



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:33 AM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

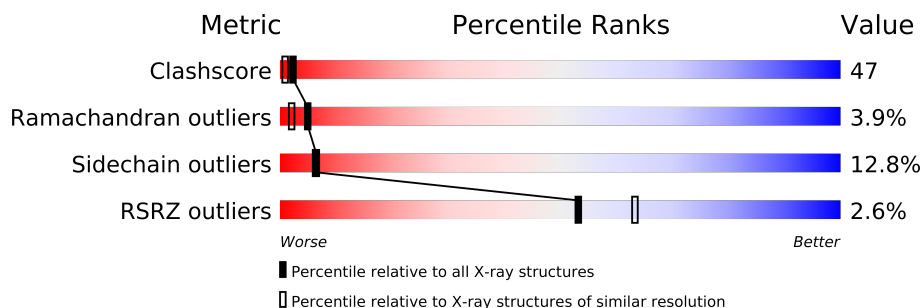
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	545	
1	B	545	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	A	703	-	X
3	MG	B	704	-	X
4	IOD	A	814	-	X
4	IOD	A	816	-	X
4	IOD	B	811	-	X
5	MPD	B	1601	-	X

2 Entry composition i

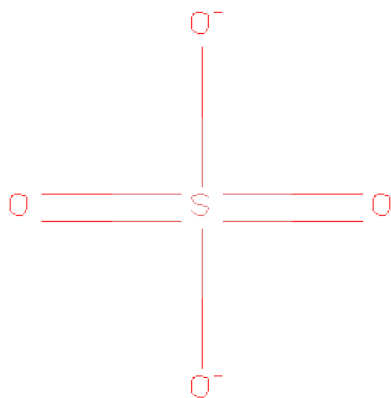
There are 6 unique types of molecules in this entry. The entry contains 8949 atoms, of which 0 are hydrogen and 0 are deuterium.

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		

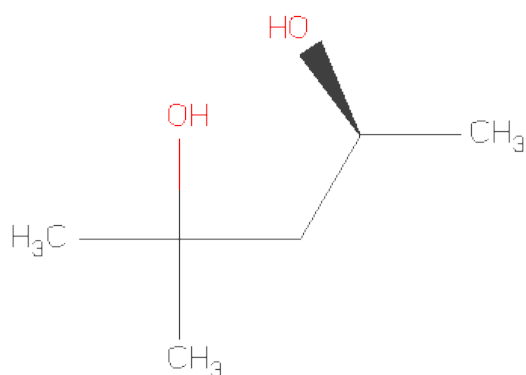
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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.

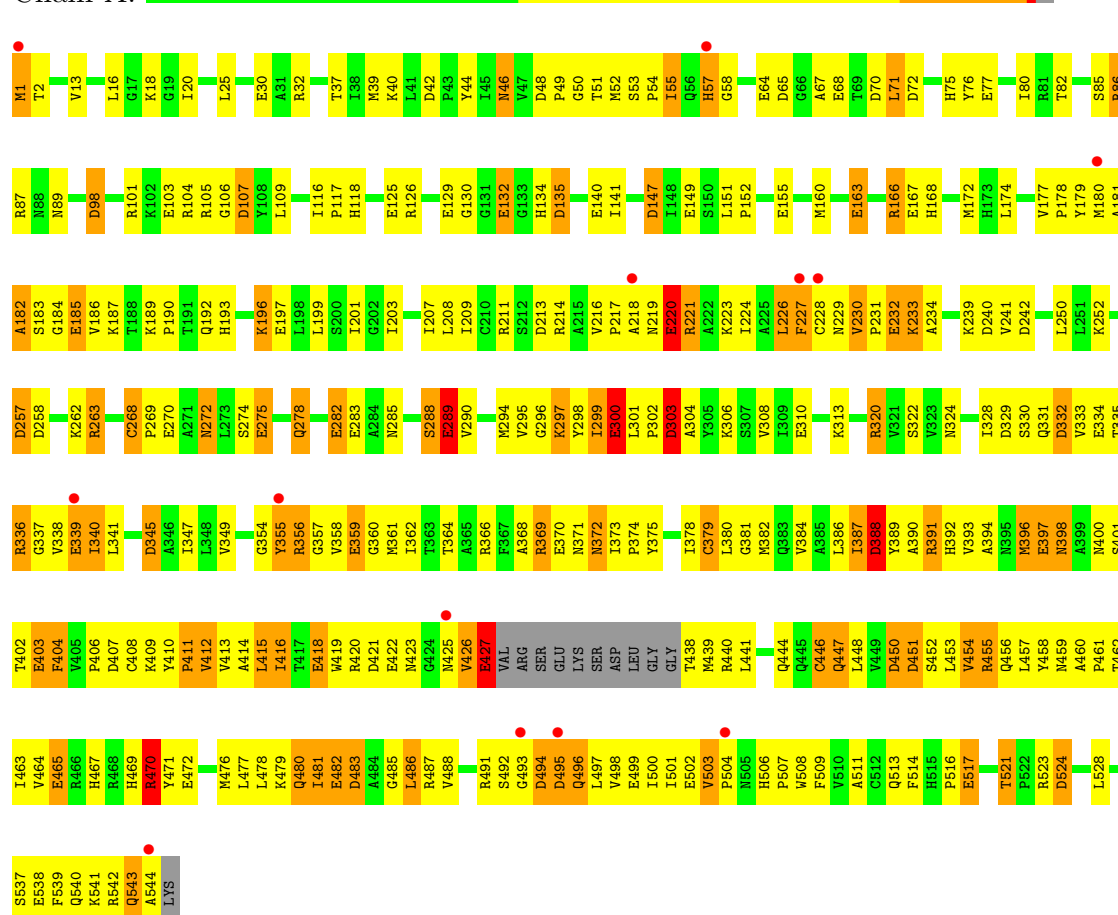
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	268	Total 268	O 268	0	0
6	B	281	Total 281	O 281	0	0

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 errors 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.

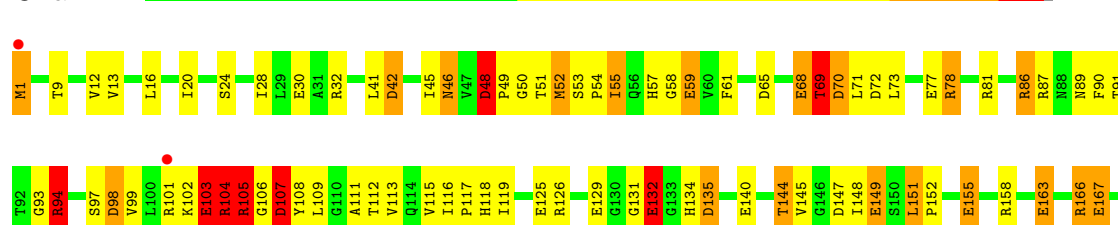
• Molecule 1: CTP synthase

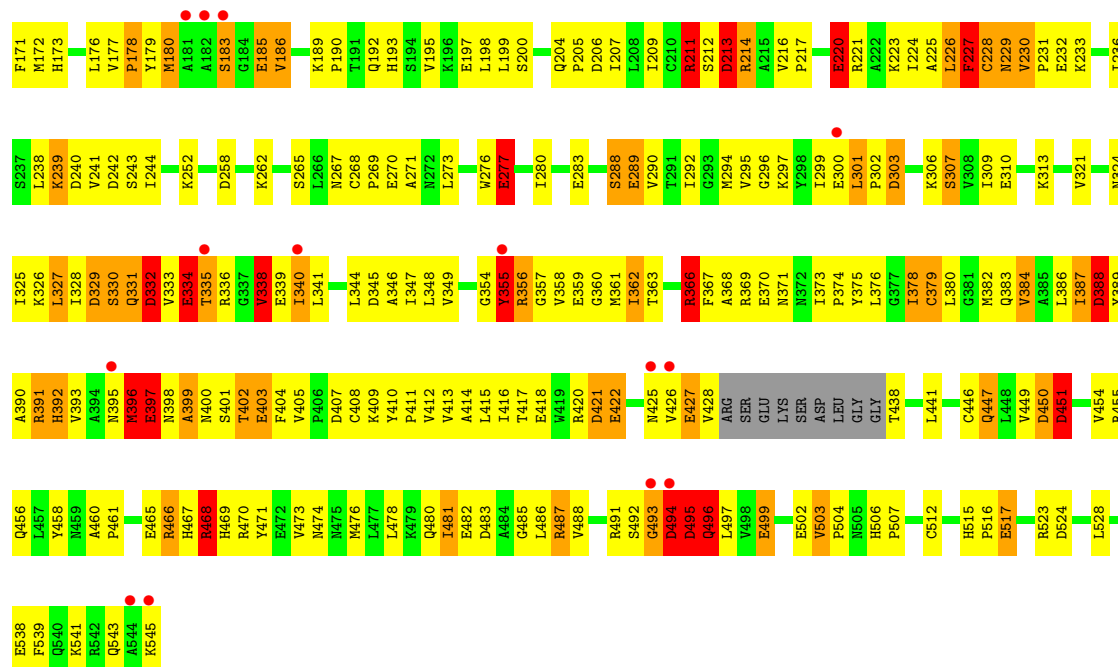
Chain A:



• Molecule 1: CTP synthase

Chain B:





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 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 V. 5-F	Depositor
R, R_{free}	0.214 , 0.281 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 109.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 101775 reflections	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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 47.

All (784) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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:H	1:B:46:ASN:HD22	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:H	1:B:46:ASN:ND2	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:B:396:MET:HA	1:B:410:TYR:CD1	2.15	0.81
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: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
1:B:391:ARG:HG3	1:B:399:ALA:HB3	1.62	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:331:GLN:O	1:B:334:GLU:HG3	1.85	0.75
1:A:86:ARG:CA	1:A:86:ARG:HH11	2.00	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:341:LEU:O	1:B:344:LEU:HG	1.88	0.73
1:B:213:ASP:CB	1:B:214:ARG:HG2	2.18	0.73
1:B:449:VAL:HG21	1:B:488:VAL:O	1.88	0.73
1:A:447:GLN:HG3	1:A:462:THR:HG22	1.71	0.73
1:A:54:PRO:O	1:A:301:LEU:HD23	1.89	0.73
1:A:409:LYS:HD3	1:A:410:TYR:CD1	2.24	0.73
1:A:347:ILE:CD1	1:A:368:ALA:HB2	2.18	0.73
1:A:86:ARG:NH1	1:A:86:ARG:N	2.37	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:213:ASP:CB	1:B:214:ARG:HE	2.03	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:A:332:ASP:HA	1:A:335:THR:HB	1.73	0.71
1:B:414:ALA:HA	1:B:471:TYR:HD2	1.54	0.71
1:A:86:ARG:HH11	1:A:86:ARG:N	1.88	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:B:326:LYS:HE2	1:B:328:ILE:CD1	2.14	0.70
1:A:224:ILE:HG23	1:A:229:ASN:HD22	1.55	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:B:402:THR:HG23	1:B:414:ALA:HB2	1.74	0.69
1:A:427:GLU:HA	1:A:427:GLU:OE1	1.92	0.69
1:A:86:ARG:NH1	1:A:86:ARG:H	1.91	0.69
1:B:108:TYR:CD2	1:B:118:HIS:HD2	2.10	0.69
1:A:290:VAL:O	1:A:324:ASN:HB2	1.93	0.69
1:A:448:LEU:HD11	1:A:463:ILE:HG21	1.73	0.68
1:B:421:ASP:HB3	1:B:425:ASN:H	1.58	0.68
1:A:448:LEU:HD22	1:A:454:VAL:CG1	2.23	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
1:A:86:ARG:HD3	6:A:1016:HOH:O	1.92	0.68
1:A:488:VAL:HG11	1:A:491:ARG:NE	2.08	0.68
1:B:180:MET:HB3	1:B:183:SER:CB	2.23	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:333:VAL:HG11	1:B:360:GLY:O	1.94	0.68
1:B:223:LYS:O	1:B:227:PHE:HB2	1.94	0.68
1:A:460:ALA:HB1	1:A:461:PRO:HD2	1.76	0.68
1:A:521:THR:HG22	1:A:524:ASP:N	1.99	0.67
1:B:224:ILE:HG23	1:B:229:ASN:ND2	2.10	0.67
1:A:382:MET:HE2	1:A:501:ILE:HG23	1.75	0.67
1:B:224:ILE:O	1:B:229:ASN:ND2	2.25	0.67
1:A:412:VAL:HG13	1:A:477:LEU:HB2	1.77	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:B:216:VAL:HG12	1:B:221:ARG:CG	2.24	0.67
1:A:539:PHE:HA	1:A:542:ARG:NH2	2.10	0.67
1:B:108:TYR:CE2	1:B:118:HIS:HD2	2.12	0.66
1:B:220:GLU:OE2	1:B:220:GLU:N	2.29	0.66
1:B:334:GLU:HG2	1:B:360:GLY:N	2.10	0.66
1:B:224:ILE:C	1:B:229:ASN:HD22	1.97	0.66
1:A:49:PRO:HA	1:A:52:MET:HE2	1.77	0.66
1:B:68:GLU:O	1:B:86:ARG:NH2	2.28	0.66
1:A:345:ASP:HA	1:A:539:PHE:CE2	2.30	0.66
1:A:2:THR:HG21	1:A:168:HIS:CE1	2.30	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:N	1:B:46:ASN:ND2	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:355:TYR:HB2	1:B:404:PHE:CD2	2.32	0.65
1:B:107:ASP:N	1:B:107:ASP:OD2	2.30	0.65
1:A:372:ASN:HD22	1:A:506:HIS:CD2	2.15	0.64
1:B:180:MET:HB3	1:B:183:SER:HB3	1.78	0.64
1:B:104:ARG:O	1:B:105:ARG:HB3	1.96	0.64
1:A:278:GLN:NE2	1:A:282:GLU:OE2	2.29	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:224:ILE:O	1:A:229:ASN:HB2	1.96	0.64
1:B:408:CYS:N	1:B:420:ARG:NH2	2.44	0.64
1:A:516:PRO:HD2	1:A:517:GLU:OE1	1.97	0.64
1:A:223:LYS:NZ	6:A:979:HOH:O	2.30	0.64
1:B:468:ARG:NH1	1:B:468:ARG:HG2	2.06	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: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:B:49:PRO:CA	1:B:52:MET:HE3	2.25	0.63
1:A:394:ALA:HB1	1:A:396:MET:HE2	1.80	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:B:421:ASP:N	1:B:476:MET:HE1	2.13	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: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:B:482:GLU:O	1:B:485:GLY:N	2.29	0.62
1:A:189:LYS:HB3	1:A:190:PRO:HD3	1.81	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:332:ASP:O	1:B:336:ARG:N	2.26	0.62
1:B:151:LEU:HB2	1:B:152:PRO:HD3	1.82	0.62
1:A:421:ASP:OD1	1:A:425:ASN:HB2	1.99	0.61
1:B:333:VAL:HG12	1:B:360:GLY:HA2	1.82	0.61
1:B:211:ARG:NH1	1:B:238:LEU:O	2.32	0.61
1:A:486:LEU:HG	1:A:487:ARG:N	2.14	0.61
1:A:285:ASN:O	1:A:320:ARG:HD2	2.01	0.61
1:B:395:ASN:ND2	1:B:410:TYR:OH	2.27	0.61
1:B:112:THR:N	6:B:1838:HOH:O	2.31	0.61
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: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:B:183:SER:CB	1:B:185:GLU:HG2	2.31	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:183:SER:HB3	1:B:185:GLU:HG2	1.80	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:B:395:ASN:O	1:B:396:MET:C	2.38	0.60
1:A:402:THR:CG2	1:A:414:ALA:HB2	2.31	0.60
1:B:371:ASN:N	1:B:371:ASN:HD22	1.99	0.60
1:B:331:GLN:O	1:B:332:ASP:C	2.39	0.60
1:A:396:MET:HE3	1:A:480:GLN:HG2	1.81	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:B:409:LYS:HE2	1:B:422:GLU:HB2	1.82	0.60
1:B:224:ILE:O	1:B:229:ASN:HB2	2.02	0.60
1:A:252:LYS:HE3	6:A:817:HOH:O	2.02	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:A:174:LEU:HG	1:A:209:ILE:HB	1.82	0.60
1:B:541:LYS:HE3	6:B:1742:HOH:O	2.01	0.60
1:B:517:GLU:N	1:B:517:GLU:OE2	2.31	0.60
1:A:413:VAL:HG12	1:A:471:TYR:HB3	1.82	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:B:333:VAL:HG12	1:B:334:GLU:N	2.16	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:46:ASN:N	1:B:46:ASN:HD22	1.96	0.59
1:A:439:MET:HB2	1:A:470:ARG:NH1	2.16	0.59
1:A:289:GLU:HB2	1:A:322:SER:HB3	1.84	0.59
1:A:313:LYS:NZ	6:A:1045:HOH:O	2.30	0.59
1:B:295:VAL:HG13	1:B:328:ILE:HG22	1.82	0.59
1:A:541:LYS:O	1:A:542:ARG:C	2.40	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:355:TYR:CD1	1:B:358:VAL:HB	2.38	0.59
1:B:333:VAL:HA	1:B:340:ILE:HD11	1.84	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:A:387:ILE:HG22	1:A:388:ASP:N	2.17	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:325:ILE:HG22	1:B:327:LEU:CD2	2.34	0.58
1:A:379:CYS:O	1:A:382:MET:N	2.34	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:A:116:ILE:HD11	1:A:155:GLU:HG2	1.85	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:330:SER:HB2	1:B:357:GLY:O	2.05	0.57
1:B:238:LEU:HD21	5:B:1601:MPD:H51	1.86	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:B:102:LYS:HB3	1:B:108:TYR:CE1	2.39	0.56
1:A:183:SER:OG	1:A:185:GLU:HG2	2.05	0.56
1:B:473:VAL:HB	6:B:1622:HOH:O	2.05	0.56
1:B:52:MET:HB3	1:B:57:HIS:CG	2.41	0.56
1:B:382:MET:HE3	1:B:512:CYS:HA	1.86	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: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:387:ILE:O	1:A:388:ASP:C	2.42	0.56
1:B:213:ASP:HB3	1:B:214:ARG:NE	2.16	0.56
1:A:452:SER:OG	1:A:455:ARG:HB2	2.06	0.56
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:355:TYR:O	1:A:356:ARG:C	2.44	0.55
1:B:387:ILE:O	1:B:389:TYR:N	2.39	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:A:117:PRO:HD2	1:A:118:HIS:CE1	2.41	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:440:ARG:HH21	1:A:469:HIS:CE1	2.25	0.55
1:A:347:ILE:HD12	1:A:368:ALA:CB	2.37	0.55
1:B:488:VAL:HG11	1:B:491:ARG:CZ	2.36	0.55
1:A:441:LEU:HA	1:A:467:HIS:O	2.06	0.55
1:B:455:ARG:HD2	1:B:455:ARG:O	2.06	0.55
1:B:186:VAL:HG21	1:B:220:GLU:HG2	1.89	0.55
1:B:421:ASP:CB	1:B:425:ASN:H	2.18	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: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:B:409:LYS:HD3	1:B:410:TYR:CE1	2.42	0.54
1:A:1:MET:O	1:A:2:THR:C	2.46	0.54
1:B:539:PHE:CE2	1:B:543:GLN:HG3	2.43	0.54
1:A:398:ASN:N	1:A:398:ASN:OD1	2.39	0.54
1:B:387:ILE:O	1:B:388:ASP:C	2.44	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:275:GLU:OE1	1:A:523:ARG:HD2	2.07	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:B:226:LEU:O	1:B:228:CYS:O	2.25	0.54
1:A:486:LEU:HG	1:A:487:ARG:H	1.72	0.54
1:A:391:ARG:O	1:A:393:VAL:N	2.41	0.54
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:C	1:B:71:LEU:HD12	2.28	0.54
1:A:422:GLU:N	1:A:422:GLU:OE2	2.29	0.54
1:B:49:PRO:HG2	1:B:69:THR:CA	2.38	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:396:MET:HE1	1:A:480:GLN:HG2	1.89	0.54
1:A:199:LEU:HD23	1:A:203:ILE:O	2.08	0.54
1:A:71:LEU:C	1:A:71:LEU:HD12	2.28	0.54
1:A:355:TYR:O	1:A:358:VAL:HG23	2.08	0.53
1:A:54:PRO:CA	1:A:58:GLY:N	2.71	0.53
1:A:420:ARG:HG3	1:A:421:ASP:H	1.71	0.53
1:B:403:GLU:HG3	1:B:471:TYR:CE1	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:416:ILE:HG23	1:A:419:TRP:CH2	2.43	0.53
1:A:333:VAL:HA	1:A:340:ILE:CD1	2.37	0.53
1:B:331:GLN:HA	1:B:334:GLU:OE2	2.08	0.53
1:A:241:VAL:HA	4:A:812:IOD:I	2.79	0.53
1:A:18:LYS:HE3	1:A:141:ILE:O	2.07	0.53
1:A:409:LYS:O	1:A:422:GLU:HA	2.09	0.53
1:B:488:VAL:HG11	1:B:491:ARG:NE	2.23	0.53
1:B:155:GLU:CD	1:B:158:ARG:HH21	2.11	0.53
1:B:486:LEU:HG	1:B:487:ARG:N	2.22	0.53
1:A:20:ILE:HG13	6:A:908:HOH:O	2.08	0.53
1:B:332:ASP:O	1:B:333:VAL:C	2.47	0.53
1:A:86:ARG:CG	1:A:86:ARG:HH11	2.22	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:A:211:ARG:CZ	5:A:601:MPD:H53	2.38	0.53
1:B:301:LEU:C	1:B:301:LEU:HD12	2.29	0.53
1:B:441:LEU:CD2	1:B:468:ARG:HD2	2.39	0.53
1:B:393:VAL:O	1:B:393:VAL:HG12	2.09	0.53
1:A:226:LEU:O	1:A:227:PHE:C	2.44	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:B:224:ILE:O	1:B:225:ALA:C	2.46	0.52
1:A:46:ASN:H	1:A:46:ASN:ND2	2.06	0.52
1:B:325:ILE:HG22	1:B:327:LEU:HD23	1.90	0.52
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:355:TYR:O	1:A:356:ARG:O	2.27	0.52
1:B:415:LEU:HD21	1:B:471:TYR:CD1	2.44	0.52
1:A:488:VAL:HG11	1:A:491:ARG:CZ	2.39	0.52
1:B:331:GLN:O	1:B:333:VAL:N	2.43	0.52
1:A:39:MET:HE1	1:A:130:GLY:HA3	1.92	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: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:492:SER:O	1:B:493:GLY:O	2.29	0.51
1:B:355:TYR:HD1	1:B:358:VAL:HB	1.75	0.51
1:B:412:VAL:HG13	1:B:413:VAL:HG23	1.92	0.51
1:B:390:ALA:HB1	1:B:396:MET:HG2	1.91	0.51
1:B:301:LEU:HD12	1:B:302:PRO:CD	2.40	0.51
1:A:389:TYR:HD2	1:A:481:ILE:CG2	2.23	0.51
1:A:233:LYS:HG2	1:A:233:LYS:O	2.10	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:B:495:ASP:O	1:B:496:GLN:O	2.29	0.51
1:A:379:CYS:O	1:A:380:LEU:C	2.49	0.51
1:B:155:GLU:OE2	1:B:158:ARG:NH2	2.36	0.51
1:A:464:VAL:C	1:A:465:GLU:HG2	2.31	0.51
1:A:272:ASN:C	1:A:272:ASN:HD22	2.12	0.51
1:A:355:TYR:CD1	1:A:404:PHE:CG	2.99	0.51
1:B:268:CYS:HB2	1:B:269:PRO:CD	2.35	0.51
1:B:131:GLY:O	1:B:134:HIS:HD2	1.93	0.51
1:B:409:LYS:O	1:B:411:PRO:HD3	2.11	0.51
1:A:357:GLY:O	1:A:360:GLY:N	2.43	0.51
1:B:361:MET:HB3	1:B:384:VAL:HG21	1.93	0.51
1:A:448:LEU:HD22	1:A:454:VAL:HG13	1.93	0.51
1:A:337:GLY:C	1:A:339:GLU:H	2.15	0.51
1:B:53:SER:O	1:B:55:ILE:O	2.29	0.51
1:B:225:ALA:O	1:B:230:VAL:N	2.44	0.51
1:B:147:ASP:HB2	6:B:1785:HOH:O	2.10	0.51
1:B:499:GLU:O	1:B:512:CYS:HA	2.11	0.50
1:B:426:VAL:CG1	1:B:427:GLU:N	2.74	0.50
1:B:355:TYR:CB	1:B:404:PHE:CD2	2.94	0.50
1:A:86:ARG:HH11	1:A:86:ARG:H	1.53	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:478:LEU:O	1:A:482:GLU:HG3	2.10	0.50
1:A:179:TYR:CD2	1:A:214:ARG:NH2	2.80	0.50
1:B:366:ARG:HA	1:B:388:ASP:OD2	2.12	0.50
1:B:108:TYR:CD2	1:B:118:HIS:CD2	2.98	0.50
1:A:289:GLU:CB	1:A:322:SER:HB3	2.42	0.50
1:A:263:ARG:O	1:A:263:ARG:HG3	2.10	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:B:405:VAL:HG12	1:B:405:VAL:O	2.12	0.50
1:B:295:VAL:HA	1:B:328:ILE:O	2.10	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:A:166:ARG:HB2	1:A:263:ARG:HH21	1.76	0.50
1:B:212:SER:HB3	1:B:214:ARG:O	2.12	0.50
1:A:179:TYR:CE1	1:A:214:ARG:NH1	2.80	0.50
1:B:395:ASN:ND2	1:B:410:TYR:CZ	2.80	0.50
1:A:409:LYS:HD3	1:A:410:TYR:CE1	2.47	0.50
1:B:447:GLN:NE2	1:B:493:GLY:H	2.09	0.50
1:A:268:CYS:CB	1:A:269:PRO:HD2	2.41	0.50
1:A:341:LEU:HD23	1:A:341:LEU:N	2.26	0.50
1:B:420:ARG:HA	1:B:425:ASN:O	2.11	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: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:B:389:TYR:CE2	1:B:486:LEU:HB2	2.47	0.49
1:A:403:GLU:HB2	1:A:471:TYR:CE2	2.47	0.49
1:B:392:HIS:CD2	1:B:392:HIS:N	2.80	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:A:179:TYR:HE2	1:A:181:ALA:HA	1.78	0.49
1:B:388:ASP:OD1	1:B:389:TYR:N	2.45	0.49
1:A:469:HIS:CE1	1:A:513:GLN:NE2	2.79	0.49
1:B:369:ARG:NH1	1:B:393:VAL:HG21	2.26	0.49
1:A:413:VAL:CG1	1:A:471:TYR:HB3	2.42	0.49
1:A:336:ARG:HH21	1:A:340:ILE:HG22	1.76	0.49
1:B:415:LEU:N	1:B:415:LEU:HD23	2.26	0.49
1:B:329:ASP:O	1:B:330:SER:C	2.50	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:HG	1:A:301:LEU:O	2.10	0.49
1:A:44:TYR:CE1	1:A:52:MET:HE1	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:299:ILE:CG2	1:B:327:LEU:HB3	2.41	0.49
1:A:382:MET:HE3	1:A:500:ILE:HA	1.95	0.49
1:B:373:ILE:HG23	1:B:374:PRO:HD2	1.95	0.49
1:B:69:THR:CG2	1:B:73:LEU:HD22	2.43	0.49
1:B:227:PHE:C	1:B:228:CYS:O	2.46	0.49
1:B:379:CYS:O	1:B:380:LEU:C	2.50	0.48
1:A:448:LEU:HD11	1:A:463:ILE:HG23	1.93	0.48
1:B:378:ILE:CD1	1:B:516:PRO:HD2	2.42	0.48
1:B:415:LEU:CD2	1:B:471:TYR:CD2	2.97	0.48
1:A:454:VAL:HG22	1:A:528:LEU:HD21	1.96	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:B:380:LEU:O	1:B:383:GLN:HB2	2.13	0.48
1:A:517:GLU:OE1	1:A:517:GLU:N	2.46	0.48
1:B:12:VAL:HG11	1:B:176:LEU:HB3	1.94	0.48
1:A:361:MET:HB2	1:A:384:VAL:CG2	2.42	0.48
1:B:189:LYS:HB3	1:B:190:PRO:CD	2.35	0.48
1:A:179:TYR:OH	1:A:184:GLY:HA2	2.13	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:B:227:PHE:O	1:B:228:CYS:O	2.31	0.48
1:A:503:VAL:HA	1:A:504:PRO:HD3	1.68	0.48
1:B:172:MET:HG2	1:B:209:ILE:HD12	1.96	0.48
1:B:493:GLY:O	1:B:494:ASP:OD1	2.32	0.48
1:B:369:ARG:NH1	1:B:393:VAL:CG2	2.77	0.48
1:A:298:TYR:O	1:A:300:GLU:N	2.47	0.48
1:A:403:GLU:HB2	1:A:471:TYR:CD2	2.48	0.48
1:A:415:LEU:HD21	1:A:471:TYR:CE2	2.49	0.48
1:B:97:SER:O	1:B:101:ARG:HD2	2.14	0.48
1:A:494:ASP:C	1:A:496:GLN:H	2.17	0.48
1:B:492:SER:HB2	1:B:499:GLU:OE2	2.14	0.47
1:A:375:TYR:HB3	1:A:509:PHE:CD1	2.49	0.47
1:A:355:TYR:HD1	1:A:404:PHE:CD2	2.32	0.47
1:A:420:ARG:CG	1:A:421:ASP:N	2.77	0.47
1:B:294:MET:CE	1:B:309:ILE:HG13	2.44	0.47
1:A:347:ILE:HD13	1:A:368:ALA:HB2	1.92	0.47
1:B:211:ARG:NE	5:B:1601:MPD:H53	2.29	0.47
1:B:506:HIS:CE1	1:B:507:PRO:HD2	2.49	0.47
1:B:172:MET:HG2	1:B:209:ILE:CD1	2.44	0.47
1:B:301:LEU:HD11	1:B:303:ASP:HB2	1.97	0.47
1:B:441:LEU:HA	1:B:467:HIS:O	2.14	0.47
1:A:506:HIS:CD2	1:A:507:PRO:HD2	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:378:ILE:HD13	1:B:516:PRO:CD	2.44	0.47
1:A:495:ASP:HB3	1:A:497:LEU:HD12	1.94	0.47
1:A:163:GLU:HG2	4:A:803:IOD:I	2.85	0.47
1:A:272:ASN:ND2	1:A:274:SER:H	2.13	0.47
1:A:25:LEU:HD22	1:A:172:MET:HE1	1.97	0.47
1:A:44:TYR:CE1	1:A:52:MET:CE	2.97	0.47
1:A:369:ARG:HH21	1:A:388:ASP:CG	2.18	0.47
1:A:67:ALA:HB2	1:A:86:ARG:CB	2.45	0.47
1:A:221:ARG:O	1:A:224:ILE:N	2.48	0.47
1:B:151:LEU:HB2	1:B:152:PRO:CD	2.45	0.47
1:A:285:ASN:O	1:A:320:ARG:NH1	2.47	0.47
1:B:277:GLU:H	1:B:277:GLU:HG2	1.62	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:A:106:GLY:O	1:A:109:LEU:HD23	2.15	0.47
1:B:54:PRO:HA	1:B:58:GLY:O	2.14	0.47
1:A:297:LYS:HG2	6:A:1048:HOH:O	2.15	0.47
1:B:355:TYR:CB	1:B:404:PHE:HD2	2.25	0.47
1:A:444:GLN:HB2	1:A:467:HIS:CE1	2.50	0.47
1:A:151:LEU:N	1:A:152:PRO:CD	2.78	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:379:CYS:HB3	1:B:380:LEU:H	1.43	0.46
1:B:289:GLU:HG3	1:B:324:ASN:ND2	2.29	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
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:B:396:MET:HE1	1:B:480:GLN:CG	2.45	0.46
1:B:402:THR:CG2	1:B:414:ALA:HB2	2.42	0.46
1:B:296:GLY:O	1:B:329:ASP:HA	2.16	0.46
1:A:55:ILE:N	1:A:55:ILE:CD1	2.79	0.46
1:A:207:ILE:HA	1:A:234:ALA:HB1	1.96	0.46
1:B:93:GLY:O	1:B:97:SER:HB2	2.15	0.46
1:B:503:VAL:HG12	1:B:503:VAL:O	2.13	0.46
1:B:230:VAL:O	1:B:230:VAL:HG12	2.16	0.46
1:A:543:GLN:O	1:A:544:ALA:HB2	2.16	0.46
1:A:396:MET:O	1:A:397:GLU:C	2.53	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:313:LYS:HZ3	1:A:313:LYS:HB3	1.81	0.46
1:A:40:LYS:HB3	1:A:89:ASN:HD22	1.81	0.46
1:A:13:VAL:HG23	1:A:16:LEU:HD21	1.97	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:B:106:GLY:O	1:B:109:LEU:N	2.35	0.46
1:B:86:ARG:HD3	1:B:86:ARG:HA	1.68	0.45
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:A:300:GLU:O	1:A:302:PRO:HD3	2.16	0.45
1:A:409:LYS:H	1:A:420:ARG:NH2	2.13	0.45
1:B:355:TYR:HA	1:B:404:PHE:CD2	2.51	0.45
1:A:362:ILE:HA	1:A:384:VAL:HG13	1.97	0.45
1:A:18:LYS:HE2	1:A:140:GLU:HG2	1.98	0.45
1:A:458:TYR:O	1:A:459:ASN:C	2.52	0.45
1:A:382:MET:CE	1:A:500:ILE:HA	2.46	0.45
1:B:488:VAL:CG1	1:B:491:ARG:NH2	2.79	0.45
1:B:78:ARG:NH1	1:B:307:SER:OG	2.48	0.45
1:A:340:ILE:HG12	1:A:341:LEU:N	2.31	0.45
1:B:45:ILE:O	1:B:46:ASN:C	2.51	0.45
1:A:537:SER:O	1:A:540:GLN:HB3	2.16	0.45
1:A:272:ASN:ND2	1:A:274:SER:OG	2.36	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:382:MET:HE3	1:A:511:ALA:O	2.16	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:301:LEU:HD21	1:A:303:ASP:HB2	1.97	0.45
1:A:86:ARG:HH22	1:A:87:ARG:HH11	1.64	0.45
1:A:230:VAL:N	1:A:231:PRO:CD	2.80	0.45
1:B:252:LYS:HE3	1:B:271:ALA:HB3	1.97	0.45
1:A:75:HIS:O	1:A:76:TYR:C	2.53	0.45
1:B:163:GLU:HG2	4:B:804:IOD:I	2.87	0.45
1:A:506:HIS:ND1	1:A:507:PRO:HD2	2.32	0.45
1:A:359:GLU:HA	1:A:362:ILE:HD12	1.98	0.45
1:B:341:LEU:HB2	1:B:367:PHE:CE2	2.52	0.45
1:A:390:ALA:CB	1:A:481:ILE:HD13	2.47	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:421:ASP:N	1:B:476:MET:CE	2.80	0.44
1:B:338:VAL:HG13	1:B:338:VAL:O	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:244:ILE:HG23	6:B:1763:HOH:O	2.17	0.44
1:B:69:THR:HG23	1:B:70:ASP:N	2.33	0.44
1:B:103:GLU:OE1	1:B:104:ARG:HG2	2.17	0.44
1:B:494:ASP:CG	1:B:495:ASP:N	2.70	0.44
1:B:421:ASP:CB	1:B:425:ASN:N	2.80	0.44
1:A:86:ARG:CG	1:A:86:ARG:NH1	2.80	0.44
1:B:506:HIS:ND1	1:B:507:PRO:CD	2.78	0.44
1:B:426:VAL:HG13	1:B:427:GLU:N	2.33	0.44
1:A:181:ALA:O	1:A:182:ALA:O	2.34	0.44
1:B:167:GLU:HB2	6:B:1789:HOH:O	2.17	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:228:CYS:HB2	6:B:1722:HOH:O	2.17	0.44
1:B:179:TYR:C	1:B:179:TYR:CD2	2.90	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:414:ALA:HA	1:A:471:TYR:HD2	1.83	0.44
1:A:400:ASN:O	1:A:411:PRO:HA	2.18	0.44
1:A:415:LEU:HD21	1:A:471:TYR:CZ	2.53	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:382:MET:HA	1:A:511:ALA:HB1	1.98	0.44
1:A:219:ASN:HB2	6:A:942:HOH:O	2.16	0.44
1:B:396:MET:CA	1:B:410:TYR:CD1	2.96	0.44
1:A:494:ASP:C	1:A:496:GLN:N	2.71	0.44
1:A:239:LYS:HD3	4:A:801:IOD:I	2.88	0.44
1:B:341:LEU:O	1:B:344:LEU:CG	2.64	0.44
1:A:540:GLN:OE1	1:A:541:LYS:HG2	2.17	0.43
1:A:229:ASN:C	1:A:231:PRO:HD3	2.38	0.43
1:B:301:LEU:HD12	1:B:303:ASP:H	1.83	0.43
1:B:224:ILE:CG2	1:B:229:ASN:ND2	2.79	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:A:296:GLY:C	1:A:299:ILE:HG12	2.39	0.43
1:B:294:MET:HB3	1:B:327:LEU:HD22	1.99	0.43
1:A:208:LEU:HD12	1:A:231:PRO:HG2	1.99	0.43
1:A:1:MET:HE1	1:A:135:ASP:N	2.33	0.43
1:B:171:PHE:N	1:B:206:ASP:OD2	2.50	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:B:487:ARG:HG3	6:B:1855:HOH:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:61:PHE:HB3	1:B:69:THR:HG22	1.99	0.43
1:A:49:PRO:C	1:A:51:THR:H	2.22	0.43
1:B:468:ARG:CG	1:B:468:ARG:NH1	2.77	0.43
1:B:86:ARG:HD3	1:B:86:ARG:O	2.17	0.43
1:A:349:VAL:HG12	1:A:381:GLY:HA3	1.95	0.43
1:B:276:TRP:O	1:B:280:ILE:HG13	2.18	0.43
1:A:335:THR:HG22	1:A:336:ARG:N	2.33	0.43
1:B:378:ILE:HD12	1:B:516:PRO:HD2	1.99	0.43
1:B:386:LEU:HA	1:B:386:LEU:HD12	1.81	0.43
1:B:398:ASN:O	1:B:399:ALA:C	2.56	0.43
1:B:397:GLU:N	1:B:410:TYR:CD1	2.87	0.43
1:B:189:LYS:O	1:B:192:GLN:HB2	2.19	0.43
1:A:345:ASP:HA	1:A:539:PHE:HD2	1.78	0.43
1:A:362:ILE:HG12	1:A:387:ILE:HG21	2.00	0.43
1:A:378:ILE:HG23	1:A:514:PHE:O	2.18	0.43
1:A:402:THR:CG2	1:A:414:ALA:CB	2.97	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:325:ILE:HG22	1:B:327:LEU:HD21	2.00	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: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:A:2:THR:HG21	1:A:168:HIS:NE2	2.34	0.43
1:A:166:ARG:HB2	1:A:263:ARG:NH2	2.34	0.43
1:A:471:TYR:C	1:A:472:GLU:HG2	2.40	0.42
1:A:178:PRO:HD2	1:A:187:LYS:O	2.18	0.42
1:B:86:ARG:HH12	1:B:89:ASN:CB	2.30	0.42
1:A:390:ALA:HA	1:A:481:ILE:HG23	2.01	0.42
1:B:148:ILE:HG13	1:B:149:GLU:OE1	2.19	0.42
1:A:179:TYR:CG	1:A:214:ARG:CZ	3.02	0.42
1:A:25:LEU:HD22	1:A:172:MET:CE	2.48	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:A:216:VAL:HG12	1:A:221:ARG:CG	2.47	0.42
1:B:454:VAL:HG12	1:B:528:LEU:HD21	2.00	0.42
1:B:388:ASP:O	1:B:392:HIS:N	2.53	0.42
1:A:421:ASP:OD2	1:A:425:ASN:N	2.47	0.42
1:B:230:VAL:N	1:B:231:PRO:CD	2.82	0.42
1:B:209:ILE:HG13	1:B:236:ILE:HB	2.00	0.42
1:A:207:ILE:HG12	1:A:234:ALA:HB1	2.00	0.42
1:B:389:TYR:HD2	1:B:481:ILE:HG22	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:386:LEU:HA	1:A:386:LEU:HD12	1.82	0.42
1:B:101:ARG:O	1:B:102:LYS:C	2.58	0.42
1:A:487:ARG:O	1:A:501:ILE:HA	2.20	0.42
1:A:217:PRO:O	1:A:219:ASN:N	2.52	0.42
1:B:295:VAL:HG22	1:B:328:ILE:CG2	2.50	0.42
1:A:335:THR:CG2	1:A:336:ARG:HG3	2.26	0.42
1:B:49:PRO:C	1:B:51:THR:H	2.23	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: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:CG	1:B:214:ARG:CZ	3.03	0.42
1:A:98:ASP:OD2	6:A:934:HOH:O	2.22	0.42
1:B:515:HIS:HA	1:B:516:PRO:HD2	1.90	0.42
1:A:179:TYR:CE2	1:A:181:ALA:HA	2.55	0.42
1:B:528:LEU:HA	1:B:528:LEU:HD23	1.69	0.42
1:A:192:GLN:HG2	1:A:228:CYS:HB3	2.01	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:483:ASP:C	1:A:485:GLY:H	2.24	0.42
1:A:420:ARG:O	1:A:476:MET:SD	2.78	0.42
1:B:268:CYS:CB	1:B:269:PRO:CD	2.96	0.42
1:A:446:CYS:SG	1:A:447:GLN:N	2.92	0.42
1:B:378:ILE:HD13	1:B:516:PRO:CG	2.49	0.42
1:A:76:TYR:N	1:A:76:TYR:CD2	2.86	0.42
1:B:24:SER:O	1:B:28:ILE:HG13	2.19	0.42
1:B:441:LEU:HD21	1:B:468:ARG:HD2	2.02	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:91:THR:HG23	6:B:1759:HOH:O	2.20	0.41
1:A:241:VAL:HG11	1:A:250:LEU:CD1	2.50	0.41
1:B:458:TYR:CE1	1:B:528:LEU:HG	2.55	0.41
1:B:389:TYR:O	1:B:390:ALA:C	2.58	0.41
1:A:411:PRO:HG3	1:A:420:ARG:NH2	2.35	0.41
1:B:301:LEU:CD1	1:B:302:PRO:HD2	2.46	0.41
1:B:151:LEU:CB	1:B:152:PRO:CD	2.98	0.41
1:A:457:LEU:HD23	1:A:457:LEU:HA	1.78	0.41
1:A:366:ARG:NH1	6:A:890:HOH:O	2.52	0.41
1:B:348:LEU:HA	1:B:376:LEU:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:320:ARG:HH11	1:A:320:ARG:HD2	1.73	0.41
1:B:290:VAL:HG22	1:B:321:VAL:HG11	2.02	0.41
1:B:172:MET:HG3	1:B:207:ILE:HB	2.02	0.41
1:B:488:VAL:CG1	1:B:491:ARG:CZ	2.99	0.41
1:A:262:LYS:HD2	4:A:805:IOD:I	2.90	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:360:GLY:O	1:B:363:THR:HB	2.21	0.41
1:B:297:LYS:HZ3	1:B:354:GLY:HA3	1.84	0.41
1:A:354:GLY:O	1:A:356:ARG:N	2.53	0.41
1:B:390:ALA:HB1	1:B:396:MET:CB	2.51	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:A:241:VAL:CG1	1:A:250:LEU:HD11	2.51	0.41
1:B:368:ALA:HB1	1:B:375:TYR:HB2	2.01	0.41
1:B:192:GLN:HG2	6:B:1722:HOH:O	2.20	0.41
1:A:542:ARG:HD3	1:A:542:ARG:HH11	1.74	0.41
1:A:439:MET:HE3	1:A:469:HIS:C	2.40	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:415:LEU:CD2	1:B:471:TYR:CG	3.03	0.41
1:B:421:ASP:HB2	1:B:425:ASN:HB2	2.03	0.41
1:A:415:LEU:HD23	1:A:415:LEU:N	2.35	0.41
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:116:ILE:CD1	1:A:155:GLU:HG2	2.50	0.41
1:A:402:THR:HG23	1:A:402:THR:H	1.61	0.41
1:B:195:VAL:HG11	1:B:229:ASN:HA	2.02	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:1:MET:HE1	1:A:134:HIS:C	2.41	0.41
1:A:39:MET:HE1	1:A:130:GLY:CA	2.51	0.41
1:B:172:MET:SD	1:B:209:ILE:HD11	2.61	0.41
1:A:80:ILE:HD12	1:A:82:THR:HB	2.02	0.41
1:A:54:PRO:C	1:A:58:GLY:N	2.74	0.40
1:A:406:PRO:O	1:A:420:ARG:NH1	2.27	0.40
1:A:334:GLU:HG3	1:A:360:GLY:CA	2.51	0.40
1:A:2:THR:HG21	1:A:168:HIS:CD2	2.56	0.40
1:B:402:THR:CG2	1:B:414:ALA:CB	2.99	0.40
1:B:116:ILE:HA	1:B:117:PRO:HA	1.83	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:220:GLU:CD	1:B:220:GLU:N	2.75	0.40
1:A:86:ARG:CA	1:A:86:ARG:NH1	2.75	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:B:415:LEU:HD23	1:B:471:TYR:CG	2.56	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:172:MET:SD	1:B:209:ILE:CD1	3.10	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%)	6	3
1	B	532/545 (98%)	467 (88%)	41 (8%)	24 (4%)	4	1
All	All	1063/1090 (98%)	936 (88%)	86 (8%)	41 (4%)	5	2

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

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Mol	Chain	Res	Type
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
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%)	9	10
1	B	454/461 (98%)	387 (85%)	67 (15%)	4	4
All	All	907/922 (98%)	791 (87%)	116 (13%)	6	6

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 chains 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	0.60	0	10,10,10	0.68	0
2	SO4	A	602	3	4,4,4	0.56	0	6,6,6	0.09	0
2	SO4	A	603	3	4,4,4	0.31	0	6,6,6	0.14	0
5	MPD	B	1601	-	7,7,7	0.52	0	10,10,10	0.39	0
2	SO4	B	1602	3	4,4,4	0.41	0	6,6,6	0.19	0
2	SO4	B	1603	3	4,4,4	0.30	0	6,6,6	0.06	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	0/0/0/0
2	SO4	A	602	3	-	0/0/0/0	0/0/0/0
2	SO4	A	603	3	-	0/0/0/0	0/0/0/0
5	MPD	B	1601	-	-	0/5/5/5	0/0/0/0
2	SO4	B	1602	3	-	0/0/0/0	0/0/0/0
2	SO4	B	1603	3	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	534/545 (97%)	-0.09	13 (2%) 56 66	31, 55, 93, 100	1 (0%)
1	B	536/545 (98%)	-0.06	16 (2%) 48 58	32, 54, 93, 100	1 (0%)
All	All	1070/1090 (98%)	-0.07	29 (2%) 53 62	31, 54, 93, 100	2 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	PHE	6.6
1	B	545	LYS	5.2
1	A	228	CYS	4.8
1	B	494	ASP	4.7
1	B	182	ALA	3.6
1	B	101	ARG	3.5
1	B	544	ALA	3.5
1	A	355	TYR	3.4
1	A	1	MET	3.3
1	A	493	GLY	3.2
1	B	181	ALA	3.1
1	A	180	MET	3.0
1	B	395	ASN	3.0
1	B	1	MET	2.8
1	B	493	GLY	2.6
1	A	57[A]	HIS	2.6
1	B	340	ILE	2.6
1	B	335	THR	2.5
1	B	355	TYR	2.5
1	A	544	ALA	2.5
1	B	183	SER	2.4
1	B	426	VAL	2.4
1	B	425	ASN	2.3
1	B	300	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	218	ALA	2.2
1	A	425	ASN	2.1
1	A	504	PRO	2.1
1	A	339	GLU	2.1
1	A	495	ASP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MG	A	703	1/1	0.28	9.20	92,92,92,92	0
4	IOD	A	814	1/1	0.18	7.11	89,89,89,89	1
3	MG	B	704	1/1	0.21	5.11	91,91,91,91	0
4	IOD	A	816	1/1	0.15	2.68	90,90,90,90	1
5	MPD	B	1601	8/8	0.19	2.42	57,79,87,88	0
4	IOD	B	811	1/1	0.12	2.41	72,72,72,72	1
2	SO4	B	1602	5/5	0.21	1.38	54,60,70,89	0
5	MPD	A	601	8/8	0.19	0.77	50,80,92,100	0
2	SO4	A	602	5/5	0.18	0.53	65,72,82,88	0
4	IOD	B	815	1/1	0.11	0.45	76,76,76,76	1
2	SO4	A	603	5/5	0.17	0.42	68,83,90,91	0
2	SO4	B	1603	5/5	0.17	0.41	57,65,92,93	0
4	IOD	B	809	1/1	0.14	0.33	77,77,77,77	1
4	IOD	A	807	1/1	0.12	0.09	63,63,63,63	1
4	IOD	B	810	1/1	0.08	-0.32	76,76,76,76	1
4	IOD	A	812	1/1	0.08	-1.14	72,72,72,72	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	IOD	A	813	1/1	0.07	-1.18	69,69,69,69	1
4	IOD	A	805	1/1	0.06	-1.40	64,64,64,64	1
4	IOD	A	806	1/1	0.06	-1.54	72,72,72,72	1
4	IOD	B	808	1/1	0.07	-1.65	73,73,73,73	1
4	IOD	B	804	1/1	0.06	-1.93	73,73,73,73	0
4	IOD	A	803	1/1	0.05	-1.97	72,72,72,72	0
4	IOD	B	802	1/1	0.05	-1.99	69,69,69,69	0
4	IOD	A	801	1/1	0.06	-2.37	72,72,72,72	0
3	MG	B	701	1/1	0.10	-3.12	64,64,64,64	0
3	MG	A	702	1/1	0.05	-4.64	47,47,47,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.