (0.1%)	1.89	707/45648 (1.5%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	ASP	C-N	-7.99	1.25	1.34
1	C	479	ASP	C-N	-6.78	1.25	1.33
1	A	928	PRO	N-CA	-5.88	1.40	1.47
1	C	703	PRO	N-CA	-5.62	1.40	1.47
1	A	927	THR	C-O	-5.47	1.18	1.24
1	D	681	GLU	CD-OE2	5.38	1.35	1.25
1	C	170	GLU	CD-OE2	5.36	1.35	1.25
1	D	280	ASP	CG-OD2	5.35	1.35	1.25
1	C	599	ARG	NE-CZ	5.35	1.39	1.33
1	D	479	ASP	C-N	-5.34	1.28	1.34
1	A	572	ASP	CG-OD2	5.26	1.35	1.25
1	A	681	GLU	CD-OE2	5.23	1.35	1.25
1	C	931	PHE	CA-CB	5.14	1.60	1.53
1	D	908	ASP	CG-OD2	5.13	1.35	1.25
1	A	162	GLY	CA-C	5.12	1.56	1.51
1	D	473	ARG	NE-CZ	5.11	1.38	1.33
1	A	479	ASP	CA-CB	5.05	1.59	1.53
1	A	224	ASP	CA-C	-5.00	1.46	1.52
1	A	249	GLU	CD-OE2	5.00	1.34	1.25

All (707) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	363	HIS	CA-CB-CG	-12.62	101.18	113.80
1	A	790	ASP	CA-CB-CG	-11.60	101.00	112.60
1	B	363	HIS	CA-CB-CG	-10.99	102.81	113.80
1	A	583	ASN	CA-CB-CG	-10.58	102.02	112.60
1	B	737	ILE	N-CA-CB	10.28	122.61	111.61
1	A	63	PHE	CA-CB-CG	-10.08	103.72	113.80
1	C	601	PHE	CA-CB-CG	-9.91	103.89	113.80
1	B	869	ASP	CA-CB-CG	-9.83	102.77	112.60
1	D	844	HIS	CA-CB-CG	-9.80	104.00	113.80
1	C	110	ASN	CA-CB-CG	-9.76	102.84	112.60
1	C	13	ARG	NE-CZ-NH2	-9.53	110.62	119.20
1	A	687	GLN	CA-C-N	9.28	131.44	119.84
1	A	687	GLN	C-N-CA	9.28	131.44	119.84
1	D	931	PHE	CA-CB-CG	-9.20	104.60	113.80
1	A	18	ASN	O-C-N	9.02	126.68	121.27
1	B	890	GLN	N-CA-CB	-8.91	96.88	109.97
1	B	68	ALA	CA-C-N	-8.88	116.20	122.59
1	B	68	ALA	C-N-CA	-8.88	116.20	122.59
1	D	297	ASN	CA-CB-CG	-8.80	103.80	112.60
1	C	592	PHE	CA-CB-CG	-8.77	105.03	113.80
1	C	614	HIS	N-CA-C	-8.77	100.04	110.13
1	A	113	PHE	CA-CB-CG	-8.77	105.03	113.80
1	B	113	PHE	CA-CB-CG	-8.63	105.17	113.80
1	C	747	PHE	CA-CB-CG	8.62	122.42	113.80
1	D	832	ASP	CA-CB-CG	-8.60	104.00	112.60
1	C	184	LEU	CB-CA-C	-8.55	95.05	109.50
1	A	689	GLU	CA-C-N	8.51	132.90	120.90
1	A	689	GLU	C-N-CA	8.51	132.90	120.90
1	C	382	ASN	CA-CB-CG	-8.48	104.12	112.60
1	A	685	LEU	O-C-N	8.40	127.19	121.14
1	A	363	HIS	CA-CB-CG	-8.35	105.45	113.80
1	D	78	LEU	CB-CA-C	-8.34	100.56	110.15
1	D	893	GLU	CB-CG-CD	8.28	126.67	112.60
1	B	360	HIS	CA-CB-CG	-8.24	105.56	113.80
1	A	770	ILE	N-CA-CB	8.21	122.25	111.90
1	A	115	PRO	CB-CA-C	-8.15	100.94	111.46
1	C	614	HIS	N-CA-CB	8.12	118.67	109.49
1	D	878	HIS	CA-CB-CG	-8.11	105.69	113.80
1	A	659	ASP	CB-CA-C	-8.05	99.87	111.95
1	B	63	PHE	CA-CB-CG	-8.04	105.76	113.80
1	C	958	ASN	N-CA-CB	8.02	125.65	111.69
1	C	634	GLN	N-CA-C	-7.99	103.09	112.92
1	C	249	GLU	N-CA-C	7.99	121.47	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	736	ALA	N-CA-C	7.99	120.26	108.60
1	C	690	SER	N-CA-C	7.87	118.34	108.19
1	D	363	HIS	CA-CB-CG	-7.87	105.93	113.80
1	C	82	ASP	CA-CB-CG	-7.86	104.74	112.60
1	B	233	ASP	CA-C-N	-7.80	110.27	122.67
1	B	233	ASP	C-N-CA	-7.80	110.27	122.67
1	C	570	TRP	N-CA-C	7.79	119.46	110.97
1	C	684	GLU	CB-CA-C	-7.78	98.18	109.84
1	D	746	ASP	N-CA-C	7.72	120.80	109.07
1	D	601	PHE	CA-CB-CG	-7.69	106.11	113.80
1	A	231	PHE	CA-CB-CG	-7.64	106.16	113.80
1	A	499	ILE	CA-C-N	-7.63	114.45	122.85
1	A	499	ILE	C-N-CA	-7.63	114.45	122.85
1	D	18	ASN	O-C-N	7.63	125.85	121.27
1	D	63	PHE	CA-C-N	7.62	127.27	119.19
1	D	63	PHE	C-N-CA	7.62	127.27	119.19
1	B	166	ARG	N-CA-C	7.59	122.67	112.88
1	D	974	HIS	CA-CB-CG	-7.50	106.30	113.80
1	A	438	GLU	CA-CB-CG	-7.47	99.16	114.10
1	A	512	PHE	CA-CB-CG	-7.45	106.35	113.80
1	C	1007	PHE	CA-CB-CG	-7.44	106.36	113.80
1	C	479	ASP	CA-C-N	7.43	127.14	119.56
1	C	479	ASP	C-N-CA	7.43	127.14	119.56
1	A	722	LEU	CA-C-O	7.42	122.24	117.94
1	C	13	ARG	NH1-CZ-NH2	7.42	128.94	119.30
1	B	988	GLY	N-CA-C	-7.41	103.28	112.77
1	D	312	VAL	CA-C-O	7.41	128.17	120.39
1	D	90	TRP	N-CA-C	7.41	121.23	111.75
1	B	725	ASN	CA-CB-CG	-7.37	105.23	112.60
1	C	345	ASN	CA-CB-CG	-7.36	105.24	112.60
1	A	77	ASP	CA-CB-CG	-7.35	105.25	112.60
1	C	226	HIS	CA-CB-CG	-7.33	106.47	113.80
1	A	816	TYR	CA-C-N	-7.33	111.08	122.37
1	A	816	TYR	C-N-CA	-7.33	111.08	122.37
1	B	964	GLN	CA-C-O	7.32	128.37	120.10
1	C	339	ASN	CA-CB-CG	-7.31	105.29	112.60
1	D	147	ASN	N-CA-CB	-7.31	99.08	110.55
1	A	632	SER	N-CA-CB	7.29	122.75	110.87
1	A	553	TRP	CA-CB-CG	-7.28	99.77	113.60
1	B	433	LEU	CA-C-O	7.28	125.40	118.34
1	A	18	ASN	CA-C-N	7.27	126.97	119.56
1	A	18	ASN	C-N-CA	7.27	126.97	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1018	LEU	N-CA-CB	-7.23	98.07	111.52
1	A	97	ALA	N-CA-C	7.22	119.78	110.39
1	C	113	PHE	CA-CB-CG	-7.21	106.59	113.80
1	D	75	GLU	N-CA-CB	7.20	120.99	110.26
1	D	221	GLN	N-CA-CB	-7.17	100.23	111.56
1	B	890	GLN	N-CA-C	7.17	120.88	110.28
1	A	746	ASP	CB-CA-C	-7.16	94.84	111.09
1	D	513	PRO	CB-CA-C	-7.15	101.61	110.98
1	B	823	LEU	N-CA-C	-7.14	105.09	113.88
1	D	113	PHE	CA-CB-CG	-7.11	106.69	113.80
1	A	659	ASP	CA-CB-CG	-7.09	105.50	112.60
1	A	997	ASP	CA-CB-CG	-7.08	105.52	112.60
1	D	798	ALA	CA-C-N	7.04	130.20	120.63
1	D	798	ALA	C-N-CA	7.04	130.20	120.63
1	D	316	HIS	CA-CB-CG	-7.03	106.77	113.80
1	C	910	LEU	CA-C-N	-7.00	110.19	120.28
1	C	910	LEU	C-N-CA	-7.00	110.19	120.28
1	B	818	ALA	N-CA-CB	7.00	120.40	109.83
1	A	127	PHE	CA-CB-CG	-7.00	106.80	113.80
1	B	737	ILE	CB-CA-C	6.98	117.84	110.37
1	A	688	PRO	N-CA-C	6.98	126.84	112.47
1	D	330	VAL	CB-CA-C	-6.97	100.31	110.63
1	A	956	GLN	CA-C-N	-6.95	110.47	121.87
1	A	956	GLN	C-N-CA	-6.95	110.47	121.87
1	D	447	ASP	N-CA-C	6.95	121.93	113.38
1	D	869	ASP	CA-CB-CG	-6.93	105.67	112.60
1	B	326	GLU	N-CA-C	-6.93	99.21	109.81
1	B	691	ALA	N-CA-C	-6.92	101.90	110.41
1	B	730	LEU	CA-C-N	6.92	128.49	119.84
1	B	730	LEU	C-N-CA	6.92	128.49	119.84
1	D	431	ARG	NE-CZ-NH2	-6.91	112.98	119.20
1	C	653	HIS	N-CA-CB	6.91	121.69	110.43
1	A	375	ASP	CA-CB-CG	-6.91	105.69	112.60
1	C	506	VAL	N-CA-C	6.90	116.99	110.30
1	D	283	GLY	CA-C-N	6.89	128.30	122.17
1	D	283	GLY	C-N-CA	6.89	128.30	122.17
1	C	809	ARG	NE-CZ-NH1	6.88	128.38	121.50
1	D	231	PHE	CA-CB-CG	-6.86	106.94	113.80
1	D	864	MET	CA-C-N	-6.86	113.25	122.72
1	D	864	MET	C-N-CA	-6.86	113.25	122.72
1	A	878	HIS	CA-CB-CG	-6.84	106.96	113.80
1	A	613	PRO	CB-CA-C	-6.83	102.03	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	920	LEU	O-C-N	6.80	126.06	121.71
1	D	143	PHE	CA-CB-CG	-6.80	107.00	113.80
1	C	869	ASP	CA-CB-CG	-6.79	105.81	112.60
1	B	638	VAL	CB-CA-C	-6.78	101.62	110.84
1	C	540	HIS	CA-CB-CG	-6.78	107.02	113.80
1	A	601	PHE	CA-CB-CG	-6.78	107.02	113.80
1	D	748	CYS	N-CA-CB	6.77	121.20	110.57
1	C	598	ASP	CA-CB-CG	-6.77	105.83	112.60
1	C	685	LEU	N-CA-CB	6.76	119.89	110.01
1	A	360	HIS	CA-CB-CG	-6.76	107.04	113.80
1	B	661	LYS	CA-C-O	6.76	124.32	119.32
1	B	332	PHE	CA-CB-CG	-6.74	107.06	113.80
1	C	497	ASP	CA-CB-CG	-6.74	105.86	112.60
1	C	931	PHE	CB-CA-C	6.74	116.84	110.17
1	A	554	GLN	CB-CG-CD	6.74	124.05	112.60
1	B	671	ASP	CA-C-N	-6.74	114.32	123.14
1	B	671	ASP	C-N-CA	-6.74	114.32	123.14
1	C	682	LEU	CA-C-N	6.73	126.70	120.03
1	C	682	LEU	C-N-CA	6.73	126.70	120.03
1	C	844	HIS	CA-CB-CG	-6.73	107.07	113.80
1	C	859	ASP	CA-C-N	6.72	128.60	120.13
1	C	859	ASP	C-N-CA	6.72	128.60	120.13
1	B	818	ALA	CB-CA-C	6.71	120.85	109.72
1	C	790	ASP	CA-CB-CG	-6.71	105.89	112.60
1	C	320	GLY	CA-C-N	-6.70	112.74	122.19
1	C	320	GLY	C-N-CA	-6.70	112.74	122.19
1	C	949	HIS	N-CA-C	6.69	120.96	110.32
1	B	69	VAL	N-CA-C	6.68	114.51	107.76
1	D	614	HIS	N-CA-C	-6.67	101.43	110.36
1	D	660	GLY	N-CA-C	-6.66	107.15	115.08
1	B	764	PHE	CA-CB-CG	-6.66	107.14	113.80
1	D	382	ASN	CA-CB-CG	-6.65	105.95	112.60
1	D	278	ILE	CA-C-N	-6.64	113.95	121.85
1	D	278	ILE	C-N-CA	-6.64	113.95	121.85
1	A	853	ARG	NE-CZ-NH2	-6.64	113.23	119.20
1	A	722	LEU	CB-CA-C	-6.63	107.52	117.07
1	D	781	ARG	N-CA-CB	-6.63	99.31	111.37
1	B	93	HIS	CA-CB-CG	-6.61	107.19	113.80
1	B	846	GLY	CA-C-N	-6.61	113.34	122.93
1	B	846	GLY	C-N-CA	-6.61	113.34	122.93
1	D	30	HIS	CA-CB-CG	-6.61	107.19	113.80
1	D	369	GLU	N-CA-C	6.61	118.15	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	765	LEU	N-CA-C	-6.60	99.64	109.15
1	B	313	VAL	CB-CA-C	-6.60	102.02	111.19
1	C	216	HIS	CA-CB-CG	-6.59	107.21	113.80
1	C	634	GLN	CA-C-N	-6.58	113.84	123.05
1	C	634	GLN	C-N-CA	-6.58	113.84	123.05
1	A	610	ASP	CA-CB-CG	-6.57	106.03	112.60
1	D	731	PRO	N-CA-CB	6.56	109.43	103.33
1	D	161	TYR	N-CA-CB	-6.56	99.33	111.53
1	B	931	PHE	CA-CB-CG	-6.55	107.25	113.80
1	B	39	SER	CA-CB-OG	-6.54	98.01	111.10
1	D	162	GLY	CA-C-N	6.53	133.78	122.82
1	D	162	GLY	C-N-CA	6.53	133.78	122.82
1	B	889	ALA	CA-C-O	6.52	127.33	120.42
1	B	948	PRO	CB-CA-C	-6.52	101.65	110.52
1	B	614	HIS	N-CA-C	-6.50	101.64	110.36
1	D	255	ARG	NE-CZ-NH1	6.50	128.00	121.50
1	B	636	ILE	N-CA-CB	6.49	118.78	110.99
1	C	553	TRP	CA-CB-CG	-6.49	101.27	113.60
1	D	164	ASP	N-CA-CB	6.48	121.45	110.49
1	B	30	HIS	CA-CB-CG	-6.48	107.32	113.80
1	A	869	ASP	N-CA-CB	6.48	120.94	110.77
1	D	662	PRO	N-CA-CB	6.48	109.02	103.19
1	D	255	ARG	NE-CZ-NH2	-6.46	113.38	119.20
1	B	20	GLY	N-CA-C	-6.45	106.87	115.32
1	A	725	ASN	CA-CB-CG	-6.45	106.15	112.60
1	D	820	ALA	N-CA-C	6.45	119.73	108.52
1	C	878	HIS	CA-CB-CG	-6.44	107.36	113.80
1	D	770	ILE	N-CA-CB	6.44	120.02	111.90
1	B	127	PHE	CA-CB-CG	-6.44	107.36	113.80
1	D	395	HIS	CA-CB-CG	-6.44	107.36	113.80
1	B	737	ILE	N-CA-C	6.43	114.89	107.89
1	A	147	ASN	N-CA-CB	-6.42	100.47	110.55
1	B	877	PRO	N-CA-CB	6.42	109.03	103.31
1	B	614	HIS	N-CA-CB	6.41	117.18	109.74
1	B	958	ASN	N-CA-CB	6.41	123.45	111.53
1	A	100	TYR	N-CA-CB	6.41	122.48	110.56
1	B	267	VAL	N-CA-C	6.40	117.18	110.72
1	D	477	SER	CB-CA-C	-6.39	100.80	110.90
1	B	728	VAL	N-CA-C	-6.39	106.55	112.43
1	D	571	VAL	N-CA-C	6.39	117.68	108.48
1	B	84	VAL	N-CA-CB	-6.36	104.40	112.60
1	D	363	HIS	N-CA-C	6.35	121.04	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	648	ASP	N-CA-C	6.35	119.96	112.72
1	A	164	ASP	N-CA-CB	6.33	121.19	110.49
1	D	683	PRO	CB-CA-C	-6.33	102.96	111.12
1	A	519	SER	N-CA-C	-6.32	101.33	110.24
1	A	433	LEU	CA-C-O	6.30	124.45	118.34
1	D	829	THR	N-CA-CB	6.29	120.90	110.52
1	C	447	ASP	N-CA-C	6.28	121.09	113.17
1	D	519	SER	N-CA-C	-6.28	101.38	110.24
1	B	441	THR	N-CA-C	6.26	118.11	111.28
1	B	310	ARG	NE-CZ-NH2	-6.26	113.56	119.20
1	C	680	ILE	CA-C-N	-6.26	114.08	122.72
1	C	680	ILE	C-N-CA	-6.26	114.08	122.72
1	B	634	GLN	N-CA-C	-6.26	104.12	112.94
1	A	614	HIS	N-CA-C	-6.25	101.98	110.36
1	A	226	HIS	CA-C-N	-6.24	115.45	123.19
1	A	226	HIS	C-N-CA	-6.24	115.45	123.19
1	B	916	ASP	CA-CB-CG	-6.24	106.36	112.60
1	D	746	ASP	CA-CB-CG	-6.23	106.37	112.60
1	A	968	MET	CB-CA-C	-6.22	98.73	110.67
1	A	78	LEU	N-CA-CB	6.22	119.09	110.01
1	D	988	GLY	N-CA-C	-6.22	104.53	113.86
1	A	85	VAL	CB-CA-C	-6.22	103.07	111.15
1	B	479	ASP	CA-C-N	6.22	125.91	119.82
1	B	479	ASP	C-N-CA	6.22	125.91	119.82
1	C	684	GLU	CB-CG-CD	6.21	123.16	112.60
1	B	965	GLN	CA-CB-CG	-6.21	101.69	114.10
1	B	996	ASP	N-CA-CB	6.20	119.36	110.06
1	B	323	ILE	N-CA-C	-6.20	105.78	111.67
1	D	688	PRO	N-CA-C	-6.20	99.70	112.47
1	C	1005	ALA	N-CA-C	6.20	118.84	111.71
1	C	294	ASN	CA-CB-CG	-6.19	106.41	112.60
1	C	729	THR	N-CA-CB	6.19	120.56	110.17
1	D	958	ASN	N-CA-CB	6.18	123.02	111.53
1	D	100	TYR	N-CA-CB	6.18	120.78	110.53
1	A	684	GLU	CA-C-N	-6.17	112.65	124.01
1	A	684	GLU	C-N-CA	-6.17	112.65	124.01
1	C	735	HIS	CA-CB-CG	6.17	119.97	113.80
1	C	729	THR	O-C-N	6.17	130.22	123.13
1	A	735	HIS	N-CA-C	-6.16	104.34	112.72
1	B	687	GLN	C-N-CD	-6.16	99.75	125.00
1	D	274	PHE	CA-CB-CG	-6.16	107.64	113.80
1	A	408	TYR	N-CA-CB	-6.16	100.92	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	TRP	CA-C-N	-6.15	113.71	122.94
1	A	456	TRP	C-N-CA	-6.15	113.71	122.94
1	D	583	ASN	CA-C-O	6.15	124.70	119.66
1	D	483	PRO	CB-CA-C	-6.13	102.92	110.95
1	B	949	HIS	CB-CA-C	-6.12	99.71	109.80
1	C	776	LEU	N-CA-C	6.11	119.50	109.72
1	D	516	PRO	CB-CA-C	-6.11	102.94	110.95
1	A	968	MET	CA-C-N	-6.11	111.33	122.38
1	A	968	MET	C-N-CA	-6.11	111.33	122.38
1	B	659	ASP	CA-CB-CG	-6.11	106.49	112.60
1	D	553	TRP	CA-CB-CG	-6.10	102.00	113.60
1	A	784	PHE	CA-CB-CG	-6.10	107.70	113.80
1	A	974	HIS	CA-CB-CG	-6.09	107.71	113.80
1	D	439	ARG	CA-C-O	6.08	126.96	119.97
1	D	556	PHE	CB-CA-C	-6.07	100.72	110.79
1	D	798	ALA	O-C-N	6.07	128.40	122.09
1	C	578	TYR	N-CA-CB	6.06	120.87	110.68
1	A	1010	SER	CA-CB-OG	-6.05	98.99	111.10
1	B	78	LEU	CA-C-N	6.04	126.20	119.32
1	B	78	LEU	C-N-CA	6.04	126.20	119.32
1	C	608	PHE	CA-C-O	-6.04	114.87	121.87
1	B	234	ASP	CA-CB-CG	-6.03	106.57	112.60
1	C	846	GLY	CA-C-N	-6.03	114.40	122.72
1	C	846	GLY	C-N-CA	-6.03	114.40	122.72
1	D	93	HIS	N-CA-C	-6.02	105.58	113.17
1	D	648	ASP	CA-CB-CG	-6.02	106.58	112.60
1	A	184	LEU	CB-CA-C	-6.01	99.23	109.51
1	C	147	ASN	N-CA-CB	-6.01	101.11	110.55
1	C	306	PRO	N-CA-CB	6.01	106.46	102.25
1	C	917	ARG	CD-NE-CZ	-6.01	115.99	124.40
1	B	442	ARG	NE-CZ-NH2	-5.99	113.81	119.20
1	B	519	SER	N-CA-C	-5.99	101.80	110.24
1	B	553	TRP	CA-CB-CG	-5.99	102.22	113.60
1	B	858	ILE	N-CA-CB	5.99	119.00	111.46
1	C	917	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	A	722	LEU	N-CA-C	-5.98	103.88	108.78
1	D	320	GLY	CA-C-N	-5.97	113.77	122.19
1	D	320	GLY	C-N-CA	-5.97	113.77	122.19
1	C	842	TRP	CE2-CD2-CE3	5.96	124.76	118.80
1	B	420	MET	CA-C-N	-5.96	117.66	122.85
1	B	420	MET	C-N-CA	-5.96	117.66	122.85
1	C	804	ASN	CA-CB-CG	5.96	118.56	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	HIS	CA-C-O	5.95	126.36	120.17
1	B	832	ASP	N-CA-CB	-5.95	101.16	110.98
1	D	890	GLN	CB-CG-CD	-5.94	102.50	112.60
1	B	140	ARG	CA-C-N	-5.94	115.44	123.10
1	B	140	ARG	C-N-CA	-5.94	115.44	123.10
1	B	868	VAL	N-CA-C	5.93	116.41	107.75
1	D	989	PHE	CA-CB-CG	-5.93	107.86	113.80
1	B	298	PRO	CB-CA-C	-5.93	103.64	111.23
1	C	370	GLN	CB-CG-CD	5.93	122.68	112.60
1	D	759	ASN	CA-CB-CG	-5.93	106.67	112.60
1	D	915	PHE	CA-CB-CG	-5.93	107.87	113.80
1	D	686	PRO	N-CA-CB	5.92	108.96	103.39
1	C	305	ILE	O-C-N	5.92	127.85	121.10
1	C	209	PHE	CA-CB-CG	-5.92	107.88	113.80
1	B	855	THR	N-CA-CB	5.91	121.70	111.00
1	A	767	GLN	OE1-CD-NE2	5.91	128.51	122.60
1	B	77	ASP	N-CA-C	5.90	119.03	110.42
1	A	383	ASN	N-CA-C	5.90	120.42	113.23
1	C	913	ALA	CA-C-N	-5.89	113.43	122.62
1	C	913	ALA	C-N-CA	-5.89	113.43	122.62
1	C	249	GLU	CA-C-N	-5.89	113.00	121.42
1	C	249	GLU	C-N-CA	-5.89	113.00	121.42
1	A	57	GLU	N-CA-C	5.88	118.25	109.25
1	D	948	PRO	CB-CA-C	-5.88	102.16	111.04
1	D	418	GLU	CA-CB-CG	-5.88	102.35	114.10
1	A	166	ARG	N-CA-C	5.87	120.45	112.88
1	B	884	LEU	CB-CA-C	-5.85	97.19	110.07
1	B	685	LEU	C-N-CD	-5.85	101.00	125.00
1	C	71	GLU	CA-C-O	5.85	126.57	119.49
1	B	819	GLU	N-CA-CB	-5.85	101.39	110.57
1	A	18	ASN	CB-CA-C	-5.84	104.09	110.98
1	A	997	ASP	CB-CG-OD2	-5.84	104.97	118.40
1	B	235	PHE	CA-CB-CG	-5.84	107.96	113.80
1	A	98	PRO	CB-CA-C	-5.83	103.34	110.98
1	B	211	ASP	N-CA-C	5.83	117.82	110.24
1	C	829	THR	N-CA-CB	5.83	120.48	110.68
1	D	817	GLN	CB-CG-CD	-5.83	102.68	112.60
1	B	1007	PHE	CA-CB-CG	-5.83	107.97	113.80
1	D	727	SER	CA-C-N	-5.83	115.67	122.14
1	D	727	SER	C-N-CA	-5.83	115.67	122.14
1	D	129	VAL	N-CA-CB	-5.83	104.36	112.52
1	C	725	ASN	CB-CA-C	-5.82	101.37	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	684	GLU	CA-C-N	-5.81	112.76	121.83
1	C	684	GLU	C-N-CA	-5.81	112.76	121.83
1	A	643	LEU	CA-C-N	-5.81	113.19	122.08
1	A	643	LEU	C-N-CA	-5.81	113.19	122.08
1	A	188	VAL	N-CA-C	5.81	116.47	107.99
1	C	110	ASN	CA-C-O	5.80	128.11	120.16
1	B	583	ASN	CA-C-O	5.80	125.58	120.19
1	A	771	GLY	N-CA-C	-5.80	99.44	113.18
1	B	84	VAL	O-C-N	-5.80	116.89	122.97
1	C	274	PHE	CA-CB-CG	-5.80	108.00	113.80
1	D	770	ILE	N-CA-C	-5.80	98.06	107.28
1	D	106	PRO	CB-CA-C	-5.79	102.71	110.88
1	D	209	PHE	CA-CB-CG	-5.79	108.01	113.80
1	D	113	PHE	O-C-N	5.79	129.42	122.94
1	A	327	ALA	CB-CA-C	-5.78	100.56	110.95
1	B	672	VAL	N-CA-CB	-5.76	103.46	111.41
1	A	101	THR	N-CA-CB	5.76	120.85	110.83
1	A	591	ASP	CA-CB-CG	-5.75	106.84	112.60
1	A	502	MET	N-CA-CB	5.75	119.62	110.65
1	B	508	GLU	N-CA-C	5.75	118.11	108.96
1	B	897	TRP	CA-C-O	5.75	127.54	121.33
1	C	782	ASP	CA-CB-CG	-5.75	106.85	112.60
1	D	66	PRO	N-CA-CB	5.75	109.60	103.39
1	C	71	GLU	CB-CG-CD	5.75	122.37	112.60
1	B	297	ASN	CB-CA-C	-5.74	105.31	110.71
1	D	63	PHE	O-C-N	5.74	126.03	121.55
1	C	737	ILE	CA-C-N	5.74	125.75	119.90
1	C	737	ILE	C-N-CA	5.74	125.75	119.90
1	A	118	ASN	N-CA-CB	-5.73	100.94	111.03
1	C	893	GLU	N-CA-C	5.72	117.60	111.36
1	D	932	PRO	N-CA-C	5.72	120.06	111.14
1	D	728	VAL	N-CA-C	-5.71	107.70	113.47
1	B	274	PHE	CA-CB-CG	-5.71	108.09	113.80
1	C	843	GLN	O-C-N	5.71	130.07	123.17
1	B	320	GLY	CA-C-N	-5.71	114.85	122.72
1	B	320	GLY	C-N-CA	-5.71	114.85	122.72
1	D	414	ASN	CA-CB-CG	5.70	118.30	112.60
1	B	447	ASP	N-CA-C	5.70	120.35	113.17
1	C	136	GLU	CB-CA-C	-5.69	97.54	110.07
1	A	787	ALA	CA-C-N	5.69	125.70	119.90
1	A	787	ALA	C-N-CA	5.69	125.70	119.90
1	B	592	PHE	CA-CB-CG	-5.69	108.11	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	PHE	CA-CB-CG	-5.69	108.11	113.80
1	C	243	GLU	CA-CB-CG	-5.69	102.73	114.10
1	D	527	PRO	N-CA-CB	5.68	109.22	103.25
1	B	788	PRO	N-CA-C	5.68	120.52	111.26
1	C	18	ASN	CA-C-N	5.67	125.77	119.87
1	C	18	ASN	C-N-CA	5.67	125.77	119.87
1	B	128	ASN	O-C-N	5.67	129.62	123.10
1	D	323	ILE	N-CA-C	-5.67	106.28	111.67
1	D	469	ASP	CA-C-O	5.66	126.42	120.42
1	D	436	MET	CA-C-O	5.66	126.41	120.42
1	B	355	ASN	CB-CA-C	-5.65	99.98	109.53
1	C	319	ASP	N-CA-C	-5.65	106.23	113.01
1	C	875	ASP	CA-CB-CG	-5.65	106.95	112.60
1	A	770	ILE	N-CA-C	-5.64	98.31	107.28
1	C	737	ILE	N-CA-CB	5.64	119.10	111.21
1	C	625	GLN	CA-C-O	-5.63	115.58	121.55
1	B	317	THR	CA-CB-OG1	-5.63	101.15	109.60
1	C	110	ASN	CA-C-N	5.63	126.18	120.38
1	C	110	ASN	C-N-CA	5.63	126.18	120.38
1	C	91	GLN	CA-C-O	5.63	126.44	119.97
1	B	670	LEU	CA-C-N	-5.62	113.08	122.92
1	B	670	LEU	C-N-CA	-5.62	113.08	122.92
1	C	100	TYR	N-CA-CB	5.62	119.96	110.46
1	C	934	GLU	N-CA-C	-5.62	101.98	110.24
1	A	570	TRP	N-CA-C	5.62	117.27	111.03
1	D	788	PRO	N-CA-C	5.62	120.42	111.26
1	A	128	ASN	N-CA-CB	-5.61	101.48	110.63
1	A	368	ASP	CA-CB-CG	-5.61	106.99	112.60
1	A	777	LEU	N-CA-CB	5.61	118.66	110.47
1	B	987	ASP	N-CA-C	5.61	118.10	109.07
1	B	98	PRO	CB-CA-C	-5.60	103.61	110.95
1	A	327	ALA	CA-C-O	-5.60	115.28	121.28
1	B	232	ASN	N-CA-CB	5.60	118.11	110.38
1	B	845	GLN	CB-CG-CD	5.60	122.11	112.60
1	B	225	PHE	N-CA-CB	5.59	120.89	110.99
1	B	948	PRO	N-CA-C	-5.59	108.86	114.68
1	A	519	SER	N-CA-CB	-5.59	100.80	109.69
1	C	782	ASP	CB-CA-C	-5.59	99.62	109.62
1	B	842	TRP	CE2-CD2-CE3	5.59	124.39	118.80
1	B	730	LEU	O-C-N	5.59	126.38	121.18
1	C	527	PRO	N-CA-CB	5.58	108.21	103.19
1	B	646	HIS	CA-CB-CG	-5.58	108.22	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	289	VAL	CA-C-O	-5.58	116.28	120.96
1	C	454	ILE	CA-C-O	5.57	124.25	118.96
1	A	160	GLY	O-C-N	5.56	130.02	123.62
1	C	825	CYS	O-C-N	-5.56	117.95	123.62
1	D	78	LEU	CA-C-N	5.55	126.78	119.84
1	D	78	LEU	C-N-CA	5.55	126.78	119.84
1	B	680	ILE	CA-C-N	-5.54	114.37	122.19
1	B	680	ILE	C-N-CA	-5.54	114.37	122.19
1	B	729	THR	N-CA-C	5.54	117.26	108.67
1	C	469	ASP	CA-CB-CG	-5.54	107.06	112.60
1	B	610	ASP	CA-CB-CG	-5.53	107.07	112.60
1	B	854	LYS	N-CA-C	5.53	118.09	109.52
1	B	116	THR	CA-C-O	5.53	126.32	119.79
1	B	463	GLY	CA-C-N	-5.53	114.21	122.39
1	B	463	GLY	C-N-CA	-5.53	114.21	122.39
1	C	733	ALA	N-CA-C	5.53	117.70	109.25
1	A	967	LEU	CA-C-O	5.52	126.41	120.55
1	A	644	PHE	CA-C-O	-5.52	112.26	118.55
1	A	843	GLN	CA-C-N	-5.52	113.14	121.86
1	A	843	GLN	C-N-CA	-5.52	113.14	121.86
1	C	252	ASP	CA-CB-CG	-5.52	107.08	112.60
1	B	567	VAL	CB-CA-C	-5.51	103.67	111.28
1	A	890	GLN	N-CA-C	5.51	118.27	110.50
1	A	417	THR	CA-C-O	5.51	127.71	121.32
1	B	410	VAL	N-CA-C	-5.51	99.81	107.80
1	A	735	HIS	CA-CB-CG	-5.51	108.29	113.80
1	C	232	ASN	N-CA-CB	5.50	118.78	110.42
1	B	475	ILE	N-CA-CB	5.50	116.98	110.55
1	D	296	GLU	CA-C-O	-5.50	114.60	120.92
1	C	387	VAL	CA-C-N	-5.49	115.42	123.00
1	C	387	VAL	C-N-CA	-5.49	115.42	123.00
1	C	298	PRO	CB-CA-C	-5.49	104.20	111.23
1	C	400	THR	CB-CA-C	5.49	119.50	110.88
1	A	395	HIS	N-CA-CB	-5.49	101.36	109.98
1	B	345	ASN	CA-CB-CG	-5.49	107.11	112.60
1	C	450	HIS	CA-C-O	5.49	123.68	119.46
1	A	277	GLU	CB-CG-CD	5.48	121.92	112.60
1	D	418	GLU	N-CA-C	5.48	117.96	111.33
1	B	840	HIS	CB-CA-C	-5.48	98.26	109.38
1	C	395	HIS	ND1-CG-CD2	5.48	111.58	106.10
1	D	787	ALA	N-CA-C	-5.48	99.53	109.44
1	A	787	ALA	N-CA-C	-5.47	98.60	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	ASN	CA-CB-CG	-5.47	107.13	112.60
1	B	771	GLY	N-CA-C	-5.47	100.21	113.18
1	A	781	ARG	N-CA-CB	-5.47	102.03	111.55
1	C	627	PHE	CA-CB-CG	-5.46	108.34	113.80
1	A	481	SER	N-CA-C	5.46	119.80	113.20
1	C	287	ASP	CA-CB-CG	-5.46	107.14	112.60
1	A	520	ILE	N-CA-C	5.45	116.18	110.62
1	A	759	ASN	CA-CB-CG	-5.45	107.15	112.60
1	C	685	LEU	CB-CA-C	5.45	116.07	109.85
1	D	922	LEU	N-CA-C	5.45	116.91	111.07
1	B	532	PRO	CB-CA-C	-5.45	103.82	110.95
1	B	947	GLY	O-C-N	-5.44	116.33	121.77
1	A	799	THR	N-CA-CB	-5.44	101.96	110.44
1	C	321	THR	CA-CB-OG1	-5.44	101.44	109.60
1	D	47	PRO	N-CA-CB	5.44	108.08	103.35
1	B	473	ARG	CD-NE-CZ	5.44	132.01	124.40
1	A	178	ARG	NE-CZ-NH2	-5.43	114.31	119.20
1	D	453	VAL	CA-C-N	-5.43	116.11	122.14
1	D	453	VAL	C-N-CA	-5.43	116.11	122.14
1	C	448	ARG	CA-C-N	-5.42	113.97	122.65
1	C	448	ARG	C-N-CA	-5.42	113.97	122.65
1	D	92	MET	N-CA-CB	5.42	119.39	110.39
1	A	365	GLN	CA-CB-CG	-5.42	103.26	114.10
1	C	729	THR	CA-C-N	5.42	128.79	121.20
1	C	729	THR	C-N-CA	5.42	128.79	121.20
1	A	469	ASP	CA-CB-CG	-5.42	107.18	112.60
1	D	997	ASP	CA-CB-CG	-5.42	107.19	112.60
1	A	576	ILE	N-CA-CB	5.41	116.43	110.53
1	C	97	ALA	CA-C-O	5.41	124.74	120.19
1	C	499	ILE	CA-C-N	-5.41	116.83	122.89
1	C	499	ILE	C-N-CA	-5.41	116.83	122.89
1	B	634	GLN	CB-CG-CD	-5.40	103.42	112.60
1	D	257	THR	CA-C-N	-5.40	116.07	123.14
1	D	257	THR	C-N-CA	-5.40	116.07	123.14
1	D	982	THR	N-CA-C	5.40	117.21	108.41
1	A	447	ASP	N-CA-C	5.40	120.53	113.30
1	B	442	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	B	586	SER	O-C-N	5.39	129.33	123.13
1	C	742	THR	CA-CB-OG1	5.39	117.68	109.60
1	C	482	ARG	CB-CA-C	-5.39	100.02	108.91
1	D	410	VAL	N-CA-CB	5.38	118.14	111.41
1	C	42	ALA	N-CA-C	-5.38	105.41	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ASP	CA-CB-CG	-5.38	107.22	112.60
1	B	685	LEU	CB-CA-C	5.38	115.28	110.44
1	B	46	ARG	CD-NE-CZ	-5.38	116.87	124.40
1	C	877	PRO	N-CA-CB	5.38	108.03	103.35
1	D	118	ASN	N-CA-CB	-5.38	101.57	111.03
1	C	366	VAL	N-CA-CB	5.37	116.97	110.95
1	B	39	SER	N-CA-C	5.37	117.21	111.36
1	C	613	PRO	CA-C-N	-5.36	113.79	122.48
1	C	613	PRO	C-N-CA	-5.36	113.79	122.48
1	A	988	GLY	N-CA-C	-5.35	105.83	113.86
1	C	667	GLU	CB-CG-CD	-5.35	103.50	112.60
1	A	968	MET	N-CA-CB	-5.35	101.98	110.28
1	C	635	THR	N-CA-C	5.35	117.25	108.52
1	A	571	VAL	N-CA-C	5.35	116.18	108.48
1	B	164	ASP	N-CA-CB	5.34	119.51	110.49
1	A	483	PRO	CB-CA-C	-5.34	104.23	111.12
1	B	702	GLN	O-C-N	5.34	126.21	121.19
1	B	779	PRO	CB-CA-C	-5.33	104.24	111.12
1	B	750	GLU	CB-CA-C	5.33	119.54	109.37
1	D	614	HIS	N-CA-CB	5.32	115.91	109.74
1	B	78	LEU	CA-C-O	5.32	124.02	119.66
1	B	818	ALA	CA-C-O	5.32	127.04	121.19
1	C	924	ASP	CA-CB-CG	-5.31	107.29	112.60
1	D	559	TYR	CB-CA-C	-5.31	103.79	109.85
1	C	127	PHE	CA-CB-CG	-5.31	108.49	113.80
1	A	986	ILE	CB-CA-C	-5.31	104.41	110.73
1	C	16	TRP	CA-C-N	-5.30	113.79	123.34
1	C	16	TRP	C-N-CA	-5.30	113.79	123.34
1	A	155	ASN	CA-CB-CG	-5.30	107.30	112.60
1	A	410	VAL	N-CA-CB	5.30	118.34	111.67
1	B	563	GLN	N-CA-C	5.29	119.24	112.26
1	D	214	LEU	N-CA-CB	5.29	119.57	110.68
1	A	922	LEU	CA-C-O	5.29	126.56	120.90
1	D	497	ASP	CA-CB-CG	-5.29	107.31	112.60
1	A	504	ALA	N-CA-C	-5.28	102.46	110.28
1	C	788	PRO	N-CA-CB	5.28	108.03	103.27
1	D	360	HIS	CA-C-N	5.28	125.09	119.28
1	D	360	HIS	C-N-CA	5.28	125.09	119.28
1	D	968	MET	CB-CA-C	-5.28	100.53	110.67
1	A	37	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	A	82	ASP	CA-CB-CG	-5.28	107.32	112.60
1	B	388	ARG	NE-CZ-NH1	5.28	126.78	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	433	LEU	CA-C-O	5.28	123.18	118.33
1	C	729	THR	N-CA-C	5.27	117.34	108.96
1	D	165	SER	CA-C-N	-5.27	114.25	122.37
1	D	165	SER	C-N-CA	-5.27	114.25	122.37
1	B	441	THR	CA-CB-OG1	-5.27	101.70	109.60
1	B	834	VAL	N-CA-CB	5.27	118.68	111.41
1	A	877	PRO	CB-CA-C	-5.26	104.67	111.46
1	C	566	PHE	CA-CB-CG	-5.26	108.54	113.80
1	A	737	ILE	N-CA-CB	5.26	118.58	111.21
1	B	748	CYS	CA-C-N	-5.25	116.26	123.14
1	B	748	CYS	C-N-CA	-5.25	116.26	123.14
1	A	858	ILE	CA-C-N	-5.25	112.90	123.09
1	A	858	ILE	C-N-CA	-5.25	112.90	123.09
1	B	412	GLU	N-CA-C	5.25	117.46	108.90
1	C	20	GLY	N-CA-C	-5.25	106.33	113.37
1	A	352	ARG	N-CA-C	-5.24	98.75	108.24
1	B	965	GLN	OE1-CD-NE2	5.24	127.84	122.60
1	D	156	GLY	CA-C-N	-5.24	115.49	122.72
1	D	156	GLY	C-N-CA	-5.24	115.49	122.72
1	D	593	GLY	N-CA-C	-5.24	108.02	115.30
1	B	686	PRO	CB-CA-C	-5.24	102.92	111.56
1	C	735	HIS	N-CA-C	-5.24	107.19	113.21
1	D	570	TRP	CA-C-N	-5.23	115.84	123.06
1	D	570	TRP	C-N-CA	-5.23	115.84	123.06
1	A	772	ASP	N-CA-CB	-5.23	102.36	110.98
1	D	495	ALA	CA-C-N	-5.23	113.38	122.37
1	D	495	ALA	C-N-CA	-5.23	113.38	122.37
1	C	738	PRO	CB-CA-C	-5.22	104.92	111.56
1	D	673	ALA	N-CA-CB	-5.22	102.57	109.78
1	B	37	ARG	N-CA-C	-5.22	105.62	112.41
1	C	177	LEU	N-CA-CB	-5.22	102.49	110.42
1	D	785	THR	CA-CB-OG1	-5.22	101.78	109.60
1	A	138	GLN	CA-C-N	-5.21	115.65	123.00
1	A	138	GLN	C-N-CA	-5.21	115.65	123.00
1	A	675	GLN	CA-CB-CG	-5.21	103.67	114.10
1	A	832	ASP	CA-CB-CG	-5.21	107.39	112.60
1	C	809	ARG	CD-NE-CZ	5.21	131.69	124.40
1	D	777	LEU	N-CA-CB	5.21	118.07	110.47
1	B	833	ALA	N-CA-CB	-5.20	103.45	111.46
1	D	98	PRO	N-CA-C	-5.20	103.00	111.68
1	A	210	ARG	N-CA-CB	5.20	119.69	111.43
1	D	1001	PRO	N-CA-CB	5.20	107.87	103.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	472	TYR	N-CA-C	-5.19	105.51	111.07
1	A	691	ALA	N-CA-C	5.19	117.41	110.35
1	A	801	ILE	CA-CB-CG1	-5.19	101.58	110.40
1	D	815	HIS	CA-C-N	-5.19	112.06	121.14
1	D	815	HIS	C-N-CA	-5.19	112.06	121.14
1	A	401	LEU	N-CA-CB	5.19	117.53	110.01
1	D	65	ALA	O-C-N	5.19	126.43	121.71
1	D	765	LEU	N-CA-C	-5.18	99.76	110.80
1	B	779	PRO	N-CA-CB	5.18	108.26	103.39
1	C	416	GLU	CA-CB-CG	-5.18	103.74	114.10
1	A	209	PHE	N-CA-C	5.18	119.70	113.17
1	B	299	LYS	N-CA-C	-5.18	101.33	109.25
1	B	823	LEU	N-CA-CB	5.18	117.48	110.59
1	A	207	GLY	N-CA-C	5.18	118.06	111.85
1	A	750	GLU	CA-CB-CG	-5.17	103.75	114.10
1	C	559	TYR	CB-CA-C	-5.17	104.20	110.15
1	B	237	ARG	CB-CA-C	-5.17	98.08	109.56
1	B	384	PHE	CA-CB-CG	-5.17	108.63	113.80
1	B	559	TYR	CB-CA-C	-5.17	103.95	109.85
1	B	790	ASP	CA-CB-CG	-5.17	107.43	112.60
1	C	711	ALA	N-CA-C	-5.17	102.73	110.23
1	A	964	GLN	N-CA-C	-5.17	105.65	111.28
1	C	722	LEU	CA-C-O	5.17	120.94	117.94
1	D	279	ILE	CB-CG1-CD1	-5.16	102.96	113.80
1	A	626	PHE	CA-CB-CG	-5.16	108.64	113.80
1	B	629	PHE	CA-CB-CG	-5.16	108.64	113.80
1	D	890	GLN	N-CA-CB	-5.16	102.39	109.97
1	D	489	GLY	O-C-N	-5.15	116.84	122.41
1	D	736	ALA	N-CA-C	5.15	118.10	109.96
1	A	684	GLU	N-CA-CB	5.15	117.60	109.83
1	B	866	ILE	CA-C-N	-5.15	115.73	122.99
1	B	866	ILE	C-N-CA	-5.15	115.73	122.99
1	C	761	GLN	CB-CG-CD	5.14	121.34	112.60
1	C	977	HIS	CA-CB-CG	-5.14	108.66	113.80
1	B	516	PRO	CB-CA-C	-5.14	104.49	111.12
1	D	78	LEU	O-C-N	5.14	127.66	121.29
1	B	721	ARG	CB-CA-C	-5.14	100.85	109.53
1	C	670	LEU	CB-CA-C	-5.13	101.28	109.75
1	D	1004	SER	CA-CB-OG	-5.13	100.83	111.10
1	D	39	SER	N-CA-C	5.13	116.87	111.28
1	C	728	VAL	N-CA-C	-5.12	107.30	112.17
1	C	730	LEU	CA-C-O	5.12	123.41	119.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	57	GLU	CB-CA-C	-5.12	101.89	110.29
1	B	842	TRP	CB-CA-C	-5.12	101.79	110.19
1	A	700	VAL	N-CA-CB	5.12	117.91	111.46
1	C	957	PHE	CA-CB-CG	-5.12	108.69	113.80
1	B	355	ASN	CA-CB-CG	-5.11	107.49	112.60
1	B	746	ASP	CB-CA-C	-5.11	98.22	109.56
1	A	705	ALA	CA-C-O	-5.11	115.95	121.87
1	D	769	TRP	CB-CA-C	-5.10	99.02	109.38
1	D	612	THR	CA-C-N	-5.10	115.31	120.31
1	D	612	THR	C-N-CA	-5.10	115.31	120.31
1	D	648	ASP	N-CA-C	5.10	119.22	113.15
1	A	349	LEU	N-CA-C	5.09	117.25	110.53
1	B	150	PHE	CA-CB-CG	-5.09	108.71	113.80
1	D	499	ILE	N-CA-C	-5.09	101.00	108.54
1	B	1004	SER	CA-CB-OG	-5.09	100.92	111.10
1	C	682	LEU	O-C-N	5.09	127.23	121.53
1	A	232	ASN	OD1-CG-ND2	5.09	127.69	122.60
1	A	900	LEU	CA-C-N	-5.09	113.88	121.87
1	A	900	LEU	C-N-CA	-5.09	113.88	121.87
1	A	141	ILE	CA-C-N	-5.08	115.76	122.98
1	A	141	ILE	C-N-CA	-5.08	115.76	122.98
1	B	237	ARG	CA-CB-CG	-5.08	103.93	114.10
1	A	546	LEU	CA-C-N	-5.08	115.13	120.31
1	A	546	LEU	C-N-CA	-5.08	115.13	120.31
1	B	360	HIS	CA-C-O	5.07	124.72	119.86
1	D	339	ASN	CA-CB-CG	-5.07	107.53	112.60
1	D	450	HIS	CA-C-N	-5.07	113.82	119.19
1	D	450	HIS	C-N-CA	-5.07	113.82	119.19
1	C	112	PRO	CA-C-N	-5.06	111.90	122.07
1	C	112	PRO	C-N-CA	-5.06	111.90	122.07
1	A	1006	GLU	CG-CD-OE2	-5.06	106.77	118.40
1	B	98	PRO	N-CA-C	-5.06	103.82	111.41
1	B	102	ASN	CA-CB-CG	5.06	117.66	112.60
1	C	210	ARG	N-CA-CB	5.06	120.35	111.55
1	B	134	LEU	CA-C-N	-5.05	113.00	120.28
1	B	134	LEU	C-N-CA	-5.05	113.00	120.28
1	C	429	ASP	CB-CA-C	-5.05	105.17	110.17
1	A	869	ASP	CA-CB-CG	-5.05	107.55	112.60
1	B	447	ASP	N-CA-CB	-5.05	103.02	110.49
1	C	739	HIS	ND1-CG-CD2	5.05	111.15	106.10
1	C	351	ILE	N-CA-C	5.05	115.60	107.98
1	A	539	ALA	CB-CA-C	-5.05	104.32	112.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	747	PHE	N-CA-C	-5.05	100.29	108.52
1	A	772	ASP	CA-C-N	-5.04	115.76	122.72
1	A	772	ASP	C-N-CA	-5.04	115.76	122.72
1	C	842	TRP	CB-CG-CD2	-5.04	119.74	126.80
1	C	489	GLY	CA-C-N	-5.04	114.23	122.40
1	C	489	GLY	C-N-CA	-5.04	114.23	122.40
1	A	510	GLN	CA-C-O	5.04	126.70	121.00
1	C	241	GLU	CB-CG-CD	-5.04	104.03	112.60
1	C	568	TRP	CB-CA-C	-5.04	102.57	110.79
1	A	634	GLN	CA-C-N	-5.04	116.05	123.00
1	A	634	GLN	C-N-CA	-5.04	116.05	123.00
1	C	303	ALA	N-CA-C	-5.04	106.64	112.89
1	B	759	ASN	CA-CB-CG	5.04	117.64	112.60
1	B	875	ASP	CA-CB-CG	-5.04	107.56	112.60
1	A	29	ALA	O-C-N	-5.03	117.27	122.96
1	A	181	GLU	N-CA-C	5.03	116.95	109.25
1	A	562	LEU	CA-C-N	-5.03	115.08	122.83
1	A	562	LEU	C-N-CA	-5.03	115.08	122.83
1	D	194	GLY	N-CA-C	-5.03	106.65	113.24
1	D	818	ALA	CA-C-N	5.03	129.94	123.00
1	D	818	ALA	C-N-CA	5.03	129.94	123.00
1	A	606	LEU	CA-C-O	5.02	125.54	119.31
1	C	950	GLN	CA-CB-CG	-5.02	104.05	114.10
1	D	612	THR	N-CA-C	-5.02	103.70	109.93
1	B	776	LEU	N-CA-C	5.02	117.67	109.59
1	C	431	ARG	CA-CB-CG	-5.02	104.07	114.10
1	C	768	MET	N-CA-CB	5.01	120.10	111.13
1	B	685	LEU	CA-C-O	5.01	123.77	119.71
1	A	556	PHE	CA-CB-CG	5.01	118.81	113.80
1	C	300	LEU	CA-C-N	-5.01	114.67	122.09
1	C	300	LEU	C-N-CA	-5.01	114.67	122.09
1	B	123	TYR	N-CA-CB	5.01	118.79	110.63
1	C	576	ILE	CB-CA-C	-5.01	104.35	111.21
1	B	632	SER	N-CA-CB	5.00	118.36	110.71

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	8124	0	7715	212	0
1	B	8124	0	7715	245	0
1	C	8124	0	7715	251	0
1	D	8124	0	7715	206	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	68	0	102	15	0
4	B	76	0	114	17	0
4	C	92	0	138	21	0
4	D	92	0	138	25	0
5	A	871	0	0	19	0
5	B	864	0	0	20	0
5	C	838	0	0	17	0
5	D	891	0	0	24	0
All	All	36314	0	31352	921	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (921) 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:D:804:ASN:ND2	1:D:809:ARG:HH21	1.32	1.26
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.42	1.18
1:C:634:GLN:H	1:C:634:GLN:NE2	1.46	1.11
1:B:744:GLU:HB2	1:B:745:MET:HE3	1.21	1.11
1:C:765:LEU:HD21	1:C:768:MET:HE2	1.33	1.09
1:B:804:ASN:ND2	1:B:809:ARG:HH21	1.51	1.06
1:B:367:MET:HE1	1:B:371:THR:HG22	1.39	1.03
1:A:600:GLN:H	1:A:600:GLN:HE21	1.07	1.01
1:D:651:LEU:HD11	1:D:653:HIS:CE1	1.97	0.99
1:D:292:ARG:HH12	4:D:8412:DMS:H23	1.27	0.97
1:A:157:ARG:HG3	1:A:157:ARG:HH11	1.29	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:737:ILE:HD12	1:C:738:PRO:HD2	1.47	0.96
1:B:804:ASN:HD22	1:B:809:ARG:HH21	1.06	0.96
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.49	0.94
1:C:634:GLN:HE21	1:C:634:GLN:N	1.65	0.93
1:C:634:GLN:H	1:C:634:GLN:HE21	0.94	0.92
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.52	0.90
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.53	0.90
1:C:781:ARG:HG2	1:C:781:ARG:HH11	1.38	0.89
1:D:651:LEU:C	1:D:651:LEU:HD12	1.97	0.89
1:A:473:ARG:NH1	1:A:476:LYS:HB2	1.88	0.88
1:C:356:ARG:HH22	1:C:367:MET:HE2	1.39	0.88
1:B:655:MET:HE2	1:B:665:SER:HB3	1.53	0.87
1:C:827:ALA:HA	1:C:836:ILE:HD13	1.56	0.87
1:B:744:GLU:CB	1:B:745:MET:HE3	2.05	0.86
1:C:765:LEU:CD2	1:C:768:MET:HE2	2.05	0.86
1:A:292:ARG:HH12	4:A:8412:DMS:H23	1.38	0.86
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.58	0.86
1:D:128:ASN:HB3	1:D:180:GLY:O	1.76	0.86
1:B:863:GLN:HG3	1:B:1021:CYS:HB3	1.58	0.84
1:B:581:ASN:HB2	1:B:583:ASN:HD22	1.43	0.84
1:D:629:PHE:O	1:D:630:ARG:HD3	1.77	0.84
1:B:730:LEU:HD12	1:B:730:LEU:H	1.40	0.84
1:B:744:GLU:HB2	1:B:745:MET:CE	2.06	0.83
1:B:804:ASN:HD22	1:B:809:ARG:NH2	1.76	0.83
1:C:633:GLY:HA3	1:C:634:GLN:HE21	1.44	0.81
1:A:615:PRO:O	1:A:618:THR:HG22	1.81	0.79
1:B:634:GLN:HG2	1:B:682:LEU:O	1.81	0.79
1:C:687:GLN:HE21	1:C:687:GLN:HA	1.47	0.79
1:A:787:ALA:HA	1:A:968:MET:HG3	1.64	0.79
1:B:634:GLN:CG	1:B:682:LEU:HB2	2.11	0.79
1:C:634:GLN:NE2	1:C:634:GLN:N	2.27	0.79
1:C:785:THR:O	1:C:881:ARG:HD2	1.83	0.78
1:C:41:GLU:HG2	5:C:4002:HOH:O	1.83	0.78
1:B:600:GLN:H	1:B:600:GLN:HE21	1.31	0.78
1:A:804:ASN:OD1	1:A:809:ARG:NH2	2.16	0.78
1:D:105:TYR:O	4:D:8419:DMS:H23	1.84	0.78
5:B:4700:HOH:O	4:C:8420:DMS:H22	1.84	0.77
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.66	0.77
4:A:8602:DMS:H13	5:A:4610:HOH:O	1.84	0.77
1:D:653:HIS:ND1	1:D:701:VAL:HG21	2.00	0.76
1:C:132:SER:HB2	4:C:8504:DMS:H12	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:595:THR:HA	1:D:596:PRO:C	2.09	0.76
1:D:581:ASN:HD22	1:D:583:ASN:HD22	1.30	0.76
1:A:367:MET:HB3	1:A:372:MET:HE3	1.68	0.76
1:A:965:GLN:O	1:A:969:GLU:HG3	1.86	0.75
1:A:277:GLU:H	1:A:277:GLU:CD	1.93	0.74
1:C:748:CYS:C	1:C:749:ILE:HD12	2.13	0.74
1:C:356:ARG:NH2	1:C:367:MET:HE2	2.02	0.73
1:A:292:ARG:HH12	4:A:8412:DMS:C2	2.00	0.73
1:D:107:ILE:CA	4:D:8419:DMS:H21	2.18	0.73
1:B:131:GLU:O	1:B:135:GLN:HG2	1.88	0.72
1:B:615:PRO:O	1:B:618:THR:HG22	1.88	0.72
1:C:367:MET:HB3	1:C:372:MET:HE2	1.71	0.72
1:A:1022:GLN:HG2	1:A:1023:LYS:N	2.04	0.72
1:B:132:SER:HA	1:B:135:GLN:HG2	1.70	0.72
1:A:178:ARG:HD2	5:A:4741:HOH:O	1.88	0.72
1:C:356:ARG:HD2	1:C:379:MET:CE	2.19	0.72
1:A:887:GLN:NE2	1:A:980:GLU:O	2.22	0.72
1:B:356:ARG:HD2	1:B:379:MET:HE1	1.70	0.71
4:D:8703:DMS:H21	5:D:4835:HOH:O	1.90	0.71
1:C:243:GLU:OE2	1:C:245:GLN:NE2	2.20	0.71
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.73	0.71
1:A:824:GLN:HG2	1:A:825:CYS:N	2.04	0.71
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.73	0.71
1:D:107:ILE:N	4:D:8419:DMS:H21	2.06	0.71
1:A:473:ARG:HH11	1:A:476:LYS:HB2	1.54	0.70
1:B:595:THR:HA	1:B:596:PRO:C	2.16	0.70
1:C:613:PRO:HB3	1:C:617:LEU:HD23	1.73	0.70
1:D:133:TRP:NE1	4:D:8703:DMS:H23	2.07	0.70
1:D:1022:GLN:HE21	1:D:1023:LYS:N	1.89	0.70
1:D:277:GLU:CD	1:D:277:GLU:H	1.99	0.70
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.26	0.69
1:A:292:ARG:NH1	4:A:8412:DMS:H23	2.08	0.69
1:D:367:MET:HB3	1:D:372:MET:HE2	1.74	0.69
1:A:599:ARG:HH11	1:A:600:GLN:NE2	1.89	0.69
1:C:799:THR:O	1:C:800:ARG:HG2	1.92	0.69
1:A:183:ARG:HD3	5:A:4302:HOH:O	1.92	0.69
1:A:243:GLU:OE2	1:A:245:GLN:NE2	2.24	0.69
1:C:615:PRO:O	1:C:618:THR:HG22	1.92	0.69
1:C:651:LEU:HD12	1:C:651:LEU:O	1.93	0.69
1:A:599:ARG:HG3	1:A:600:GLN:NE2	2.08	0.68
1:B:316:HIS:CD2	4:B:8406:DMS:H23	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:755:ARG:HG2	1:C:769:TRP:CE3	2.29	0.68
1:D:316:HIS:HA	1:D:323:ILE:HD13	1.75	0.68
1:D:577:LYS:O	1:D:584:PRO:HA	1.92	0.68
1:B:251:ARG:CD	4:B:8416:DMS:H23	2.23	0.68
1:C:633:GLY:HA3	1:C:634:GLN:NE2	2.08	0.68
1:A:920:LEU:HB3	1:A:921:PRO:HD2	1.74	0.68
1:A:843:GLN:HG2	1:A:848:THR:HA	1.76	0.68
1:C:878:HIS:HD2	5:C:4094:HOH:O	1.76	0.68
1:B:701:VAL:HG22	1:B:714:ILE:HG12	1.75	0.67
1:B:687:GLN:NE2	1:B:687:GLN:HA	2.10	0.67
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.75	0.67
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.16	0.67
1:C:131:GLU:HG3	1:C:135:GLN:NE2	2.09	0.67
1:C:651:LEU:HD12	1:C:651:LEU:C	2.19	0.67
1:C:843:GLN:NE2	1:C:848:THR:OG1	2.27	0.67
1:D:887:GLN:NE2	1:D:980:GLU:O	2.27	0.67
1:A:595:THR:HA	1:A:596:PRO:C	2.20	0.67
1:B:132:SER:HA	1:B:135:GLN:CG	2.24	0.67
4:D:8419:DMS:H22	5:D:4366:HOH:O	1.94	0.67
1:A:128:ASN:HA	1:A:180:GLY:O	1.94	0.67
1:A:685:LEU:HD23	5:A:4839:HOH:O	1.94	0.67
1:B:1018:LEU:HD23	1:B:1019:VAL:N	2.08	0.67
1:A:168:PRO:O	1:A:442:ARG:NH2	2.28	0.66
1:B:316:HIS:CG	4:B:8406:DMS:H23	2.28	0.66
1:B:262:GLN:HE21	1:B:262:GLN:C	2.03	0.66
1:A:252:ASP:CG	4:A:8416:DMS:H12	2.20	0.66
1:A:98:PRO:HB2	1:A:203:TRP:CE3	2.30	0.66
1:B:296:GLU:HB2	4:B:8601:DMS:O	1.94	0.66
1:B:200:GLN:HG2	1:B:391:HIS:HB2	1.77	0.66
1:D:781:ARG:NH1	5:D:4692:HOH:O	2.27	0.66
1:D:1022:GLN:HE21	1:D:1022:GLN:C	2.04	0.66
1:B:367:MET:HE1	1:B:371:THR:CG2	2.20	0.66
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.77	0.66
1:D:473:ARG:HH11	1:D:476:LYS:HB2	1.60	0.66
1:C:653:HIS:ND1	1:C:667:GLU:HG2	2.11	0.66
4:D:8411:DMS:H11	5:D:4286:HOH:O	1.96	0.66
1:C:781:ARG:HG2	1:C:781:ARG:NH1	2.11	0.66
1:B:655:MET:CE	1:B:665:SER:HB3	2.24	0.65
1:A:600:GLN:HE21	1:A:600:GLN:N	1.89	0.65
1:C:646:HIS:HB3	5:C:4747:HOH:O	1.96	0.65
1:C:658:LEU:HG	1:C:661:LYS:NZ	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:659:ASP:OD2	1:B:692:GLY:HA3	1.97	0.65
1:B:878:HIS:HD2	5:B:4087:HOH:O	1.79	0.65
1:C:827:ALA:HA	1:C:836:ILE:CD1	2.25	0.65
1:C:802:ASP:O	1:C:808:GLU:HG3	1.96	0.65
1:B:132:SER:HA	1:B:135:GLN:CD	2.21	0.65
1:B:581:ASN:HB2	1:B:583:ASN:ND2	2.10	0.65
1:C:92:MET:HE2	1:C:92:MET:HA	1.79	0.65
1:D:292:ARG:HH12	4:D:8412:DMS:C2	2.07	0.65
1:D:660:GLY:O	1:D:662:PRO:HD3	1.97	0.65
1:D:1022:GLN:NE2	1:D:1023:LYS:HG2	2.11	0.65
1:B:117:GLU:HB2	5:B:4415:HOH:O	1.95	0.65
1:C:1020:TRP:HD1	1:C:1021:CYS:N	1.95	0.65
1:A:252:ASP:OD2	4:A:8416:DMS:H12	1.97	0.65
1:A:746:ASP:HA	1:A:760:ARG:HG3	1.79	0.64
1:D:63:PHE:HB3	1:D:64:PRO:HD2	1.79	0.64
1:B:251:ARG:HD2	4:B:8416:DMS:H23	1.80	0.64
1:D:102:ASN:HB3	4:D:8506:DMS:H11	1.79	0.64
1:D:749:ILE:HD12	1:D:749:ILE:N	2.13	0.64
1:C:765:LEU:HD21	1:C:768:MET:CE	2.20	0.64
1:D:573:GLN:HB2	1:D:602:CYS:O	1.98	0.63
1:B:181:GLU:OE2	1:B:181:GLU:HA	1.98	0.63
1:D:973:ARG:O	4:D:8423:DMS:H12	1.98	0.63
1:C:754:LYS:NZ	1:C:1022:GLN:OE1	2.32	0.63
1:C:687:GLN:HA	1:C:687:GLN:NE2	2.13	0.63
1:D:658:LEU:O	1:D:661:LYS:HG3	1.99	0.63
1:B:381:GLN:O	1:B:621:LYS:HE3	1.98	0.63
1:C:573:GLN:HB2	1:C:602:CYS:O	1.99	0.63
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.28	0.63
1:D:106:PRO:C	4:D:8419:DMS:H21	2.24	0.62
1:D:893:GLU:HG2	1:D:894:ARG:CD	2.28	0.62
1:B:634:GLN:NE2	1:B:683:PRO:O	2.31	0.62
1:C:633:GLY:CA	1:C:634:GLN:HE21	2.11	0.62
1:D:360:HIS:CE1	1:D:362:LEU:HB2	2.34	0.62
4:A:8403:DMS:H12	5:A:4076:HOH:O	2.00	0.62
1:C:653:HIS:CE1	1:C:667:GLU:HG2	2.34	0.62
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.33	0.62
1:B:377:LEU:CD2	1:B:708:TRP:HA	2.29	0.62
1:B:651:LEU:HD22	1:B:651:LEU:O	1.99	0.62
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.00	0.62
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.81	0.62
1:B:637:GLU:CD	1:B:677:LYS:HD3	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:768:MET:HE1	1:C:1020:TRP:CH2	2.34	0.62
1:D:88:SER:HA	1:D:366:VAL:HG21	1.80	0.62
1:A:646:HIS:ND1	5:A:4723:HOH:O	2.23	0.61
1:C:986:ILE:HG21	1:C:1018:LEU:HD21	1.82	0.61
1:B:1020:TRP:HD1	1:B:1021:CYS:N	1.96	0.61
1:A:249:GLU:OE2	1:A:251:ARG:NH2	2.32	0.61
4:B:8404:DMS:H12	5:B:4593:HOH:O	2.01	0.61
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.81	0.61
1:B:634:GLN:HE21	1:B:683:PRO:C	2.07	0.61
1:C:997:ASP:HB2	1:C:999:TRP:CZ2	2.36	0.61
1:D:133:TRP:HE1	4:D:8703:DMS:C2	2.13	0.61
1:D:737:ILE:HD13	1:D:832:ASP:HA	1.83	0.61
1:A:754:LYS:NZ	5:A:4760:HOH:O	2.34	0.60
1:A:824:GLN:NE2	1:A:837:THR:HG22	2.16	0.60
1:B:233:ASP:HA	4:B:8417:DMS:H13	1.83	0.60
1:C:890:GLN:OE1	1:C:948:PRO:HD3	2.01	0.60
1:D:133:TRP:HE1	4:D:8703:DMS:H23	1.65	0.60
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.83	0.60
1:A:686:PRO:C	1:A:688:PRO:HD3	2.26	0.60
1:D:788:PRO:HD2	1:D:968:MET:HG3	1.84	0.60
1:B:890:GLN:HB2	5:B:4808:HOH:O	2.00	0.60
1:C:655:MET:HE2	1:C:664:ALA:O	2.01	0.60
1:B:334:GLU:OE1	1:B:336:ARG:NH1	2.30	0.60
1:A:75:GLU:OE1	1:A:75:GLU:HA	2.01	0.60
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.66	0.60
1:B:755:ARG:HD3	5:B:4833:HOH:O	2.00	0.60
1:B:262:GLN:HE21	1:B:263:GLY:N	1.99	0.60
1:C:833:ALA:HB1	1:C:858:ILE:O	2.01	0.60
1:B:797:GLU:O	1:B:801:ILE:HD13	2.02	0.60
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.37	0.60
1:D:653:HIS:CE1	1:D:701:VAL:HG21	2.37	0.60
1:B:52:ARG:NH1	5:B:4602:HOH:O	2.34	0.59
1:C:634:GLN:H	1:C:634:GLN:CD	1.95	0.59
1:A:873:ALA:O	1:A:876:THR:HG22	2.02	0.59
1:C:614:HIS:HB3	1:C:615:PRO:HD2	1.84	0.59
1:B:596:PRO:HB3	5:B:4714:HOH:O	2.02	0.59
1:D:896:ASN:HB2	1:D:919:ASP:OD2	2.02	0.59
1:B:499:ILE:HD11	1:B:529:GLU:CD	2.27	0.59
1:D:746:ASP:HA	1:D:760:ARG:HG3	1.84	0.59
1:A:742:THR:HG22	1:A:743:SER:N	2.16	0.59
1:C:292:ARG:HG3	1:C:292:ARG:HH11	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:703:PRO:HG2	4:D:8425:DMS:H12	1.84	0.59
1:B:114:VAL:HB	1:B:115:PRO:HD2	1.84	0.59
1:D:745:MET:HE1	1:D:761:GLN:NE2	2.18	0.59
1:A:533:LEU:C	1:A:533:LEU:HD23	2.28	0.59
1:A:878:HIS:HD2	5:A:4073:HOH:O	1.86	0.59
4:A:8404:DMS:H12	5:A:4344:HOH:O	2.03	0.59
1:B:37:ARG:HH12	4:B:8504:DMS:H21	1.67	0.58
1:B:132:SER:CA	1:B:135:GLN:HG2	2.32	0.58
1:C:46:ARG:NH2	5:C:4002:HOH:O	2.27	0.58
1:C:377:LEU:CD2	1:C:708:TRP:HA	2.33	0.58
1:C:809:ARG:HH22	1:C:1001:PRO:HB3	1.67	0.58
1:A:577:LYS:O	1:A:584:PRO:HA	2.03	0.58
1:A:648:ASP:OD2	5:A:4772:HOH:O	2.17	0.58
1:B:128:ASN:HB2	5:B:4776:HOH:O	2.04	0.58
1:B:863:GLN:HG3	1:B:1021:CYS:CB	2.31	0.58
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.38	0.58
1:A:863:GLN:NE2	1:A:952:ARG:HH22	2.01	0.58
1:D:584:PRO:HD2	5:D:4674:HOH:O	2.03	0.58
1:D:893:GLU:HG2	1:D:894:ARG:HD2	1.84	0.58
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.84	0.58
1:C:797:GLU:O	1:C:801:ILE:HD13	2.03	0.58
1:B:88:SER:HA	1:B:366:VAL:HG21	1.85	0.58
1:D:240:LEU:HD23	1:D:240:LEU:C	2.28	0.58
1:A:688:PRO:O	1:A:689:GLU:HB2	2.03	0.58
1:B:739:HIS:ND1	1:B:750:GLU:OE1	2.37	0.58
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.86	0.58
1:C:768:MET:O	1:C:775:GLN:N	2.32	0.58
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.39	0.58
1:A:737:ILE:C	1:A:737:ILE:HD13	2.29	0.58
1:D:1022:GLN:O	1:D:1022:GLN:HG3	2.02	0.58
1:C:572:ASP:HB3	1:C:603:MET:HG2	1.86	0.57
1:B:131:GLU:OE2	1:B:134:LEU:HB2	2.05	0.57
1:D:767:GLN:NE2	1:D:774:LYS:HZ3	2.02	0.57
1:B:241:GLU:HG3	1:B:292:ARG:HG2	1.85	0.57
1:B:878:HIS:CE1	1:B:1010:SER:HB3	2.40	0.57
1:C:250:LEU:O	1:C:251:ARG:HD3	2.05	0.57
1:C:595:THR:HA	1:C:596:PRO:C	2.28	0.57
1:D:237:ARG:HH11	1:D:237:ARG:HG2	1.69	0.57
1:A:587:ALA:HB1	1:A:591:ASP:HB2	1.86	0.57
1:A:844:HIS:CE1	1:A:845:GLN:HG3	2.39	0.57
1:A:861:SER:OG	1:A:863:GLN:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:ARG:HH11	1:B:600:GLN:NE2	2.03	0.57
1:C:334:GLU:OE1	1:C:336:ARG:NH1	2.36	0.57
1:D:622:HIS:O	1:D:625:GLN:HG3	2.05	0.57
1:D:1022:GLN:O	1:D:1023:LYS:HB2	2.05	0.57
1:B:824:GLN:HG2	1:B:825:CYS:N	2.19	0.56
1:C:70:PRO:HG2	1:C:78:LEU:HD21	1.87	0.56
1:D:896:ASN:OD1	1:D:917:ARG:NH1	2.35	0.56
1:C:533:LEU:C	1:C:533:LEU:HD23	2.29	0.56
1:D:292:ARG:NH1	4:D:8412:DMS:H23	2.10	0.56
1:A:132:SER:HA	1:A:135:GLN:HG3	1.87	0.56
1:B:360:HIS:HE1	1:B:362:LEU:HB2	1.71	0.56
1:D:893:GLU:HG2	1:D:894:ARG:HG2	1.87	0.56
1:A:372:MET:HE1	1:A:395:HIS:HB3	1.87	0.56
1:A:947:GLY:O	1:A:1023:LYS:HE3	2.05	0.56
1:B:533:LEU:HD23	1:B:533:LEU:C	2.30	0.56
1:C:750:GLU:OE2	1:C:755:ARG:HD2	2.04	0.56
1:A:599:ARG:HG3	1:A:600:GLN:HE21	1.68	0.56
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.86	0.56
1:A:84:VAL:HA	4:A:8414:DMS:O	2.06	0.56
1:A:347:LYS:HE3	5:A:4259:HOH:O	2.06	0.56
1:D:360:HIS:HE1	1:D:362:LEU:HB2	1.69	0.56
1:A:71:GLU:HG2	5:A:4655:HOH:O	2.06	0.56
1:A:613:PRO:HB3	1:A:617:LEU:HD23	1.88	0.56
1:B:127:PHE:O	1:B:182:ASN:N	2.36	0.56
1:C:1023:LYS:HE3	1:C:1023:LYS:HA	1.88	0.56
1:D:651:LEU:HD12	1:D:651:LEU:O	2.03	0.56
1:B:243:GLU:OE2	1:B:245:GLN:NE2	2.37	0.56
1:B:131:GLU:OE1	1:B:179:ALA:HB2	2.06	0.55
1:B:360:HIS:ND1	1:B:361:PRO:HD2	2.21	0.55
1:B:797:GLU:O	1:B:800:ARG:N	2.37	0.55
1:C:708:TRP:CH2	4:C:8403:DMS:H13	2.40	0.55
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.06	0.55
1:A:584:PRO:HD2	5:A:4628:HOH:O	2.06	0.55
1:B:662:PRO:C	1:B:663:LEU:HD23	2.31	0.55
1:C:781:ARG:HH11	1:C:781:ARG:CG	2.16	0.55
1:D:765:LEU:HD21	1:D:768:MET:SD	2.45	0.55
1:D:770:ILE:HD12	1:D:775:GLN:CD	2.31	0.55
1:A:358:GLU:C	1:A:367:MET:HE3	2.31	0.55
1:D:133:TRP:CD1	4:D:8703:DMS:H23	2.41	0.55
1:D:317:THR:HG23	1:D:323:ILE:HD11	1.87	0.55
1:A:651:LEU:HD23	1:A:703:PRO:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:LYS:O	4:C:8403:DMS:H11	2.06	0.55
1:B:356:ARG:HH22	1:B:367:MET:HE2	1.72	0.55
1:B:658:LEU:N	1:B:661:LYS:O	2.39	0.55
1:B:822:LEU:HD21	1:B:825:CYS:HB2	1.89	0.55
1:C:652:LEU:HD11	1:C:698:VAL:HB	1.88	0.55
1:A:684:GLU:HG2	1:A:685:LEU:N	2.21	0.55
1:B:37:ARG:NH1	4:B:8504:DMS:H21	2.21	0.55
1:A:88:SER:HA	1:A:366:VAL:HG21	1.89	0.55
1:D:135:GLN:C	1:D:136:GLU:HG2	2.31	0.55
1:D:770:ILE:HD12	1:D:775:GLN:NE2	2.22	0.55
1:C:930:VAL:HA	1:C:973:ARG:HD3	1.89	0.55
1:D:628:GLN:HB3	5:D:4561:HOH:O	2.07	0.54
1:B:356:ARG:HD2	1:B:379:MET:CE	2.36	0.54
1:B:737:ILE:HD11	5:B:4803:HOH:O	2.07	0.54
1:C:962:TYR:OH	4:C:8423:DMS:H21	2.08	0.54
1:D:316:HIS:HA	1:D:323:ILE:CD1	2.38	0.54
1:D:738:PRO:HB3	1:D:751:LEU:HB2	1.89	0.54
1:A:252:ASP:HB2	4:A:8416:DMS:O	2.06	0.54
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.42	0.54
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.42	0.54
1:A:472:TYR:O	1:A:476:LYS:HG2	2.08	0.54
1:B:708:TRP:CZ2	4:B:8403:DMS:H13	2.42	0.54
1:C:658:LEU:O	1:C:659:ASP:C	2.47	0.54
1:D:117:GLU:HB2	5:D:4434:HOH:O	2.07	0.54
1:A:738:PRO:HG3	1:A:751:LEU:HD22	1.89	0.54
1:B:231:PHE:O	4:B:8417:DMS:H23	2.08	0.54
1:A:360:HIS:HE1	1:A:362:LEU:HD12	1.73	0.54
1:C:768:MET:HE1	1:C:1020:TRP:CZ3	2.43	0.54
1:C:88:SER:HA	1:C:366:VAL:HG21	1.90	0.54
1:A:685:LEU:HB3	1:A:686:PRO:CD	2.36	0.54
1:B:763:GLY:HA3	1:B:822:LEU:HD13	1.91	0.54
1:D:288:ARG:NH1	5:D:4461:HOH:O	2.30	0.54
1:C:658:LEU:HD11	1:C:692:GLY:HA3	1.91	0.53
1:A:753:ASN:OD1	1:A:753:ASN:N	2.40	0.53
1:C:734:SER:C	1:C:736:ALA:H	2.16	0.53
1:C:782:ASP:HA	1:C:884:LEU:HD23	1.90	0.53
1:C:749:ILE:HD12	1:C:749:ILE:N	2.21	0.53
1:A:200:GLN:HG2	1:A:391:HIS:HB2	1.90	0.53
1:B:625:GLN:NE2	5:B:4216:HOH:O	2.32	0.53
1:B:1017:GLN:HB2	5:B:4804:HOH:O	2.09	0.53
1:B:117:GLU:OE1	1:B:117:GLU:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:VAL:HG13	1:C:87:PRO:HA	1.90	0.53
1:C:499:ILE:HD11	1:C:529:GLU:CD	2.33	0.53
1:C:733:ALA:O	1:C:734:SER:C	2.51	0.53
1:C:764:PHE:CE1	1:C:781:ARG:NH1	2.77	0.53
1:D:773:LYS:HD2	1:D:774:LYS:O	2.08	0.53
1:A:355:ASN:OD1	1:A:388:ARG:HD3	2.09	0.53
1:B:437:SER:HB2	1:B:471:LEU:HD21	1.89	0.53
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.22	0.53
1:D:965:GLN:O	1:D:969:GLU:HG3	2.09	0.53
1:B:585:TRP:CE3	1:B:974:HIS:CE1	2.97	0.53
1:D:730:LEU:HD12	1:D:730:LEU:H	1.73	0.53
1:A:660:GLY:O	1:A:662:PRO:HD3	2.08	0.53
1:D:277:GLU:OE2	4:D:8412:DMS:H22	2.09	0.53
1:A:599:ARG:HH11	1:A:600:GLN:HE22	1.58	0.52
1:B:13:ARG:HG3	1:C:13:ARG:NH1	2.23	0.52
1:D:1017:GLN:HB2	5:D:4874:HOH:O	2.09	0.52
1:B:52:ARG:O	1:B:213:SER:HB2	2.08	0.52
1:B:71:GLU:H	1:B:71:GLU:CD	2.17	0.52
1:B:842:TRP:C	1:B:843:GLN:HG3	2.33	0.52
1:A:625:GLN:NE2	5:A:4201:HOH:O	2.35	0.52
1:A:725:ASN:HB2	5:A:4834:HOH:O	2.10	0.52
1:D:997:ASP:HB2	1:D:999:TRP:CZ2	2.45	0.52
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.91	0.52
1:A:797:GLU:O	1:A:801:ILE:HD13	2.09	0.52
1:D:79:PRO:HG2	1:D:80:GLU:OE2	2.10	0.52
1:B:317:THR:OG1	1:B:319:ASP:OD1	2.27	0.52
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.92	0.52
1:A:892:ALA:HB3	1:A:946:TYR:CE1	2.45	0.52
1:B:777:LEU:HG	1:B:889:ALA:HA	1.91	0.52
1:C:396:PRO:HG3	5:C:4147:HOH:O	2.10	0.52
1:C:499:ILE:HD11	1:C:529:GLU:CG	2.38	0.52
1:C:930:VAL:O	1:C:932:PRO:HD3	2.10	0.52
1:D:878:HIS:CE1	1:D:1010:SER:HB3	2.44	0.52
1:B:360:HIS:CE1	1:B:361:PRO:HD2	2.45	0.52
1:D:237:ARG:HG2	1:D:237:ARG:NH1	2.25	0.52
1:D:891:VAL:HG23	1:D:981:GLY:HA2	1.91	0.52
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.78	0.52
1:B:91:GLN:HG2	1:B:98:PRO:HA	1.92	0.52
1:C:756:TRP:CD2	1:C:858:ILE:HD13	2.45	0.52
1:C:972:HIS:HB3	1:C:974:HIS:HD1	1.75	0.52
1:D:802:ASP:O	1:D:808:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:878:HIS:HD2	5:D:4110:HOH:O	1.93	0.52
1:C:127:PHE:N	1:C:127:PHE:CD2	2.78	0.52
1:C:178:ARG:HD2	5:C:4783:HOH:O	2.10	0.52
1:D:893:GLU:CG	1:D:894:ARG:HD2	2.40	0.52
1:A:127:PHE:N	1:A:127:PHE:CD2	2.77	0.51
1:D:651:LEU:C	1:D:651:LEU:CD1	2.74	0.51
1:A:683:PRO:O	1:A:685:LEU:HG	2.09	0.51
1:C:577:LYS:O	1:C:584:PRO:HA	2.09	0.51
1:C:767:GLN:HG3	1:C:768:MET:N	2.26	0.51
1:D:356:ARG:HH22	1:D:367:MET:HE2	1.76	0.51
4:D:8423:DMS:H11	5:D:4553:HOH:O	2.10	0.51
1:A:129:VAL:N	1:A:180:GLY:O	2.41	0.51
1:B:655:MET:HE2	1:B:664:ALA:O	2.09	0.51
1:C:579:ASP:OD1	1:C:583:ASN:HB2	2.09	0.51
1:A:499:ILE:HG22	1:A:501:PRO:HD3	1.92	0.51
1:C:805:ALA:O	1:C:806:TRP:C	2.52	0.51
1:B:86:VAL:HG13	1:B:87:PRO:HA	1.92	0.51
1:B:635:THR:HG23	1:B:681:GLU:OE1	2.10	0.51
1:B:251:ARG:HD3	4:B:8416:DMS:H23	1.90	0.51
1:C:1020:TRP:CD1	1:C:1021:CYS:N	2.77	0.51
1:A:997:ASP:HB2	1:A:999:TRP:CZ2	2.46	0.51
1:B:730:LEU:HD12	1:B:730:LEU:N	2.17	0.51
1:A:157:ARG:HG3	1:A:157:ARG:NH1	2.05	0.51
1:A:800:ARG:CZ	1:A:800:ARG:HB2	2.36	0.51
1:B:685:LEU:O	1:B:686:PRO:C	2.52	0.51
1:B:824:GLN:OE1	1:B:837:THR:HG22	2.11	0.51
1:D:145:GLY:HA2	5:D:4107:HOH:O	2.10	0.51
4:D:8404:DMS:H23	5:D:4164:HOH:O	2.10	0.51
1:A:745:MET:HE1	1:A:761:GLN:HE21	1.75	0.51
1:B:577:LYS:O	1:B:584:PRO:HA	2.11	0.51
1:D:521:LYS:HE2	5:D:4453:HOH:O	2.11	0.51
1:C:579:ASP:CG	1:C:583:ASN:HB2	2.36	0.50
1:C:708:TRP:CZ2	4:C:8403:DMS:H13	2.46	0.50
1:C:745:MET:O	1:C:746:ASP:OD1	2.29	0.50
1:D:843:GLN:HA	1:D:847:LYS:O	2.11	0.50
1:D:890:GLN:HG3	1:D:891:VAL:N	2.25	0.50
1:B:629:PHE:HA	1:B:637:GLU:O	2.11	0.50
1:D:896:ASN:HD21	1:D:917:ARG:HD2	1.77	0.50
1:A:125:LEU:O	1:A:183:ARG:HA	2.12	0.50
1:B:319:ASP:OD1	1:B:321:THR:N	2.42	0.50
1:D:638:VAL:O	1:D:677:LYS:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:SER:O	1:B:135:GLN:HG3	2.12	0.50
1:B:241:GLU:HG3	1:B:292:ARG:CG	2.42	0.50
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.46	0.50
1:B:930:VAL:HA	1:B:973:ARG:HD3	1.94	0.50
1:C:844:HIS:HD2	5:C:4734:HOH:O	1.95	0.50
1:A:756:TRP:CD2	1:A:858:ILE:HD13	2.47	0.50
1:B:127:PHE:CD2	1:B:127:PHE:N	2.80	0.50
1:C:829:THR:HG22	1:C:830:LEU:N	2.25	0.50
1:D:785:THR:HB	1:D:816:TYR:CE2	2.47	0.50
1:A:40:GLU:HA	1:A:40:GLU:OE1	2.11	0.50
1:A:154:CYS:O	1:A:155:ASN:C	2.54	0.50
1:B:651:LEU:C	1:B:651:LEU:CD2	2.85	0.50
1:C:141:ILE:CD1	1:C:184:LEU:HD11	2.42	0.50
1:A:249:GLU:OE2	1:A:251:ARG:NE	2.43	0.50
1:B:873:ALA:O	1:B:876:THR:HG22	2.11	0.50
1:B:910:LEU:C	1:B:910:LEU:HD12	2.37	0.50
1:D:1020:TRP:HD1	1:D:1021:CYS:N	2.10	0.50
1:B:79:PRO:HD2	1:B:80:GLU:OE2	2.12	0.49
1:B:826:THR:OG1	1:B:837:THR:HB	2.12	0.49
1:B:1020:TRP:CD1	1:B:1021:CYS:N	2.79	0.49
1:D:755:ARG:HG3	1:D:769:TRP:HB2	1.94	0.49
1:A:376:ILE:HD12	1:A:401:LEU:HB3	1.94	0.49
1:C:100:TYR:CE1	1:C:602:CYS:HB3	2.47	0.49
1:C:367:MET:HE1	1:C:371:THR:CG2	2.41	0.49
1:A:668:VAL:HG12	1:A:669:PRO:O	2.12	0.49
1:A:742:THR:CG2	1:A:743:SER:N	2.74	0.49
1:C:416:GLU:HA	1:C:460:ASN:O	2.11	0.49
1:C:625:GLN:NE2	5:C:4225:HOH:O	2.40	0.49
1:A:699:ARG:NH1	5:A:4837:HOH:O	2.45	0.49
1:A:112:PRO:HD2	1:A:113:PHE:CE1	2.48	0.49
1:B:788:PRO:HD2	1:B:968:MET:HB2	1.94	0.49
1:B:804:ASN:ND2	1:B:809:ARG:NH2	2.35	0.49
1:C:178:ARG:O	1:C:178:ARG:HG2	2.12	0.49
1:C:287:ASP:OD1	1:C:287:ASP:N	2.37	0.49
1:D:277:GLU:HA	5:D:4563:HOH:O	2.13	0.49
1:D:827:ALA:HB2	1:D:836:ILE:CD1	2.42	0.49
1:A:128:ASN:HB2	5:A:4769:HOH:O	2.11	0.49
1:B:658:LEU:O	1:B:661:LYS:HG3	2.13	0.49
1:D:630:ARG:NH1	5:D:4561:HOH:O	2.46	0.49
1:A:1022:GLN:NE2	1:A:1023:LYS:O	2.46	0.49
1:C:356:ARG:CD	1:C:379:MET:HE1	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:675:GLN:HG3	5:D:4760:HOH:O	2.11	0.49
1:B:805:ALA:O	1:B:809:ARG:HG3	2.13	0.49
1:B:942:ARG:HA	1:B:953:GLY:O	2.13	0.49
1:B:569:ASP:O	1:B:605:GLY:HA2	2.12	0.49
1:B:786:ARG:HG2	1:B:880:ALA:HB1	1.95	0.49
1:C:624:GLN:NE2	5:C:4043:HOH:O	2.46	0.49
1:C:730:LEU:N	1:C:730:LEU:HD23	2.28	0.49
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.48	0.49
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.47	0.49
1:B:658:LEU:O	1:B:659:ASP:C	2.54	0.49
1:B:731:PRO:O	1:B:732:ALA:HB2	2.12	0.49
1:C:578:TYR:CE2	1:C:584:PRO:HB3	2.48	0.49
1:C:854:LYS:HD3	1:C:868:VAL:HG22	1.95	0.49
1:A:948:PRO:O	1:A:1022:GLN:HG2	2.12	0.48
1:B:797:GLU:O	1:B:800:ARG:C	2.56	0.48
1:C:778:THR:HG23	1:C:887:GLN:HB3	1.95	0.48
1:D:767:GLN:NE2	1:D:774:LYS:NZ	2.61	0.48
1:A:230:ARG:NH1	1:A:241:GLU:HG3	2.28	0.48
1:A:253:TYR:CD1	1:A:253:TYR:C	2.91	0.48
1:A:755:ARG:NH2	1:A:772:ASP:HA	2.28	0.48
1:B:634:GLN:HG2	1:B:682:LEU:C	2.37	0.48
1:D:130:ASP:O	1:D:131:GLU:C	2.56	0.48
1:A:832:ASP:OD1	1:A:832:ASP:N	2.45	0.48
1:C:230:ARG:HB3	5:C:4785:HOH:O	2.12	0.48
1:D:893:GLU:HG2	1:D:894:ARG:CG	2.43	0.48
1:D:427:THR:HG21	1:D:462:SER:HB3	1.94	0.48
1:D:650:GLU:HB3	1:D:670:LEU:HD12	1.94	0.48
1:A:147:ASN:HA	1:A:148:SER:HA	1.58	0.48
1:A:580:GLU:OE1	1:A:580:GLU:HA	2.14	0.48
1:A:599:ARG:HG3	1:A:600:GLN:H	1.79	0.48
1:A:702:GLN:O	1:A:712:GLY:N	2.44	0.48
1:B:513:PRO:O	1:B:514:ALA:HB3	2.12	0.48
1:A:835:LEU:HD11	1:A:855:THR:HB	1.95	0.48
1:B:819:GLU:H	1:B:819:GLU:HG2	1.30	0.48
1:C:569:ASP:O	1:C:605:GLY:HA2	2.13	0.48
1:C:571:VAL:CG2	1:C:609:ALA:HA	2.43	0.48
1:D:476:LYS:NZ	5:D:4087:HOH:O	2.46	0.48
1:A:80:GLU:OE1	1:A:80:GLU:N	2.29	0.48
1:B:433:LEU:O	1:B:433:LEU:HD12	2.13	0.48
1:B:683:PRO:O	1:B:685:LEU:HG	2.13	0.48
1:D:893:GLU:O	1:D:893:GLU:HG3	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.96	0.48
1:B:730:LEU:HA	1:B:731:PRO:HD3	1.77	0.48
1:C:347:LYS:HE3	5:C:4277:HOH:O	2.14	0.48
1:C:741:THR:N	1:C:748:CYS:O	2.35	0.48
1:D:142:ILE:CG1	1:D:170:GLU:HG2	2.35	0.48
1:A:685:LEU:CB	1:A:686:PRO:HD2	2.40	0.48
1:B:128:ASN:HB2	1:B:181:GLU:OE2	2.14	0.48
1:B:786:ARG:HG2	1:B:880:ALA:CB	2.44	0.48
1:C:781:ARG:NH1	1:C:781:ARG:CG	2.76	0.48
1:C:806:TRP:HA	1:C:809:ARG:HE	1.78	0.48
1:A:146:VAL:HG11	1:A:150:PHE:CD2	2.49	0.47
1:A:767:GLN:HG3	1:A:768:MET:N	2.28	0.47
1:A:991:MET:HE2	1:A:1003:VAL:HG21	1.96	0.47
1:B:360:HIS:ND1	1:B:362:LEU:N	2.49	0.47
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.49	0.47
1:C:781:ARG:HD3	5:C:4276:HOH:O	2.14	0.47
4:C:8412:DMS:H12	5:C:4348:HOH:O	2.13	0.47
1:D:629:PHE:C	1:D:630:ARG:HD3	2.40	0.47
1:D:833:ALA:HB1	1:D:858:ILE:O	2.14	0.47
1:A:126:THR:HA	1:A:182:ASN:O	2.14	0.47
1:B:305:ILE:HD11	1:B:645:ARG:HB3	1.96	0.47
1:D:316:HIS:HB2	1:D:321:THR:O	2.14	0.47
1:D:804:ASN:HD22	1:D:809:ARG:HH21	0.58	0.47
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.49	0.47
1:C:533:LEU:HD23	1:C:534:ILE:N	2.30	0.47
1:C:780:LEU:C	1:C:781:ARG:HG3	2.38	0.47
1:D:476:LYS:HD2	5:D:4236:HOH:O	2.15	0.47
1:A:635:THR:HG22	1:A:636:ILE:N	2.29	0.47
1:B:74:LEU:HD22	1:B:153:TRP:CG	2.49	0.47
1:B:128:ASN:HA	1:B:180:GLY:O	2.14	0.47
1:D:272:ALA:HB1	1:D:273:PRO:HD2	1.97	0.47
1:D:437:SER:O	1:D:441:THR:HG23	2.14	0.47
1:D:788:PRO:CD	1:D:968:MET:HG3	2.45	0.47
1:A:424:ASN:O	1:A:425:ARG:C	2.57	0.47
1:B:377:LEU:O	1:B:381:GLN:HG3	2.15	0.47
1:C:65:ALA:HB1	1:C:66:PRO:HD2	1.96	0.47
1:C:251:ARG:HD2	4:C:8416:DMS:H23	1.97	0.47
1:C:375:ASP:O	1:C:379:MET:HG3	2.14	0.47
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.50	0.47
1:A:685:LEU:O	1:A:687:GLN:OE1	2.33	0.47
1:B:131:GLU:O	1:B:131:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:830:LEU:HD12	1:B:833:ALA:HB3	1.96	0.47
1:C:651:LEU:C	1:C:651:LEU:CD1	2.88	0.47
1:D:142:ILE:HG12	1:D:170:GLU:CG	2.35	0.47
1:A:35:SER:HB2	1:A:217:LYS:HD3	1.95	0.47
1:B:661:LYS:NZ	5:B:4774:HOH:O	2.47	0.47
1:C:685:LEU:CB	1:C:686:PRO:HD2	2.41	0.47
1:C:699:ARG:NH1	5:C:4741:HOH:O	2.47	0.47
1:D:510:GLN:OE1	5:D:4667:HOH:O	2.20	0.47
1:A:103:VAL:HG22	1:A:418:GLU:OE2	2.15	0.47
1:A:734:SER:C	1:A:736:ALA:H	2.22	0.47
1:B:914:CYS:HB2	5:B:4378:HOH:O	2.15	0.47
1:C:809:ARG:NH2	1:C:1001:PRO:HG3	2.30	0.47
1:A:685:LEU:CB	1:A:686:PRO:CD	2.92	0.46
1:A:770:ILE:HD12	1:A:775:GLN:CD	2.39	0.46
1:B:131:GLU:O	1:B:135:GLN:N	2.38	0.46
1:B:730:LEU:H	1:B:730:LEU:CD1	2.13	0.46
1:C:367:MET:HE1	1:C:371:THR:HG22	1.96	0.46
1:D:305:ILE:HD11	1:D:645:ARG:HB3	1.97	0.46
1:D:640:SER:O	1:D:675:GLN:HA	2.15	0.46
1:D:873:ALA:O	1:D:876:THR:HG22	2.14	0.46
1:C:433:LEU:N	1:C:434:PRO:CD	2.78	0.46
1:D:785:THR:O	1:D:881:ARG:HD2	2.15	0.46
1:A:115:PRO:HB2	1:A:117:GLU:O	2.16	0.46
1:A:826:THR:OG1	1:A:837:THR:HB	2.15	0.46
1:B:147:ASN:HA	1:B:148:SER:HA	1.60	0.46
1:B:670:LEU:HA	1:B:670:LEU:HD23	1.63	0.46
1:B:685:LEU:HA	1:B:686:PRO:HD3	1.61	0.46
1:B:965:GLN:NE2	5:B:4822:HOH:O	2.48	0.46
1:C:808:GLU:OE1	1:C:808:GLU:HA	2.15	0.46
1:D:251:ARG:NH1	5:D:4790:HOH:O	2.48	0.46
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.15	0.46
1:B:46:ARG:HB3	1:B:47:PRO:HD2	1.98	0.46
1:D:646:HIS:NE2	1:D:671:ASP:OD1	2.48	0.46
1:A:45:ASP:O	4:A:8501:DMS:H13	2.16	0.46
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.51	0.46
1:B:133:TRP:CE3	1:B:216:HIS:HB2	2.51	0.46
1:C:110:ASN:N	1:C:111:PRO:HD3	2.31	0.46
1:A:945:ASN:HB3	1:A:1023:LYS:NZ	2.31	0.46
1:B:262:GLN:CA	1:B:262:GLN:NE2	2.79	0.46
1:C:49:GLN:HB2	1:C:50:GLN:OE1	2.15	0.46
1:A:372:MET:HE1	1:A:395:HIS:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:TRP:CD2	1:B:42:ALA:HA	2.50	0.46
1:C:132:SER:CB	4:C:8504:DMS:H12	2.42	0.46
1:C:233:ASP:OD1	1:C:234:ASP:N	2.49	0.46
1:C:292:ARG:HG3	1:C:292:ARG:NH1	2.31	0.46
1:A:433:LEU:N	1:A:434:PRO:CD	2.79	0.46
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.78	0.46
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.79	0.46
1:C:22:THR:OG1	1:C:438:GLU:OE2	2.33	0.46
1:C:178:ARG:HE	1:C:178:ARG:HB3	1.16	0.46
1:C:240:LEU:C	1:C:240:LEU:HD23	2.40	0.46
1:C:655:MET:SD	1:C:656:VAL:N	2.89	0.46
1:D:114:VAL:HB	1:D:115:PRO:HD2	1.97	0.46
1:B:352:ARG:HG2	1:B:553:TRP:CH2	2.50	0.46
1:C:706:THR:OG1	1:C:709:SER:N	2.48	0.46
1:A:658:LEU:O	1:A:659:ASP:C	2.56	0.45
1:D:250:LEU:C	1:D:251:ARG:HG2	2.40	0.45
1:A:262:GLN:HE22	1:A:299:LYS:HG3	1.81	0.45
1:A:768:MET:HE1	1:A:1020:TRP:CH2	2.52	0.45
1:B:360:HIS:CE1	1:B:362:LEU:H	2.29	0.45
1:B:854:LYS:NZ	5:B:4016:HOH:O	2.47	0.45
1:C:649:ASN:HA	4:C:8425:DMS:C1	2.47	0.45
1:C:658:LEU:HG	1:C:661:LYS:HZ1	1.81	0.45
1:C:658:LEU:HG	1:C:661:LYS:HZ2	1.81	0.45
1:D:78:LEU:HA	1:D:78:LEU:HD23	1.66	0.45
1:A:600:GLN:HB2	1:A:603:MET:CE	2.46	0.45
1:B:654:TRP:O	1:B:665:SER:HB2	2.16	0.45
1:B:1018:LEU:HD23	1:B:1018:LEU:C	2.41	0.45
1:C:305:ILE:HA	1:C:306:PRO:HD2	1.82	0.45
1:C:806:TRP:CD2	1:C:991:MET:HE1	2.52	0.45
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.51	0.45
1:B:651:LEU:HD22	1:B:651:LEU:C	2.40	0.45
1:C:824:GLN:CG	1:C:825:CYS:N	2.78	0.45
1:D:158:TRP:CZ2	1:D:160:GLY:HA2	2.52	0.45
1:A:127:PHE:N	1:A:182:ASN:O	2.46	0.45
1:A:200:GLN:CG	1:A:391:HIS:HB2	2.46	0.45
1:A:734:SER:OG	1:A:860:GLY:HA3	2.16	0.45
1:D:106:PRO:C	4:D:8419:DMS:C2	2.90	0.45
1:A:320:GLY:O	4:A:8406:DMS:H21	2.15	0.45
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.98	0.45
1:D:79:PRO:HD2	1:D:80:GLU:OE2	2.17	0.45
1:B:46:ARG:HB3	1:B:47:PRO:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:TRP:CG	1:B:569:ASP:HB3	2.52	0.45
1:C:824:GLN:HG2	1:C:825:CYS:N	2.31	0.45
1:C:890:GLN:HG3	1:C:891:VAL:N	2.30	0.45
1:D:301:TRP:CH2	1:D:452:SER:HA	2.52	0.45
1:C:829:THR:HG22	1:C:830:LEU:O	2.16	0.45
1:A:166:ARG:HG3	1:A:392:TYR:CB	2.47	0.44
1:C:339:ASN:O	1:D:527:PRO:HB3	2.17	0.44
1:C:724:GLU:O	1:D:847:LYS:NZ	2.49	0.44
1:D:94:GLY:HA2	5:D:4199:HOH:O	2.17	0.44
1:D:107:ILE:C	4:D:8419:DMS:H21	2.42	0.44
1:A:45:ASP:OD1	4:A:8501:DMS:H11	2.17	0.44
1:D:446:ARG:NE	1:D:447:ASP:OD1	2.47	0.44
1:A:959:ILE:HD13	1:A:959:ILE:HG21	1.65	0.44
1:B:340:GLY:O	1:B:561:ARG:HG2	2.18	0.44
1:C:92:MET:HE2	1:C:92:MET:CA	2.46	0.44
1:A:577:LYS:HD3	1:A:587:ALA:HB2	2.00	0.44
1:A:890:GLN:HG3	1:A:891:VAL:N	2.32	0.44
1:B:662:PRO:O	1:B:663:LEU:HD23	2.18	0.44
1:B:769:TRP:CD1	1:B:774:LYS:HG3	2.52	0.44
1:C:32:PRO:HB2	4:C:8404:DMS:H13	1.99	0.44
1:C:510:GLN:HB3	1:C:512:PHE:CZ	2.53	0.44
1:D:653:HIS:CD2	1:D:667:GLU:HB3	2.53	0.44
1:D:957:PHE:CD1	1:D:957:PHE:C	2.94	0.44
1:B:959:ILE:HA	1:B:983:TRP:O	2.18	0.44
1:B:1022:GLN:CG	1:B:1023:LYS:N	2.80	0.44
1:C:649:ASN:HA	4:C:8425:DMS:H12	1.98	0.44
1:C:968:MET:O	1:C:968:MET:HG3	2.18	0.44
4:C:8417:DMS:H22	5:C:4570:HOH:O	2.17	0.44
1:D:107:ILE:N	4:D:8419:DMS:C2	2.78	0.44
1:D:192:SER:O	1:D:195:SER:HB2	2.18	0.44
1:D:433:LEU:HB3	1:D:434:PRO:HD3	1.99	0.44
1:D:962:TYR:CE2	1:D:976:LEU:HB3	2.53	0.44
1:A:433:LEU:N	1:A:434:PRO:HD2	2.32	0.44
1:B:75:GLU:HA	1:B:75:GLU:OE1	2.17	0.44
1:B:433:LEU:HD12	1:B:433:LEU:C	2.41	0.44
1:D:595:THR:OG1	1:D:596:PRO:HA	2.18	0.44
1:A:99:ILE:HB	1:A:204:ARG:HB2	1.99	0.44
1:A:473:ARG:HH12	1:A:477:SER:N	2.15	0.44
1:B:801:ILE:HD13	1:B:801:ILE:N	2.33	0.44
1:B:843:GLN:HG2	1:B:848:THR:HA	2.00	0.44
5:B:4578:HOH:O	4:C:8420:DMS:H12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:GLN:CD	1:C:50:GLN:N	2.75	0.44
1:C:610:ASP:O	1:C:611:ARG:HB2	2.17	0.44
1:C:743:SER:HB3	5:C:4618:HOH:O	2.18	0.44
1:D:518:TRP:O	1:D:519:SER:C	2.61	0.44
1:D:808:GLU:HA	1:D:811:LYS:HD3	2.00	0.44
1:A:990:HIS:HD2	1:A:991:MET:O	2.00	0.44
1:B:814:GLY:HA3	1:B:844:HIS:CG	2.52	0.44
1:C:580:GLU:H	1:C:580:GLU:HG3	1.54	0.44
1:C:1023:LYS:HA	1:C:1023:LYS:CE	2.48	0.44
1:D:243:GLU:OE2	1:D:245:GLN:NE2	2.42	0.44
1:A:103:VAL:HG22	1:A:418:GLU:CD	2.43	0.44
1:A:577:LYS:HD2	1:A:592:PHE:CE2	2.53	0.44
1:B:772:ASP:OD1	1:B:773:LYS:HD3	2.18	0.44
1:C:111:PRO:HA	1:C:112:PRO:HA	1.71	0.44
1:C:755:ARG:HH11	1:C:755:ARG:HD3	1.64	0.44
1:D:130:ASP:OD1	1:D:132:SER:OG	2.30	0.44
1:D:376:ILE:CD1	1:D:401:LEU:HB3	2.48	0.44
1:D:1022:GLN:HE22	1:D:1023:LYS:HG2	1.80	0.44
1:A:118:ASN:HA	1:A:119:PRO:HD2	1.83	0.43
1:B:852:SER:HA	1:B:870:VAL:HG22	2.00	0.43
1:C:806:TRP:CE2	1:C:991:MET:HE1	2.53	0.43
1:A:765:LEU:HD21	1:A:768:MET:HE2	2.00	0.43
1:C:126:THR:HA	1:C:182:ASN:O	2.18	0.43
1:C:132:SER:OG	4:C:8504:DMS:H11	2.18	0.43
1:C:147:ASN:HA	1:C:148:SER:HA	1.80	0.43
1:C:614:HIS:HB3	1:C:615:PRO:CD	2.46	0.43
1:D:78:LEU:HB3	1:D:80:GLU:OE2	2.18	0.43
1:D:653:HIS:ND1	1:D:701:VAL:CG2	2.74	0.43
1:A:752:GLY:C	1:A:754:LYS:H	2.25	0.43
1:B:642:TYR:O	1:B:675:GLN:OE1	2.36	0.43
1:C:679:LEU:HD23	1:C:679:LEU:HA	1.76	0.43
1:C:737:ILE:CD1	1:C:738:PRO:HD2	2.32	0.43
1:C:1006:GLU:HG2	1:C:1007:PHE:CD1	2.53	0.43
1:B:183:ARG:HB3	5:B:4316:HOH:O	2.18	0.43
1:B:299:LYS:HE2	5:B:4633:HOH:O	2.18	0.43
1:D:754:LYS:C	1:D:755:ARG:HG2	2.42	0.43
1:B:360:HIS:CG	1:B:361:PRO:HD2	2.52	0.43
1:B:393:PRO:HD3	1:B:412:GLU:O	2.17	0.43
1:B:639:THR:OG1	1:B:677:LYS:HG2	2.19	0.43
1:C:608:PHE:CE1	1:C:614:HIS:HD2	2.36	0.43
1:D:827:ALA:CB	1:D:836:ILE:CD1	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1022:GLN:C	1:D:1022:GLN:NE2	2.74	0.43
1:A:649:ASN:HA	4:A:8425:DMS:H12	2.00	0.43
1:A:755:ARG:HH22	1:A:772:ASP:HA	1.84	0.43
1:A:1020:TRP:C	1:A:1020:TRP:CD1	2.96	0.43
1:B:261:TRP:CZ3	1:B:266:GLN:HB2	2.54	0.43
1:C:131:GLU:OE1	1:C:179:ALA:HB2	2.19	0.43
1:C:823:LEU:O	1:D:730:LEU:HD21	2.18	0.43
1:B:377:LEU:HD22	1:B:708:TRP:CA	2.47	0.43
1:C:107:ILE:HA	4:C:8419:DMS:H22	2.01	0.43
1:C:600:GLN:HB2	1:C:603:MET:HE2	2.00	0.43
1:D:581:ASN:HD22	1:D:583:ASN:ND2	2.07	0.43
1:D:890:GLN:HB2	5:D:4743:HOH:O	2.17	0.43
1:A:780:LEU:HA	1:A:886:CYS:HB3	2.00	0.43
1:A:830:LEU:HD12	1:A:833:ALA:HB3	2.01	0.43
1:A:930:VAL:HA	1:A:973:ARG:HD3	2.00	0.43
1:B:486:TYR:CZ	1:B:488:GLY:HA3	2.54	0.43
1:B:578:TYR:HA	1:B:583:ASN:O	2.18	0.43
1:C:989:PHE:CE1	1:C:1014:TYR:HB3	2.54	0.43
1:D:379:MET:HE1	1:D:387:VAL:HB	2.00	0.43
1:D:745:MET:HE1	1:D:761:GLN:HB2	2.01	0.43
1:D:968:MET:HE3	1:D:968:MET:HB2	1.78	0.43
1:A:460:ASN:O	1:A:461:GLU:C	2.62	0.43
1:B:43:ARG:HD2	1:B:261:TRP:CD2	2.53	0.43
1:B:395:HIS:ND1	1:B:396:PRO:HD2	2.34	0.43
1:B:663:LEU:HD23	1:B:663:LEU:N	2.34	0.43
1:B:748:CYS:C	1:B:749:ILE:HD12	2.43	0.43
1:B:961:ARG:NE	1:B:981:GLY:O	2.49	0.43
1:C:100:TYR:CZ	1:C:602:CYS:HB3	2.53	0.43
1:C:579:ASP:OD1	1:C:583:ASN:N	2.42	0.43
1:C:759:ASN:HB3	1:C:762:SER:OG	2.19	0.43
1:D:827:ALA:HB2	1:D:836:ILE:HD12	2.01	0.43
1:A:50:GLN:N	1:A:50:GLN:CD	2.77	0.43
1:B:32:PRO:HB2	4:B:8404:DMS:H13	2.01	0.43
1:B:486:TYR:CE2	1:B:488:GLY:HA3	2.54	0.43
1:B:965:GLN:HA	1:B:968:MET:HE3	2.01	0.43
1:C:262:GLN:O	1:C:263:GLY:C	2.60	0.43
1:D:769:TRP:HA	1:D:773:LYS:O	2.19	0.43
1:A:486:TYR:CE2	1:A:488:GLY:HA3	2.54	0.42
1:A:649:ASN:OD1	1:A:703:PRO:HD2	2.19	0.42
1:B:59:ARG:HA	1:B:59:ARG:HD2	1.88	0.42
1:C:651:LEU:CD1	1:C:653:HIS:CE1	2.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:997:ASP:HB2	1:C:999:TRP:CE2	2.54	0.42
1:D:479:ASP:HA	1:D:480:PRO:HD2	1.80	0.42
1:D:595:THR:HA	1:D:596:PRO:O	2.17	0.42
1:D:746:ASP:CA	1:D:760:ARG:HG3	2.48	0.42
1:A:801:ILE:HD13	1:A:801:ILE:HA	1.71	0.42
1:A:823:LEU:O	1:B:730:LEU:HD23	2.19	0.42
1:B:215:LEU:HD21	1:B:217:LYS:HD3	2.01	0.42
1:B:395:HIS:ND1	1:B:395:HIS:C	2.77	0.42
1:C:479:ASP:HA	1:C:480:PRO:HD3	1.51	0.42
1:C:499:ILE:HG22	1:C:501:PRO:HD3	2.01	0.42
1:D:663:LEU:HD22	1:D:663:LEU:HA	1.84	0.42
1:A:554:GLN:CD	1:A:554:GLN:C	2.88	0.42
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.82	0.42
1:B:637:GLU:OE2	1:B:677:LYS:HD3	2.18	0.42
1:B:686:PRO:C	1:B:687:GLN:O	2.61	0.42
1:C:525:SER:O	1:C:526:LEU:C	2.61	0.42
1:D:211:ASP:HB3	5:D:4335:HOH:O	2.18	0.42
1:D:359:HIS:CD2	1:D:573:GLN:HA	2.55	0.42
1:D:748:CYS:C	1:D:749:ILE:HD12	2.44	0.42
1:A:736:ALA:HB1	1:A:751:LEU:HD11	2.01	0.42
1:B:118:ASN:O	1:B:119:PRO:C	2.60	0.42
1:B:262:GLN:NE2	1:B:263:GLY:N	2.67	0.42
1:B:872:VAL:O	1:B:873:ALA:C	2.61	0.42
1:C:45:ASP:O	4:C:8501:DMS:H13	2.19	0.42
1:A:844:HIS:O	1:A:845:GLN:C	2.62	0.42
1:B:320:GLY:HA2	4:B:8406:DMS:O	2.19	0.42
1:C:395:HIS:ND1	1:C:395:HIS:C	2.77	0.42
1:C:487:GLU:O	1:C:491:ALA:N	2.50	0.42
1:C:872:VAL:O	1:C:873:ALA:C	2.61	0.42
1:D:518:TRP:CD1	1:D:526:LEU:HD11	2.55	0.42
1:D:583:ASN:HA	1:D:584:PRO:HD3	1.75	0.42
1:A:226:HIS:O	1:A:242:ALA:HA	2.19	0.42
1:A:255:ARG:HD3	1:A:273:PRO:HA	2.01	0.42
1:B:167:LEU:HD23	1:B:167:LEU:HA	1.94	0.42
1:B:475:ILE:O	1:B:476:LYS:C	2.61	0.42
1:C:262:GLN:HE21	1:C:262:GLN:HB3	1.56	0.42
1:C:734:SER:CB	1:C:860:GLY:HA3	2.50	0.42
1:C:768:MET:HB2	1:C:775:GLN:HB2	2.02	0.42
1:C:799:THR:H	1:C:799:THR:HG23	1.41	0.42
1:C:894:ARG:NE	1:C:919:ASP:OD1	2.50	0.42
1:A:745:MET:HE1	1:A:761:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:PHE:O	4:C:8417:DMS:H12	2.20	0.42
1:C:304:GLU:C	1:C:305:ILE:HG13	2.43	0.42
1:C:651:LEU:CD1	1:C:653:HIS:ND1	2.82	0.42
1:D:157:ARG:NH1	1:D:175:ALA:O	2.52	0.42
1:D:200:GLN:HG2	1:D:391:HIS:HB2	2.01	0.42
1:D:737:ILE:CD1	1:D:832:ASP:HA	2.47	0.42
1:D:898:LEU:HD12	1:D:898:LEU:HA	1.82	0.42
1:A:670:LEU:HD23	1:A:670:LEU:HA	1.83	0.42
1:A:817:GLN:HE21	1:A:817:GLN:HB3	1.24	0.42
1:B:499:ILE:HD11	1:B:529:GLU:CG	2.49	0.42
1:A:127:PHE:O	1:A:182:ASN:N	2.33	0.42
4:A:8425:DMS:H22	5:A:4695:HOH:O	2.19	0.42
1:C:26:ARG:HD2	1:C:169:SER:HA	2.01	0.42
1:C:200:GLN:HG2	1:C:391:HIS:HB2	2.01	0.42
1:C:957:PHE:HA	1:C:985:ASN:O	2.20	0.42
1:A:13:ARG:HB3	1:A:14:ARG:H	1.59	0.42
1:A:863:GLN:HE22	1:A:952:ARG:HH22	1.66	0.42
1:B:646:HIS:CE1	1:B:673:ALA:HA	2.55	0.42
1:B:658:LEU:HG	1:B:659:ASP:OD2	2.20	0.42
1:B:731:PRO:HB2	1:B:732:ALA:H	1.69	0.42
1:C:895:VAL:O	1:C:919:ASP:HA	2.19	0.42
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.55	0.42
1:D:340:GLY:O	1:D:561:ARG:HG2	2.20	0.42
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.55	0.42
1:A:114:VAL:HB	1:A:115:PRO:HD2	2.02	0.41
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.55	0.41
1:B:114:VAL:HB	1:B:115:PRO:CD	2.49	0.41
1:B:261:TRP:CH2	1:B:266:GLN:HB2	2.55	0.41
1:B:360:HIS:ND1	1:B:360:HIS:C	2.78	0.41
1:C:114:VAL:HB	1:C:115:PRO:HD2	2.02	0.41
1:D:598:ASP:CG	4:D:8506:DMS:H12	2.45	0.41
1:A:103:VAL:HG13	1:A:418:GLU:HG2	2.02	0.41
1:A:157:ARG:NH1	1:A:157:ARG:CG	2.81	0.41
1:A:769:TRP:HA	1:A:773:LYS:O	2.20	0.41
1:C:107:ILE:CA	4:C:8419:DMS:H22	2.50	0.41
1:C:241:GLU:HG3	1:C:290:THR:CG2	2.51	0.41
1:C:940:GLY:O	5:C:4357:HOH:O	2.22	0.41
1:D:639:THR:OG1	1:D:677:LYS:HD3	2.19	0.41
1:D:869:ASP:OD1	1:D:1015:HIS:ND1	2.42	0.41
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.55	0.41
1:B:200:GLN:CG	1:B:391:HIS:HB2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:863:GLN:HG2	1:B:1019:VAL:CG1	2.50	0.41
1:A:354:VAL:CG1	1:A:379:MET:HE3	2.51	0.41
1:A:598:ASP:C	1:A:599:ARG:HG2	2.45	0.41
1:B:986:ILE:HG23	1:B:986:ILE:O	2.20	0.41
1:C:63:PHE:HB3	1:C:64:PRO:HD2	2.02	0.41
1:D:323:ILE:HD12	1:D:323:ILE:N	2.35	0.41
1:B:178:ARG:O	1:B:178:ARG:HG3	2.17	0.41
1:B:190:ARG:HG2	1:B:191:TRP:CE2	2.54	0.41
1:B:758:PHE:CZ	1:B:765:LEU:HD13	2.55	0.41
1:C:138:GLN:HA	1:C:174:SER:OG	2.20	0.41
1:A:768:MET:HE1	1:A:1020:TRP:CE2	2.55	0.41
1:C:279:ILE:HA	1:C:279:ILE:HD13	1.78	0.41
1:C:629:PHE:HA	1:C:637:GLU:O	2.20	0.41
1:A:241:GLU:OE2	1:A:292:ARG:NE	2.46	0.41
1:A:518:TRP:O	1:A:519:SER:C	2.62	0.41
1:A:696:LEU:HD23	1:A:720:TRP:CE3	2.55	0.41
1:B:673:ALA:O	1:B:674:PRO:C	2.63	0.41
1:B:869:ASP:OD1	1:B:1015:HIS:ND1	2.36	0.41
1:C:658:LEU:CG	1:C:661:LYS:NZ	2.83	0.41
1:C:670:LEU:HD23	1:C:670:LEU:HA	1.65	0.41
1:D:577:LYS:HB3	1:D:577:LYS:HE3	1.81	0.41
1:D:736:ALA:HB1	1:D:737:ILE:H	1.69	0.41
1:D:896:ASN:HA	1:D:918:TRP:O	2.21	0.41
1:B:110:ASN:N	1:B:111:PRO:HD3	2.36	0.41
1:C:133:TRP:NE1	4:C:8504:DMS:H21	2.34	0.41
1:C:778:THR:HG23	1:C:887:GLN:CB	2.50	0.41
1:C:825:CYS:HA	1:C:837:THR:O	2.21	0.41
1:C:972:HIS:HB3	1:C:974:HIS:ND1	2.35	0.41
1:D:36:TRP:CD2	1:D:42:ALA:HA	2.56	0.41
1:D:354:VAL:HG12	1:D:379:MET:HE3	2.03	0.41
1:A:73:TRP:O	1:A:183:ARG:NH2	2.47	0.41
1:A:411:ASP:OD2	1:A:447:ASP:OD2	2.38	0.41
1:A:699:ARG:HD3	1:A:714:ILE:HD12	2.03	0.41
1:A:701:VAL:HG22	1:A:714:ILE:HD13	2.03	0.41
1:B:63:PHE:HB3	1:B:64:PRO:HD2	2.02	0.41
1:B:262:GLN:NE2	1:B:262:GLN:HA	2.35	0.41
1:B:367:MET:CE	1:B:371:THR:HG22	2.30	0.41
1:B:674:PRO:O	1:B:675:GLN:HB2	2.21	0.41
1:B:785:THR:O	1:B:881:ARG:HD2	2.21	0.41
1:B:907:PRO:HG2	1:B:990:HIS:O	2.21	0.41
1:C:143:PHE:O	1:C:168:PRO:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:LEU:HA	1:C:471:LEU:HD23	1.83	0.41
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.56	0.41
1:C:562:LEU:HD23	1:C:562:LEU:HA	1.95	0.41
1:C:633:GLY:C	1:C:634:GLN:HE21	2.23	0.41
1:C:768:MET:HE3	1:C:776:LEU:HD21	2.01	0.41
1:D:225:PHE:HA	1:D:243:GLU:O	2.21	0.41
1:D:354:VAL:CG1	1:D:379:MET:HE3	2.50	0.41
1:B:347:LYS:HG3	1:B:644:PHE:CE2	2.55	0.41
1:B:777:LEU:HD23	1:B:777:LEU:HA	1.87	0.41
1:C:608:PHE:CD1	1:C:614:HIS:HD2	2.39	0.41
1:D:147:ASN:HA	1:D:148:SER:HA	1.52	0.41
1:D:907:PRO:HG2	1:D:990:HIS:O	2.20	0.41
1:D:1004:SER:O	1:D:1005:ALA:C	2.64	0.41
1:A:230:ARG:NH1	1:A:241:GLU:CD	2.79	0.40
1:B:133:TRP:NE1	4:B:8504:DMS:H12	2.36	0.40
1:B:736:ALA:O	1:B:860:GLY:HA3	2.22	0.40
1:C:118:ASN:O	1:C:119:PRO:C	2.64	0.40
1:C:743:SER:O	1:C:744:GLU:C	2.63	0.40
1:D:963:SER:OG	1:D:966:GLN:HB2	2.22	0.40
1:A:372:MET:HE2	5:A:4191:HOH:O	2.21	0.40
1:A:486:TYR:CZ	1:A:488:GLY:HA3	2.56	0.40
1:A:668:VAL:HG11	1:A:680:ILE:HD13	2.02	0.40
1:A:750:GLU:CG	1:A:751:LEU:N	2.84	0.40
1:A:920:LEU:HB3	1:A:921:PRO:CD	2.46	0.40
1:C:89:ASN:O	1:C:92:MET:HB2	2.21	0.40
1:C:333:ARG:O	1:C:333:ARG:HG2	2.13	0.40
1:C:622:HIS:CE1	4:C:8402:DMS:C1	3.04	0.40
1:D:949:HIS:HB2	1:D:951:TRP:CH2	2.55	0.40
1:A:101:THR:HG23	1:A:204:ARG:NH2	2.37	0.40
1:A:502:MET:HB2	1:A:503:TYR:CD1	2.56	0.40
1:A:910:LEU:C	1:A:910:LEU:HD12	2.47	0.40
1:C:316:HIS:HB2	1:C:321:THR:O	2.21	0.40
1:C:559:TYR:CE2	1:D:522:LYS:HA	2.56	0.40
1:C:972:HIS:CB	1:C:974:HIS:CE1	3.04	0.40
1:D:780:LEU:HA	1:D:886:CYS:HB3	2.04	0.40
1:D:807:VAL:HG13	1:D:808:GLU:N	2.36	0.40
1:A:573:GLN:HB2	1:A:602:CYS:O	2.22	0.40
1:B:32:PRO:HG2	5:B:4208:HOH:O	2.22	0.40
1:B:55:ASN:O	4:B:8408:DMS:H11	2.22	0.40
1:B:824:GLN:O	1:B:838:THR:HA	2.22	0.40
1:C:189:LEU:HA	1:C:189:LEU:HD23	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:TRP:O	1:C:478:VAL:HG13	2.22	0.40
1:C:655:MET:HE2	1:C:665:SER:HB3	2.02	0.40
1:D:36:TRP:HH2	4:D:8404:DMS:H21	1.85	0.40
1:B:894:ARG:HE	1:B:894:ARG:HB3	1.72	0.40
1:B:973:ARG:O	4:B:8423:DMS:H12	2.21	0.40
1:C:767:GLN:CG	1:C:768:MET:N	2.85	0.40
1:D:63:PHE:CD1	1:D:69:VAL:HG22	2.56	0.40
1:D:959:ILE:HG21	1:D:959:ILE:HD13	1.78	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	1009/1023 (99%)	963 (95%)	44 (4%)	2 (0%)	43	37
1	B	1009/1023 (99%)	965 (96%)	36 (4%)	8 (1%)	16	9
1	C	1009/1023 (99%)	961 (95%)	47 (5%)	1 (0%)	48	43
1	D	1009/1023 (99%)	958 (95%)	48 (5%)	3 (0%)	36	30
All	All	4036/4092 (99%)	3847 (95%)	175 (4%)	14 (0%)	36	30

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	688	PRO
1	B	690	SER
1	B	731	PRO
1	A	689	GLU
1	D	688	PRO
1	B	732	ALA
1	B	733	ALA

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Mol	Chain	Res	Type
1	D	733	ALA
1	A	164	ASP
1	B	164	ASP
1	B	686	PRO
1	B	687	GLN
1	D	540	HIS
1	C	164	ASP

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	864/875 (99%)	823 (95%)	41 (5%)	23	17
1	B	864/875 (99%)	809 (94%)	55 (6%)	16	9
1	C	864/875 (99%)	812 (94%)	52 (6%)	17	10
1	D	864/875 (99%)	817 (95%)	47 (5%)	20	12
All	All	3456/3500 (99%)	3261 (94%)	195 (6%)	19	12

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	78	LEU
1	A	117	GLU
1	A	131	GLU
1	A	157	ARG
1	A	178	ARG
1	A	250	LEU
1	A	267	VAL
1	A	277	GLU
1	A	344	LEU
1	A	431	ARG
1	A	478	VAL
1	A	519	SER
1	A	546	LEU

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Mol	Chain	Res	Type
1	A	600	GLN
1	A	632	SER
1	A	634	GLN
1	A	655	MET
1	A	661	LYS
1	A	663	LEU
1	A	667	GLU
1	A	670	LEU
1	A	671	ASP
1	A	672	VAL
1	A	684	GLU
1	A	714	ILE
1	A	729	THR
1	A	735	HIS
1	A	737	ILE
1	A	773	LYS
1	A	774	LYS
1	A	797	GLU
1	A	799	THR
1	A	800	ARG
1	A	817	GLN
1	A	819	GLU
1	A	824	GLN
1	A	885	ASN
1	A	958	ASN
1	A	969	GLU
1	A	1023	LYS
1	B	13	ARG
1	B	80	GLU
1	B	117	GLU
1	B	130	ASP
1	B	181	GLU
1	B	230	ARG
1	B	251	ARG
1	B	262	GLN
1	B	264	GLU
1	B	277	GLU
1	B	279	ILE
1	B	344	LEU
1	B	362	LEU
1	B	370	GLN
1	B	395	HIS

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Mol	Chain	Res	Type
1	B	400	THR
1	B	478	VAL
1	B	519	SER
1	B	546	LEU
1	B	580	GLU
1	B	595	THR
1	B	600	GLN
1	B	604	ASN
1	B	630	ARG
1	B	635	THR
1	B	636	ILE
1	B	651	LEU
1	B	655	MET
1	B	661	LYS
1	B	667	GLU
1	B	685	LEU
1	B	687	GLN
1	B	689	GLU
1	B	730	LEU
1	B	737	ILE
1	B	745	MET
1	B	748	CYS
1	B	750	GLU
1	B	766	SER
1	B	769	TRP
1	B	773	LYS
1	B	797	GLU
1	B	799	THR
1	B	800	ARG
1	B	801	ILE
1	B	819	GLU
1	B	824	GLN
1	B	845	GLN
1	B	847	LYS
1	B	863	GLN
1	B	956	GLN
1	B	968	MET
1	B	969	GLU
1	B	1018	LEU
1	B	1023	LYS
1	C	13	ARG
1	C	75	GLU

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Mol	Chain	Res	Type
1	C	76	CYS
1	C	80	GLU
1	C	135	GLN
1	C	136	GLU
1	C	178	ARG
1	C	249	GLU
1	C	262	GLN
1	C	264	GLU
1	C	278	ILE
1	C	333	ARG
1	C	344	LEU
1	C	370	GLN
1	C	395	HIS
1	C	400	THR
1	C	478	VAL
1	C	519	SER
1	C	546	LEU
1	C	580	GLU
1	C	581	ASN
1	C	634	GLN
1	C	655	MET
1	C	663	LEU
1	C	672	VAL
1	C	681	GLU
1	C	687	GLN
1	C	699	ARG
1	C	710	GLU
1	C	730	LEU
1	C	734	SER
1	C	735	HIS
1	C	737	ILE
1	C	745	MET
1	C	749	ILE
1	C	750	GLU
1	C	773	LYS
1	C	781	ARG
1	C	789	LEU
1	C	799	THR
1	C	800	ARG
1	C	801	ILE
1	C	819	GLU
1	C	824	GLN

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Mol	Chain	Res	Type
1	C	854	LYS
1	C	881	ARG
1	C	922	LEU
1	C	956	GLN
1	C	968	MET
1	C	986	ILE
1	C	1022	GLN
1	C	1023	LYS
1	D	13	ARG
1	D	49	GLN
1	D	71	GLU
1	D	76	CYS
1	D	80	GLU
1	D	108	THR
1	D	128	ASN
1	D	129	VAL
1	D	230	ARG
1	D	237	ARG
1	D	277	GLU
1	D	370	GLN
1	D	390	SER
1	D	519	SER
1	D	546	LEU
1	D	581	ASN
1	D	632	SER
1	D	651	LEU
1	D	655	MET
1	D	663	LEU
1	D	667	GLU
1	D	672	VAL
1	D	681	GLU
1	D	682	LEU
1	D	684	GLU
1	D	685	LEU
1	D	689	GLU
1	D	699	ARG
1	D	730	LEU
1	D	735	HIS
1	D	745	MET
1	D	755	ARG
1	D	772	ASP
1	D	773	LYS

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Mol	Chain	Res	Type
1	D	774	LYS
1	D	799	THR
1	D	800	ARG
1	D	819	GLU
1	D	824	GLN
1	D	845	GLN
1	D	871	GLU
1	D	893	GLU
1	D	956	GLN
1	D	986	ILE
1	D	1017	GLN
1	D	1018	LEU
1	D	1022	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	GLN
1	A	363	HIS
1	A	394	ASN
1	A	445	GLN
1	A	485	GLN
1	A	600	GLN
1	A	614	HIS
1	A	624	GLN
1	A	761	GLN
1	A	775	GLN
1	A	817	GLN
1	A	824	GLN
1	A	844	HIS
1	A	863	GLN
1	A	878	HIS
1	A	977	HIS
1	A	1017	GLN
1	B	262	GLN
1	B	394	ASN
1	B	554	GLN
1	B	583	ASN
1	B	600	GLN
1	B	624	GLN
1	B	646	HIS
1	B	653	HIS

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Mol	Chain	Res	Type
1	B	675	GLN
1	B	757	GLN
1	B	804	ASN
1	B	817	GLN
1	B	843	GLN
1	B	844	HIS
1	B	878	HIS
1	B	885	ASN
1	B	965	GLN
1	B	977	HIS
1	B	1017	GLN
1	C	135	GLN
1	C	163	GLN
1	C	226	HIS
1	C	262	GLN
1	C	363	HIS
1	C	374	GLN
1	C	394	ASN
1	C	485	GLN
1	C	510	GLN
1	C	583	ASN
1	C	614	HIS
1	C	624	GLN
1	C	634	GLN
1	C	646	HIS
1	C	687	GLN
1	C	783	GLN
1	C	804	ASN
1	C	824	GLN
1	C	843	GLN
1	C	878	HIS
1	D	135	GLN
1	D	266	GLN
1	D	394	ASN
1	D	485	GLN
1	D	583	ASN
1	D	614	HIS
1	D	761	GLN
1	D	767	GLN
1	D	804	ASN
1	D	878	HIS
1	D	903	GLN

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Mol	Chain	Res	Type
1	D	977	HIS
1	D	1022	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 108 ligands modelled in this entry, 26 are monoatomic - leaving 82 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
4	DMS	C	8401	-	3,3,3	1.63	1 (33%)	3,3,3	0.29	0
4	DMS	C	8425	3	3,3,3	1.53	1 (33%)	3,3,3	0.33	0
4	DMS	C	8419	-	3,3,3	0.80	0	3,3,3	0.31	0
4	DMS	C	8402	-	3,3,3	1.42	1 (33%)	3,3,3	0.09	0
4	DMS	D	8402	-	3,3,3	0.63	0	3,3,3	0.48	0
4	DMS	D	8508	-	3,3,3	1.04	0	3,3,3	0.27	0
4	DMS	C	8420	-	3,3,3	1.74	1 (33%)	3,3,3	0.07	0
4	DMS	C	8501	-	3,3,3	1.39	0	3,3,3	0.47	0
4	DMS	D	8420	-	3,3,3	1.60	1 (33%)	3,3,3	0.27	0
4	DMS	C	8506	-	3,3,3	1.65	1 (33%)	3,3,3	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	B	8416	-	3,3,3	0.85	0	3,3,3	0.36	0
4	DMS	D	8703	-	3,3,3	0.75	0	3,3,3	0.48	0
4	DMS	D	8421	-	3,3,3	0.55	0	3,3,3	0.12	0
4	DMS	B	8411	-	3,3,3	1.22	1 (33%)	3,3,3	0.23	0
4	DMS	A	8404	-	3,3,3	1.24	0	3,3,3	0.46	0
4	DMS	D	8501	-	3,3,3	0.53	0	3,3,3	0.35	0
4	DMS	B	8421	-	3,3,3	0.71	0	3,3,3	0.59	0
4	DMS	B	8409	-	3,3,3	1.71	1 (33%)	3,3,3	0.38	0
4	DMS	D	8401	-	3,3,3	1.39	1 (33%)	3,3,3	0.85	0
4	DMS	C	8404	-	3,3,3	1.50	1 (33%)	3,3,3	1.18	1 (33%)
4	DMS	D	8425	3	3,3,3	0.45	0	3,3,3	0.34	0
4	DMS	B	8402	-	3,3,3	0.80	0	3,3,3	0.53	0
4	DMS	D	8419	-	3,3,3	1.37	1 (33%)	3,3,3	0.91	0
4	DMS	A	8411	-	3,3,3	0.70	0	3,3,3	0.10	0
4	DMS	B	8508	-	3,3,3	1.68	1 (33%)	3,3,3	0.91	0
4	DMS	C	8421	-	3,3,3	0.52	0	3,3,3	0.19	0
4	DMS	D	8404	-	3,3,3	1.19	0	3,3,3	0.16	0
4	DMS	D	8408	-	3,3,3	0.57	0	3,3,3	0.32	0
4	DMS	D	8405	-	3,3,3	1.17	0	3,3,3	1.12	0
4	DMS	B	8408	-	3,3,3	0.77	0	3,3,3	1.40	1 (33%)
4	DMS	A	8405	-	3,3,3	1.62	1 (33%)	3,3,3	0.22	0
4	DMS	B	8504	-	3,3,3	0.98	0	3,3,3	0.64	0
4	DMS	C	8602	-	3,3,3	1.69	1 (33%)	3,3,3	0.23	0
4	DMS	A	8403	-	3,3,3	2.05	2 (66%)	3,3,3	0.72	0
4	DMS	D	8412	-	3,3,3	0.89	0	3,3,3	0.40	0
4	DMS	A	8409	-	3,3,3	1.60	1 (33%)	3,3,3	0.19	0
4	DMS	D	8705	-	3,3,3	0.28	0	3,3,3	1.08	0
4	DMS	C	8416	-	3,3,3	0.77	0	3,3,3	0.44	0
4	DMS	B	8403	-	3,3,3	1.78	1 (33%)	3,3,3	0.31	0
4	DMS	D	8411	-	3,3,3	0.87	0	3,3,3	0.13	0
4	DMS	B	8414	-	3,3,3	0.72	0	3,3,3	0.46	0
4	DMS	A	8416	-	3,3,3	1.07	0	3,3,3	0.50	0
4	DMS	A	8602	-	3,3,3	1.18	0	3,3,3	0.20	0
4	DMS	A	8414	-	3,3,3	0.83	0	3,3,3	0.19	0
4	DMS	C	8411	-	3,3,3	1.22	0	3,3,3	0.38	0
4	DMS	A	8412	-	3,3,3	0.88	0	3,3,3	0.46	0
4	DMS	B	8412	-	3,3,3	1.22	0	3,3,3	0.25	0
4	DMS	C	8423	-	3,3,3	0.55	0	3,3,3	0.45	0
4	DMS	C	8409	-	3,3,3	0.93	0	3,3,3	0.27	0
4	DMS	D	8409	-	3,3,3	1.27	1 (33%)	3,3,3	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	A	8425	3	3,3,3	1.08	0	3,3,3	0.19	0
4	DMS	B	8601	-	3,3,3	1.20	0	3,3,3	0.45	0
4	DMS	B	8423	-	3,3,3	0.89	0	3,3,3	0.55	0
4	DMS	C	8414	-	3,3,3	0.95	0	3,3,3	0.24	0
4	DMS	B	8417	-	3,3,3	0.46	0	3,3,3	0.27	0
4	DMS	A	8421	-	3,3,3	1.11	0	3,3,3	0.23	0
4	DMS	C	8601	-	3,3,3	1.93	1 (33%)	3,3,3	0.64	0
4	DMS	C	8417	-	3,3,3	0.11	0	3,3,3	0.50	0
4	DMS	B	8425	3	3,3,3	1.71	1 (33%)	3,3,3	0.20	0
4	DMS	A	8501	-	3,3,3	1.46	0	3,3,3	0.52	0
4	DMS	A	8504	-	3,3,3	0.48	0	3,3,3	0.33	0
4	DMS	D	8701	-	3,3,3	1.77	1 (33%)	3,3,3	1.00	0
4	DMS	A	8402	-	3,3,3	1.34	0	3,3,3	0.33	0
4	DMS	D	8406	-	3,3,3	1.14	0	3,3,3	0.65	0
4	DMS	C	8504	-	3,3,3	0.45	0	3,3,3	0.29	0
4	DMS	D	8414	-	3,3,3	0.42	0	3,3,3	0.08	0
4	DMS	C	8408	-	3,3,3	1.17	0	3,3,3	0.54	0
4	DMS	B	8404	-	3,3,3	0.36	0	3,3,3	0.66	0
4	DMS	D	8416	-	3,3,3	1.22	1 (33%)	3,3,3	0.23	0
4	DMS	A	8401	-	3,3,3	0.56	0	3,3,3	0.34	0
4	DMS	D	8506	-	3,3,3	1.96	1 (33%)	3,3,3	0.44	0
4	DMS	C	8403	-	3,3,3	1.61	1 (33%)	3,3,3	0.26	0
4	DMS	D	8403	-	3,3,3	2.03	1 (33%)	3,3,3	0.36	0
4	DMS	C	8407	-	3,3,3	2.22	2 (66%)	3,3,3	0.21	0
4	DMS	B	8406	-	3,3,3	0.67	0	3,3,3	0.27	0
4	DMS	C	8412	-	3,3,3	0.55	0	3,3,3	0.45	0
4	DMS	B	8401	-	3,3,3	1.12	0	3,3,3	0.56	0
4	DMS	C	8405	-	3,3,3	1.72	1 (33%)	3,3,3	0.30	0
4	DMS	A	8408	-	3,3,3	0.36	0	3,3,3	0.10	0
4	DMS	A	8406	-	3,3,3	0.78	0	3,3,3	0.93	0
4	DMS	B	8405	-	3,3,3	1.76	1 (33%)	3,3,3	0.34	0
4	DMS	D	8423	-	3,3,3	1.15	0	3,3,3	0.27	0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	8506	DMS	O-S	3.26	1.71	1.50
4	C	8601	DMS	C2-S	3.25	1.99	1.76
4	B	8405	DMS	O-S	2.94	1.69	1.50
4	D	8403	DMS	C2-S	2.87	1.96	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8409	DMS	O-S	2.85	1.69	1.50
4	B	8403	DMS	C2-S	2.78	1.95	1.76
4	B	8425	DMS	O-S	2.76	1.68	1.50
4	C	8420	DMS	O-S	2.74	1.68	1.50
4	C	8405	DMS	C1-S	2.71	1.95	1.76
4	A	8409	DMS	O-S	2.62	1.67	1.50
4	A	8403	DMS	C2-S	2.62	1.94	1.76
4	C	8602	DMS	C2-S	-2.56	1.57	1.76
4	C	8425	DMS	O-S	2.50	1.66	1.50
4	A	8405	DMS	O-S	2.47	1.66	1.50
4	B	8508	DMS	C1-S	2.46	1.93	1.76
4	C	8404	DMS	C2-S	2.42	1.93	1.76
4	C	8407	DMS	O-S	2.42	1.66	1.50
4	C	8401	DMS	O-S	2.40	1.66	1.50
4	D	8420	DMS	C1-S	2.40	1.93	1.76
4	C	8506	DMS	C1-S	2.40	1.93	1.76
4	A	8403	DMS	O-S	2.31	1.65	1.50
4	D	8419	DMS	C2-S	-2.30	1.59	1.76
4	C	8407	DMS	C2-S	2.23	1.92	1.76
4	C	8403	DMS	C2-S	2.20	1.91	1.76
4	C	8402	DMS	C2-S	2.18	1.91	1.76
4	D	8409	DMS	O-S	2.14	1.64	1.50
4	D	8701	DMS	C1-S	2.12	1.91	1.76
4	D	8401	DMS	O-S	2.11	1.64	1.50
4	B	8411	DMS	C1-S	2.07	1.90	1.76
4	D	8416	DMS	O-S	2.00	1.63	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	8408	DMS	C2-S-C1	2.42	110.81	98.42
4	C	8404	DMS	C2-S-C1	2.02	108.77	98.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

38 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	8425	DMS	2	0
4	C	8419	DMS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	8402	DMS	1	0
4	C	8420	DMS	2	0
4	C	8501	DMS	1	0
4	B	8416	DMS	3	0
4	D	8703	DMS	5	0
4	A	8404	DMS	1	0
4	C	8404	DMS	1	0
4	D	8425	DMS	1	0
4	D	8419	DMS	8	0
4	D	8404	DMS	2	0
4	B	8408	DMS	1	0
4	B	8504	DMS	3	0
4	A	8403	DMS	1	0
4	D	8412	DMS	4	0
4	C	8416	DMS	1	0
4	B	8403	DMS	1	0
4	D	8411	DMS	1	0
4	A	8416	DMS	3	0
4	A	8602	DMS	1	0
4	A	8414	DMS	1	0
4	A	8412	DMS	3	0
4	C	8423	DMS	1	0
4	A	8425	DMS	2	0
4	B	8601	DMS	1	0
4	B	8423	DMS	1	0
4	B	8417	DMS	2	0
4	C	8417	DMS	2	0
4	A	8501	DMS	2	0
4	C	8504	DMS	4	0
4	B	8404	DMS	2	0
4	D	8506	DMS	2	0
4	C	8403	DMS	3	0
4	B	8406	DMS	3	0
4	C	8412	DMS	1	0
4	A	8406	DMS	1	0
4	D	8423	DMS	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1011/1023 (98%)	-0.60	12 (1%) 76 78	9, 22, 53, 100	0
1	B	1011/1023 (98%)	-0.50	15 (1%) 72 73	11, 23, 54, 100	0
1	C	1011/1023 (98%)	-0.53	11 (1%) 78 80	10, 23, 55, 99	0
1	D	1011/1023 (98%)	-0.57	14 (1%) 73 75	10, 23, 53, 100	0
All	All	4044/4092 (98%)	-0.55	52 (1%) 75 76	9, 23, 54, 100	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	685	LEU	4.3
1	A	686	PRO	4.3
1	D	734	SER	4.1
1	C	736	ALA	3.9
1	B	745	MET	3.7
1	C	733	ALA	3.7
1	B	730	LEU	3.4
1	A	772	ASP	3.4
1	A	688	PRO	3.4
1	C	730	LEU	3.2
1	C	731	PRO	3.2
1	D	733	ALA	3.1
1	A	732	ALA	3.1
1	C	829	THR	3.0
1	B	733	ALA	3.0
1	A	731	PRO	3.0
1	A	735	HIS	2.9
1	B	731	PRO	2.8
1	D	1023	LYS	2.8
1	D	686	PRO	2.8
1	A	1023	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	686	PRO	2.8
1	D	735	HIS	2.7
1	B	732	ALA	2.7
1	D	736	ALA	2.7
1	D	685	LEU	2.7
1	C	735	HIS	2.7
1	D	634	GLN	2.7
1	B	735	HIS	2.7
1	C	734	SER	2.7
1	A	730	LEU	2.6
1	D	799	THR	2.6
1	D	730	LEU	2.6
1	D	732	ALA	2.6
1	C	1023	LYS	2.5
1	C	737	ILE	2.5
1	C	732	ALA	2.4
1	A	687	GLN	2.4
1	D	688	PRO	2.4
1	A	733	ALA	2.3
1	A	799	THR	2.3
1	A	800	ARG	2.3
1	B	845	GLN	2.3
1	B	684	GLU	2.2
1	B	1023	LYS	2.2
1	B	663	LEU	2.2
1	B	130	ASP	2.2
1	C	799	THR	2.2
1	B	181	GLU	2.1
1	D	755	ARG	2.1
1	D	731	PRO	2.1
1	B	729	THR	2.1

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 ⓘ

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
4	DMS	A	8416	4/4	0.79	0.20	36,66,91,100	0
4	DMS	B	8406	4/4	0.85	0.22	38,56,100,100	0
4	DMS	C	8506	4/4	0.85	0.19	51,54,73,100	0
4	DMS	C	8407	4/4	0.86	0.19	24,32,100,100	0
4	DMS	A	8421	4/4	0.86	0.19	68,73,83,100	0
4	DMS	B	8508	4/4	0.87	0.17	46,49,56,100	0
2	MG	A	3005	1/1	0.88	0.10	44,44,44,44	0
4	DMS	A	8406	4/4	0.88	0.13	26,35,53,78	0
4	DMS	D	8420	4/4	0.88	0.21	39,58,78,100	0
4	DMS	D	8416	4/4	0.88	0.16	49,54,72,100	0
4	DMS	D	8703	4/4	0.88	0.20	31,67,78,79	0
4	DMS	C	8416	4/4	0.89	0.16	65,77,100,100	0
4	DMS	C	8421	4/4	0.89	0.17	52,71,78,100	0
4	DMS	D	8421	4/4	0.89	0.17	51,71,100,100	0
4	DMS	B	8417	4/4	0.89	0.13	27,30,49,75	0
4	DMS	A	8501	4/4	0.90	0.10	28,32,54,59	0
4	DMS	B	8414	4/4	0.91	0.15	26,59,70,100	0
4	DMS	B	8416	4/4	0.91	0.11	37,39,76,100	0
4	DMS	A	8414	4/4	0.91	0.16	49,55,92,97	0
4	DMS	C	8417	4/4	0.91	0.12	24,40,50,61	0
4	DMS	D	8423	4/4	0.91	0.18	36,56,77,100	0
4	DMS	B	8423	4/4	0.91	0.16	53,53,74,80	0
4	DMS	B	8421	4/4	0.92	0.12	34,52,77,100	0
4	DMS	D	8414	4/4	0.92	0.16	43,63,100,100	0
4	DMS	A	8602	4/4	0.92	0.21	57,95,100,100	0
3	NA	D	3104	1/1	0.92	0.08	44,44,44,44	0
4	DMS	B	8408	4/4	0.92	0.15	29,44,44,67	0
4	DMS	D	8506	4/4	0.92	0.17	60,82,100,100	0
4	DMS	C	8601	4/4	0.92	0.12	33,41,60,73	0
4	DMS	D	8705	4/4	0.92	0.11	36,42,50,52	0
3	NA	B	3104	1/1	0.93	0.08	39,39,39,39	0
4	DMS	C	8504	4/4	0.93	0.16	43,75,100,100	0
4	DMS	A	8504	4/4	0.93	0.19	27,49,100,100	0
4	DMS	C	8420	4/4	0.93	0.16	42,62,86,100	0
4	DMS	D	8409	4/4	0.94	0.11	41,44,46,57	0
4	DMS	B	8504	4/4	0.94	0.11	36,38,60,100	0
4	DMS	B	8404	4/4	0.94	0.09	29,30,56,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DMS	D	8419	4/4	0.94	0.12	47,59,83,92	0
4	DMS	C	8423	4/4	0.94	0.12	53,55,57,75	0
4	DMS	A	8411	4/4	0.94	0.14	30,45,54,100	0
3	NA	C	3104	1/1	0.94	0.07	36,36,36,36	0
4	DMS	D	8508	4/4	0.94	0.13	41,50,71,78	0
4	DMS	A	8425	4/4	0.94	0.12	37,39,60,70	0
4	DMS	C	8419	4/4	0.94	0.16	61,79,85,100	0
4	DMS	C	8409	4/4	0.95	0.10	46,50,57,63	0
4	DMS	C	8414	4/4	0.95	0.16	26,46,100,100	0
4	DMS	C	8425	4/4	0.95	0.16	37,50,100,100	0
3	NA	D	3103	1/1	0.95	0.05	35,35,35,35	0
2	MG	A	3105	1/1	0.95	0.05	32,32,32,32	0
4	DMS	A	8412	4/4	0.95	0.11	39,39,50,100	0
4	DMS	C	8602	4/4	0.95	0.16	22,65,100,100	0
4	DMS	C	8408	4/4	0.95	0.10	23,41,44,44	0
4	DMS	D	8403	4/4	0.95	0.11	31,32,49,67	0
4	DMS	D	8404	4/4	0.95	0.13	22,40,56,100	0
4	DMS	A	8409	4/4	0.96	0.10	39,42,46,48	0
4	DMS	B	8409	4/4	0.96	0.08	33,37,37,47	0
4	DMS	C	8412	4/4	0.96	0.17	39,43,96,100	0
4	DMS	B	8425	4/4	0.96	0.07	30,33,44,55	0
3	NA	A	3104	1/1	0.96	0.04	32,32,32,32	0
4	DMS	A	8404	4/4	0.96	0.10	25,37,51,61	0
4	DMS	D	8425	4/4	0.96	0.14	13,26,31,59	4
4	DMS	D	8501	4/4	0.96	0.10	42,42,53,66	0
4	DMS	B	8601	4/4	0.96	0.12	44,57,68,100	0
4	DMS	C	8403	4/4	0.96	0.08	23,30,41,44	0
3	NA	C	3103	1/1	0.96	0.06	37,37,37,37	0
4	DMS	D	8406	4/4	0.96	0.10	24,25,33,49	0
4	DMS	A	8408	4/4	0.97	0.10	32,37,50,100	0
2	MG	D	3001	1/1	0.97	0.03	26,26,26,26	0
4	DMS	C	8501	4/4	0.97	0.07	25,30,42,49	0
4	DMS	C	8411	4/4	0.97	0.09	38,38,50,72	0
4	DMS	A	8405	4/4	0.97	0.08	28,38,39,40	0
4	DMS	B	8411	4/4	0.97	0.10	22,42,43,100	0
4	DMS	B	8412	4/4	0.97	0.11	32,46,48,78	0
4	DMS	B	8403	4/4	0.97	0.08	33,35,41,47	0
4	DMS	A	8403	4/4	0.97	0.11	32,36,46,67	0
4	DMS	C	8404	4/4	0.97	0.07	18,24,38,50	0
4	DMS	B	8405	4/4	0.97	0.10	38,52,53,63	0
4	DMS	D	8408	4/4	0.97	0.09	23,36,40,100	0
3	NA	D	3101	1/1	0.98	0.03	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	3001	1/1	0.98	0.07	21,21,21,21	0
4	DMS	D	8405	4/4	0.98	0.07	29,31,31,36	0
3	NA	B	3101	1/1	0.98	0.08	29,29,29,29	0
4	DMS	A	8401	4/4	0.98	0.07	14,19,31,33	0
4	DMS	A	8402	4/4	0.98	0.06	14,28,31,58	0
4	DMS	D	8411	4/4	0.98	0.09	26,29,43,100	0
4	DMS	C	8402	4/4	0.98	0.06	14,28,30,30	0
3	NA	B	3103	1/1	0.98	0.04	25,25,25,25	0
2	MG	B	3002	1/1	0.98	0.05	18,18,18,18	0
4	DMS	C	8405	4/4	0.98	0.07	23,36,39,47	0
3	NA	C	3101	1/1	0.98	0.04	30,30,30,30	0
2	MG	A	3002	1/1	0.98	0.06	23,23,23,23	0
3	NA	A	3101	1/1	0.98	0.06	30,30,30,30	0
4	DMS	B	8401	4/4	0.98	0.05	18,20,29,33	0
4	DMS	B	8402	4/4	0.98	0.06	15,23,29,33	0
4	DMS	D	8701	4/4	0.98	0.10	21,32,32,55	0
4	DMS	D	8401	4/4	0.98	0.05	20,20,27,29	0
4	DMS	D	8402	4/4	0.98	0.07	15,32,33,35	0
2	MG	A	3001	1/1	0.99	0.02	30,30,30,30	0
4	DMS	C	8401	4/4	0.99	0.06	19,21,33,54	0
3	NA	B	3102	1/1	0.99	0.03	19,19,19,19	0
3	NA	D	3102	1/1	0.99	0.02	18,18,18,18	0
2	MG	D	3002	1/1	0.99	0.06	17,17,17,17	0
2	MG	C	3001	1/1	0.99	0.04	20,20,20,20	0
3	NA	A	3103	1/1	0.99	0.03	27,27,27,27	0
4	DMS	D	8412	4/4	0.99	0.07	26,34,45,50	0
3	NA	C	3102	1/1	0.99	0.02	18,18,18,18	0
2	MG	C	3002	1/1	0.99	0.03	17,17,17,17	0
3	NA	A	3102	1/1	1.00	0.03	14,14,14,14	0

6.5 Other polymers ⓘ

There are no such residues in this entry.