



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 06:04 am BST

PDB ID : 1S1M
Title : Crystal Structure of E. Coli CTP Synthetase
Authors : Endrizzi, J.A.; Kim, H.; Anderson, P.M.; Baldwin, E.P.
Deposited on : 2004-01-06
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

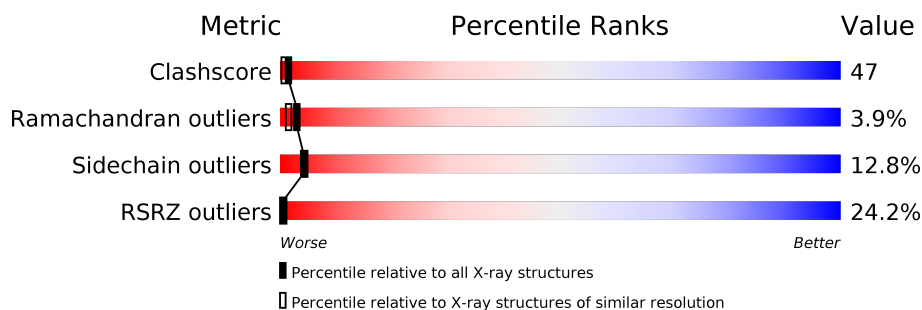
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	545	
1	B	545	

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
3	MG	A	703	-	-	-	X
3	MG	B	704	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IOD	A	803	-	-	X	-
4	IOD	A	806	-	-	X	-
4	IOD	A	814	-	-	X	-
4	IOD	B	808	-	-	X	-
4	IOD	B	815	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8949 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 CTP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	5	1	0
			4167	2633	729	784	21			
1	B	536	Total	C	N	O	S	5	0	0
			4177	2640	730	786	21			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

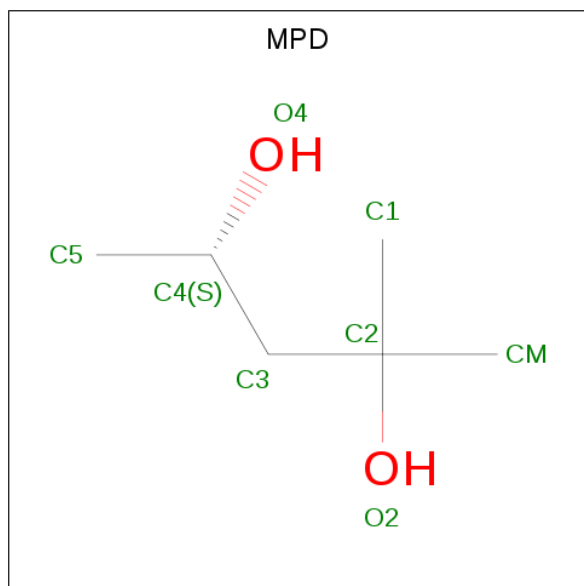
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	7	Total	I	0	0
			7	7		
4	A	9	Total	I	0	0
			9	9		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		

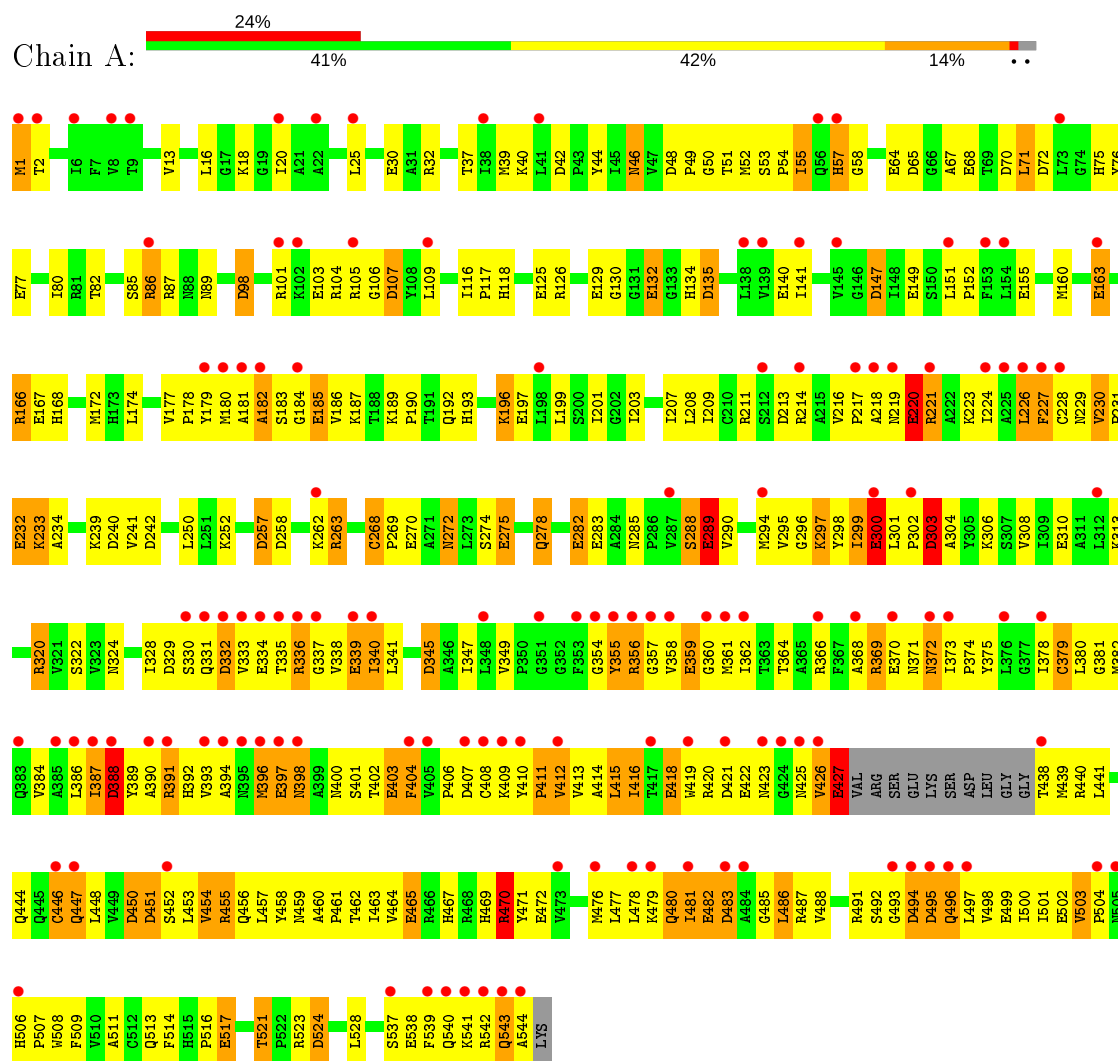
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	268	Total 268	O 268	0	0
6	B	281	Total 281	O 281	0	0

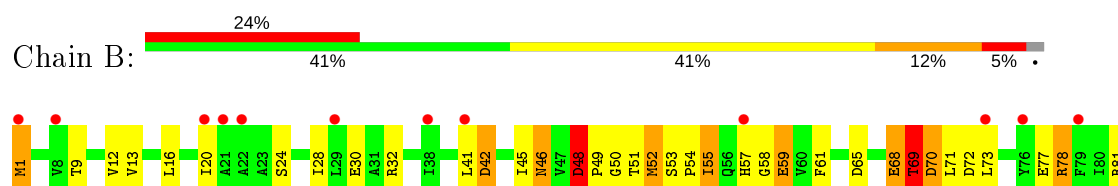
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: CTP synthase



• Molecule 1: CTP synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	165.51Å 106.81Å 130.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 38.58 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.30) 99.0 (38.58-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.29Å)	Xtriage
Refinement program	TNT version 5f	Depositor
R, R_{free}	0.214 , 0.281 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 100.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8949	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, IOD, MG, SO4

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	1.08	37/4248 (0.9%)	1.29	52/5755 (0.9%)
1	B	0.93	37/4253 (0.9%)	1.26	57/5761 (1.0%)
All	All	1.01	74/8501 (0.9%)	1.27	109/11516 (0.9%)

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57[A]	HIS	C-N	25.86	1.79	1.33
1	A	57[B]	HIS	C-N	25.86	1.79	1.33
1	A	132	GLU	CD-OE2	6.78	1.33	1.25
1	B	129	GLU	CD-OE2	6.67	1.32	1.25
1	B	427	GLU	CD-OE2	6.66	1.32	1.25
1	A	129	GLU	CD-OE2	6.58	1.32	1.25
1	A	418	GLU	CD-OE2	6.57	1.32	1.25
1	B	339	GLU	CD-OE2	6.45	1.32	1.25
1	A	499	GLU	CD-OE2	6.42	1.32	1.25
1	B	132	GLU	CD-OE2	6.35	1.32	1.25
1	B	397	GLU	CD-OE2	6.34	1.32	1.25
1	A	232	GLU	CD-OE2	6.32	1.32	1.25
1	B	197	GLU	CD-OE2	6.31	1.32	1.25
1	B	167	GLU	CD-OE2	6.30	1.32	1.25
1	B	163	GLU	CD-OE2	6.25	1.32	1.25
1	B	149	GLU	CD-OE2	6.21	1.32	1.25
1	B	220	GLU	CD-OE2	6.20	1.32	1.25
1	A	167	GLU	CD-OE2	6.17	1.32	1.25
1	B	310	GLU	CD-OE2	6.16	1.32	1.25
1	B	77	GLU	CD-OE2	6.16	1.32	1.25
1	B	232	GLU	CD-OE2	6.15	1.32	1.25
1	B	300	GLU	CD-OE2	6.13	1.32	1.25
1	B	370	GLU	CD-OE2	6.09	1.32	1.25
1	B	418	GLU	CD-OE2	6.08	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	370	GLU	CD-OE2	6.07	1.32	1.25
1	B	30	GLU	CD-OE2	6.02	1.32	1.25
1	A	427	GLU	CD-OE2	6.01	1.32	1.25
1	B	68	GLU	CD-OE2	5.97	1.32	1.25
1	A	103	GLU	CD-OE2	5.97	1.32	1.25
1	B	422	GLU	CD-OE2	5.96	1.32	1.25
1	A	77	GLU	CD-OE2	5.95	1.32	1.25
1	A	30	GLU	CD-OE2	5.95	1.32	1.25
1	B	103	GLU	CD-OE2	5.94	1.32	1.25
1	A	125	GLU	CD-OE2	5.88	1.32	1.25
1	A	149	GLU	CD-OE2	5.84	1.32	1.25
1	B	502	GLU	CD-OE2	5.84	1.32	1.25
1	A	220	GLU	CD-OE2	5.84	1.32	1.25
1	A	403	GLU	CD-OE2	5.77	1.31	1.25
1	A	397	GLU	CD-OE2	5.75	1.31	1.25
1	B	125	GLU	CD-OE2	5.75	1.31	1.25
1	B	538	GLU	CD-OE2	5.74	1.31	1.25
1	A	270	GLU	CD-OE2	5.73	1.31	1.25
1	A	482	GLU	CD-OE2	5.68	1.31	1.25
1	B	359	GLU	CD-OE2	5.67	1.31	1.25
1	A	185	GLU	CD-OE2	5.66	1.31	1.25
1	A	538	GLU	CD-OE2	5.65	1.31	1.25
1	B	270	GLU	CD-OE2	5.64	1.31	1.25
1	A	517	GLU	CD-OE2	5.64	1.31	1.25
1	B	277	GLU	CD-OE2	5.64	1.31	1.25
1	B	289	GLU	CD-OE2	5.60	1.31	1.25
1	A	163	GLU	CD-OE2	5.57	1.31	1.25
1	A	300	GLU	CD-OE2	5.54	1.31	1.25
1	A	310	GLU	CD-OE2	5.51	1.31	1.25
1	A	197	GLU	CD-OE2	5.41	1.31	1.25
1	B	185	GLU	CD-OE2	5.41	1.31	1.25
1	B	334	GLU	CD-OE2	5.41	1.31	1.25
1	B	517	GLU	CD-OE2	5.40	1.31	1.25
1	A	502	GLU	CD-OE2	5.39	1.31	1.25
1	A	289	GLU	CD-OE2	5.35	1.31	1.25
1	A	465	GLU	CD-OE2	5.31	1.31	1.25
1	A	359	GLU	CD-OE2	5.30	1.31	1.25
1	B	140	GLU	CD-OE2	5.30	1.31	1.25
1	A	275	GLU	CD-OE2	5.30	1.31	1.25
1	A	282	GLU	CD-OE2	5.30	1.31	1.25
1	B	403	GLU	CD-OE2	5.26	1.31	1.25
1	B	283	GLU	CD-OE2	5.25	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	GLU	CD-OE2	5.24	1.31	1.25
1	B	499	GLU	CD-OE2	5.23	1.31	1.25
1	A	339	GLU	CD-OE2	5.21	1.31	1.25
1	A	283	GLU	CD-OE2	5.17	1.31	1.25
1	A	64	GLU	CD-OE2	5.14	1.31	1.25
1	B	465	GLU	CD-OE2	5.11	1.31	1.25
1	B	155	GLU	CD-OE2	5.08	1.31	1.25
1	B	59	GLU	CD-OE2	5.04	1.31	1.25

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57[A]	HIS	C-N-CA	-16.73	87.17	122.30
1	A	57[B]	HIS	C-N-CA	-16.73	87.17	122.30
1	A	503	VAL	C-N-CD	-8.17	102.63	120.60
1	B	213	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	A	72	ASP	CB-CG-OD1	7.84	125.36	118.30
1	A	57[A]	HIS	O-C-N	-7.38	110.65	123.20
1	A	57[B]	HIS	O-C-N	-7.38	110.65	123.20
1	B	524	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	A	407	ASP	CB-CG-OD1	7.14	124.73	118.30
1	B	70	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	B	388	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	450	ASP	CB-CG-OD2	-6.92	112.08	118.30
1	A	107	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	A	407	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	72	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	B	483	ASP	CB-CG-OD2	-6.71	112.27	118.30
1	B	42	ASP	CB-CG-OD1	6.69	124.32	118.30
1	B	407	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	B	483	ASP	CB-CG-OD1	6.67	124.30	118.30
1	A	227	PHE	CB-CG-CD2	-6.52	116.24	120.80
1	B	135	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	B	495	ASP	CB-CG-OD2	-6.46	112.48	118.30
1	B	48	ASP	CB-CG-OD1	6.46	124.11	118.30
1	B	388	ASP	CB-CG-OD1	6.45	124.10	118.30
1	B	242	ASP	CB-CG-OD1	6.45	124.10	118.30
1	A	213	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	A	221	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	B	242	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	B	42	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	B	107	ASP	CB-CG-OD2	-6.34	112.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	ASP	CB-CG-OD2	-6.34	112.60	118.30
1	A	135	ASP	CB-CG-OD1	6.32	123.98	118.30
1	A	495	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	A	98	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	451	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	147	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	B	345	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	B	524	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	495	ASP	CB-CG-OD1	6.14	123.83	118.30
1	B	329	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	B	227	PHE	CB-CG-CD1	-6.14	116.50	120.80
1	A	258	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	A	329	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	B	70	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	48	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	48	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	B	421	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	B	332	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	107	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	483	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	A	98	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	B	303	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	B	65	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	242	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	258	ASP	CB-CG-OD1	6.01	123.71	118.30
1	B	213	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	70	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	135	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	B	329	ASP	CB-CG-OD1	5.96	123.67	118.30
1	B	355	TYR	N-CA-CB	5.88	121.19	110.60
1	B	451	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	A	524	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	303	ASP	CB-CG-OD1	5.86	123.58	118.30
1	B	258	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	A	42	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	B	466	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	240	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	A	65	ASP	CB-CG-OD1	5.82	123.54	118.30
1	B	72	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	388	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	147	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	69	THR	N-CA-CB	-5.80	99.28	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	345	ASP	CB-CG-OD2	-5.79	113.08	118.30
1	A	494	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	B	78	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	240	ASP	CB-CG-OD1	5.74	123.47	118.30
1	B	65	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	A	257	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	B	98	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	B	240	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	70	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	450	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	A	329	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	32	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	468	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	211	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	494	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	470	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	523	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	407	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	107	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	104	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	450	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	450	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	332	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	213	ASP	CB-CA-C	-5.27	99.86	110.40
1	B	94	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	366	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	345	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	483	ASP	CB-CG-OD1	5.19	122.97	118.30
1	B	87	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	503	VAL	C-N-CD	-5.15	109.26	120.60
1	B	495	ASP	CB-CG-OD1	5.15	122.93	118.30
1	B	135	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	388	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	B	402	THR	CA-CB-CG2	-5.05	105.33	112.40
1	B	303	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	332	ASP	CB-CG-OD2	-5.01	113.79	118.30

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	4167	0	4178	385	0
1	B	4177	0	4198	394	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	9	0	0	10	0
4	B	7	0	0	8	0
5	A	8	0	14	2	0
5	B	8	0	14	2	0
6	A	268	0	0	20	0
6	B	281	0	0	25	0
All	All	8949	0	8404	784	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 47.

All (784) 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:A:196:LYS:NZ	6:A:1077:HOH:O	1.61	1.28
4:A:807:IOD:I	6:A:979:HOH:O	2.25	1.24
1:B:326:LYS:HE2	1:B:328:ILE:HD11	1.24	1.16
1:B:395:ASN:HD21	1:B:480:GLN:NE2	1.46	1.11
1:A:401:SER:HB2	1:A:413:VAL:HB	1.26	1.10
4:B:811:IOD:I	6:B:1871:HOH:O	2.39	1.10
1:A:408:CYS:H	1:A:420:ARG:NH2	1.50	1.08
1:A:335:THR:HG22	1:A:336:ARG:HG3	1.34	1.08
1:A:147:ASP:HB2	6:A:867:HOH:O	1.58	1.04
1:A:521:THR:HG22	1:A:524:ASP:H	1.16	1.04
1:B:49:PRO:HA	1:B:52:MET:HE3	1.41	1.03
4:B:808:IOD:I	6:B:1754:HOH:O	2.48	1.02
1:B:401:SER:HB2	1:B:413:VAL:HB	1.44	1.00
1:A:49:PRO:HG3	6:A:1009:HOH:O	1.63	0.98
1:B:493:GLY:HA2	1:B:496:GLN:NE2	1.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ASN:HD21	1:B:480:GLN:HE21	1.12	0.94
1:B:198:LEU:HD12	1:B:205:PRO:HG3	1.51	0.93
1:A:301:LEU:HD12	1:A:302:PRO:CD	2.00	0.91
4:B:815:IOD:I	6:B:1774:HOH:O	2.60	0.90
4:A:814:IOD:I	1:B:193:HIS:HD2	2.26	0.89
1:A:408:CYS:N	1:A:420:ARG:HH22	1.71	0.89
1:A:46:ASN:HB2	1:A:52:MET:HE1	1.55	0.88
1:B:49:PRO:HA	1:B:52:MET:CE	2.04	0.88
1:B:189:LYS:HB3	1:B:190:PRO:HD3	1.53	0.88
1:B:46:ASN:HD22	1:B:46:ASN:H	1.19	0.88
1:B:326:LYS:CE	1:B:328:ILE:HD11	2.04	0.88
1:A:178:PRO:HB3	4:A:806:IOD:I	2.45	0.87
1:B:468:ARG:HG2	1:B:468:ARG:HH11	1.40	0.86
1:A:403:GLU:HG3	1:A:471:TYR:CE1	2.09	0.86
4:A:814:IOD:I	1:B:193:HIS:CD2	2.98	0.86
1:B:355:TYR:CG	1:B:404:PHE:HB3	2.10	0.86
1:A:49:PRO:HA	1:A:52:MET:CE	2.05	0.86
1:B:408:CYS:H	1:B:420:ARG:HH22	1.23	0.86
1:B:396:MET:HE1	1:B:480:GLN:HB3	1.55	0.85
1:B:493:GLY:HA2	1:B:496:GLN:HE22	1.39	0.85
1:B:344:LEU:HD12	1:B:347:ILE:HD11	1.57	0.85
1:A:301:LEU:HD12	1:A:302:PRO:HD2	1.58	0.85
1:B:117:PRO:HD2	1:B:118:HIS:CE1	2.11	0.84
1:B:46:ASN:ND2	1:B:46:ASN:H	1.69	0.84
1:B:198:LEU:CD1	1:B:205:PRO:HG3	2.08	0.84
1:B:213:ASP:HB3	1:B:214:ARG:HE	1.41	0.84
1:B:86:ARG:NH1	1:B:89:ASN:HB3	1.92	0.84
1:A:408:CYS:H	1:A:420:ARG:HH22	0.86	0.83
1:B:334:GLU:HG2	1:B:360:GLY:CA	2.08	0.83
1:B:117:PRO:HD2	1:B:118:HIS:ND1	1.93	0.83
1:A:402:THR:HG23	1:A:414:ALA:HB2	1.61	0.82
1:A:506:HIS:CG	1:A:507:PRO:HD2	2.13	0.82
1:A:521:THR:CG2	1:A:524:ASP:H	1.92	0.82
1:A:521:THR:HB	6:A:1001:HOH:O	1.77	0.81
1:B:227:PHE:O	1:B:228:CYS:C	2.15	0.81
1:B:396:MET:HA	1:B:410:TYR:CD1	2.15	0.81
1:B:268:CYS:HB2	1:B:269:PRO:HD2	1.62	0.81
4:A:806:IOD:I	1:B:178:PRO:HB3	2.51	0.81
1:A:401:SER:CB	1:A:413:VAL:HB	2.11	0.80
1:B:299:ILE:HG21	1:B:327:LEU:HB3	1.64	0.80
1:B:176:LEU:HD12	1:B:177:VAL:H	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ARG:HG3	1:B:399:ALA:HB3	1.62	0.79
1:A:349:VAL:HG12	1:A:381:GLY:HA2	1.64	0.79
1:A:409:LYS:C	1:A:411:PRO:HD3	2.03	0.79
1:A:345:ASP:HA	1:A:539:PHE:CD2	2.16	0.79
1:B:395:ASN:ND2	1:B:480:GLN:HE21	1.79	0.79
1:B:408:CYS:H	1:B:420:ARG:NH2	1.80	0.79
1:B:176:LEU:HD12	1:B:177:VAL:N	1.97	0.78
1:A:105:ARG:HG3	1:A:107:ASP:OD1	1.83	0.78
1:B:106:GLY:O	1:B:108:TYR:N	2.17	0.78
1:A:186:VAL:HG13	1:A:220:GLU:HG2	1.65	0.77
1:A:439:MET:CE	1:A:470:ARG:HG2	2.15	0.77
1:B:456:GLN:HG3	6:B:1857:HOH:O	1.84	0.76
1:A:306:LYS:NZ	6:A:1080:HOH:O	2.18	0.76
1:A:361:MET:HB2	1:A:384:VAL:HG21	1.68	0.76
1:A:54:PRO:HA	1:A:58:GLY:N	2.00	0.76
1:B:355:TYR:HB2	1:B:404:PHE:HD2	1.50	0.76
1:A:86:ARG:CB	1:A:86:ARG:HH11	2.00	0.75
1:A:349:VAL:HG12	1:A:381:GLY:CA	2.16	0.75
1:A:54:PRO:O	1:A:58:GLY:N	2.20	0.75
1:A:86:ARG:CA	1:A:86:ARG:HH11	2.00	0.75
1:B:331:GLN:O	1:B:334:GLU:HG3	1.85	0.75
1:B:506:HIS:ND1	1:B:507:PRO:HD2	2.02	0.75
1:B:213:ASP:HB3	1:B:214:ARG:HG2	1.68	0.75
1:A:448:LEU:HD11	1:A:463:ILE:CG2	2.16	0.75
1:A:347:ILE:HD12	1:A:368:ALA:HB2	1.69	0.74
1:A:401:SER:HB2	1:A:413:VAL:CB	2.12	0.74
1:B:226:LEU:HG	1:B:227:PHE:N	2.01	0.74
1:A:49:PRO:HA	1:A:52:MET:HE3	1.68	0.74
1:A:394:ALA:HB1	1:A:396:MET:CE	2.17	0.74
1:A:493:GLY:O	1:A:496:GLN:HG3	1.88	0.74
1:B:348:LEU:HD23	1:B:349:VAL:N	2.02	0.74
1:B:396:MET:HB3	1:B:399:ALA:HB2	1.70	0.74
1:B:49:PRO:HG2	1:B:69:THR:HA	1.70	0.74
1:A:423:ASN:HB2	1:A:425:ASN:HD22	1.53	0.73
1:A:421:ASP:CG	1:A:425:ASN:HB2	2.09	0.73
1:B:213:ASP:CB	1:B:214:ARG:HG2	2.18	0.73
1:B:341:LEU:O	1:B:344:LEU:HG	1.88	0.73
1:A:447:GLN:HG3	1:A:462:THR:HG22	1.71	0.73
1:B:449:VAL:HG21	1:B:488:VAL:O	1.88	0.73
1:A:347:ILE:CD1	1:A:368:ALA:HB2	2.18	0.73
1:A:409:LYS:HD3	1:A:410:TYR:CD1	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:PRO:O	1:A:301:LEU:HD23	1.89	0.73
1:A:86:ARG:N	1:A:86:ARG:NH1	2.37	0.72
1:B:229:ASN:C	1:B:231:PRO:HD3	2.10	0.72
1:B:228:CYS:O	1:B:230:VAL:N	2.23	0.72
1:A:333:VAL:HA	1:A:340:ILE:HD11	1.71	0.72
1:B:395:ASN:ND2	1:B:480:GLN:NE2	2.30	0.72
1:B:32:ARG:HD3	1:B:269:PRO:O	1.90	0.71
1:A:371:ASN:HB2	1:A:373:ILE:CD1	2.19	0.71
1:B:199:LEU:HD21	1:B:204:GLN:NE2	2.05	0.71
1:B:213:ASP:CB	1:B:214:ARG:HE	2.03	0.71
1:A:332:ASP:HA	1:A:335:THR:HB	1.73	0.71
1:A:86:ARG:N	1:A:86:ARG:HH11	1.88	0.71
1:B:414:ALA:HA	1:B:471:TYR:HD2	1.54	0.71
1:B:220:GLU:O	1:B:224:ILE:HD12	1.89	0.71
1:A:224:ILE:HG23	1:A:229:ASN:ND2	2.06	0.71
1:B:425:ASN:O	1:B:476:MET:HE1	1.90	0.70
1:B:301:LEU:HD12	1:B:302:PRO:HD2	1.73	0.70
1:A:224:ILE:HG23	1:A:229:ASN:HD22	1.55	0.70
1:B:326:LYS:HE2	1:B:328:ILE:CD1	2.14	0.70
1:A:330:SER:OG	1:A:357:GLY:HA3	1.92	0.70
1:B:313:LYS:HE3	6:B:1741:HOH:O	1.92	0.70
1:B:330:SER:HB3	1:B:361:MET:HG3	1.74	0.70
1:A:349:VAL:CG1	1:A:381:GLY:HA2	2.22	0.70
1:A:495:ASP:HB3	1:A:497:LEU:CD1	2.21	0.70
1:A:268:CYS:HB2	1:A:269:PRO:HD2	1.74	0.70
1:A:396:MET:CE	1:A:480:GLN:HG2	2.22	0.69
1:A:408:CYS:N	1:A:420:ARG:NH2	2.34	0.69
1:A:389:TYR:HD2	1:A:481:ILE:HG22	1.56	0.69
1:A:371:ASN:HB2	1:A:373:ILE:HD12	1.74	0.69
1:A:427:GLU:OE1	1:A:427:GLU:HA	1.92	0.69
1:B:402:THR:HG23	1:B:414:ALA:HB2	1.74	0.69
1:A:86:ARG:NH1	1:A:86:ARG:H	1.91	0.69
1:A:290:VAL:O	1:A:324:ASN:HB2	1.93	0.69
1:B:108:TYR:CD2	1:B:118:HIS:HD2	2.10	0.69
1:A:448:LEU:HD11	1:A:463:ILE:HG21	1.73	0.68
1:A:448:LEU:HD22	1:A:454:VAL:CG1	2.23	0.68
1:B:421:ASP:HB3	1:B:425:ASN:H	1.58	0.68
1:B:495:ASP:O	1:B:496:GLN:C	2.31	0.68
1:A:297:LYS:HE3	1:A:298:TYR:CE2	2.28	0.68
1:B:334:GLU:HG2	1:B:360:GLY:HA3	1.74	0.68
1:A:439:MET:HE3	1:A:470:ARG:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:VAL:HG11	1:A:491:ARG:NE	2.08	0.68
1:A:86:ARG:HD3	6:A:1016:HOH:O	1.92	0.68
1:B:180:MET:HB3	1:B:183:SER:CB	2.23	0.68
1:B:333:VAL:HG11	1:B:360:GLY:O	1.94	0.68
1:A:460:ALA:HB1	1:A:461:PRO:HD2	1.76	0.68
1:B:223:LYS:O	1:B:227:PHE:HB2	1.94	0.68
1:A:521:THR:HG22	1:A:524:ASP:N	1.99	0.67
1:A:382:MET:HE2	1:A:501:ILE:HG23	1.75	0.67
1:B:224:ILE:HG23	1:B:229:ASN:ND2	2.10	0.67
1:A:412:VAL:HG13	1:A:477:LEU:HB2	1.77	0.67
1:B:224:ILE:O	1:B:229:ASN:ND2	2.25	0.67
1:B:408:CYS:N	1:B:420:ARG:HH22	1.93	0.67
1:A:355:TYR:HA	1:A:404:PHE:CD2	2.30	0.67
1:B:103:GLU:O	1:B:105:ARG:N	2.27	0.67
1:A:539:PHE:HA	1:A:542:ARG:NH2	2.10	0.67
1:B:216:VAL:HG12	1:B:221:ARG:CG	2.24	0.67
1:B:108:TYR:CE2	1:B:118:HIS:HD2	2.12	0.66
1:B:220:GLU:N	1:B:220:GLU:OE2	2.29	0.66
1:B:334:GLU:HG2	1:B:360:GLY:N	2.10	0.66
1:A:49:PRO:HA	1:A:52:MET:HE2	1.77	0.66
1:B:224:ILE:C	1:B:229:ASN:HD22	1.97	0.66
1:A:2:THR:HG21	1:A:168:HIS:CE1	2.30	0.66
1:A:345:ASP:HA	1:A:539:PHE:CE2	2.30	0.66
1:B:68:GLU:O	1:B:86:ARG:NH2	2.28	0.66
1:A:216:VAL:HG12	1:A:221:ARG:HG3	1.77	0.66
1:A:492:SER:OG	1:A:493:GLY:N	2.28	0.66
1:B:292:ILE:HG12	1:B:346:ALA:HB3	1.76	0.66
1:A:301:LEU:HD11	1:A:303:ASP:H	1.60	0.66
1:A:337:GLY:O	1:A:340:ILE:HD13	1.96	0.66
1:A:301:LEU:HD12	1:A:302:PRO:N	2.10	0.66
1:A:39:MET:CE	1:A:130:GLY:HA3	2.26	0.65
1:A:413:VAL:HA	1:A:472:GLU:O	1.97	0.65
1:B:94:ARG:NH1	1:B:98:ASP:OD1	2.29	0.65
1:B:387:ILE:O	1:B:390:ALA:N	2.29	0.65
1:B:46:ASN:ND2	1:B:46:ASN:N	2.43	0.65
1:A:301:LEU:CD1	1:A:303:ASP:H	2.09	0.65
1:B:53:SER:O	1:B:57:HIS:HB3	1.96	0.65
1:B:107:ASP:N	1:B:107:ASP:OD2	2.30	0.65
1:B:355:TYR:HB2	1:B:404:PHE:CD2	2.32	0.65
1:A:278:GLN:NE2	1:A:282:GLU:OE2	2.29	0.64
1:A:372:ASN:HD22	1:A:506:HIS:CD2	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ARG:O	1:B:105:ARG:HB3	1.96	0.64
1:B:180:MET:HB3	1:B:183:SER:HB3	1.78	0.64
1:B:332:ASP:HA	1:B:335:THR:HB	1.79	0.64
1:B:86:ARG:HH12	1:B:89:ASN:HB3	1.58	0.64
1:A:224:ILE:O	1:A:229:ASN:HB2	1.96	0.64
1:A:516:PRO:HD2	1:A:517:GLU:OE1	1.97	0.64
1:B:408:CYS:N	1:B:420:ARG:NH2	2.44	0.64
1:A:223:LYS:NZ	6:A:979:HOH:O	2.30	0.64
1:B:180:MET:HE3	6:B:1604:HOH:O	1.98	0.64
1:B:289:GLU:HG3	1:B:324:ASN:HD21	1.63	0.64
1:B:468:ARG:NH1	1:B:468:ARG:HG2	2.06	0.64
1:A:369:ARG:NH2	1:A:388:ASP:OD2	2.30	0.64
1:A:403:GLU:HG3	1:A:471:TYR:CZ	2.32	0.64
1:A:439:MET:HG3	1:A:440:ARG:N	2.12	0.64
1:A:394:ALA:HB1	1:A:396:MET:HE2	1.80	0.63
1:B:49:PRO:CA	1:B:52:MET:HE3	2.25	0.63
1:A:409:LYS:H	1:A:420:ARG:HH21	1.43	0.63
1:A:85:SER:OG	1:A:87:ARG:HG2	1.98	0.63
1:A:373:ILE:HG23	1:A:374:PRO:HD2	1.81	0.63
1:B:105:ARG:HG3	1:B:107:ASP:OD2	1.98	0.63
1:A:382:MET:CE	1:A:501:ILE:HG23	2.28	0.63
1:A:389:TYR:CD2	1:A:481:ILE:HG22	2.33	0.63
1:B:421:ASP:N	1:B:476:MET:HE1	2.13	0.63
1:B:408:CYS:O	1:B:420:ARG:NH2	2.28	0.63
1:B:396:MET:HE1	1:B:480:GLN:CB	2.28	0.63
1:A:126:ARG:NH1	6:A:934:HOH:O	2.30	0.62
1:A:189:LYS:HB3	1:A:190:PRO:HD3	1.81	0.62
1:B:482:GLU:O	1:B:485:GLY:N	2.29	0.62
1:B:189:LYS:HB2	4:B:808:IOD:I	2.69	0.62
1:A:230:VAL:HG12	1:A:230:VAL:O	2.00	0.62
1:B:503:VAL:HG13	1:B:504:PRO:HD2	1.81	0.62
1:A:444:GLN:HG2	6:A:1022:HOH:O	1.99	0.62
1:B:151:LEU:HB2	1:B:152:PRO:HD3	1.82	0.62
1:B:332:ASP:O	1:B:336:ARG:N	2.26	0.62
1:A:421:ASP:OD1	1:A:425:ASN:HB2	1.99	0.61
1:B:211:ARG:NH1	1:B:238:LEU:O	2.32	0.61
1:B:333:VAL:HG12	1:B:360:GLY:HA2	1.82	0.61
1:A:285:ASN:O	1:A:320:ARG:HD2	2.01	0.61
1:A:486:LEU:HG	1:A:487:ARG:N	2.14	0.61
1:B:112:THR:N	6:B:1838:HOH:O	2.31	0.61
1:B:395:ASN:ND2	1:B:410:TYR:OH	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:LEU:N	1:B:327:LEU:HD23	2.13	0.61
1:A:439:MET:HE1	1:A:470:ARG:HG2	1.81	0.61
1:B:183:SER:HB3	1:B:185:GLU:HG2	1.80	0.61
1:B:183:SER:CB	1:B:185:GLU:HG2	2.31	0.61
1:B:396:MET:HA	1:B:410:TYR:CG	2.36	0.61
1:B:69:THR:HG21	1:B:73:LEU:HD22	1.81	0.61
1:A:410:TYR:N	1:A:411:PRO:HD3	2.14	0.61
1:A:478:LEU:HD21	1:A:498:VAL:HG21	1.81	0.61
1:B:148:ILE:HG22	1:B:151:LEU:HD11	1.83	0.61
1:A:402:THR:CG2	1:A:414:ALA:HB2	2.31	0.60
1:B:371:ASN:HD22	1:B:371:ASN:N	1.99	0.60
1:B:395:ASN:O	1:B:396:MET:C	2.38	0.60
1:A:396:MET:HE3	1:A:480:GLN:HG2	1.81	0.60
1:B:331:GLN:O	1:B:332:ASP:C	2.39	0.60
1:A:335:THR:HG22	1:A:336:ARG:CG	2.21	0.60
1:A:426:VAL:O	1:A:427:GLU:HB2	2.02	0.60
1:A:252:LYS:HE3	6:A:817:HOH:O	2.02	0.60
1:B:224:ILE:O	1:B:229:ASN:HB2	2.02	0.60
1:B:409:LYS:HE2	1:B:422:GLU:HB2	1.82	0.60
1:A:174:LEU:HG	1:A:209:ILE:HB	1.82	0.60
1:B:395:ASN:HD21	1:B:480:GLN:HE22	1.44	0.60
1:B:395:ASN:O	1:B:397:GLU:N	2.34	0.60
1:B:517:GLU:OE2	1:B:517:GLU:N	2.31	0.60
1:B:541:LYS:HE3	6:B:1742:HOH:O	2.01	0.60
1:A:413:VAL:HG12	1:A:471:TYR:HB3	1.82	0.60
1:A:390:ALA:HB2	1:A:481:ILE:CD1	2.32	0.60
1:B:148:ILE:HG22	1:B:151:LEU:CD1	2.32	0.60
1:B:333:VAL:HG12	1:B:334:GLU:N	2.16	0.60
1:B:415:LEU:HD23	1:B:471:TYR:CD2	2.37	0.60
1:B:68:GLU:OE2	1:B:468:ARG:NE	2.26	0.60
1:A:289:GLU:HB2	1:A:322:SER:HB3	1.84	0.59
1:A:439:MET:HB2	1:A:470:ARG:NH1	2.16	0.59
1:B:46:ASN:HD22	1:B:46:ASN:N	1.96	0.59
1:A:313:LYS:NZ	6:A:1045:HOH:O	2.30	0.59
1:A:541:LYS:O	1:A:542:ARG:C	2.40	0.59
1:B:295:VAL:HG13	1:B:328:ILE:HG22	1.82	0.59
1:A:193:HIS:HB3	6:B:1720:HOH:O	2.01	0.59
1:A:495:ASP:HB3	1:A:497:LEU:HD11	1.83	0.59
1:A:408:CYS:O	1:A:410:TYR:N	2.34	0.59
1:B:331:GLN:O	1:B:334:GLU:N	2.36	0.59
1:B:333:VAL:HA	1:B:340:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:TYR:CD1	1:B:358:VAL:HB	2.38	0.59
1:A:387:ILE:HG22	1:A:388:ASP:N	2.17	0.59
1:A:408:CYS:SG	1:A:411:PRO:HB3	2.43	0.59
1:B:216:VAL:HG12	1:B:221:ARG:HG3	1.85	0.59
1:B:217:PRO:O	1:B:220:GLU:N	2.35	0.59
1:A:542:ARG:O	1:A:544:ALA:N	2.29	0.58
1:A:331:GLN:O	1:A:334:GLU:HB2	2.04	0.58
1:A:39:MET:HE2	1:A:130:GLY:HA3	1.84	0.58
1:A:294:MET:HE3	1:A:308:VAL:HG11	1.84	0.58
1:A:337:GLY:O	1:A:339:GLU:N	2.37	0.58
1:A:379:CYS:O	1:A:382:MET:N	2.34	0.58
1:B:325:ILE:HG22	1:B:327:LEU:CD2	2.34	0.58
1:A:116:ILE:HD11	1:A:155:GLU:HG2	1.85	0.58
1:A:46:ASN:H	1:A:46:ASN:HD22	1.51	0.58
1:A:98:ASP:OD2	1:A:126:ARG:NH1	2.35	0.58
1:B:330:SER:O	1:B:360:GLY:HA3	2.03	0.58
1:B:401:SER:HA	1:B:413:VAL:O	2.04	0.57
1:A:294:MET:HE1	1:A:308:VAL:HB	1.86	0.57
1:B:447:GLN:HE22	1:B:493:GLY:H	1.53	0.57
1:B:41:LEU:HG	1:B:90:PHE:CZ	2.39	0.57
1:B:447:GLN:HE22	1:B:493:GLY:N	2.03	0.57
1:A:355:TYR:CD1	1:A:404:PHE:HB3	2.40	0.57
1:A:361:MET:CB	1:A:384:VAL:HG21	2.34	0.57
1:A:374:PRO:HA	1:A:508:TRP:O	2.05	0.57
1:B:238:LEU:HD21	5:B:1601:MPD:H51	1.86	0.57
1:B:330:SER:HB2	1:B:357:GLY:O	2.05	0.57
1:B:99:VAL:HG21	1:B:119:ILE:HD13	1.86	0.57
1:B:241:VAL:HA	4:B:810:IOD:I	2.75	0.57
1:A:186:VAL:HG13	1:A:220:GLU:CG	2.35	0.56
1:A:183:SER:OG	1:A:185:GLU:HG2	2.05	0.56
1:B:102:LYS:HB3	1:B:108:TYR:CE1	2.39	0.56
1:B:473:VAL:HB	6:B:1622:HOH:O	2.05	0.56
1:B:382:MET:HE3	1:B:512:CYS:HA	1.86	0.56
1:B:52:MET:HB3	1:B:57:HIS:CG	2.41	0.56
1:B:288:SER:HB2	6:B:1778:HOH:O	2.05	0.56
1:A:358:VAL:HG21	1:A:404:PHE:CE2	2.41	0.56
1:A:387:ILE:O	1:A:388:ASP:C	2.42	0.56
1:A:408:CYS:O	1:A:409:LYS:HB3	2.06	0.56
1:B:333:VAL:HG12	1:B:360:GLY:CA	2.35	0.56
1:A:452:SER:OG	1:A:455:ARG:HB2	2.06	0.56
1:B:213:ASP:HB3	1:B:214:ARG:NE	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ARG:CG	1:B:399:ALA:HB3	2.35	0.56
1:B:460:ALA:HB1	1:B:461:PRO:HD2	1.88	0.56
1:A:117:PRO:HD2	1:A:118:HIS:CE1	2.41	0.55
1:A:355:TYR:O	1:A:356:ARG:C	2.44	0.55
1:A:409:LYS:N	1:A:420:ARG:HH21	2.02	0.55
1:A:421:ASP:OD2	1:A:425:ASN:HB2	2.06	0.55
1:B:387:ILE:O	1:B:389:TYR:N	2.39	0.55
1:A:186:VAL:CG1	1:A:220:GLU:HG2	2.34	0.55
1:A:313:LYS:HB3	1:A:313:LYS:NZ	2.21	0.55
1:B:277:GLU:HG3	6:B:1699:HOH:O	2.06	0.55
1:B:290:VAL:HG22	1:B:321:VAL:CG1	2.37	0.55
1:B:355:TYR:CD2	1:B:404:PHE:HB3	2.42	0.55
1:A:347:ILE:HD12	1:A:368:ALA:CB	2.37	0.55
1:A:441:LEU:HA	1:A:467:HIS:O	2.06	0.55
1:A:440:ARG:HH21	1:A:469:HIS:CE1	2.25	0.55
1:B:455:ARG:HD2	1:B:455:ARG:O	2.06	0.55
1:B:488:VAL:HG11	1:B:491:ARG:CZ	2.36	0.55
1:B:186:VAL:HG21	1:B:220:GLU:HG2	1.89	0.55
1:B:211:ARG:HB3	1:B:211:ARG:CZ	2.37	0.55
1:B:273:LEU:O	1:B:277:GLU:HG2	2.07	0.55
1:B:421:ASP:CB	1:B:425:ASN:H	2.18	0.55
1:A:332:ASP:O	1:A:336:ARG:N	2.37	0.55
1:B:289:GLU:CG	1:B:324:ASN:HD21	2.19	0.55
1:A:151:LEU:N	1:A:152:PRO:HD2	2.22	0.55
1:A:297:LYS:O	1:A:300:GLU:OE2	2.25	0.54
1:A:1:MET:O	1:A:2:THR:C	2.46	0.54
1:A:398:ASN:N	1:A:398:ASN:OD1	2.39	0.54
1:B:409:LYS:HD3	1:B:410:TYR:CE1	2.42	0.54
1:B:539:PHE:CE2	1:B:543:GLN:HG3	2.43	0.54
1:B:387:ILE:O	1:B:388:ASP:C	2.44	0.54
1:A:275:GLU:OE1	1:A:523:ARG:HD2	2.07	0.54
1:A:331:GLN:HG2	1:A:334:GLU:OE1	2.08	0.54
1:B:216:VAL:CG1	1:B:221:ARG:HG2	2.37	0.54
1:A:336:ARG:NH2	1:A:340:ILE:HG22	2.23	0.54
1:B:180:MET:HG2	1:B:183:SER:H	1.72	0.54
1:A:177:VAL:CG1	1:A:186:VAL:HG23	2.36	0.54
1:A:481:ILE:O	1:A:482:GLU:C	2.45	0.54
1:B:539:PHE:O	1:B:543:GLN:HG2	2.07	0.54
1:A:391:ARG:O	1:A:393:VAL:N	2.41	0.54
1:A:486:LEU:HG	1:A:487:ARG:H	1.72	0.54
1:B:226:LEU:O	1:B:228:CYS:O	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:THR:N	6:B:1759:HOH:O	2.25	0.54
1:A:390:ALA:O	1:A:394:ALA:HB3	2.07	0.54
1:A:40:LYS:HB3	1:A:89:ASN:ND2	2.22	0.54
1:B:415:LEU:HD21	1:B:471:TYR:CE1	2.42	0.54
1:B:506:HIS:CG	1:B:507:PRO:HD2	2.42	0.54
1:B:71:LEU:HD12	1:B:71:LEU:C	2.28	0.54
1:A:199:LEU:HD23	1:A:203:ILE:O	2.08	0.54
1:A:422:GLU:OE2	1:A:422:GLU:N	2.29	0.54
1:A:396:MET:HE1	1:A:480:GLN:HG2	1.89	0.54
1:A:71:LEU:HD12	1:A:71:LEU:C	2.28	0.54
1:B:49:PRO:HG2	1:B:69:THR:CA	2.38	0.54
1:A:355:TYR:O	1:A:358:VAL:HG23	2.08	0.53
1:A:420:ARG:HG3	1:A:421:ASP:H	1.71	0.53
1:A:54:PRO:CA	1:A:58:GLY:N	2.71	0.53
1:B:403:GLU:HG3	1:B:471:TYR:CE1	2.43	0.53
1:A:416:ILE:HG23	1:A:419:TRP:CH2	2.43	0.53
1:B:179:TYR:CD2	1:B:214:ARG:NH2	2.75	0.53
1:B:516:PRO:HD2	1:B:517:GLU:OE2	2.07	0.53
1:A:18:LYS:HE3	1:A:141:ILE:O	2.07	0.53
1:A:333:VAL:HA	1:A:340:ILE:CD1	2.37	0.53
1:A:241:VAL:HA	4:A:812:IOD:I	2.79	0.53
1:B:331:GLN:HA	1:B:334:GLU:OE2	2.08	0.53
1:A:409:LYS:O	1:A:422:GLU:HA	2.09	0.53
1:B:155:GLU:CD	1:B:158:ARG:HH21	2.11	0.53
1:B:488:VAL:HG11	1:B:491:ARG:NE	2.23	0.53
1:A:20:ILE:HG13	6:A:908:HOH:O	2.08	0.53
1:B:486:LEU:HG	1:B:487:ARG:N	2.22	0.53
1:A:86:ARG:CG	1:A:86:ARG:HH11	2.22	0.53
1:B:332:ASP:O	1:B:333:VAL:C	2.47	0.53
1:A:211:ARG:CZ	5:A:601:MPD:H53	2.38	0.53
1:B:216:VAL:HG12	1:B:221:ARG:HG2	1.90	0.53
1:B:216:VAL:O	1:B:221:ARG:NH1	2.38	0.53
1:B:301:LEU:C	1:B:301:LEU:HD12	2.29	0.53
1:A:226:LEU:O	1:A:227:PHE:C	2.44	0.53
1:B:393:VAL:O	1:B:393:VAL:HG12	2.09	0.53
1:B:441:LEU:CD2	1:B:468:ARG:HD2	2.39	0.53
1:A:288:SER:HB3	6:A:999:HOH:O	2.08	0.53
1:B:166:ARG:NH2	6:B:1830:HOH:O	2.42	0.53
1:A:46:ASN:H	1:A:46:ASN:ND2	2.06	0.52
1:B:224:ILE:O	1:B:225:ALA:C	2.46	0.52
1:B:325:ILE:HG22	1:B:327:LEU:HD23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:ASP:O	1:B:451:ASP:HB2	2.09	0.52
1:A:53:SER:O	1:A:57[B]:HIS:HB3	2.09	0.52
1:A:401:SER:HA	1:A:413:VAL:O	2.08	0.52
1:B:416:ILE:HD11	1:B:497:LEU:HD21	1.91	0.52
1:B:382:MET:HE3	1:B:499:GLU:O	2.10	0.52
1:A:409:LYS:O	1:A:411:PRO:HD3	2.09	0.52
1:A:444:GLN:HB2	1:A:467:HIS:ND1	2.24	0.52
1:B:111:ALA:HB1	6:B:1838:HOH:O	2.09	0.52
1:B:193:HIS:NE2	6:B:1720:HOH:O	2.25	0.52
1:A:355:TYR:O	1:A:356:ARG:O	2.27	0.52
1:A:488:VAL:HG11	1:A:491:ARG:CZ	2.39	0.52
1:B:415:LEU:HD21	1:B:471:TYR:CD1	2.44	0.52
1:A:233:LYS:HB3	6:A:1067:HOH:O	2.09	0.52
1:A:295:VAL:HA	1:A:328:ILE:O	2.10	0.52
1:A:39:MET:HE1	1:A:130:GLY:HA3	1.92	0.52
1:B:331:GLN:O	1:B:333:VAL:N	2.43	0.52
1:B:98:ASP:OD2	1:B:126:ARG:NH2	2.35	0.52
1:A:394:ALA:HB1	1:A:396:MET:HE3	1.89	0.52
1:B:183:SER:OG	1:B:185:GLU:OE2	2.27	0.52
1:A:362:ILE:HG13	1:A:384:VAL:HG22	1.92	0.51
1:A:453:LEU:O	1:A:456:GLN:HB2	2.10	0.51
1:A:420:ARG:HG3	1:A:421:ASP:N	2.24	0.51
1:B:355:TYR:HD1	1:B:358:VAL:HB	1.75	0.51
1:B:492:SER:O	1:B:493:GLY:O	2.29	0.51
1:B:412:VAL:HG13	1:B:413:VAL:HG23	1.92	0.51
1:B:301:LEU:HD12	1:B:302:PRO:CD	2.40	0.51
1:B:390:ALA:HB1	1:B:396:MET:HG2	1.91	0.51
1:A:233:LYS:HG2	1:A:233:LYS:O	2.10	0.51
1:A:389:TYR:HD2	1:A:481:ILE:CG2	2.23	0.51
1:A:160:MET:HG2	4:A:803:IOD:I	2.80	0.51
1:B:371:ASN:N	1:B:371:ASN:ND2	2.58	0.51
1:A:272:ASN:C	1:A:272:ASN:HD22	2.12	0.51
1:A:379:CYS:O	1:A:380:LEU:C	2.49	0.51
1:A:464:VAL:C	1:A:465:GLU:HG2	2.31	0.51
1:B:155:GLU:OE2	1:B:158:ARG:NH2	2.36	0.51
1:B:495:ASP:O	1:B:496:GLN:O	2.29	0.51
1:A:355:TYR:CD1	1:A:404:PHE:CG	2.99	0.51
1:B:131:GLY:O	1:B:134:HIS:HD2	1.93	0.51
1:B:268:CYS:HB2	1:B:269:PRO:CD	2.35	0.51
1:A:357:GLY:O	1:A:360:GLY:N	2.43	0.51
1:A:448:LEU:HD22	1:A:454:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:MET:HB3	1:B:384:VAL:HG21	1.93	0.51
1:B:409:LYS:O	1:B:411:PRO:HD3	2.11	0.51
1:A:337:GLY:C	1:A:339:GLU:H	2.15	0.51
1:B:147:ASP:HB2	6:B:1785:HOH:O	2.10	0.51
1:B:225:ALA:O	1:B:230:VAL:N	2.44	0.51
1:B:53:SER:O	1:B:55:ILE:O	2.29	0.51
1:B:426:VAL:CG1	1:B:427:GLU:N	2.74	0.50
1:B:499:GLU:O	1:B:512:CYS:HA	2.11	0.50
1:B:355:TYR:CB	1:B:404:PHE:CD2	2.94	0.50
1:A:179:TYR:CD2	1:A:214:ARG:NH2	2.80	0.50
1:A:478:LEU:O	1:A:482:GLU:HG3	2.10	0.50
1:A:86:ARG:HH11	1:A:86:ARG:H	1.53	0.50
1:A:263:ARG:O	1:A:263:ARG:HG3	2.10	0.50
1:A:289:GLU:CB	1:A:322:SER:HB3	2.42	0.50
1:B:108:TYR:CD2	1:B:118:HIS:CD2	2.98	0.50
1:B:366:ARG:HA	1:B:388:ASP:OD2	2.12	0.50
1:B:405:VAL:HG12	1:B:405:VAL:O	2.12	0.50
1:B:413:VAL:O	1:B:414:ALA:HB2	2.10	0.50
1:B:48:ASP:OD1	1:B:50:GLY:N	2.42	0.50
1:A:166:ARG:HB2	1:A:263:ARG:HH21	1.76	0.50
1:A:331:GLN:HG2	6:A:1069:HOH:O	2.11	0.50
1:A:331:GLN:O	1:A:335:THR:N	2.36	0.50
1:B:295:VAL:HA	1:B:328:ILE:O	2.10	0.50
1:A:179:TYR:CE1	1:A:214:ARG:NH1	2.80	0.50
1:B:212:SER:HB3	1:B:214:ARG:O	2.12	0.50
1:A:268:CYS:CB	1:A:269:PRO:HD2	2.41	0.50
1:A:409:LYS:HD3	1:A:410:TYR:CE1	2.47	0.50
1:B:395:ASN:ND2	1:B:410:TYR:CZ	2.80	0.50
1:B:447:GLN:NE2	1:B:493:GLY:H	2.09	0.50
1:A:341:LEU:HD23	1:A:341:LEU:N	2.26	0.50
1:B:179:TYR:CE1	1:B:214:ARG:NH1	2.80	0.50
1:B:299:ILE:O	1:B:299:ILE:HG22	2.11	0.50
1:B:420:ARG:HA	1:B:425:ASN:O	2.11	0.50
1:B:86:ARG:NH1	1:B:89:ASN:O	2.45	0.49
1:A:355:TYR:CD1	1:A:404:PHE:CD2	2.99	0.49
1:A:403:GLU:HB2	1:A:471:TYR:CE2	2.47	0.49
1:B:389:TYR:CE2	1:B:486:LEU:HB2	2.47	0.49
1:A:179:TYR:HE2	1:A:181:ALA:HA	1.78	0.49
1:A:177:VAL:HG12	1:A:186:VAL:HG23	1.93	0.49
1:A:201:ILE:CD1	1:A:203:ILE:HD12	2.42	0.49
1:B:392:HIS:CD2	1:B:392:HIS:N	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:HIS:CE1	1:A:513:GLN:NE2	2.79	0.49
1:B:388:ASP:OD1	1:B:389:TYR:N	2.45	0.49
1:B:369:ARG:NH1	1:B:393:VAL:HG21	2.26	0.49
1:A:336:ARG:HH21	1:A:340:ILE:HG22	1.76	0.49
1:A:413:VAL:CG1	1:A:471:TYR:HB3	2.42	0.49
1:B:329:ASP:O	1:B:330:SER:C	2.50	0.49
1:B:415:LEU:N	1:B:415:LEU:HD23	2.26	0.49
1:A:488:VAL:HG11	1:A:491:ARG:HE	1.77	0.49
1:B:115:VAL:O	1:B:119:ILE:HB	2.13	0.49
1:A:301:LEU:O	1:A:301:LEU:HG	2.10	0.49
1:A:44:TYR:CE1	1:A:52:MET:HE1	2.47	0.49
1:A:382:MET:HE3	1:A:500:ILE:HA	1.95	0.49
1:B:299:ILE:CG2	1:B:327:LEU:HB3	2.41	0.49
1:B:373:ILE:HG23	1:B:374:PRO:HD2	1.95	0.49
1:B:227:PHE:C	1:B:228:CYS:O	2.46	0.49
1:B:69:THR:CG2	1:B:73:LEU:HD22	2.43	0.49
1:A:448:LEU:HD11	1:A:463:ILE:HG23	1.93	0.48
1:B:379:CYS:O	1:B:380:LEU:C	2.50	0.48
1:B:378:ILE:CD1	1:B:516:PRO:HD2	2.42	0.48
1:A:454:VAL:HG22	1:A:528:LEU:HD21	1.96	0.48
1:B:415:LEU:CD2	1:B:471:TYR:CD2	2.97	0.48
1:A:355:TYR:CD1	1:A:404:PHE:CB	2.96	0.48
1:A:413:VAL:O	1:A:414:ALA:HB2	2.13	0.48
1:A:517:GLU:OE1	1:A:517:GLU:N	2.46	0.48
1:B:380:LEU:O	1:B:383:GLN:HB2	2.13	0.48
1:A:361:MET:HB2	1:A:384:VAL:CG2	2.42	0.48
1:B:12:VAL:HG11	1:B:176:LEU:HB3	1.94	0.48
1:A:179:TYR:OH	1:A:184:GLY:HA2	2.13	0.48
1:B:189:LYS:HB3	1:B:190:PRO:CD	2.35	0.48
1:A:416:ILE:HA	1:A:419:TRP:CE2	2.49	0.48
1:B:81:ARG:HB2	6:B:1816:HOH:O	2.14	0.48
1:A:503:VAL:HA	1:A:504:PRO:HD3	1.68	0.48
1:B:227:PHE:O	1:B:228:CYS:O	2.31	0.48
1:B:172:MET:HG2	1:B:209:ILE:HD12	1.96	0.48
1:B:369:ARG:NH1	1:B:393:VAL:CG2	2.77	0.48
1:B:493:GLY:O	1:B:494:ASP:OD1	2.32	0.48
1:A:298:TYR:O	1:A:300:GLU:N	2.47	0.48
1:A:415:LEU:HD21	1:A:471:TYR:CE2	2.49	0.48
1:A:403:GLU:HB2	1:A:471:TYR:CD2	2.48	0.48
1:A:494:ASP:C	1:A:496:GLN:H	2.17	0.48
1:B:97:SER:O	1:B:101:ARG:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:TYR:HB3	1:A:509:PHE:CD1	2.49	0.47
1:B:492:SER:HB2	1:B:499:GLU:OE2	2.14	0.47
1:A:355:TYR:HD1	1:A:404:PHE:CD2	2.32	0.47
1:A:347:ILE:HD13	1:A:368:ALA:HB2	1.92	0.47
1:A:420:ARG:CG	1:A:421:ASP:N	2.77	0.47
1:B:211:ARG:NE	5:B:1601:MPD:H53	2.29	0.47
1:B:294:MET:CE	1:B:309:ILE:HG13	2.44	0.47
1:B:172:MET:HG2	1:B:209:ILE:CD1	2.44	0.47
1:B:506:HIS:CE1	1:B:507:PRO:HD2	2.49	0.47
1:B:301:LEU:HD11	1:B:303:ASP:HB2	1.97	0.47
1:A:506:HIS:CD2	1:A:507:PRO:HD2	2.50	0.47
1:B:441:LEU:HA	1:B:467:HIS:O	2.14	0.47
1:B:378:ILE:HD13	1:B:516:PRO:CD	2.44	0.47
1:A:163:GLU:HG2	4:A:803:IOD:I	2.85	0.47
1:A:25:LEU:HD22	1:A:172:MET:HE1	1.97	0.47
1:A:272:ASN:ND2	1:A:274:SER:H	2.13	0.47
1:A:495:ASP:HB3	1:A:497:LEU:HD12	1.94	0.47
1:A:221:ARG:O	1:A:224:ILE:N	2.48	0.47
1:A:369:ARG:HH21	1:A:388:ASP:CG	2.18	0.47
1:A:44:TYR:CE1	1:A:52:MET:CE	2.97	0.47
1:A:67:ALA:HB2	1:A:86:ARG:CB	2.45	0.47
1:B:151:LEU:HB2	1:B:152:PRO:CD	2.45	0.47
1:B:277:GLU:H	1:B:277:GLU:HG2	1.62	0.47
1:A:285:ASN:O	1:A:320:ARG:NH1	2.47	0.47
1:A:106:GLY:O	1:A:109:LEU:HD23	2.15	0.47
1:B:229:ASN:C	1:B:230:VAL:HG23	2.35	0.47
1:B:515:HIS:HB3	1:B:517:GLU:CD	2.35	0.47
1:B:54:PRO:HA	1:B:58:GLY:O	2.14	0.47
1:A:151:LEU:N	1:A:152:PRO:CD	2.78	0.47
1:A:297:LYS:HG2	6:A:1048:HOH:O	2.15	0.47
1:A:444:GLN:HB2	1:A:467:HIS:CE1	2.50	0.47
1:B:355:TYR:CB	1:B:404:PHE:HD2	2.25	0.47
1:A:372:ASN:ND2	1:A:506:HIS:CD2	2.82	0.46
1:B:13:VAL:HG23	1:B:16:LEU:HG	1.97	0.46
1:A:302:PRO:O	1:A:304:ALA:N	2.48	0.46
1:A:341:LEU:CD1	1:A:364:THR:HG23	2.45	0.46
1:A:46:ASN:HB2	1:A:52:MET:CE	2.35	0.46
1:B:289:GLU:HG3	1:B:324:ASN:ND2	2.29	0.46
1:B:379:CYS:HB3	1:B:380:LEU:H	1.43	0.46
1:B:493:GLY:HA2	1:B:496:GLN:CD	2.33	0.46
1:B:426:VAL:HG13	1:B:427:GLU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:PHE:O	1:B:229:ASN:ND2	2.48	0.46
1:B:42:ASP:O	1:B:91:THR:HA	2.15	0.46
1:A:294:MET:CE	1:A:308:VAL:HG11	2.44	0.46
1:A:207:ILE:HA	1:A:234:ALA:HB1	1.96	0.46
1:A:55:ILE:N	1:A:55:ILE:CD1	2.79	0.46
1:B:296:GLY:O	1:B:329:ASP:HA	2.16	0.46
1:B:402:THR:CG2	1:B:414:ALA:HB2	2.42	0.46
1:B:396:MET:HE1	1:B:480:GLN:CG	2.45	0.46
1:B:503:VAL:HG12	1:B:503:VAL:O	2.13	0.46
1:B:93:GLY:O	1:B:97:SER:HB2	2.15	0.46
1:A:13:VAL:HG23	1:A:16:LEU:HD21	1.97	0.46
1:A:313:LYS:HZ3	1:A:313:LYS:HB3	1.81	0.46
1:A:396:MET:O	1:A:397:GLU:C	2.53	0.46
1:A:543:GLN:O	1:A:544:ALA:HB2	2.16	0.46
1:A:40:LYS:HB3	1:A:89:ASN:HD22	1.81	0.46
1:B:230:VAL:O	1:B:230:VAL:HG12	2.16	0.46
1:B:106:GLY:O	1:B:109:LEU:N	2.35	0.46
1:B:224:ILE:CA	1:B:229:ASN:HD22	2.28	0.46
1:B:495:ASP:HB3	1:B:497:LEU:HG	1.98	0.46
1:A:537:SER:O	1:A:541:LYS:HG3	2.16	0.45
1:B:9:THR:O	1:B:173:HIS:HA	2.16	0.45
1:B:86:ARG:HA	1:B:86:ARG:HD3	1.68	0.45
1:A:18:LYS:HE2	1:A:140:GLU:HG2	1.98	0.45
1:A:300:GLU:O	1:A:302:PRO:HD3	2.16	0.45
1:A:362:ILE:HA	1:A:384:VAL:HG13	1.97	0.45
1:A:409:LYS:H	1:A:420:ARG:NH2	2.13	0.45
1:A:458:TYR:O	1:A:459:ASN:C	2.52	0.45
1:B:355:TYR:HA	1:B:404:PHE:CD2	2.51	0.45
1:A:382:MET:CE	1:A:500:ILE:HA	2.46	0.45
1:B:78:ARG:NH1	1:B:307:SER:OG	2.48	0.45
1:B:488:VAL:CG1	1:B:491:ARG:NH2	2.79	0.45
1:A:272:ASN:ND2	1:A:274:SER:OG	2.36	0.45
1:A:340:ILE:HG12	1:A:341:LEU:N	2.31	0.45
1:A:537:SER:O	1:A:540:GLN:HB3	2.16	0.45
1:B:45:ILE:O	1:B:46:ASN:C	2.51	0.45
1:A:189:LYS:N	1:A:190:PRO:CD	2.79	0.45
1:A:272:ASN:ND2	1:A:272:ASN:C	2.70	0.45
1:A:382:MET:HE3	1:A:511:ALA:O	2.16	0.45
1:A:414:ALA:HB1	1:A:418:GLU:OE1	2.17	0.45
1:B:189:LYS:N	1:B:190:PRO:CD	2.80	0.45
1:A:301:LEU:HD21	1:A:303:ASP:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:VAL:N	1:A:231:PRO:CD	2.80	0.45
1:A:75:HIS:O	1:A:76:TYR:C	2.53	0.45
1:A:86:ARG:HH22	1:A:87:ARG:HH11	1.64	0.45
1:B:163:GLU:HG2	4:B:804:IOD:I	2.87	0.45
1:B:252:LYS:HE3	1:B:271:ALA:HB3	1.97	0.45
1:A:359:GLU:HA	1:A:362:ILE:HD12	1.98	0.45
1:A:506:HIS:ND1	1:A:507:PRO:HD2	2.32	0.45
1:A:390:ALA:CB	1:A:481:ILE:HD13	2.47	0.45
1:B:341:LEU:HB2	1:B:367:PHE:CE2	2.52	0.45
1:B:216:VAL:HA	1:B:217:PRO:HD3	1.74	0.45
1:B:355:TYR:CD1	1:B:404:PHE:HB3	2.50	0.45
1:A:420:ARG:CG	1:A:421:ASP:H	2.28	0.44
1:B:244:ILE:HG23	6:B:1763:HOH:O	2.17	0.44
1:B:338:VAL:HG13	1:B:338:VAL:O	2.17	0.44
1:B:421:ASP:N	1:B:476:MET:CE	2.80	0.44
1:B:103:GLU:OE1	1:B:104:ARG:HG2	2.17	0.44
1:B:69:THR:HG23	1:B:70:ASP:N	2.33	0.44
1:A:181:ALA:O	1:A:182:ALA:O	2.34	0.44
1:A:86:ARG:CG	1:A:86:ARG:NH1	2.80	0.44
1:B:167:GLU:HB2	6:B:1789:HOH:O	2.17	0.44
1:B:421:ASP:CB	1:B:425:ASN:N	2.80	0.44
1:B:426:VAL:HG13	1:B:427:GLU:N	2.33	0.44
1:B:494:ASP:CG	1:B:495:ASP:N	2.70	0.44
1:B:506:HIS:ND1	1:B:507:PRO:CD	2.78	0.44
1:A:415:LEU:HG	1:A:418:GLU:CD	2.37	0.44
1:A:302:PRO:C	1:A:304:ALA:N	2.71	0.44
1:B:179:TYR:C	1:B:179:TYR:CD2	2.90	0.44
1:B:228:CYS:HB2	6:B:1722:HOH:O	2.17	0.44
1:A:400:ASN:O	1:A:411:PRO:HA	2.18	0.44
1:A:414:ALA:HA	1:A:471:TYR:HD2	1.83	0.44
1:B:366:ARG:HB2	1:B:388:ASP:OD2	2.18	0.44
1:B:478:LEU:O	1:B:481:ILE:N	2.50	0.44
1:A:219:ASN:HB2	6:A:942:HOH:O	2.16	0.44
1:A:415:LEU:HD21	1:A:471:TYR:CZ	2.53	0.44
1:A:382:MET:HA	1:A:511:ALA:HB1	1.98	0.44
1:B:118:HIS:N	1:B:118:HIS:ND1	2.56	0.44
1:B:267:ASN:O	1:B:268:CYS:HB3	2.17	0.44
1:A:239:LYS:HD3	4:A:801:IOD:I	2.88	0.44
1:A:494:ASP:C	1:A:496:GLN:N	2.71	0.44
1:B:396:MET:CA	1:B:410:TYR:CD1	2.96	0.44
1:B:341:LEU:O	1:B:344:LEU:CG	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASN:C	1:A:231:PRO:HD3	2.38	0.43
1:A:540:GLN:OE1	1:A:541:LYS:HG2	2.17	0.43
1:B:301:LEU:HD12	1:B:303:ASP:H	1.83	0.43
5:A:601:MPD:O2	5:A:601:MPD:O4	2.30	0.43
1:B:1:MET:HG3	1:B:135:ASP:OD1	2.18	0.43
1:B:224:ILE:CG2	1:B:229:ASN:ND2	2.79	0.43
1:A:1:MET:HE1	1:A:135:ASP:N	2.33	0.43
1:A:208:LEU:HD12	1:A:231:PRO:HG2	1.99	0.43
1:A:296:GLY:C	1:A:299:ILE:HG12	2.39	0.43
1:B:171:PHE:N	1:B:206:ASP:OD2	2.50	0.43
1:B:294:MET:HB3	1:B:327:LEU:HD22	1.99	0.43
1:B:545:LYS:HB3	6:B:1809:HOH:O	2.19	0.43
1:A:303:ASP:N	1:A:303:ASP:OD2	2.52	0.43
1:A:302:PRO:C	1:A:304:ALA:H	2.21	0.43
1:A:349:VAL:HG12	1:A:381:GLY:HA3	1.95	0.43
1:A:49:PRO:C	1:A:51:THR:H	2.22	0.43
1:B:276:TRP:O	1:B:280:ILE:HG13	2.18	0.43
1:B:468:ARG:CG	1:B:468:ARG:NH1	2.77	0.43
1:B:487:ARG:HG3	6:B:1855:HOH:O	2.18	0.43
1:B:61:PHE:HB3	1:B:69:THR:HG22	1.99	0.43
1:B:86:ARG:O	1:B:86:ARG:HD3	2.17	0.43
1:A:335:THR:HG22	1:A:336:ARG:N	2.33	0.43
1:B:386:LEU:HD12	1:B:386:LEU:HA	1.81	0.43
1:B:378:ILE:HD12	1:B:516:PRO:HD2	1.99	0.43
1:A:345:ASP:HA	1:A:539:PHE:HD2	1.78	0.43
1:A:378:ILE:HG23	1:A:514:PHE:O	2.18	0.43
1:A:362:ILE:HG12	1:A:387:ILE:HG21	2.00	0.43
1:B:189:LYS:O	1:B:192:GLN:HB2	2.19	0.43
1:B:397:GLU:N	1:B:410:TYR:CD1	2.87	0.43
1:B:398:ASN:O	1:B:399:ALA:C	2.56	0.43
1:A:402:THR:CG2	1:A:414:ALA:CB	2.97	0.43
1:B:325:ILE:HG22	1:B:327:LEU:HD21	2.00	0.43
1:B:382:MET:HE3	1:B:512:CYS:CA	2.48	0.43
1:B:420:ARG:HG3	1:B:421:ASP:O	2.19	0.43
1:B:102:LYS:HB3	1:B:108:TYR:HE1	1.84	0.43
1:B:113:VAL:HG13	1:B:118:HIS:CG	2.54	0.43
1:B:396:MET:HA	1:B:410:TYR:CE1	2.54	0.43
1:B:421:ASP:N	1:B:425:ASN:O	2.50	0.43
1:A:166:ARG:HB2	1:A:263:ARG:NH2	2.34	0.43
1:A:2:THR:HG21	1:A:168:HIS:NE2	2.34	0.43
1:A:25:LEU:HD22	1:A:172:MET:CE	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:PRO:HD2	1:A:187:LYS:O	2.18	0.42
1:A:179:TYR:CG	1:A:214:ARG:CZ	3.02	0.42
1:A:390:ALA:HA	1:A:481:ILE:HG23	2.01	0.42
1:A:471:TYR:C	1:A:472:GLU:HG2	2.40	0.42
1:B:148:ILE:HG13	1:B:149:GLU:OE1	2.19	0.42
1:B:86:ARG:HH12	1:B:89:ASN:CB	2.30	0.42
1:A:216:VAL:HG12	1:A:221:ARG:CG	2.47	0.42
1:A:408:CYS:SG	1:A:411:PRO:CB	3.07	0.42
1:B:379:CYS:O	1:B:382:MET:N	2.46	0.42
1:B:454:VAL:HG12	1:B:528:LEU:HD21	2.00	0.42
1:A:207:ILE:HG12	1:A:234:ALA:HB1	2.00	0.42
1:A:421:ASP:OD2	1:A:425:ASN:N	2.47	0.42
1:B:209:ILE:HG13	1:B:236:ILE:HB	2.00	0.42
1:B:230:VAL:N	1:B:231:PRO:CD	2.82	0.42
1:B:388:ASP:O	1:B:392:HIS:N	2.53	0.42
1:A:386:LEU:HA	1:A:386:LEU:HD12	1.82	0.42
1:B:389:TYR:HD2	1:B:481:ILE:HG22	1.85	0.42
1:B:466:ARG:HG3	4:B:815:IOD:I	2.90	0.42
1:B:94:ARG:NH1	1:B:97:SER:HB3	2.33	0.42
1:A:217:PRO:O	1:A:219:ASN:N	2.52	0.42
1:A:487:ARG:O	1:A:501:ILE:HA	2.20	0.42
1:B:101:ARG:O	1:B:102:LYS:C	2.58	0.42
1:A:335:THR:CG2	1:A:336:ARG:HG3	2.26	0.42
1:B:295:VAL:HG22	1:B:328:ILE:CG2	2.50	0.42
1:B:49:PRO:C	1:B:51:THR:H	2.23	0.42
1:A:177:VAL:CG1	1:A:186:VAL:CG2	2.98	0.42
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.62	0.42
1:B:144:THR:O	1:B:145:VAL:C	2.57	0.42
1:B:179:TYR:CD1	1:B:214:ARG:NH1	2.87	0.42
1:B:330:SER:HB3	1:B:361:MET:CG	2.47	0.42
1:A:179:TYR:CE2	1:A:181:ALA:HA	2.55	0.42
1:A:192:GLN:HG2	1:A:228:CYS:HB3	2.01	0.42
1:A:98:ASP:OD2	6:A:934:HOH:O	2.22	0.42
1:B:179:TYR:CG	1:B:214:ARG:CZ	3.03	0.42
1:B:515:HIS:HA	1:B:516:PRO:HD2	1.90	0.42
1:B:528:LEU:HA	1:B:528:LEU:HD23	1.69	0.42
1:A:483:ASP:C	1:A:485:GLY:H	2.24	0.42
1:B:390:ALA:C	1:B:396:MET:HB2	2.41	0.42
1:B:474:ASN:OD1	1:B:476:MET:HB2	2.20	0.42
1:A:420:ARG:O	1:A:476:MET:SD	2.78	0.42
1:A:446:CYS:SG	1:A:447:GLN:N	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:TYR:N	1:A:76:TYR:CD2	2.86	0.42
1:B:268:CYS:CB	1:B:269:PRO:CD	2.96	0.42
1:B:24:SER:O	1:B:28:ILE:HG13	2.19	0.42
1:B:378:ILE:HD13	1:B:516:PRO:CG	2.49	0.42
1:A:241:VAL:HG11	1:A:250:LEU:CD1	2.50	0.41
1:A:371:ASN:CB	1:A:373:ILE:HD12	2.47	0.41
1:A:37:THR:HB	1:A:134:HIS:CE1	2.54	0.41
1:B:441:LEU:HD21	1:B:468:ARG:HD2	2.02	0.41
1:B:458:TYR:CE1	1:B:528:LEU:HG	2.55	0.41
1:B:91:THR:HG23	6:B:1759:HOH:O	2.20	0.41
1:A:366:ARG:NH1	6:A:890:HOH:O	2.52	0.41
1:A:411:PRO:HG3	1:A:420:ARG:NH2	2.35	0.41
1:A:457:LEU:HD23	1:A:457:LEU:HA	1.78	0.41
1:B:151:LEU:CB	1:B:152:PRO:CD	2.98	0.41
1:B:301:LEU:CD1	1:B:302:PRO:HD2	2.46	0.41
1:B:389:TYR:O	1:B:390:ALA:C	2.58	0.41
1:A:320:ARG:HH11	1:A:320:ARG:HD2	1.73	0.41
1:B:172:MET:HG3	1:B:207:ILE:HB	2.02	0.41
1:B:290:VAL:HG22	1:B:321:VAL:HG11	2.02	0.41
1:B:348:LEU:HA	1:B:376:LEU:O	2.21	0.41
1:A:262:LYS:HD2	4:A:805:IOD:I	2.90	0.41
1:B:488:VAL:CG1	1:B:491:ARG:CZ	2.99	0.41
1:A:297:LYS:HZ1	1:A:354:GLY:HA3	1.86	0.41
1:B:226:LEU:O	1:B:228:CYS:N	2.53	0.41
1:B:297:LYS:HZ3	1:B:354:GLY:HA3	1.84	0.41
1:B:360:GLY:O	1:B:363:THR:HB	2.21	0.41
1:A:241:VAL:CG1	1:A:250:LEU:HD11	2.51	0.41
1:A:354:GLY:O	1:A:356:ARG:N	2.53	0.41
1:A:454:VAL:HG11	1:A:500:ILE:HD13	2.03	0.41
1:A:455:ARG:HD3	1:A:455:ARG:O	2.20	0.41
1:B:368:ALA:HB1	1:B:375:TYR:HB2	2.01	0.41
1:B:390:ALA:HB1	1:B:396:MET:CB	2.51	0.41
1:A:439:MET:HE3	1:A:469:HIS:C	2.40	0.41
1:A:542:ARG:HD3	1:A:542:ARG:HH11	1.74	0.41
1:B:192:GLN:HG2	6:B:1722:HOH:O	2.20	0.41
1:A:297:LYS:C	1:A:299:ILE:H	2.23	0.41
1:A:341:LEU:HD11	1:A:364:THR:HG23	2.02	0.41
1:B:421:ASP:HB2	1:B:425:ASN:HB2	2.03	0.41
1:B:415:LEU:CD2	1:B:471:TYR:CG	3.03	0.41
1:A:116:ILE:CD1	1:A:155:GLU:HG2	2.50	0.41
1:A:415:LEU:HD23	1:A:415:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ALA:HB2	1:A:481:ILE:HD12	2.03	0.41
1:A:491:ARG:HA	1:A:497:LEU:O	2.21	0.41
1:A:39:MET:HE1	1:A:130:GLY:CA	2.51	0.41
1:A:1:MET:HE1	1:A:134:HIS:C	2.41	0.41
1:A:402:THR:HG23	1:A:402:THR:H	1.61	0.41
1:A:80:ILE:HD12	1:A:82:THR:HB	2.02	0.41
1:B:195:VAL:HG11	1:B:229:ASN:HA	2.02	0.41
1:B:172:MET:SD	1:B:209:ILE:HD11	2.61	0.41
1:B:220:GLU:O	1:B:223:LYS:HB3	2.21	0.41
1:B:358:VAL:O	1:B:362:ILE:HD12	2.21	0.41
1:A:2:THR:HG21	1:A:168:HIS:CD2	2.56	0.40
1:A:334:GLU:HG3	1:A:360:GLY:CA	2.51	0.40
1:A:406:PRO:O	1:A:420:ARG:NH1	2.27	0.40
1:A:54:PRO:C	1:A:58:GLY:N	2.74	0.40
1:B:116:ILE:HA	1:B:117:PRO:HA	1.83	0.40
1:B:402:THR:CG2	1:B:414:ALA:CB	2.99	0.40
1:B:515:HIS:HB3	1:B:517:GLU:OE1	2.22	0.40
1:B:239:LYS:HB3	4:B:802:IOD:I	2.92	0.40
1:A:224:ILE:CG2	1:A:229:ASN:HD22	2.29	0.40
1:A:460:ALA:HB1	1:A:461:PRO:CD	2.48	0.40
1:A:86:ARG:CA	1:A:86:ARG:NH1	2.75	0.40
1:B:220:GLU:CD	1:B:220:GLU:N	2.75	0.40
1:B:172:MET:SD	1:B:209:ILE:CD1	3.10	0.40
1:B:334:GLU:H	1:B:334:GLU:HG3	1.50	0.40
1:B:348:LEU:C	1:B:348:LEU:HD23	2.42	0.40
1:B:415:LEU:HD23	1:B:471:TYR:CG	2.56	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	531/545 (97%)	469 (88%)	45 (8%)	17 (3%)	4	2
1	B	532/545 (98%)	467 (88%)	41 (8%)	24 (4%)	2	1
All	All	1063/1090 (98%)	936 (88%)	86 (8%)	41 (4%)	3	1

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	ALA
1	A	230	VAL
1	A	232	GLU
1	A	338	VAL
1	A	356	ARG
1	A	391	ARG
1	A	392	HIS
1	A	411	PRO
1	B	105	ARG
1	B	107	ASP
1	B	151	LEU
1	B	355	TYR
1	B	356	ARG
1	B	396	MET
1	B	494	ASP
1	A	299	ILE
1	A	300	GLU
1	A	387	ILE
1	A	543	GLN
1	B	103	GLU
1	B	104	ARG
1	B	227	PHE
1	B	229	ASN
1	B	331	GLN
1	B	387	ILE
1	B	388	ASP
1	B	391	ARG
1	B	397	GLU
1	B	399	ALA
1	B	493	GLY
1	A	132	GLU
1	A	218	ALA
1	A	355	TYR
1	B	132	GLU
1	B	332	ASP

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Mol	Chain	Res	Type
1	B	338	VAL
1	B	335	THR
1	B	496	GLN
1	A	50	GLY
1	A	303	ASP
1	B	230	VAL

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	453/461 (98%)	404 (89%)	49 (11%)	6	7
1	B	454/461 (98%)	387 (85%)	67 (15%)	3	3
All	All	907/922 (98%)	791 (87%)	116 (13%)	4	4

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	46	ASN
1	A	55	ILE
1	A	71	LEU
1	A	86	ARG
1	A	101	ARG
1	A	166	ARG
1	A	180	MET
1	A	196	LYS
1	A	220	GLU
1	A	226	LEU
1	A	233	LYS
1	A	257	ASP
1	A	263	ARG
1	A	268	CYS
1	A	272	ASN
1	A	278	GLN

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Mol	Chain	Res	Type
1	A	288	SER
1	A	289	GLU
1	A	297	LYS
1	A	320	ARG
1	A	336	ARG
1	A	340	ILE
1	A	369	ARG
1	A	372	ASN
1	A	379	CYS
1	A	388	ASP
1	A	396	MET
1	A	398	ASN
1	A	404	PHE
1	A	412	VAL
1	A	415	LEU
1	A	416	ILE
1	A	426	VAL
1	A	427	GLU
1	A	438	THR
1	A	446	CYS
1	A	447	GLN
1	A	450	ASP
1	A	451	ASP
1	A	454	VAL
1	A	455	ARG
1	A	470	ARG
1	A	479	LYS
1	A	480	GLN
1	A	481	ILE
1	A	486	LEU
1	A	496	GLN
1	A	521	THR
1	B	1	MET
1	B	20	ILE
1	B	46	ASN
1	B	48	ASP
1	B	52	MET
1	B	55	ILE
1	B	59	GLU
1	B	69	THR
1	B	86	ARG
1	B	94	ARG

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Mol	Chain	Res	Type
1	B	104	ARG
1	B	105	ARG
1	B	107	ASP
1	B	132	GLU
1	B	144	THR
1	B	166	ARG
1	B	178	PRO
1	B	180	MET
1	B	183	SER
1	B	186	VAL
1	B	200	SER
1	B	211	ARG
1	B	213	ASP
1	B	214	ARG
1	B	220	GLU
1	B	226	LEU
1	B	227	PHE
1	B	228	CYS
1	B	233	LYS
1	B	239	LYS
1	B	243	SER
1	B	262	LYS
1	B	265	SER
1	B	277	GLU
1	B	288	SER
1	B	301	LEU
1	B	306	LYS
1	B	307	SER
1	B	327	LEU
1	B	330	SER
1	B	332	ASP
1	B	334	GLU
1	B	338	VAL
1	B	340	ILE
1	B	356	ARG
1	B	362	ILE
1	B	366	ARG
1	B	378	ILE
1	B	379	CYS
1	B	384	VAL
1	B	388	ASP
1	B	392	HIS

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Mol	Chain	Res	Type
1	B	396	MET
1	B	400	ASN
1	B	417	THR
1	B	428	VAL
1	B	438	THR
1	B	446	CYS
1	B	447	GLN
1	B	451	ASP
1	B	468	ARG
1	B	469	HIS
1	B	470	ARG
1	B	481	ILE
1	B	487	ARG
1	B	495	ASP
1	B	496	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	75	HIS
1	A	134	HIS
1	A	229	ASN
1	A	272	ASN
1	A	285	ASN
1	A	372	ASN
1	A	383	GLN
1	A	425	ASN
1	A	447	GLN
1	A	469	HIS
1	A	513	GLN
1	B	46	ASN
1	B	75	HIS
1	B	118	HIS
1	B	134	HIS
1	B	192	GLN
1	B	193	HIS
1	B	204	GLN
1	B	229	ASN
1	B	272	ASN
1	B	324	ASN
1	B	371	ASN

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Mol	Chain	Res	Type
1	B	392	HIS
1	B	447	GLN
1	B	469	HIS
1	B	480	GLN
1	B	496	GLN
1	B	543	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 20 are monoatomic - leaving 6 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	$\# Z > 2$
5	MPD	A	601	-	7,7,7	0.65	0	9,10,10	0.70	0
2	SO4	A	602	3	4,4,4	0.40	0	6,6,6	0.07	0
2	SO4	A	603	3	4,4,4	0.31	0	6,6,6	0.08	0
5	MPD	B	1601	-	7,7,7	0.57	0	9,10,10	0.43	0
2	SO4	B	1603	3	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	B	1602	3	4,4,4	0.26	0	6,6,6	0.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	A	601	-	-	0/5/5/5	-
5	MPD	B	1601	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1601	MPD	O2-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	MPD	2	0
5	B	1601	MPD	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	57:HIS	C	58:GLY	N	1.79

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	534/545 (97%)	1.39	130 (24%) 0 0	31, 55, 93, 100	1 (0%)
1	B	536/545 (98%)	1.38	129 (24%) 0 0	32, 54, 93, 100	1 (0%)
All	All	1070/1090 (98%)	1.39	259 (24%) 0 0	31, 54, 93, 100	2 (0%)

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	493	GLY	9.9
1	B	544	ALA	8.2
1	A	228	CYS	8.0
1	A	227	PHE	7.7
1	B	493	GLY	7.3
1	B	395	ASN	7.3
1	A	1	MET	7.2
1	B	218	ALA	7.2
1	B	494	ASP	7.0
1	B	545	LYS	6.8
1	B	228	CYS	6.5
1	A	218	ALA	6.5
1	B	184	GLY	6.4
1	B	219	ASN	6.3
1	A	180	MET	6.2
1	A	544	ALA	6.2
1	B	335	THR	6.1
1	A	390	ALA	6.1
1	A	335	THR	5.9
1	B	101	ARG	5.8
1	B	181	ALA	5.7
1	B	1	MET	5.5
1	B	180	MET	5.5
1	A	355	TYR	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	179	TYR	5.4
1	A	494	ASP	5.3
1	B	408	CYS	5.2
1	A	219	ASN	5.2
1	A	405	VAL	5.1
1	B	405	VAL	4.9
1	A	543	GLN	4.9
1	A	425	ASN	4.8
1	B	182	ALA	4.7
1	B	425	ASN	4.7
1	B	421	ASP	4.7
1	A	2	THR	4.7
1	A	362	ILE	4.6
1	B	360	GLY	4.5
1	A	339	GLU	4.5
1	A	226	LEU	4.4
1	B	355	TYR	4.4
1	A	504	PRO	4.4
1	A	334	GLU	4.3
1	A	496	GLN	4.3
1	A	300	GLU	4.3
1	A	407	ASP	4.3
1	A	366	ARG	4.2
1	A	397	GLU	4.2
1	B	336	ARG	4.2
1	B	410	TYR	4.2
1	A	181	ALA	4.2
1	B	334	GLU	4.1
1	A	57[A]	HIS	4.1
1	A	423	ASN	4.1
1	B	227	PHE	4.1
1	B	179	TYR	4.1
1	B	485	GLY	4.1
1	A	331	GLN	4.0
1	B	105	ARG	4.0
1	B	183	SER	4.0
1	A	337	GLY	4.0
1	A	360	GLY	4.0
1	A	386	LEU	3.9
1	A	395	ASN	3.9
1	B	300	GLU	3.9
1	B	333	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	106	GLY	3.8
1	B	339	GLU	3.8
1	A	408	CYS	3.8
1	A	217	PRO	3.8
1	B	481	ILE	3.7
1	B	226	LEU	3.7
1	B	394	ALA	3.7
1	A	426	VAL	3.7
1	B	185	GLU	3.6
1	A	540	GLN	3.6
1	B	390	ALA	3.6
1	B	504	PRO	3.6
1	A	378	ILE	3.6
1	B	423	ASN	3.6
1	A	505	ASN	3.6
1	A	393	VAL	3.5
1	B	217	PRO	3.5
1	B	419	TRP	3.5
1	A	105	ARG	3.4
1	B	396	MET	3.4
1	B	492	SER	3.4
1	A	404	PHE	3.4
1	A	333	VAL	3.4
1	B	424	GLY	3.3
1	A	141	ILE	3.3
1	A	541	LYS	3.2
1	A	368	ALA	3.2
1	B	172	MET	3.2
1	A	410	TYR	3.2
1	B	198	LEU	3.2
1	A	495	ASP	3.2
1	B	98	ASP	3.2
1	B	363	THR	3.1
1	B	438	THR	3.1
1	B	426	VAL	3.1
1	B	407	ASP	3.1
1	B	354	GLY	3.1
1	A	481	ILE	3.1
1	B	104	ARG	3.0
1	B	38	ILE	3.0
1	B	267	ASN	3.0
1	A	332	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	483	ASP	3.0
1	A	417	THR	3.0
1	A	424	GLY	3.0
1	A	438	THR	3.0
1	B	409	LYS	2.9
1	A	484	ALA	2.9
1	B	340	ILE	2.9
1	A	198	LEU	2.9
1	B	478	LEU	2.9
1	B	496	GLN	2.9
1	B	138	LEU	2.9
1	A	396	MET	2.9
1	A	312	LEU	2.8
1	B	225	ALA	2.8
1	B	366	ARG	2.8
1	B	76	TYR	2.8
1	A	473	VAL	2.8
1	B	541	LYS	2.8
1	A	225	ALA	2.8
1	A	478	LEU	2.8
1	B	376	LEU	2.8
1	B	337	GLY	2.8
1	B	331	GLN	2.8
1	A	184	GLY	2.8
1	B	261	CYS	2.8
1	A	421	ASP	2.7
1	A	22	ALA	2.7
1	A	101	ARG	2.7
1	A	212	SER	2.7
1	A	452	SER	2.7
1	A	145	VAL	2.7
1	A	539	PHE	2.7
1	A	542	ARG	2.7
1	A	506	HIS	2.7
1	B	115	VAL	2.7
1	A	348	LEU	2.6
1	A	446	CYS	2.6
1	A	336	ARG	2.6
1	B	8	VAL	2.6
1	B	22	ALA	2.6
1	B	404	PHE	2.6
1	B	299	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	41	LEU	2.6
1	A	151	LEU	2.6
1	A	354	GLY	2.6
1	A	8	VAL	2.5
1	B	107	ASP	2.5
1	B	387	ILE	2.5
1	A	419	TRP	2.5
1	B	368	ALA	2.5
1	B	332	ASP	2.5
1	A	138	LEU	2.5
1	B	542	ARG	2.5
1	A	358	VAL	2.5
1	A	361	MET	2.5
1	B	20	ILE	2.5
1	A	376	LEU	2.5
1	B	256	LEU	2.5
1	B	506	HIS	2.5
1	B	306	LYS	2.5
1	B	79	PHE	2.5
1	B	145	VAL	2.5
1	B	21	ALA	2.5
1	B	220	GLU	2.5
1	A	25	LEU	2.5
1	B	233	LYS	2.4
1	A	447	GLN	2.4
1	B	268	CYS	2.4
1	B	329	ASP	2.4
1	B	308	VAL	2.4
1	A	6	ILE	2.4
1	B	452	SER	2.4
1	A	302	PRO	2.4
1	A	357	GLY	2.4
1	B	221	ARG	2.4
1	A	409	LYS	2.4
1	B	378	ILE	2.4
1	B	414	ALA	2.4
1	A	182	ALA	2.4
1	A	391	ARG	2.4
1	B	174	LEU	2.4
1	B	312	LEU	2.4
1	A	224	ILE	2.3
1	A	73	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	428	VAL	2.3
1	A	154	LEU	2.3
1	A	353	PHE	2.3
1	A	109	LEU	2.3
1	B	386	LEU	2.3
1	B	398	ASN	2.3
1	B	495	ASP	2.3
1	A	372	ASN	2.3
1	B	208	LEU	2.3
1	A	294	MET	2.3
1	A	497	LEU	2.3
1	B	212	SER	2.3
1	B	482	GLU	2.3
1	A	153	PHE	2.3
1	A	388	ASP	2.3
1	A	356	ARG	2.2
1	B	132	GLU	2.2
1	B	229	ASN	2.2
1	A	56	GLN	2.2
1	B	41	LEU	2.2
1	B	73	LEU	2.2
1	B	109	LEU	2.2
1	B	57	HIS	2.2
1	B	451	ASP	2.2
1	A	102	LYS	2.2
1	A	412	VAL	2.2
1	B	230	VAL	2.2
1	A	385	ALA	2.2
1	A	340	ILE	2.2
1	B	163	GLU	2.2
1	A	262	LYS	2.2
1	B	139	VAL	2.2
1	B	529	PHE	2.2
1	B	417	THR	2.2
1	A	387	ILE	2.2
1	A	214	ARG	2.2
1	B	29	LEU	2.2
1	B	251	LEU	2.2
1	B	486	LEU	2.2
1	A	330	SER	2.2
1	B	223	LYS	2.2
1	B	391	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	221	ARG	2.1
1	A	163	GLU	2.1
1	A	383	GLN	2.1
1	B	372	ASN	2.1
1	A	394	ALA	2.1
1	A	479	LYS	2.1
1	A	537	SER	2.1
1	B	403	GLU	2.1
1	A	86	ARG	2.1
1	A	373	ILE	2.1
1	B	505	ASN	2.1
1	A	476	MET	2.1
1	B	171	PHE	2.1
1	A	38	ILE	2.1
1	B	361	MET	2.1
1	A	370	GLU	2.1
1	B	141	ILE	2.1
1	A	20	ILE	2.0
1	A	398	ASN	2.0
1	B	397	GLU	2.0
1	A	351	GLY	2.0
1	A	139	VAL	2.0
1	A	287	VAL	2.0
1	A	9	THR	2.0
1	B	97	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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(\AA^2)	Q<0.9
3	MG	A	703	1/1	0.42	0.43	92,92,92,92	0
4	IOD	A	814	1/1	0.72	0.28	89,89,89,89	1
3	MG	B	704	1/1	0.76	0.42	91,91,91,91	0
5	MPD	A	601	8/8	0.87	0.31	50,80,92,100	0
5	MPD	B	1601	8/8	0.87	0.32	57,79,87,88	0
3	MG	B	701	1/1	0.88	0.19	64,64,64,64	0
4	IOD	A	807	1/1	0.90	0.17	63,63,63,63	1
4	IOD	A	816	1/1	0.93	0.23	90,90,90,90	1
2	SO4	B	1602	5/5	0.93	0.20	54,60,70,89	0
4	IOD	B	810	1/1	0.94	0.13	76,76,76,76	1
4	IOD	B	809	1/1	0.94	0.21	77,77,77,77	1
4	IOD	A	806	1/1	0.94	0.14	72,72,72,72	1
2	SO4	A	603	5/5	0.94	0.20	68,83,90,91	0
4	IOD	A	813	1/1	0.95	0.13	69,69,69,69	1
2	SO4	A	602	5/5	0.95	0.21	65,72,82,88	0
4	IOD	A	805	1/1	0.97	0.10	64,64,64,64	1
2	SO4	B	1603	5/5	0.97	0.19	57,65,92,93	0
4	IOD	B	802	1/1	0.98	0.09	69,69,69,69	0
4	IOD	B	815	1/1	0.98	0.19	76,76,76,76	1
3	MG	A	702	1/1	0.98	0.21	47,47,47,47	0
4	IOD	A	812	1/1	0.98	0.14	72,72,72,72	1
4	IOD	B	811	1/1	0.98	0.25	72,72,72,72	1
4	IOD	A	801	1/1	0.98	0.10	72,72,72,72	0
4	IOD	B	804	1/1	0.99	0.10	73,73,73,73	0
4	IOD	B	808	1/1	0.99	0.12	73,73,73,73	1
4	IOD	A	803	1/1	0.99	0.09	72,72,72,72	0

6.5 Other polymers ⓘ

There are no such residues in this entry.