



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:54 AM UTC

PDB ID : 2ONH / pdb_00002onh
Title : Crystal Structure of of limonene synthase with 2-fluorolinalyl diphosphate(FLPP)
Authors : Hyatt, D.C.; Youn, B.; Croteau, R.; Kang, C.
Deposited on : 2007-01-24
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

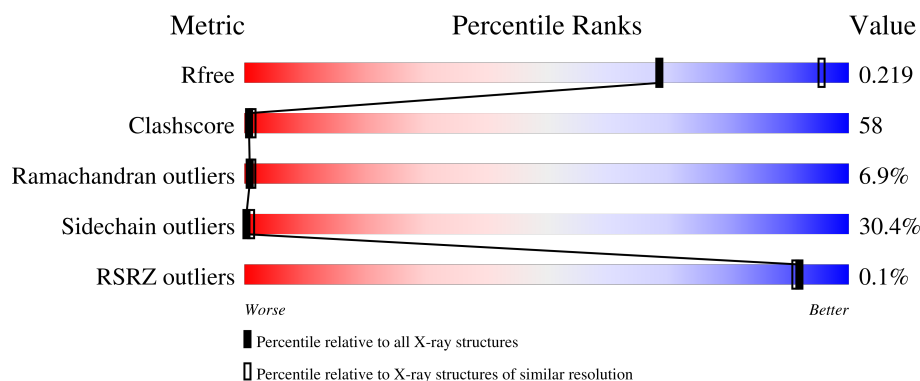
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	543	 20% 41% 32% 7%
1	B	543	 23% 42% 27% 8%

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	F3P	A	600	-	-	X	-
3	F3P	B	1600	-	-	X	-
4	BTB	A	604	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9165 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 4S-limonene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	0	0
			4497	2873	761	843	20			
1	B	543	Total	C	N	O	S	0	0	0
			4497	2873	761	843	20			

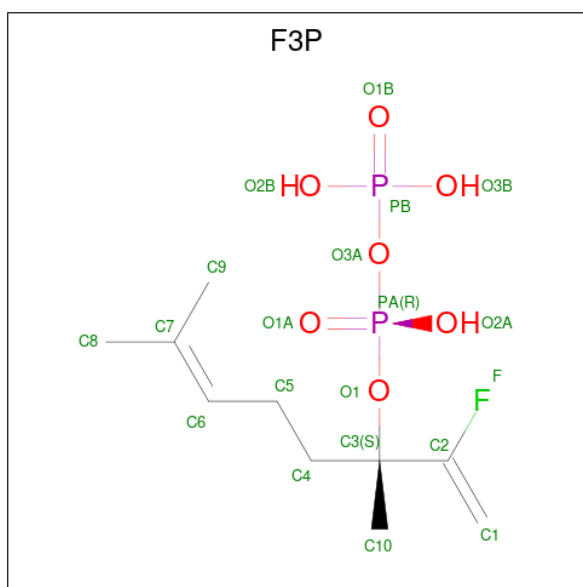
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	MET	GLU	engineered mutation	UNP Q40322
B	57	MET	GLU	engineered mutation	UNP Q40322

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

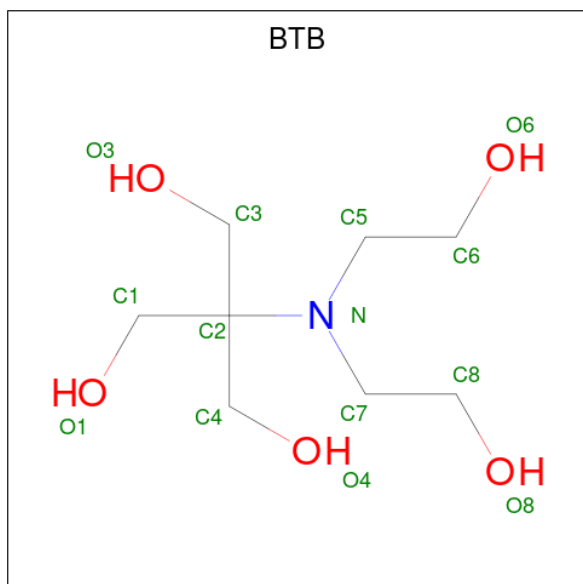
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mn	0	0
			3	3		
2	B	3	Total	Mn	0	0
			3	3		

- Molecule 3 is (3S)-2-fluoro-3,7-dimethylocta-1,6-dien-3-yl trihydrogen diphosphate (CCD ID: F3P) (formula: C₁₀H₁₉FO₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	O	P	0	0
			20	10	1	7	2		
3	B	1	Total	C	F	O	P	0	0
			20	10	1	7	2		

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

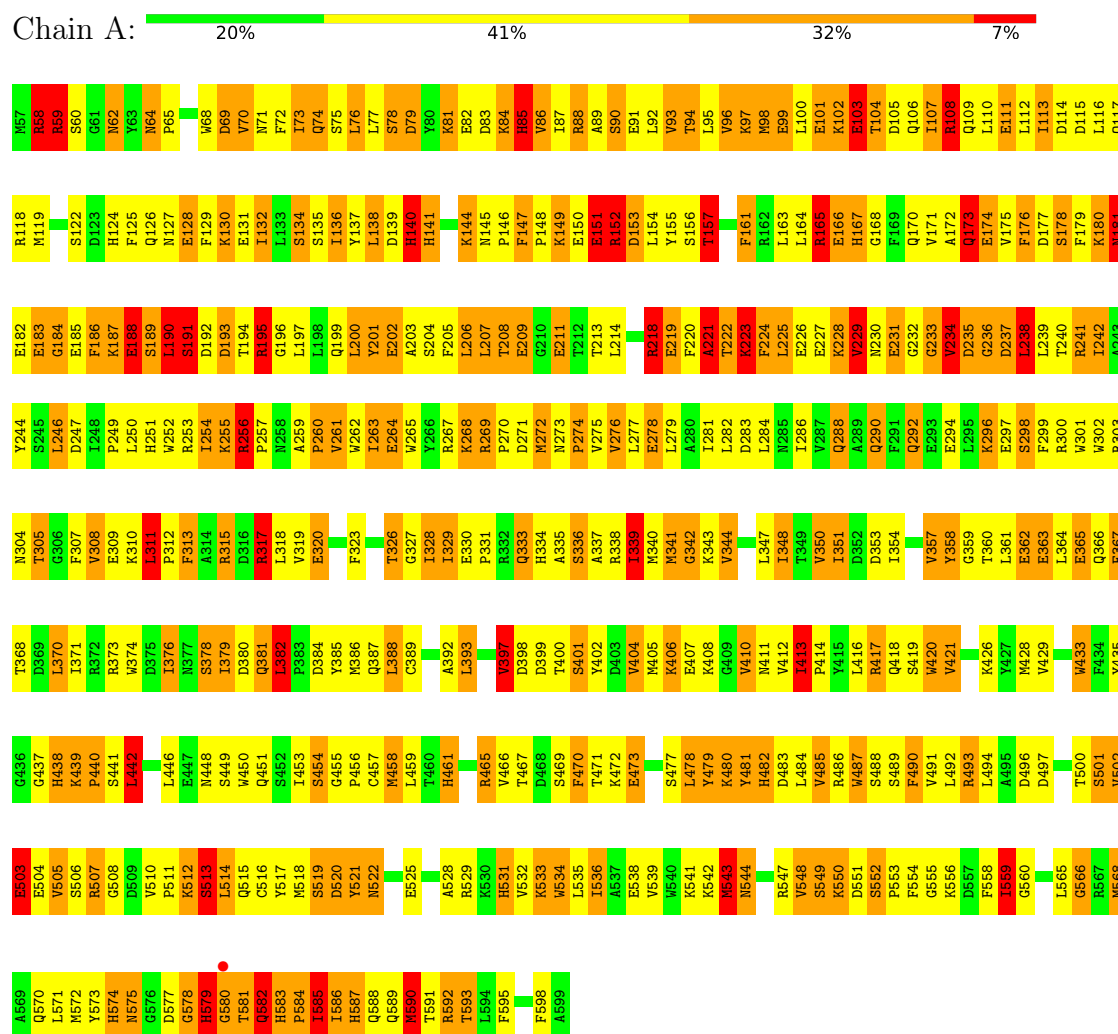
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	58	Total 58	O 58	0	0
5	B	53	Total 53	O 53	0	0

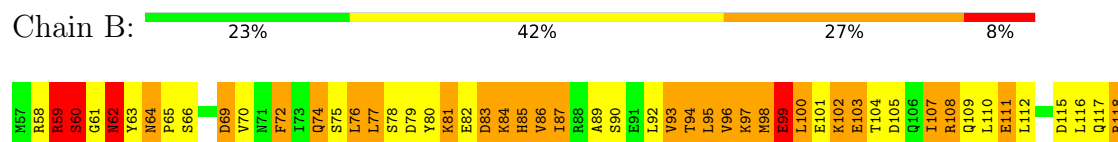
3 Residue-property plots

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

• Molecule 1: 4S-limonene synthase



• Molecule 1: 4S-limonene synthase





4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	198.66Å 198.66Å 122.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 10.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.70) 91.0 (10.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.61Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.206 , 0.234 0.217 , 0.219	Depositor DCC
R_{free} test set	3309 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.487 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9165	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: F3P, BTB, MN

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	1.47	80/4609 (1.7%)	1.65	124/6237 (2.0%)
1	B	1.44	66/4609 (1.4%)	1.62	100/6237 (1.6%)
All	All	1.46	146/9218 (1.6%)	1.63	224/12474 (1.8%)

All (146) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	539	VAL	CA-CB	-10.83	1.42	1.54
1	A	413	ILE	CA-CB	10.55	1.61	1.53
1	A	368	THR	C-N	9.92	1.47	1.33
1	B	404	VAL	CA-CB	-9.77	1.43	1.54
1	A	368	THR	C-O	9.32	1.35	1.24
1	A	351	ILE	CA-CB	-9.31	1.42	1.54
1	A	348	ILE	CA-CB	-9.06	1.44	1.54
1	A	482	HIS	N-CA	-8.81	1.35	1.46
1	B	368	THR	CA-CB	-7.99	1.40	1.53
1	A	487	TRP	CG-CD2	-7.88	1.29	1.43
1	A	461	HIS	CG-ND1	-7.86	1.29	1.38
1	B	171	VAL	CA-CB	7.62	1.64	1.54
1	B	413	ILE	CA-CB	7.23	1.63	1.54
1	A	485	VAL	N-CA	-7.14	1.38	1.46
1	B	482	HIS	N-CA	-7.11	1.37	1.46
1	A	485	VAL	CA-CB	-7.06	1.46	1.54
1	A	339	ILE	CA-CB	-7.06	1.46	1.54
1	A	482	HIS	CG-ND1	-7.04	1.30	1.38
1	A	108	ARG	NE-CZ	6.92	1.40	1.33
1	A	421	VAL	CA-CB	-6.91	1.46	1.54
1	A	85	HIS	CG-ND1	-6.79	1.30	1.38
1	B	500	THR	CA-CB	6.66	1.64	1.53
1	A	397	VAL	N-CA	-6.61	1.38	1.46
1	B	470	PHE	N-CA	-6.57	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	LYS	N-CA	-6.53	1.38	1.46
1	B	453	ILE	CA-CB	6.51	1.62	1.54
1	B	96	VAL	CA-CB	-6.51	1.44	1.54
1	A	559	ILE	CA-CB	6.29	1.65	1.54
1	B	124	HIS	ND1-CE1	6.27	1.38	1.32
1	A	482	HIS	CB-CG	-6.25	1.41	1.50
1	A	344	VAL	CA-CB	-6.24	1.47	1.54
1	A	531	HIS	CG-ND1	-6.23	1.31	1.38
1	B	461	HIS	CG-ND1	-6.18	1.31	1.38
1	A	251	HIS	CG-ND1	-6.13	1.31	1.38
1	A	141	HIS	ND1-CE1	6.09	1.38	1.32
1	B	574	HIS	ND1-CE1	6.08	1.38	1.32
1	A	478	LEU	N-CA	-6.05	1.39	1.46
1	A	482	HIS	CE1-NE2	6.04	1.38	1.32
1	B	482	HIS	CG-ND1	-6.04	1.31	1.38
1	A	218	ARG	NE-CZ	6.02	1.39	1.33
1	B	583	HIS	ND1-CE1	6.02	1.38	1.32
1	A	574	HIS	ND1-CE1	6.00	1.38	1.32
1	A	86	VAL	CA-CB	-5.99	1.46	1.54
1	A	458	MET	N-CA	-5.98	1.39	1.46
1	B	400	THR	CA-CB	-5.97	1.43	1.53
1	A	593	THR	CA-CB	5.97	1.63	1.53
1	B	108	ARG	NE-CZ	5.94	1.39	1.33
1	B	141	HIS	ND1-CE1	5.91	1.38	1.32
1	B	141	HIS	CE1-NE2	5.89	1.38	1.32
1	A	141	HIS	CE1-NE2	5.88	1.38	1.32
1	A	221	ALA	N-CA	-5.88	1.38	1.46
1	B	467	THR	N-CA	-5.87	1.39	1.46
1	B	351	ILE	CA-CB	-5.86	1.46	1.54
1	A	400	THR	CA-CB	-5.86	1.44	1.53
1	A	579	HIS	CE1-NE2	5.85	1.38	1.32
1	B	167	HIS	CE1-NE2	5.85	1.38	1.32
1	B	579	HIS	CE1-NE2	5.83	1.38	1.32
1	B	583	HIS	CE1-NE2	5.83	1.38	1.32
1	B	150	GLU	N-CA	5.81	1.53	1.46
1	B	491	VAL	CA-CB	-5.81	1.47	1.54
1	B	482	HIS	CE1-NE2	5.79	1.38	1.32
1	B	574	HIS	CE1-NE2	5.79	1.38	1.32
1	B	140	HIS	CE1-NE2	5.77	1.38	1.32
1	A	574	HIS	CE1-NE2	5.76	1.38	1.32
1	B	438	HIS	CG-ND1	-5.76	1.31	1.38
1	B	419	SER	N-CA	-5.76	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	HIS	ND1-CE1	5.74	1.38	1.32
1	B	587	HIS	ND1-CE1	5.73	1.38	1.32
1	A	514	LEU	N-CA	-5.73	1.39	1.46
1	A	140	HIS	CG-ND1	-5.72	1.31	1.38
1	A	124	HIS	ND1-CE1	5.72	1.38	1.32
1	B	140	HIS	ND1-CE1	5.71	1.38	1.32
1	B	85	HIS	CE1-NE2	5.70	1.38	1.32
1	A	587	HIS	CE1-NE2	5.70	1.38	1.32
1	A	140	HIS	CE1-NE2	5.69	1.38	1.32
1	B	579	HIS	ND1-CE1	5.69	1.38	1.32
1	A	348	ILE	N-CA	-5.69	1.40	1.46
1	A	247	ASP	N-CA	5.68	1.53	1.46
1	B	247	ASP	N-CA	5.68	1.53	1.46
1	A	276	VAL	N-CA	-5.68	1.40	1.46
1	A	334	HIS	CE1-NE2	5.64	1.38	1.32
1	A	334	HIS	CG-ND1	-5.64	1.32	1.38
1	A	579	HIS	ND1-CE1	5.62	1.38	1.32
1	A	438	HIS	CE1-NE2	5.59	1.38	1.32
1	B	478	LEU	N-CA	-5.59	1.39	1.46
1	B	531	HIS	ND1-CE1	5.57	1.38	1.32
1	B	124	HIS	CE1-NE2	5.56	1.38	1.32
1	B	432	ARG	NE-CZ	5.56	1.39	1.33
1	B	167	HIS	ND1-CE1	5.54	1.38	1.32
1	B	320	GLU	N-CA	-5.53	1.39	1.46
1	B	166	GLU	N-CA	-5.53	1.39	1.46
1	A	587	HIS	ND1-CE1	5.52	1.38	1.32
1	A	583	HIS	ND1-CE1	5.52	1.38	1.32
1	A	124	HIS	CE1-NE2	5.50	1.38	1.32
1	A	140	HIS	ND1-CE1	5.50	1.38	1.32
1	A	420	TRP	CG-CD2	-5.49	1.33	1.43
1	B	438	HIS	ND1-CE1	5.49	1.38	1.32
1	B	438	HIS	CE1-NE2	5.48	1.38	1.32
1	B	251	HIS	CE1-NE2	5.47	1.38	1.32
1	A	73	ILE	N-CA	-5.46	1.39	1.46
1	B	368	THR	N-CA	-5.45	1.39	1.46
1	B	475	VAL	C-N	-5.45	1.26	1.33
1	B	587	HIS	CE1-NE2	5.44	1.38	1.32
1	A	251	HIS	ND1-CE1	5.44	1.38	1.32
1	A	481	TYR	N-CA	-5.43	1.39	1.46
1	A	167	HIS	ND1-CE1	5.43	1.38	1.32
1	A	317	ARG	N-CA	-5.41	1.39	1.46
1	A	85	HIS	CE1-NE2	5.41	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	334	HIS	CE1-NE2	5.40	1.38	1.32
1	B	251	HIS	CG-ND1	-5.40	1.32	1.38
1	A	97	LYS	N-CA	-5.39	1.39	1.46
1	A	166	GLU	N-CA	-5.39	1.39	1.46
1	A	167	HIS	CE1-NE2	5.39	1.38	1.32
1	B	85	HIS	CG-ND1	-5.39	1.32	1.38
1	B	474	THR	CA-CB	-5.35	1.45	1.53
1	A	583	HIS	CE1-NE2	5.33	1.37	1.32
1	B	531	HIS	CG-ND1	-5.32	1.32	1.38
1	B	85	HIS	ND1-CE1	5.31	1.37	1.32
1	A	531	HIS	CE1-NE2	5.29	1.37	1.32
1	A	251	HIS	CE1-NE2	5.27	1.37	1.32
1	A	438	HIS	ND1-CE1	5.24	1.37	1.32
1	A	350	VAL	CA-CB	-5.23	1.48	1.54
1	B	334	HIS	ND1-CE1	5.23	1.37	1.32
1	A	473	GLU	N-CA	-5.20	1.40	1.46
1	A	348	ILE	C-O	-5.19	1.18	1.24
1	A	406	LYS	N-CA	-5.19	1.40	1.46
1	A	374	TRP	CG-CD2	-5.17	1.34	1.43
1	A	85	HIS	ND1-CE1	5.16	1.37	1.32
1	A	553	PRO	N-CA	-5.16	1.41	1.47
1	B	583	HIS	CB-CG	5.15	1.57	1.50
1	A	438	HIS	CG-ND1	-5.14	1.32	1.38
1	B	476	ASP	N-CA	-5.14	1.40	1.46
1	B	251	HIS	ND1-CE1	5.13	1.37	1.32
1	B	469	SER	C-N	-5.12	1.26	1.33
1	B	482	HIS	ND1-CE1	5.12	1.37	1.32
1	A	471	THR	CA-CB	-5.12	1.44	1.53
1	A	363	GLU	N-CA	-5.08	1.40	1.46
1	B	132	ILE	CA-CB	-5.08	1.47	1.54
1	A	157	THR	N-CA	-5.06	1.40	1.46
1	A	141	HIS	N-CA	-5.06	1.39	1.46
1	B	450	TRP	CG-CD2	-5.05	1.34	1.43
1	A	379	ILE	N-CA	-5.02	1.40	1.46
1	A	521	TYR	N-CA	-5.02	1.40	1.46
1	A	531	HIS	N-CA	-5.01	1.40	1.46
1	B	263	ILE	CA-CB	-5.01	1.46	1.54
1	B	360	THR	CA-CB	-5.01	1.45	1.53

All (224) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	GLU	CB-CG-CD	15.43	138.82	112.60
1	A	482	HIS	ND1-CG-CD2	14.23	120.33	106.10
1	B	426	LYS	CA-CB-CG	-12.87	88.35	114.10
1	A	209	GLU	CB-CG-CD	11.20	131.64	112.60
1	A	480	LYS	N-CA-C	-11.10	99.75	113.18
1	B	131	GLU	CB-CG-CD	11.07	131.42	112.60
1	B	108	ARG	CA-CB-CG	10.88	135.86	114.10
1	B	480	LYS	N-CA-C	-10.78	99.39	112.54
1	A	487	TRP	CE2-CD2-CE3	10.28	129.08	118.80
1	A	219	GLU	CB-CG-CD	10.19	129.92	112.60
1	B	482	HIS	ND1-CG-CD2	10.05	116.15	106.10
1	B	219	GLU	CB-CG-CD	9.89	129.41	112.60
1	B	85	HIS	ND1-CG-CD2	9.85	115.95	106.10
1	A	227	GLU	CB-CG-CD	9.72	129.12	112.60
1	B	191	SER	N-CA-C	-9.50	101.70	113.20
1	A	85	HIS	ND1-CG-CD2	9.04	115.14	106.10
1	B	118	ARG	CA-CB-CG	-8.93	96.24	114.10
1	A	342	GLY	N-CA-C	-8.83	101.95	112.64
1	B	342	GLY	N-CA-C	-8.82	102.15	112.73
1	A	103	GLU	CB-CG-CD	-8.70	97.81	112.60
1	A	311	LEU	CA-C-N	8.67	129.41	120.04
1	A	311	LEU	C-N-CA	8.67	129.41	120.04
1	B	311	LEU	CA-C-N	8.66	128.88	119.87
1	B	311	LEU	C-N-CA	8.66	128.88	119.87
1	A	401	SER	CA-CB-OG	-8.29	94.51	111.10
1	B	187	LYS	CA-CB-CG	-8.27	97.56	114.10
1	B	251	HIS	ND1-CG-CD2	8.15	114.25	106.10
1	A	238	LEU	N-CA-C	-8.14	103.86	113.88
1	B	531	HIS	ND1-CG-CD2	8.09	114.19	106.10
1	A	74	GLN	CA-CB-CG	-8.07	97.96	114.10
1	A	108	ARG	CA-CB-CG	8.00	130.10	114.10
1	B	443	GLU	CB-CG-CD	8.00	126.19	112.60
1	B	579	HIS	ND1-CG-CD2	7.97	114.07	106.10
1	A	102	LYS	N-CA-C	-7.96	103.78	113.97
1	A	531	HIS	ND1-CG-CD2	7.96	114.06	106.10
1	B	320	GLU	CB-CG-CD	7.94	126.10	112.60
1	B	588	GLN	CB-CG-CD	7.91	126.04	112.60
1	A	278	GLU	CA-CB-CG	-7.88	98.34	114.10
1	B	542	LYS	CB-CG-CD	-7.87	93.19	111.30
1	B	438	HIS	ND1-CG-CD2	7.76	113.86	106.10
1	B	459	LEU	N-CA-C	7.73	119.49	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	HIS	ND1-CG-CD2	7.71	113.81	106.10
1	B	596	GLU	CB-CG-CD	7.66	125.63	112.60
1	A	578	GLY	N-CA-C	-7.63	105.48	115.47
1	A	139	ASP	N-CA-C	-7.54	101.16	111.56
1	A	438	HIS	ND1-CG-CD2	7.46	113.56	106.10
1	A	236	GLY	N-CA-C	-7.46	95.51	113.18
1	A	223	LYS	N-CA-C	-7.42	103.19	111.28
1	B	576	GLY	N-CA-C	-7.42	99.50	111.59
1	B	582	GLN	CA-CB-CG	-7.41	99.28	114.10
1	B	543	MET	CG-SD-CE	-7.35	84.72	100.90
1	A	326	THR	N-CA-C	-7.34	104.13	113.23
1	B	219	GLU	CA-CB-CG	7.28	128.67	114.10
1	A	211	GLU	CA-CB-CG	-7.18	99.74	114.10
1	B	188	GLU	CB-CG-CD	7.16	124.77	112.60
1	A	170	GLN	CB-CG-CD	7.15	124.76	112.60
1	B	493	ARG	CA-CB-CG	-7.12	99.86	114.10
1	A	579	HIS	ND1-CG-CD2	7.11	113.21	106.10
1	B	103	GLU	CB-CG-CD	-7.11	100.52	112.60
1	A	251	HIS	ND1-CG-CD2	7.07	113.17	106.10
1	A	165	ARG	CA-CB-CG	-7.06	99.98	114.10
1	B	420	TRP	CG-CD1-NE1	-7.05	101.03	110.20
1	A	74	GLN	CB-CG-CD	7.00	124.50	112.60
1	A	487	TRP	CG-CD2-CE3	-6.97	126.93	133.90
1	B	543	MET	CA-CB-CG	-6.96	100.19	114.10
1	A	473	GLU	N-CA-C	-6.85	103.50	110.97
1	A	334	HIS	ND1-CG-CD2	6.82	112.92	106.10
1	A	140	HIS	ND1-CG-CD2	6.81	112.91	106.10
1	B	524	SER	CA-CB-OG	-6.81	97.48	111.10
1	A	503	GLU	CB-CG-CD	6.79	124.14	112.60
1	A	315	ARG	CB-CG-CD	-6.74	95.80	111.30
1	B	501	SER	CA-CB-OG	-6.72	97.66	111.10
1	A	151	GLU	CB-CG-CD	6.71	124.01	112.60
1	A	559	ILE	CB-CG1-CD1	-6.71	99.71	113.80
1	A	410	VAL	N-CA-C	6.70	119.17	108.85
1	A	59	ARG	CA-CB-CG	6.70	127.50	114.10
1	A	413	ILE	CB-CG1-CD1	6.66	127.78	113.80
1	B	540	TRP	CB-CG-CD1	-6.64	116.94	126.90
1	A	585	ILE	CB-CG1-CD1	6.63	127.73	113.80
1	B	236	GLY	N-CA-C	-6.60	97.25	115.33
1	B	578	GLY	N-CA-C	-6.59	97.55	113.18
1	A	480	LYS	CA-CB-CG	6.58	127.27	114.10
1	A	173	GLN	CA-CB-CG	6.53	127.16	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	GLU	N-CA-C	-6.52	104.09	111.07
1	B	334	HIS	ND1-CG-CD2	6.52	112.62	106.10
1	A	99	GLU	CB-CG-CD	6.48	123.62	112.60
1	A	320	GLU	CB-CG-CD	6.47	123.60	112.60
1	A	252	TRP	CE2-CD2-CE3	6.42	125.22	118.80
1	A	195	ARG	CA-CB-CG	6.42	126.93	114.10
1	B	146	PRO	CA-N-CD	-6.41	103.03	112.00
1	A	503	GLU	CA-CB-CG	6.39	126.89	114.10
1	B	480	LYS	CA-CB-CG	6.39	126.87	114.10
1	A	482	HIS	CB-CG-CD2	-6.36	122.93	131.20
1	A	246	LEU	CD1-CG-CD2	-6.30	96.94	110.80
1	A	590	MET	CG-SD-CE	-6.30	87.05	100.90
1	B	313	PHE	N-CA-C	-6.29	105.56	113.18
1	B	128	GLU	N-CA-C	-6.28	104.06	111.03
1	A	574	HIS	ND1-CG-CD2	6.27	112.37	106.10
1	B	123	ASP	N-CA-C	6.25	118.09	111.28
1	B	253	ARG	CA-CB-CG	6.23	126.57	114.10
1	A	64	ASN	CA-C-N	6.23	125.99	119.76
1	A	64	ASN	C-N-CA	6.23	125.99	119.76
1	B	534	TRP	CB-CG-CD1	-6.19	117.62	126.90
1	B	430	GLU	CB-CG-CD	6.19	123.12	112.60
1	A	313	PHE	N-CA-C	-6.16	105.25	112.89
1	A	479	TYR	N-CA-C	6.16	120.40	113.01
1	B	244	TYR	N-CA-C	-6.15	104.21	111.03
1	A	328	ILE	N-CA-C	6.15	117.70	111.00
1	B	534	TRP	CG-CD2-CE3	6.14	140.04	133.90
1	B	420	TRP	CD1-CG-CD2	6.13	116.11	106.30
1	A	549	SER	CA-CB-OG	-6.12	98.87	111.10
1	B	461	HIS	ND1-CG-CD2	6.11	112.21	106.10
1	A	459	LEU	N-CA-C	6.10	118.73	111.71
1	A	341	MET	CA-CB-CG	-6.07	101.95	114.10
1	A	482	HIS	CG-ND1-CE1	-6.06	98.99	109.30
1	B	99	GLU	CB-CG-CD	6.06	122.90	112.60
1	B	241	ARG	CA-CB-CG	-6.04	102.01	114.10
1	A	487	TRP	CD2-CE2-CZ2	-6.04	116.36	122.40
1	A	583	HIS	ND1-CG-CD2	6.00	112.10	106.10
1	A	191	SER	CA-CB-OG	5.99	123.08	111.10
1	A	374	TRP	CD1-CG-CD2	5.99	115.89	106.30
1	B	298	SER	CA-CB-OG	5.97	123.05	111.10
1	A	450	TRP	CG-CD2-CE3	5.97	139.87	133.90
1	B	553	PRO	N-CA-C	-5.97	105.88	114.18
1	A	543	MET	CA-CB-CG	-5.94	102.21	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ASP	N-CA-C	-5.91	105.65	112.92
1	A	102	LYS	CA-CB-CG	-5.90	102.30	114.10
1	B	582	GLN	CB-CG-CD	5.89	122.61	112.60
1	A	184	GLY	N-CA-C	-5.89	106.97	115.27
1	B	378	SER	N-CA-C	-5.88	105.81	112.87
1	B	595	PHE	N-CA-C	5.86	120.22	112.72
1	B	225	LEU	N-CA-C	-5.86	104.08	111.11
1	A	161	PHE	N-CA-C	-5.84	104.55	111.03
1	A	487	TRP	NE1-CE2-CD2	5.84	114.99	107.40
1	B	515	GLN	CB-CG-CD	5.83	122.51	112.60
1	A	433	TRP	CB-CG-CD2	-5.83	118.64	126.80
1	A	482	HIS	CG-CD2-NE2	-5.79	101.41	107.20
1	B	487	TRP	CE2-CD2-CE3	5.78	124.58	118.80
1	A	406	LYS	CA-CB-CG	-5.78	102.54	114.10
1	A	566	GLY	N-CA-C	-5.78	105.50	112.49
1	A	128	GLU	CB-CG-CD	5.77	122.42	112.60
1	A	419	SER	CA-CB-OG	-5.76	99.59	111.10
1	A	170	GLN	CA-CB-CG	5.73	125.57	114.10
1	B	324	TRP	CB-CG-CD1	-5.72	118.32	126.90
1	A	420	TRP	CE2-CD2-CE3	5.68	124.48	118.80
1	B	141	HIS	ND1-CG-CD2	5.66	111.75	106.10
1	B	549	SER	CA-CB-OG	-5.66	99.79	111.10
1	B	198	LEU	N-CA-C	-5.65	106.06	113.12
1	B	450	TRP	CD1-CG-CD2	5.65	115.33	106.30
1	A	298	SER	CA-CB-OG	5.60	122.30	111.10
1	A	124	HIS	ND1-CG-CD2	5.59	111.69	106.10
1	B	167	HIS	ND1-CG-CD2	5.57	111.67	106.10
1	B	266	TYR	CB-CG-CD1	-5.54	112.48	120.80
1	B	550	LYS	CB-CG-CD	5.54	124.04	111.30
1	A	378	SER	N-CA-C	-5.53	104.38	113.50
1	A	188	GLU	CB-CG-CD	5.53	122.00	112.60
1	B	450	TRP	CG-CD1-NE1	-5.51	103.04	110.20
1	B	452	SER	CA-CB-OG	-5.46	100.18	111.10
1	A	450	TRP	CG-CD1-NE1	-5.46	103.10	110.20
1	B	412	VAL	CG1-CB-CG2	-5.45	98.80	110.80
1	A	367	PHE	N-CA-C	-5.42	105.27	111.07
1	A	448	ASN	N-CA-C	-5.42	106.35	113.12
1	A	542	LYS	CB-CG-CD	-5.42	98.84	111.30
1	B	309	GLU	CB-CG-CD	5.41	121.80	112.60
1	B	208	THR	CA-C-O	-5.41	114.94	121.32
1	A	374	TRP	CG-CD1-NE1	-5.40	103.18	110.20
1	A	519	SER	CA-CB-OG	-5.38	100.34	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	HIS	ND1-CG-CD2	5.38	111.48	106.10
1	A	381	GLN	CB-CG-CD	-5.38	103.46	112.60
1	B	288	GLN	CB-CG-CD	-5.37	103.47	112.60
1	B	237	ASP	N-CA-C	-5.37	105.12	110.97
1	A	583	HIS	CA-C-N	5.36	126.54	119.84
1	A	583	HIS	C-N-CA	5.36	126.54	119.84
1	A	488	SER	CA-CB-OG	-5.35	100.40	111.10
1	A	568	MET	CA-CB-CG	-5.34	103.41	114.10
1	B	413	ILE	CB-CG1-CD1	5.33	124.99	113.80
1	B	326	THR	N-CA-C	-5.32	105.65	111.82
1	A	433	TRP	CD1-CG-CD2	5.32	114.81	106.30
1	A	336	SER	CA-CB-OG	-5.30	100.49	111.10
1	B	178	SER	CA-CB-OG	5.30	121.71	111.10
1	B	256	ARG	CA-CB-CG	-5.30	103.50	114.10
1	B	358	TYR	CB-CG-CD2	-5.29	112.86	120.80
1	B	540	TRP	CG-CD2-CE3	5.29	139.19	133.90
1	B	161	PHE	N-CA-C	-5.29	105.21	110.97
1	A	480	LYS	CA-C-O	5.28	125.87	119.11
1	B	358	TYR	CD1-CG-CD2	5.27	126.01	118.10
1	A	442	LEU	CD1-CG-CD2	-5.26	99.22	110.80
1	A	233	GLY	N-CA-C	-5.26	100.71	113.18
1	A	382	LEU	CD1-CG-CD2	-5.26	99.24	110.80
1	A	413	ILE	N-CA-CB	5.25	113.81	110.50
1	A	328	ILE	CB-CG1-CD1	-5.25	102.78	113.80
1	A	420	TRP	CD1-CG-CD2	5.24	114.68	106.30
1	B	441	SER	CA-CB-OG	-5.24	100.63	111.10
1	A	365	GLU	CA-CB-CG	-5.22	103.65	114.10
1	A	420	TRP	CG-CD1-NE1	-5.22	103.41	110.20
1	B	449	SER	CA-CB-OG	-5.22	100.66	111.10
1	A	450	TRP	CD1-CG-CD2	5.20	114.61	106.30
1	B	184	GLY	N-CA-C	-5.19	100.88	113.18
1	B	518	MET	CB-CG-SD	-5.18	97.15	112.70
1	A	357	VAL	CG1-CB-CG2	-5.18	99.40	110.80
1	A	256	ARG	CB-CG-CD	5.18	123.21	111.30
1	B	207	LEU	N-CA-C	5.17	118.37	110.36
1	B	487	TRP	CD2-CE2-CZ2	-5.17	117.23	122.40
1	B	556	LYS	CB-CG-CD	5.16	123.17	111.30
1	A	167	HIS	ND1-CG-CD2	5.16	111.26	106.10
1	B	458	MET	CA-CB-CG	-5.14	103.83	114.10
1	B	150	GLU	CB-CG-CD	5.13	121.32	112.60
1	B	165	ARG	CA-CB-CG	-5.12	103.86	114.10
1	A	433	TRP	CD2-CE2-CZ2	-5.12	117.28	122.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	ILE	CB-CA-C	-5.10	108.94	114.35
1	A	552	SER	CA-C-O	5.10	124.96	120.02
1	B	328	ILE	N-CA-C	-5.09	106.83	111.67
1	A	534	TRP	CB-CG-CD1	-5.06	119.31	126.90
1	A	292	GLN	CA-CB-CG	-5.06	103.98	114.10
1	A	450	TRP	CB-CG-CD1	-5.05	119.32	126.90
1	A	433	TRP	CE2-CD2-CE3	5.05	123.85	118.80
1	A	288	GLN	CB-CG-CD	-5.05	104.02	112.60
1	A	229	VAL	N-CA-C	-5.04	105.79	110.53
1	B	64	ASN	CA-C-N	5.04	127.05	120.25
1	B	64	ASN	C-N-CA	5.04	127.05	120.25
1	B	443	GLU	CA-CB-CG	-5.04	104.03	114.10
1	A	433	TRP	CG-CD1-NE1	-5.02	103.68	110.20
1	A	130	LYS	CB-CG-CD	5.01	122.83	111.30
1	B	469	SER	CA-CB-OG	-5.01	101.09	111.10

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	4497	0	4353	498	0
1	B	4497	0	4353	493	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	20	0	18	7	0
3	B	20	0	18	12	0
4	A	14	0	19	29	0
5	A	58	0	0	5	1
5	B	53	0	0	3	1
All	All	9165	0	8761	1028	1

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 58.

All (1028) 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)
4:A:604:BTB:N	4:A:604:BTB:C2	1.68	1.55
3:B:1600:F3P:H13	3:B:1600:F3P:C6	1.62	1.29
3:B:1600:F3P:H61	3:B:1600:F3P:C1	1.62	1.29
4:A:604:BTB:C7	4:A:604:BTB:H32	1.74	1.16
4:A:604:BTB:N	4:A:604:BTB:C3	2.12	1.12
3:A:600:F3P:H13	3:A:600:F3P:H61	1.20	1.11
1:B:449:SER:HB2	1:B:493:ARG:HD3	1.29	1.11
1:A:172:ALA:HB1	1:A:174:GLU:HG2	1.35	1.09
1:B:453:ILE:HD13	1:B:493:ARG:HA	1.34	1.09
3:A:600:F3P:H13	3:A:600:F3P:C6	1.82	1.09
1:B:302:TRP:HB2	1:B:318:LEU:HD13	1.30	1.09
1:A:152:ARG:HH21	1:A:178:SER:HB3	1.17	1.04
1:B:82:GLU:HG2	1:B:84:LYS:HG3	1.40	1.03
3:B:1600:F3P:H13	3:B:1600:F3P:H61	1.05	1.03
1:A:411:ASN:HD21	1:A:413:ILE:HG23	1.22	1.03
1:A:218:ARG:HG3	1:A:218:ARG:HH11	1.25	1.01
4:A:604:BTB:H32	4:A:604:BTB:H71	1.41	0.99
1:B:515:GLN:H	1:B:515:GLN:HE21	1.02	0.98
1:A:544:ASN:HD22	1:A:547:ARG:HD3	1.26	0.97
4:A:604:BTB:N	4:A:604:BTB:C1	2.27	0.97
1:B:197:LEU:HD11	1:B:220:PHE:HE2	1.26	0.96
1:B:582:GLN:OE1	1:B:582:GLN:HA	1.65	0.96
1:A:74:GLN:HG3	1:A:303:ARG:NH2	1.80	0.96
3:B:1600:F3P:H61	3:B:1600:F3P:C2	1.95	0.96
1:B:269:ARG:O	1:B:272:MET:HB3	1.66	0.96
1:A:411:ASN:ND2	1:A:413:ILE:HG23	1.81	0.96
1:A:117:GLN:HG3	1:A:129:PHE:HE1	1.33	0.93
4:A:604:BTB:N	4:A:604:BTB:C4	2.31	0.93
1:B:255:LYS:NZ	1:B:255:LYS:H	1.67	0.91
1:B:320:GLU:HB3	1:B:579:HIS:O	1.71	0.91
1:B:267:ARG:HG2	1:B:277:LEU:HD11	1.53	0.91
1:A:71:ASN:O	1:A:75:SER:HB3	1.71	0.91
1:A:235:ASP:HB2	1:A:238:LEU:HB3	1.51	0.91
1:A:333:GLN:H	1:A:333:GLN:HE21	1.01	0.90
1:A:165:ARG:HB3	1:A:206:LEU:HD12	1.53	0.90
1:A:302:TRP:HB2	1:A:318:LEU:HD13	1.54	0.90
4:A:604:BTB:C7	4:A:604:BTB:C3	2.51	0.88
4:A:604:BTB:O4	4:A:604:BTB:H62	1.73	0.87
1:A:281:ILE:HG23	1:A:598:PHE:HD1	1.39	0.87
1:B:515:GLN:HE21	1:B:515:GLN:N	1.72	0.87
1:A:543:MET:O	1:A:547:ARG:HG2	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLU:HG2	1:B:183:GLU:H	1.39	0.86
1:B:515:GLN:H	1:B:515:GLN:NE2	1.73	0.86
1:B:345:ASN:ND2	3:B:1600:F3P:H91	1.90	0.85
1:B:58:ARG:O	1:B:59:ARG:HB2	1.76	0.85
1:B:411:ASN:HD21	1:B:413:ILE:HG23	1.41	0.85
1:A:515:GLN:HB2	5:A:704:HOH:O	1.77	0.84
4:A:604:BTB:C4	4:A:604:BTB:H62	2.06	0.84
1:A:209:GLU:OE2	5:A:739:HOH:O	1.95	0.84
1:A:98:MET:HA	1:A:101:GLU:OE1	1.78	0.84
1:B:147:PHE:HA	1:B:149:LYS:HZ1	1.42	0.84
1:B:160:ALA:O	1:B:164:LEU:HB2	1.77	0.84
1:A:281:ILE:HG23	1:A:598:PHE:CD1	2.13	0.82
1:B:378:SER:HB3	1:B:381:GLN:OE1	1.78	0.82
1:A:449:SER:HB2	1:A:493:ARG:HD3	1.62	0.81
1:B:137:TYR:HA	1:B:142:TYR:HD1	1.44	0.81
1:B:575:ASN:HB2	1:B:584:PRO:HG2	1.62	0.81
1:A:446:LEU:HD13	4:A:604:BTB:H11	1.62	0.81
1:B:117:GLN:HE22	1:B:167:HIS:HE1	1.26	0.81
1:B:119:MET:HG2	1:B:262:TRP:HD1	1.43	0.81
3:B:1600:F3P:H13	3:B:1600:F3P:H62	1.60	0.81
1:B:449:SER:HB2	1:B:493:ARG:CD	2.09	0.81
1:A:79:ASP:HA	1:A:81:LYS:HE3	1.63	0.80
1:B:586:ILE:HA	1:B:589:GLN:HE21	1.44	0.80
1:B:302:TRP:CB	1:B:318:LEU:HD13	2.12	0.80
1:A:183:GLU:HB3	1:A:185:GLU:OE1	1.81	0.79
1:B:173:GLN:HG3	1:B:213:THR:HB	1.64	0.79
3:A:600:F3P:H13	3:A:600:F3P:C7	2.11	0.79
1:B:413:ILE:HG12	1:B:414:PRO:N	1.97	0.79
1:A:547:ARG:HA	1:A:559:ILE:HD13	1.65	0.79
1:A:585:ILE:HD13	1:A:585:ILE:H	1.48	0.79
1:A:152:ARG:NH2	1:A:178:SER:HB3	1.97	0.79
1:B:345:ASN:HD22	3:B:1600:F3P:C9	1.95	0.78
1:A:453:ILE:HG12	1:A:492:LEU:HG	1.66	0.78
1:B:92:LEU:HB3	1:B:279:LEU:HB2	1.63	0.78
1:A:228:LYS:HD3	1:A:233:GLY:HA3	1.64	0.78
1:A:219:GLU:O	1:A:222:THR:HG22	1.83	0.78
1:B:95:LEU:HB3	1:B:275:VAL:HG21	1.66	0.78
1:A:502:VAL:HG23	1:A:503:GLU:H	1.49	0.78
1:B:255:LYS:H	1:B:255:LYS:HZ3	1.28	0.78
1:B:411:ASN:ND2	1:B:413:ILE:HG23	1.98	0.78
1:B:130:LYS:O	1:B:134:SER:HB2	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ASP:O	1:A:118:ARG:HG2	1.83	0.77
4:A:604:BTB:N	4:A:604:BTB:H32	1.86	0.77
1:A:581:THR:O	1:A:582:GLN:HB2	1.84	0.77
1:B:61:GLY:H	1:B:357:VAL:CG1	1.97	0.77
1:A:433:TRP:CD1	1:A:438:HIS:HD1	2.02	0.77
1:B:497:ASP:OD2	1:B:512:LYS:HB3	1.84	0.76
1:B:218:ARG:CB	1:B:218:ARG:HH11	1.98	0.76
1:A:194:THR:HB	1:A:228:LYS:NZ	2.00	0.76
1:B:181:ASN:C	1:B:181:ASN:HD22	1.93	0.76
1:B:107:ILE:HG13	1:B:156:SER:HB3	1.67	0.76
1:B:119:MET:HG2	1:B:262:TRP:CD1	2.21	0.75
1:B:515:GLN:HA	1:B:518:MET:HG3	1.67	0.75
1:A:117:GLN:HG3	1:A:129:PHE:CE1	2.19	0.75
1:B:61:GLY:H	1:B:357:VAL:HG13	1.52	0.75
1:B:583:HIS:HB2	1:B:586:ILE:HB	1.67	0.75
4:A:604:BTB:C3	4:A:604:BTB:H71	2.15	0.75
1:B:345:ASN:HD21	1:B:458:MET:HE3	1.51	0.75
1:B:158:SER:HB2	1:B:199:GLN:HB3	1.69	0.75
1:A:145:ASN:OD1	1:A:174:GLU:HG3	1.85	0.75
1:A:78:SER:O	1:A:81:LYS:HG3	1.87	0.74
1:A:195:ARG:HG3	1:A:196:GLY:H	1.52	0.74
1:A:515:GLN:HA	1:A:518:MET:HE2	1.68	0.74
1:B:283:ASP:CG	1:B:332:ARG:HH22	1.95	0.74
1:B:428:MET:HE3	1:B:431:ALA:HB3	1.69	0.74
1:A:82:GLU:HB2	1:A:85:HIS:HE1	1.53	0.74
1:B:137:TYR:HB2	1:B:164:LEU:HD11	1.69	0.74
1:A:202:GLU:OE1	1:A:250:LEU:HG	1.88	0.74
1:A:87:ILE:HA	1:A:90:SER:HB2	1.71	0.73
4:A:604:BTB:C7	4:A:604:BTB:H12	2.18	0.73
1:A:135:SER:O	1:A:138:LEU:HD12	1.89	0.73
1:B:147:PHE:N	1:B:148:PRO:HD3	2.04	0.73
1:B:103:GLU:CD	1:B:104:THR:H	1.97	0.73
4:A:604:BTB:N	4:A:604:BTB:H12	2.04	0.72
1:B:267:ARG:HA	1:B:277:LEU:CD1	2.20	0.72
1:A:70:VAL:O	1:A:74:GLN:N	2.22	0.72
1:A:88:ARG:HH21	1:A:91:GLU:HG3	1.54	0.72
1:A:311:LEU:HG	1:A:313:PHE:CE2	2.25	0.72
1:B:345:ASN:ND2	3:B:1600:F3P:C9	2.53	0.72
1:A:327:GLY:HA3	1:A:568:MET:SD	2.29	0.72
1:B:324:TRP:HE1	1:B:579:HIS:HA	1.54	0.72
1:A:181:ASN:C	1:A:181:ASN:HD22	1.96	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:TRP:CD2	1:B:343:LYS:HG2	2.25	0.71
1:B:197:LEU:HD11	1:B:220:PHE:CE2	2.19	0.71
1:A:360:THR:O	1:A:364:LEU:HG	1.90	0.71
1:B:117:GLN:NE2	1:B:167:HIS:HE1	1.89	0.71
1:A:85:HIS:HB3	1:A:282:LEU:HD11	1.72	0.70
1:A:333:GLN:H	1:A:333:GLN:NE2	1.82	0.70
1:B:529:ARG:HD2	5:B:754:HOH:O	1.92	0.70
3:A:600:F3P:C2	3:A:600:F3P:H93	2.20	0.70
1:B:182:GLU:HG2	1:B:183:GLU:N	2.07	0.69
4:A:604:BTB:C2	4:A:604:BTB:C7	2.70	0.69
1:A:103:GLU:OE2	1:A:108:ARG:HD3	1.92	0.69
1:B:218:ARG:HH11	1:B:218:ARG:HB2	1.55	0.69
1:B:281:ILE:HG23	1:B:598:PHE:HD2	1.56	0.69
1:B:529:ARG:O	1:B:533:LYS:HG3	1.92	0.69
1:B:268:LYS:HD3	1:B:270:PRO:HD3	1.73	0.69
1:A:149:LYS:C	1:A:151:GLU:H	2.00	0.69
1:A:370:LEU:HD13	1:A:382:LEU:HD21	1.75	0.69
1:A:373:ARG:HG3	1:A:373:ARG:HH11	1.57	0.69
1:B:92:LEU:HD13	1:B:279:LEU:HA	1.74	0.69
1:B:147:PHE:HA	1:B:149:LYS:NZ	2.07	0.69
1:A:97:LYS:O	1:A:100:LEU:HB3	1.94	0.68
1:A:117:GLN:HE22	1:A:167:HIS:CE1	2.12	0.68
1:A:550:LYS:HE3	1:A:551:ASP:HA	1.75	0.68
4:A:604:BTB:H62	4:A:604:BTB:H42	1.74	0.68
1:A:96:VAL:HA	1:A:99:GLU:HG3	1.75	0.68
1:A:186:PHE:HD2	1:A:190:LEU:HD23	1.57	0.68
1:B:360:THR:O	1:B:364:LEU:HG	1.93	0.68
1:B:512:LYS:HB2	1:B:515:GLN:HE22	1.56	0.68
1:A:191:SER:HB2	1:A:224:PHE:CZ	2.28	0.68
1:A:194:THR:HB	1:A:228:LYS:HZ3	1.57	0.68
1:A:393:LEU:HD21	1:A:420:TRP:CD2	2.29	0.68
1:B:435:TYR:C	1:B:437:GLY:H	2.01	0.68
1:B:188:GLU:O	1:B:191:SER:HB3	1.94	0.68
1:A:234:VAL:HG23	1:A:238:LEU:HD22	1.75	0.68
1:A:177:ASP:HA	1:A:180:LYS:HD3	1.76	0.67
1:B:147:PHE:HB3	1:B:152:ARG:NH2	2.09	0.67
1:B:267:ARG:CG	1:B:277:LEU:HD11	2.23	0.67
1:A:74:GLN:HG3	1:A:303:ARG:CZ	2.24	0.67
1:A:107:ILE:HD12	1:A:110:LEU:HD12	1.76	0.67
1:A:218:ARG:HH11	1:A:218:ARG:CG	2.04	0.67
1:A:413:ILE:HG12	1:A:414:PRO:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:VAL:HG22	1:B:276:VAL:HG23	1.75	0.67
1:A:115:ASP:O	1:A:119:MET:HG3	1.94	0.67
1:A:284:LEU:HD22	1:A:598:PHE:HB2	1.76	0.67
1:B:254:ILE:HD12	1:B:254:ILE:N	2.09	0.67
4:A:604:BTB:N	4:A:604:BTB:H42	2.10	0.67
1:B:236:GLY:HA2	1:B:239:LEU:HG	1.77	0.66
1:B:89:ALA:HB2	1:B:282:LEU:HD23	1.78	0.66
1:A:269:ARG:O	1:A:272:MET:HB3	1.95	0.66
1:B:191:SER:HB2	1:B:224:PHE:CE1	2.31	0.66
1:B:96:VAL:HG23	1:B:275:VAL:HG22	1.77	0.66
1:B:82:GLU:HG2	1:B:84:LYS:CG	2.23	0.66
1:B:80:TYR:CE2	1:B:285:ASN:HB3	2.31	0.66
1:B:161:PHE:HD2	1:B:203:ALA:HB1	1.60	0.66
1:B:254:ILE:HD12	1:B:254:ILE:H	1.61	0.66
1:B:345:ASN:HD22	3:B:1600:F3P:H92	1.60	0.65
1:A:254:ILE:HG23	1:A:257:PRO:HD2	1.78	0.65
1:A:268:LYS:HE3	1:A:270:PRO:HD3	1.76	0.65
1:A:269:ARG:HH21	1:A:271:ASP:HB2	1.61	0.65
1:B:514:LEU:HD12	1:B:532:VAL:HG21	1.77	0.65
1:A:93:VAL:HG22	1:A:279:LEU:HD21	1.78	0.65
1:A:149:LYS:HA	1:A:152:ARG:NH2	2.12	0.65
1:A:317:ARG:HG3	1:A:579:HIS:CE1	2.32	0.65
1:B:121:LEU:HD21	1:B:280:ALA:HA	1.79	0.65
1:A:92:LEU:HD23	1:A:279:LEU:HA	1.80	0.64
1:B:222:THR:O	1:B:226:GLU:HB2	1.96	0.64
1:B:235:ASP:C	1:B:237:ASP:H	2.06	0.64
1:A:333:GLN:HE21	1:A:333:GLN:N	1.84	0.64
1:B:103:GLU:CD	1:B:104:THR:N	2.54	0.64
1:B:146:PRO:C	1:B:148:PRO:HD3	2.23	0.64
1:B:236:GLY:O	1:B:239:LEU:HB2	1.97	0.64
1:A:584:PRO:HB2	1:A:585:ILE:HD13	1.80	0.64
1:B:311:LEU:HD11	1:B:385:TYR:HB2	1.78	0.64
1:B:136:ILE:O	1:B:140:HIS:HB2	1.98	0.64
1:A:153:ASP:O	1:A:157:THR:HB	1.98	0.64
1:A:571:LEU:HD23	1:A:571:LEU:C	2.23	0.64
1:B:369:ASP:O	1:B:373:ARG:HG3	1.97	0.64
1:A:136:ILE:O	1:A:140:HIS:HB2	1.97	0.64
1:A:544:ASN:HA	1:A:547:ARG:HD3	1.80	0.64
1:A:191:SER:HA	1:A:224:PHE:CE2	2.33	0.63
4:A:604:BTB:C1	4:A:604:BTB:C5	2.77	0.63
1:B:363:GLU:HB3	1:B:386:MET:HE1	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:PHE:O	1:B:371:ILE:HG13	1.98	0.63
1:A:82:GLU:HB2	1:A:85:HIS:CE1	2.33	0.63
1:A:145:ASN:HB3	1:A:146:PRO:CD	2.28	0.63
1:B:256:ARG:CG	1:B:256:ARG:HH11	2.11	0.63
1:B:413:ILE:N	1:B:414:PRO:CD	2.61	0.63
1:A:98:MET:O	1:A:102:LYS:HB2	1.97	0.63
1:A:340:MET:HE3	1:A:461:HIS:HB3	1.81	0.63
1:B:105:ASP:OD1	1:B:107:ILE:HG22	1.98	0.63
1:A:188:GLU:O	1:A:191:SER:HB3	1.98	0.63
1:A:282:LEU:HG	1:A:286:ILE:HD11	1.81	0.63
1:B:72:PHE:C	1:B:72:PHE:CD2	2.77	0.63
1:B:92:LEU:HD21	1:B:278:GLU:HG2	1.78	0.62
1:B:137:TYR:HA	1:B:142:TYR:CD1	2.31	0.62
1:B:145:ASN:ND2	1:B:146:PRO:HG3	2.15	0.62
1:A:225:LEU:HD23	1:A:246:LEU:HD13	1.80	0.62
1:A:543:MET:O	1:A:543:MET:HG3	1.92	0.62
1:B:184:GLY:O	1:B:185:GLU:O	2.17	0.62
1:B:518:MET:O	1:B:522:ASN:HA	2.00	0.62
1:A:106:GLN:HG2	1:A:136:ILE:HG12	1.81	0.62
1:A:255:LYS:H	1:A:255:LYS:CD	2.13	0.62
1:A:575:ASN:OD1	1:A:586:ILE:HD13	1.98	0.62
1:A:585:ILE:HD13	1:A:585:ILE:N	2.14	0.62
1:A:117:GLN:HE22	1:A:167:HIS:HE1	1.45	0.62
1:A:413:ILE:O	1:A:417:ARG:HB2	2.00	0.62
1:A:585:ILE:H	1:A:585:ILE:CD1	2.08	0.62
1:B:86:VAL:HG12	1:B:87:ILE:N	2.14	0.62
1:A:413:ILE:N	1:A:414:PRO:CD	2.63	0.62
1:A:514:LEU:HD12	1:A:532:VAL:HG21	1.82	0.62
1:A:264:GLU:OE1	1:A:598:PHE:HZ	1.83	0.61
1:A:205:PHE:CZ	1:A:249:PRO:HG3	2.36	0.61
1:A:455:GLY:N	1:A:456:PRO:HD2	2.15	0.61
1:B:69:ASP:CG	1:B:70:VAL:N	2.57	0.61
1:B:266:TYR:HD2	1:B:277:LEU:HD12	1.64	0.61
1:A:194:THR:HG21	1:A:234:VAL:CG2	2.30	0.61
1:A:172:ALA:HB1	1:A:174:GLU:CG	2.22	0.61
1:B:255:LYS:H	1:B:255:LYS:HZ2	1.48	0.61
1:B:105:ASP:HB3	1:B:108:ARG:CD	2.31	0.61
1:A:388:LEU:HD22	1:B:402:TYR:CE1	2.36	0.61
1:B:299:PHE:HA	1:B:318:LEU:HD22	1.83	0.61
1:B:148:PRO:HB3	1:B:178:SER:OG	2.01	0.60
1:A:544:ASN:ND2	1:A:547:ARG:HD3	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ILE:HG12	1:B:414:PRO:CD	2.31	0.60
1:B:480:LYS:O	1:B:481:TYR:HB2	2.00	0.60
1:B:572:MET:HE3	1:B:579:HIS:N	2.15	0.60
1:B:60:SER:C	1:B:62:ASN:H	2.09	0.60
1:A:95:LEU:HA	1:A:98:MET:SD	2.41	0.60
1:B:89:ALA:O	1:B:93:VAL:HG23	2.01	0.60
1:B:182:GLU:C	1:B:184:GLY:H	2.08	0.60
1:A:105:ASP:C	1:A:105:ASP:OD1	2.43	0.60
1:A:197:LEU:HD21	1:A:224:PHE:CD2	2.37	0.60
1:A:435:TYR:C	1:A:437:GLY:H	2.09	0.60
1:A:100:LEU:HD13	1:A:112:LEU:HD23	1.82	0.60
1:A:566:GLY:O	1:A:570:GLN:HG3	2.02	0.60
1:A:573:TYR:OH	3:A:600:F3P:H102	2.02	0.60
1:B:385:TYR:OH	1:B:386:MET:HE3	2.02	0.60
1:A:195:ARG:HG3	1:A:196:GLY:N	2.17	0.59
1:A:544:ASN:O	1:A:548:VAL:HG22	2.01	0.59
1:B:72:PHE:C	1:B:72:PHE:HD2	2.10	0.59
1:A:106:GLN:O	1:A:109:GLN:HB2	2.01	0.59
1:A:259:ALA:O	1:A:260:PRO:C	2.43	0.59
1:A:376:ILE:O	1:A:376:ILE:HG13	2.00	0.59
1:B:583:HIS:CB	1:B:586:ILE:HB	2.32	0.59
1:A:254:ILE:HD11	1:A:327:GLY:O	2.02	0.59
1:B:168:GLY:HA2	1:B:548:VAL:HG22	1.84	0.59
1:B:177:ASP:OD2	1:B:180:LYS:HE2	2.02	0.59
1:A:137:TYR:HB2	1:A:164:LEU:CD2	2.33	0.59
1:B:222:THR:O	1:B:223:LYS:C	2.45	0.59
1:A:144:LYS:HE2	1:A:145:ASN:H	1.67	0.59
1:A:335:ALA:O	1:A:339:ILE:HG12	2.03	0.59
1:A:347:LEU:O	1:A:351:ILE:HG13	2.02	0.59
1:B:75:SER:O	1:B:76:LEU:O	2.20	0.59
1:B:413:ILE:N	1:B:414:PRO:HD3	2.18	0.59
1:B:177:ASP:C	1:B:179:PHE:H	2.11	0.59
1:A:480:LYS:O	1:A:481:TYR:HB2	2.01	0.58
1:A:529:ARG:O	1:A:533:LYS:HG3	2.03	0.58
3:A:600:F3P:C7	3:A:600:F3P:C1	2.80	0.58
1:B:584:PRO:HD2	1:B:586:ILE:HG12	1.84	0.58
1:A:544:ASN:O	1:A:547:ARG:HG3	2.03	0.58
4:A:604:BTB:H12	4:A:604:BTB:H52	1.85	0.58
1:B:125:PHE:HB3	1:B:129:PHE:CE1	2.38	0.58
1:A:181:ASN:HD21	1:A:185:GLU:H	1.49	0.58
1:A:529:ARG:HD3	5:A:797:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:VAL:HG13	1:A:176:PHE:N	2.18	0.58
1:B:166:GLU:HA	1:B:547:ARG:NH2	2.18	0.58
1:B:571:LEU:C	1:B:571:LEU:HD12	2.29	0.58
1:A:315:ARG:HB3	1:A:317:ARG:CD	2.34	0.58
1:B:145:ASN:CG	1:B:146:PRO:HD3	2.29	0.58
1:B:415:TYR:OH	1:B:472:LYS:HD3	2.04	0.58
1:A:93:VAL:O	1:A:95:LEU:N	2.37	0.58
4:A:604:BTB:H12	4:A:604:BTB:C5	2.33	0.58
1:B:92:LEU:HD13	1:B:279:LEU:CA	2.33	0.58
1:B:216:SER:O	1:B:219:GLU:HB2	2.04	0.58
1:A:315:ARG:HB3	1:A:317:ARG:HD2	1.86	0.57
1:B:61:GLY:N	1:B:357:VAL:HG13	2.17	0.57
1:B:237:ASP:HB3	1:B:241:ARG:NE	2.19	0.57
1:B:235:ASP:HB2	1:B:238:LEU:HB2	1.85	0.57
1:A:189:SER:O	1:A:190:LEU:C	2.48	0.57
1:A:534:TRP:O	1:A:538:GLU:HG2	2.04	0.57
1:B:189:SER:C	1:B:191:SER:H	2.12	0.57
1:B:310:LYS:C	1:B:312:PRO:HD3	2.29	0.57
1:A:583:HIS:CE1	1:A:585:ILE:HG12	2.39	0.57
1:B:586:ILE:HD13	1:B:589:GLN:NE2	2.20	0.57
1:A:96:VAL:HG23	1:A:275:VAL:HG12	1.87	0.57
1:A:105:ASP:HB3	1:A:108:ARG:CD	2.34	0.57
1:A:149:LYS:HB2	1:A:149:LYS:NZ	2.19	0.57
1:A:202:GLU:CD	1:A:250:LEU:HG	2.29	0.57
1:B:83:ASP:C	1:B:85:HIS:H	2.12	0.57
1:B:215:GLU:O	1:B:219:GLU:HG3	2.04	0.57
1:A:277:LEU:O	1:A:281:ILE:HG13	2.04	0.57
1:B:578:GLY:HA2	1:B:586:ILE:HG13	1.86	0.57
1:A:105:ASP:HB3	1:A:108:ARG:HD3	1.87	0.57
1:B:248:ILE:HB	1:B:253:ARG:NH1	2.20	0.57
1:B:248:ILE:O	1:B:253:ARG:NH1	2.38	0.57
1:B:80:TYR:HA	1:B:85:HIS:CD2	2.40	0.57
1:B:63:TYR:CD1	1:B:581:THR:HG23	2.39	0.57
1:B:281:ILE:HG23	1:B:598:PHE:CD2	2.40	0.57
1:B:443:GLU:HA	1:B:443:GLU:OE1	2.05	0.57
1:A:267:ARG:HG2	1:A:268:LYS:N	2.19	0.56
1:B:284:LEU:HD22	1:B:598:PHE:HB2	1.87	0.56
1:B:332:ARG:HA	1:B:338:ARG:NH2	2.19	0.56
1:B:411:ASN:HD21	1:B:413:ILE:HD13	1.70	0.56
1:A:93:VAL:HG12	1:A:94:THR:N	2.20	0.56
1:A:105:ASP:OD1	1:A:107:ILE:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASP:OD1	1:A:156:SER:N	2.38	0.56
1:A:479:TYR:C	1:A:481:TYR:N	2.60	0.56
1:A:500:THR:HG22	1:A:500:THR:O	2.05	0.56
1:B:208:THR:H	1:B:211:GLU:HG3	1.70	0.56
1:B:234:VAL:C	1:B:236:GLY:H	2.13	0.56
1:B:370:LEU:O	1:B:374:TRP:N	2.38	0.56
1:A:283:ASP:HA	1:A:286:ILE:HD12	1.88	0.56
1:B:170:GLN:HA	1:B:170:GLN:NE2	2.20	0.56
1:A:103:GLU:OE2	1:A:104:THR:N	2.37	0.56
1:A:503:GLU:O	1:A:507:ARG:HB3	2.04	0.56
4:A:604:BTB:C7	4:A:604:BTB:C1	2.81	0.56
1:B:209:GLU:O	1:B:211:GLU:N	2.38	0.56
1:B:385:TYR:CZ	1:B:386:MET:HE3	2.40	0.56
1:B:479:TYR:C	1:B:481:TYR:N	2.54	0.56
1:B:162:ARG:HG2	1:B:162:ARG:HH11	1.70	0.56
1:B:261:VAL:HA	1:B:264:GLU:HG3	1.87	0.56
1:A:329:ILE:HB	1:A:338:ARG:HD3	1.88	0.56
1:A:583:HIS:O	1:A:586:ILE:N	2.37	0.56
1:A:240:THR:O	1:A:244:TYR:N	2.34	0.56
1:B:234:VAL:O	1:B:235:ASP:HB2	2.04	0.56
1:A:98:MET:HA	1:A:101:GLU:CD	2.31	0.56
1:B:164:LEU:HD12	1:B:169:PHE:CD1	2.41	0.56
1:A:137:TYR:HB2	1:A:164:LEU:HD22	1.87	0.55
1:A:554:PHE:HB3	1:A:558:PHE:HD2	1.70	0.55
1:B:457:CYS:O	1:B:461:HIS:HD2	1.89	0.55
1:A:256:ARG:CB	1:A:257:PRO:HD3	2.35	0.55
1:A:441:SER:O	1:A:442:LEU:C	2.48	0.55
1:A:264:GLU:OE1	1:A:264:GLU:N	2.39	0.55
1:B:220:PHE:CD2	1:B:221:ALA:N	2.75	0.55
1:B:578:GLY:O	1:B:580:GLY:N	2.39	0.55
1:A:483:ASP:HB3	1:A:487:TRP:CH2	2.42	0.55
1:B:266:TYR:CD2	1:B:277:LEU:HD12	2.41	0.55
1:B:273:ASN:OD1	1:B:275:VAL:HG12	2.05	0.55
1:B:330:GLU:N	1:B:331:PRO:CD	2.70	0.55
1:B:418:GLN:O	1:B:419:SER:C	2.48	0.55
1:B:487:TRP:HA	1:B:487:TRP:CE3	2.42	0.55
1:A:95:LEU:C	1:A:97:LYS:N	2.63	0.55
1:A:302:TRP:CB	1:A:318:LEU:HD13	2.34	0.55
1:A:89:ALA:HB2	1:A:282:LEU:CD2	2.37	0.55
1:A:570:GLN:O	1:A:574:HIS:HB2	2.07	0.55
1:B:501:SER:O	1:B:505:VAL:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:TYR:HD1	1:A:164:LEU:HD13	1.71	0.55
1:A:209:GLU:CD	5:A:739:HOH:O	2.47	0.55
1:A:501:SER:O	1:A:505:VAL:HG23	2.05	0.55
1:A:82:GLU:O	1:A:85:HIS:ND1	2.32	0.55
1:A:220:PHE:HA	1:A:223:LYS:HE2	1.89	0.55
1:A:302:TRP:O	1:A:305:THR:HG23	2.06	0.55
1:B:162:ARG:HG2	1:B:162:ARG:NH1	2.22	0.55
1:B:264:GLU:HG2	1:B:598:PHE:HZ	1.72	0.55
1:B:526:ALA:O	1:B:530:LYS:HB3	2.07	0.55
1:A:323:PHE:HE1	1:A:593:THR:HG21	1.71	0.55
1:A:177:ASP:C	1:A:179:PHE:H	2.15	0.54
1:A:232:GLY:HA2	1:A:239:LEU:HD11	1.88	0.54
1:A:256:ARG:HB3	1:A:257:PRO:HD3	1.88	0.54
1:A:268:LYS:CE	1:A:270:PRO:HD3	2.36	0.54
1:B:467:THR:HG22	1:B:470:PHE:HD1	1.72	0.54
1:A:82:GLU:N	1:A:82:GLU:OE1	2.41	0.54
1:A:175:VAL:HG13	1:A:176:PHE:CD1	2.42	0.54
1:A:220:PHE:CZ	1:A:224:PHE:HE2	2.25	0.54
1:A:264:GLU:OE1	1:A:598:PHE:CZ	2.61	0.54
1:A:470:PHE:N	1:A:470:PHE:CD2	2.74	0.54
1:A:525:GLU:O	1:A:529:ARG:HB2	2.07	0.54
1:B:96:VAL:HG21	1:B:276:VAL:HA	1.90	0.54
1:A:344:VAL:O	1:A:348:ILE:HG13	2.06	0.54
1:A:413:ILE:HD13	1:A:414:PRO:HD3	1.88	0.54
1:A:583:HIS:CE1	1:A:584:PRO:HG2	2.43	0.54
1:B:470:PHE:N	1:B:470:PHE:CD1	2.75	0.54
1:A:535:LEU:O	1:A:539:VAL:HG13	2.07	0.54
1:B:187:LYS:O	1:B:190:LEU:HG	2.07	0.54
1:B:302:TRP:HB2	1:B:318:LEU:CD1	2.22	0.54
1:B:329:ILE:HG21	1:B:334:HIS:HB2	1.89	0.54
1:B:80:TYR:CD2	1:B:285:ASN:HB3	2.42	0.54
1:B:205:PHE:CE1	1:B:249:PRO:HG3	2.42	0.54
1:B:268:LYS:HD3	1:B:268:LYS:C	2.32	0.54
1:B:446:LEU:HA	1:B:449:SER:OG	2.08	0.54
1:B:583:HIS:ND1	1:B:583:HIS:N	2.56	0.54
1:A:238:LEU:HG	1:A:242:ILE:HD12	1.89	0.54
1:A:433:TRP:CG	1:A:438:HIS:HD1	2.26	0.54
1:B:531:HIS:O	1:B:532:VAL:C	2.49	0.54
1:B:585:ILE:O	1:B:586:ILE:C	2.48	0.54
1:A:501:SER:HA	1:A:512:LYS:HD2	1.89	0.54
1:A:514:LEU:CD1	1:A:532:VAL:HG21	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLU:C	1:A:184:GLY:H	2.15	0.54
1:A:559:ILE:HD12	1:A:559:ILE:O	2.08	0.54
1:B:59:ARG:O	1:B:60:SER:C	2.51	0.54
1:B:70:VAL:O	1:B:74:GLN:N	2.40	0.54
1:B:135:SER:O	1:B:136:ILE:C	2.51	0.54
1:B:267:ARG:HA	1:B:277:LEU:HD13	1.90	0.54
1:B:572:MET:HB3	1:B:578:GLY:HA3	1.89	0.54
1:A:231:GLU:HG2	1:A:232:GLY:N	2.22	0.53
1:A:401:SER:CB	1:A:413:ILE:HG22	2.38	0.53
1:B:129:PHE:CD1	1:B:129:PHE:N	2.74	0.53
1:B:311:LEU:HG	1:B:313:PHE:CE2	2.43	0.53
1:A:220:PHE:C	1:A:222:THR:H	2.15	0.53
1:A:360:THR:OG1	1:A:363:GLU:HG3	2.09	0.53
1:B:87:ILE:HA	1:B:90:SER:HB2	1.90	0.53
1:B:290:GLN:HA	1:B:290:GLN:OE1	2.08	0.53
1:B:486:ARG:NH1	1:B:490:PHE:HE2	2.06	0.53
1:A:200:LEU:HD23	1:A:221:ALA:HB2	1.89	0.53
1:B:190:LEU:C	1:B:192:ASP:H	2.15	0.53
1:A:79:ASP:HA	1:A:81:LYS:CE	2.35	0.53
1:A:119:MET:HG2	1:A:262:TRP:CD1	2.44	0.53
1:A:241:ARG:O	1:A:244:TYR:HB3	2.09	0.53
1:A:465:ARG:HH11	1:A:465:ARG:HG3	1.73	0.53
1:B:256:ARG:NH1	1:B:256:ARG:HG2	2.23	0.53
1:B:572:MET:HA	1:B:586:ILE:HD12	1.89	0.53
1:A:272:MET:O	1:A:272:MET:HE3	2.08	0.53
1:A:173:GLN:HE22	1:A:213:THR:H	1.57	0.53
1:A:234:VAL:HG23	1:A:238:LEU:CD2	2.38	0.53
1:A:311:LEU:N	1:A:312:PRO:HD3	2.24	0.53
1:A:378:SER:C	1:A:380:ASP:H	2.15	0.53
1:A:453:ILE:O	1:A:454:SER:CB	2.57	0.53
1:A:579:HIS:O	1:A:580:GLY:C	2.52	0.53
1:B:92:LEU:HD11	1:B:278:GLU:HG3	1.91	0.53
1:A:88:ARG:O	1:A:91:GLU:HG2	2.09	0.53
1:A:109:GLN:O	1:A:110:LEU:C	2.51	0.53
1:A:135:SER:O	1:A:136:ILE:C	2.52	0.53
1:B:220:PHE:HD2	1:B:221:ALA:N	2.07	0.53
1:B:369:ASP:OD1	1:B:372:ARG:NH1	2.42	0.53
1:A:255:LYS:HB2	1:A:330:GLU:OE2	2.08	0.53
1:A:378:SER:C	1:A:380:ASP:N	2.57	0.53
1:A:555:GLY:O	1:A:559:ILE:HG23	2.09	0.53
1:B:311:LEU:HG	1:B:313:PHE:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:LEU:HD22	1:A:490:PHE:HE1	1.73	0.53
1:B:497:ASP:OD2	1:B:512:LYS:HD3	2.09	0.53
1:B:500:THR:HG22	1:B:500:THR:O	2.08	0.53
1:B:92:LEU:CD1	1:B:278:GLU:HG3	2.39	0.52
1:B:98:MET:O	1:B:102:LYS:HB2	2.09	0.52
1:B:109:GLN:O	1:B:110:LEU:C	2.51	0.52
1:B:117:GLN:HE22	1:B:167:HIS:CE1	2.17	0.52
1:B:240:THR:C	1:B:242:ILE:H	2.17	0.52
1:B:377:ASN:C	1:B:379:ILE:N	2.66	0.52
1:B:401:SER:CB	1:B:413:ILE:HG22	2.39	0.52
1:B:477:SER:O	1:B:480:LYS:HG3	2.09	0.52
1:A:76:LEU:HD11	1:A:595:PHE:CE1	2.44	0.52
1:A:95:LEU:O	1:A:97:LYS:N	2.42	0.52
4:A:604:BTB:C4	4:A:604:BTB:C6	2.84	0.52
1:B:105:ASP:HB3	1:B:108:ARG:HD3	1.91	0.52
1:B:256:ARG:HH11	1:B:256:ARG:HG2	1.75	0.52
1:A:85:HIS:O	1:A:86:VAL:C	2.50	0.52
1:A:479:TYR:C	1:A:481:TYR:H	2.09	0.52
1:B:227:GLU:C	1:B:229:VAL:N	2.65	0.52
1:A:195:ARG:CG	1:A:196:GLY:H	2.22	0.52
1:A:502:VAL:HG23	1:A:503:GLU:N	2.22	0.52
1:B:79:ASP:C	1:B:81:LYS:N	2.66	0.52
1:B:146:PRO:O	1:B:147:PHE:HB2	2.09	0.52
1:B:237:ASP:C	1:B:241:ARG:HE	2.16	0.52
1:B:283:ASP:OD2	1:B:332:ARG:NH2	2.43	0.52
1:A:208:THR:C	1:A:541:LYS:HD2	2.33	0.52
4:A:604:BTB:O4	4:A:604:BTB:C6	2.54	0.52
1:B:190:LEU:O	1:B:197:LEU:HD13	2.10	0.52
1:B:317:ARG:CZ	1:B:581:THR:H	2.23	0.52
1:B:348:ILE:O	1:B:349:THR:C	2.52	0.52
1:A:83:ASP:O	1:A:87:ILE:HG13	2.10	0.52
1:A:93:VAL:C	1:A:95:LEU:N	2.65	0.52
1:A:182:GLU:C	1:A:184:GLY:N	2.65	0.52
1:A:218:ARG:HG3	1:A:218:ARG:NH1	2.05	0.52
1:B:204:SER:CB	1:B:218:ARG:HB2	2.39	0.52
1:A:457:CYS:O	1:A:461:HIS:HD2	1.93	0.52
1:A:585:ILE:N	1:A:585:ILE:CD1	2.73	0.52
1:A:177:ASP:O	1:A:180:LYS:HG2	2.09	0.52
1:A:290:GLN:OE1	1:A:294:GLU:HG3	2.09	0.52
1:B:61:GLY:H	1:B:357:VAL:HG11	1.75	0.52
1:B:351:ILE:HG12	1:B:389:CYS:SG	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:ASP:OD2	1:A:512:LYS:HD3	2.10	0.52
1:B:125:PHE:HA	1:B:128:GLU:OE1	2.09	0.52
1:A:477:SER:O	1:A:480:LYS:HG2	2.10	0.51
1:B:164:LEU:O	1:B:169:PHE:HB2	2.10	0.51
1:B:242:ILE:HG22	1:B:243:ALA:N	2.25	0.51
1:A:301:TRP:CG	1:A:343:LYS:HD3	2.45	0.51
1:A:512:LYS:O	1:A:513:SER:C	2.53	0.51
1:B:415:TYR:O	1:B:418:GLN:HB3	2.11	0.51
1:A:313:PHE:CD1	1:A:358:TYR:HB2	2.45	0.51
1:A:393:LEU:HD21	1:A:420:TRP:CG	2.45	0.51
1:A:433:TRP:CE3	1:A:440:PRO:HG3	2.44	0.51
1:A:521:TYR:N	1:A:521:TYR:CD2	2.79	0.51
1:B:147:PHE:N	1:B:148:PRO:CD	2.72	0.51
1:B:158:SER:HB3	1:B:200:LEU:HA	1.92	0.51
1:B:204:SER:HB2	1:B:218:ARG:HB2	1.92	0.51
1:A:149:LYS:C	1:A:151:GLU:N	2.62	0.51
1:B:228:LYS:HE2	1:B:234:VAL:HG11	1.93	0.51
1:B:235:ASP:C	1:B:237:ASP:N	2.67	0.51
1:B:331:PRO:HB3	1:B:333:GLN:HE21	1.75	0.51
1:B:462:ILE:O	1:B:463:PHE:C	2.53	0.51
1:B:479:TYR:C	1:B:481:TYR:H	2.12	0.51
1:A:299:PHE:HA	1:A:318:LEU:CD2	2.40	0.51
1:A:341:MET:O	1:A:342:GLY:C	2.54	0.51
1:A:465:ARG:HG3	1:A:465:ARG:NH1	2.23	0.51
1:B:225:LEU:HD23	1:B:246:LEU:HD11	1.92	0.51
1:A:261:VAL:O	1:A:264:GLU:HB2	2.11	0.51
1:B:107:ILE:CG1	1:B:156:SER:HB3	2.39	0.51
1:B:235:ASP:HB3	1:B:238:LEU:H	1.76	0.51
1:B:95:LEU:CB	1:B:275:VAL:HG21	2.40	0.51
1:B:281:ILE:HG23	1:B:598:PHE:HB3	1.93	0.51
1:B:531:HIS:O	1:B:534:TRP:N	2.44	0.51
1:A:404:VAL:HG11	1:A:412:VAL:HG21	1.93	0.51
1:A:416:LEU:HG	1:A:461:HIS:CE1	2.46	0.51
1:A:517:TYR:C	1:A:517:TYR:CD2	2.89	0.51
1:A:181:ASN:HD21	1:A:185:GLU:N	2.10	0.50
1:A:269:ARG:HH21	1:A:271:ASP:CB	2.25	0.50
1:B:105:ASP:HB3	1:B:108:ARG:HB2	1.93	0.50
1:B:187:LYS:HB2	1:B:190:LEU:HD23	1.92	0.50
1:A:511:PRO:HB3	1:A:515:GLN:CD	2.36	0.50
1:B:70:VAL:CG1	1:B:74:GLN:HG3	2.42	0.50
1:A:194:THR:HG21	1:A:234:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ALA:O	1:A:175:VAL:HG12	2.11	0.50
1:A:175:VAL:HG13	1:A:176:PHE:H	1.75	0.50
1:A:288:GLN:O	1:A:292:GLN:HG3	2.11	0.50
1:A:413:ILE:N	1:A:414:PRO:HD3	2.27	0.50
1:B:216:SER:HA	1:B:219:GLU:CG	2.42	0.50
1:B:270:PRO:C	1:B:272:MET:H	2.18	0.50
1:B:161:PHE:CD2	1:B:203:ALA:HB1	2.43	0.50
1:B:547:ARG:HG3	1:B:548:VAL:N	2.26	0.50
1:A:442:LEU:HD23	1:A:517:TYR:N	2.26	0.50
1:A:190:LEU:O	1:A:191:SER:C	2.54	0.50
1:A:311:LEU:HD23	1:A:350:VAL:CG1	2.42	0.50
1:A:483:ASP:HB3	1:A:487:TRP:CZ3	2.47	0.50
1:B:512:LYS:HG3	1:B:515:GLN:OE1	2.12	0.50
1:A:154:LEU:HD21	1:A:197:LEU:HD12	1.94	0.49
1:A:284:LEU:C	1:A:284:LEU:HD23	2.36	0.49
1:B:103:GLU:CD	1:B:108:ARG:HD3	2.38	0.49
1:B:181:ASN:C	1:B:181:ASN:ND2	2.62	0.49
1:B:487:TRP:HA	1:B:487:TRP:HE3	1.77	0.49
1:B:587:HIS:ND1	1:B:587:HIS:C	2.69	0.49
1:A:222:THR:CG2	1:A:223:LYS:N	2.75	0.49
1:A:491:VAL:O	1:A:492:LEU:C	2.54	0.49
1:B:63:TYR:HD1	1:B:581:THR:HG23	1.78	0.49
1:B:201:TYR:C	1:B:201:TYR:CD2	2.90	0.49
1:B:240:THR:O	1:B:244:TYR:N	2.45	0.49
1:A:168:GLY:HA2	1:A:548:VAL:CG1	2.42	0.49
1:A:181:ASN:C	1:A:181:ASN:ND2	2.65	0.49
1:A:201:TYR:C	1:A:201:TYR:CD2	2.91	0.49
1:A:207:LEU:C	1:A:207:LEU:HD23	2.37	0.49
1:A:513:SER:O	1:A:514:LEU:C	2.53	0.49
1:A:203:ALA:C	1:A:205:PHE:H	2.20	0.49
1:A:299:PHE:CD1	1:A:303:ARG:HD2	2.48	0.49
1:B:93:VAL:C	1:B:95:LEU:N	2.70	0.49
1:B:149:LYS:HD2	1:B:149:LYS:N	2.28	0.49
1:B:254:ILE:HB	1:B:257:PRO:HD2	1.95	0.49
1:B:259:ALA:O	1:B:260:PRO:C	2.55	0.49
1:A:73:ILE:HG21	1:A:299:PHE:CG	2.48	0.49
1:A:161:PHE:HD1	1:A:171:VAL:HG11	1.78	0.49
1:A:172:ALA:CB	1:A:174:GLU:HG2	2.24	0.49
1:B:93:VAL:O	1:B:95:LEU:N	2.46	0.49
1:B:112:LEU:HD12	1:B:112:LEU:O	2.12	0.49
1:A:220:PHE:CE1	1:A:224:PHE:CE2	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:SER:HB2	1:A:413:ILE:HG22	1.95	0.49
1:B:147:PHE:O	1:B:149:LYS:HD2	2.13	0.49
1:B:332:ARG:C	1:B:338:ARG:HH22	2.21	0.49
1:A:299:PHE:HA	1:A:318:LEU:HD22	1.95	0.48
1:A:307:PHE:O	1:A:311:LEU:N	2.39	0.48
1:A:411:ASN:HD21	1:A:413:ILE:CG2	2.10	0.48
1:B:224:PHE:O	1:B:225:LEU:C	2.56	0.48
1:B:254:ILE:H	1:B:254:ILE:CD1	2.16	0.48
1:A:264:GLU:O	1:A:265:TRP:C	2.56	0.48
1:B:69:ASP:OD1	1:B:69:ASP:C	2.55	0.48
1:B:227:GLU:O	1:B:229:VAL:N	2.46	0.48
1:B:592:ARG:HA	1:B:596:GLU:HG3	1.94	0.48
1:A:412:VAL:C	1:A:414:PRO:HD2	2.38	0.48
1:A:558:PHE:C	1:A:560:GLY:N	2.69	0.48
1:B:147:PHE:CA	1:B:149:LYS:HZ1	2.20	0.48
1:B:370:LEU:HD22	1:B:382:LEU:HD11	1.94	0.48
1:A:69:ASP:OD2	1:A:69:ASP:C	2.56	0.48
1:A:149:LYS:HA	1:A:152:ARG:CZ	2.43	0.48
1:A:544:ASN:HA	1:A:547:ARG:CG	2.43	0.48
1:B:145:ASN:OD1	1:B:146:PRO:HD3	2.13	0.48
1:B:248:ILE:O	1:B:249:PRO:C	2.56	0.48
1:B:313:PHE:CD1	1:B:358:TYR:HB2	2.48	0.48
1:B:512:LYS:HB2	1:B:515:GLN:NE2	2.26	0.48
1:B:584:PRO:HD2	1:B:586:ILE:CG1	2.43	0.48
1:B:586:ILE:HD13	1:B:589:GLN:HE21	1.77	0.48
1:B:229:VAL:HG23	1:B:230:ASN:OD1	2.13	0.48
1:B:505:VAL:HG23	1:B:506:SER:N	2.29	0.48
1:A:145:ASN:HB3	1:A:146:PRO:HD3	1.96	0.48
1:A:268:LYS:O	1:A:269:ARG:C	2.57	0.48
1:B:295:LEU:O	1:B:295:LEU:HD12	2.13	0.48
1:B:445:TYR:CD2	1:B:445:TYR:C	2.92	0.48
1:B:541:LYS:HE2	5:B:788:HOH:O	2.13	0.48
1:A:584:PRO:O	1:A:585:ILE:C	2.56	0.48
1:B:96:VAL:HG13	1:B:276:VAL:CG2	2.44	0.48
1:B:129:PHE:N	1:B:129:PHE:HD1	2.10	0.48
1:B:225:LEU:O	1:B:229:VAL:HG13	2.14	0.48
1:A:192:ASP:O	1:A:193:ASP:HB2	2.13	0.48
1:A:261:VAL:HG22	1:A:262:TRP:N	2.28	0.48
1:A:267:ARG:HB2	1:A:277:LEU:HD21	1.96	0.48
1:A:397:VAL:HG22	1:A:398:ASP:N	2.28	0.48
1:B:93:VAL:HG12	1:B:97:LYS:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:GLU:C	1:B:229:VAL:H	2.21	0.48
1:B:492:LEU:HD22	1:B:565:LEU:HD11	1.95	0.48
1:A:220:PHE:C	1:A:222:THR:N	2.71	0.48
1:A:244:TYR:OH	1:A:253:ARG:HD3	2.14	0.48
1:A:389:CYS:O	1:A:392:ALA:HB3	2.14	0.48
1:A:408:LYS:HE2	1:A:467:THR:O	2.13	0.48
1:A:547:ARG:CB	1:A:559:ILE:HD11	2.44	0.48
1:B:268:LYS:O	1:B:270:PRO:HD3	2.14	0.48
1:A:113:ILE:HG22	1:A:163:LEU:HD21	1.96	0.48
4:A:604:BTB:H32	4:A:604:BTB:C8	2.38	0.48
1:B:256:ARG:CG	1:B:256:ARG:NH1	2.74	0.48
1:B:351:ILE:O	1:B:351:ILE:HG22	2.14	0.48
1:B:521:TYR:CD2	1:B:521:TYR:N	2.82	0.48
1:A:453:ILE:O	1:A:454:SER:HB3	2.14	0.47
1:B:435:TYR:C	1:B:437:GLY:N	2.65	0.47
1:B:453:ILE:O	1:B:454:SER:CB	2.62	0.47
1:A:58:ARG:HA	1:A:58:ARG:HD2	1.42	0.47
1:A:75:SER:O	1:A:76:LEU:O	2.31	0.47
1:A:157:THR:HG21	1:A:179:PHE:HE2	1.79	0.47
1:A:577:ASP:C	1:A:579:HIS:H	2.22	0.47
1:A:583:HIS:O	1:A:586:ILE:HB	2.14	0.47
1:B:87:ILE:H	1:B:87:ILE:HG12	1.37	0.47
1:A:193:ASP:O	1:A:194:THR:C	2.57	0.47
1:B:301:TRP:CG	1:B:343:LYS:HG2	2.49	0.47
1:A:93:VAL:O	1:A:94:THR:C	2.58	0.47
1:A:188:GLU:H	1:A:188:GLU:HG3	1.35	0.47
1:B:100:LEU:C	1:B:102:LYS:H	2.22	0.47
1:B:263:ILE:HG22	1:B:263:ILE:O	2.12	0.47
1:A:435:TYR:C	1:A:437:GLY:N	2.73	0.47
1:A:496:ASP:HA	1:A:573:TYR:CG	2.48	0.47
1:B:240:THR:C	1:B:242:ILE:N	2.72	0.47
1:B:328:ILE:HG12	1:B:565:LEU:HA	1.97	0.47
1:B:332:ARG:HA	1:B:338:ARG:HH22	1.79	0.47
1:A:259:ALA:O	1:A:262:TRP:N	2.47	0.47
1:A:455:GLY:N	1:A:456:PRO:CD	2.77	0.47
1:B:173:GLN:OE1	1:B:211:GLU:HA	2.14	0.47
1:B:268:LYS:O	1:B:269:ARG:C	2.57	0.47
1:B:323:PHE:O	1:B:324:TRP:C	2.57	0.47
1:A:88:ARG:NH2	1:A:91:GLU:HG3	2.27	0.47
1:A:208:THR:O	1:A:211:GLU:HB2	2.14	0.47
1:A:410:VAL:HG21	1:A:470:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:HIS:O	1:A:532:VAL:C	2.57	0.47
1:B:177:ASP:C	1:B:179:PHE:N	2.72	0.47
1:B:348:ILE:O	1:B:352:ASP:N	2.46	0.47
1:B:401:SER:HB2	1:B:413:ILE:HG22	1.97	0.47
1:A:144:LYS:HZ3	1:A:146:PRO:HD2	1.80	0.47
1:A:147:PHE:HE2	1:A:177:ASP:OD1	1.98	0.47
1:A:189:SER:O	1:A:191:SER:N	2.48	0.47
1:A:518:MET:HG3	1:A:528:ALA:HB2	1.97	0.47
1:A:544:ASN:ND2	1:A:547:ARG:HH11	2.12	0.47
1:B:83:ASP:C	1:B:85:HIS:N	2.73	0.47
1:B:357:VAL:HG12	1:B:358:TYR:N	2.30	0.47
1:B:426:LYS:HB2	1:B:426:LYS:HE2	1.47	0.47
1:B:585:ILE:C	1:B:587:HIS:N	2.70	0.47
1:A:70:VAL:HG23	1:A:74:GLN:HG3	1.97	0.47
1:A:75:SER:O	1:A:76:LEU:C	2.57	0.47
1:A:144:LYS:HE2	1:A:146:PRO:HD2	1.96	0.47
1:A:320:GLU:HG3	1:A:590:MET:HE1	1.97	0.47
1:B:93:VAL:O	1:B:94:THR:C	2.56	0.47
1:B:259:ALA:HB3	1:B:260:PRO:CD	2.45	0.47
1:B:441:SER:O	1:B:442:LEU:C	2.58	0.47
1:B:520:ASP:HB3	1:B:521:TYR:CD2	2.50	0.47
1:A:117:GLN:C	1:A:119:MET:H	2.24	0.46
1:A:173:GLN:NE2	1:A:213:THR:H	2.14	0.46
1:A:230:ASN:N	1:A:230:ASN:HD22	2.12	0.46
1:A:161:PHE:HD1	1:A:171:VAL:CG1	2.29	0.46
1:A:260:PRO:O	1:A:263:ILE:N	2.48	0.46
1:B:301:TRP:O	1:B:305:THR:HG23	2.15	0.46
1:B:377:ASN:C	1:B:379:ILE:H	2.21	0.46
1:A:95:LEU:O	1:A:99:GLU:HG2	2.15	0.46
1:A:229:VAL:HA	1:A:239:LEU:CD1	2.45	0.46
1:A:311:LEU:HG	1:A:313:PHE:CZ	2.50	0.46
1:A:518:MET:SD	1:A:525:GLU:HB2	2.55	0.46
1:B:177:ASP:O	1:B:180:LYS:HG3	2.15	0.46
1:B:190:LEU:C	1:B:192:ASP:N	2.71	0.46
1:B:535:LEU:O	1:B:539:VAL:HG23	2.14	0.46
3:B:1600:F3P:C10	3:B:1600:F3P:O3A	2.63	0.46
1:A:337:ALA:O	1:A:341:MET:HG2	2.14	0.46
1:A:438:HIS:CD2	1:A:439:LYS:H	2.33	0.46
1:A:484:LEU:O	1:A:485:VAL:C	2.58	0.46
1:B:147:PHE:HA	1:B:149:LYS:CE	2.45	0.46
1:B:238:LEU:O	1:B:239:LEU:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:O	1:A:96:VAL:C	2.58	0.46
1:A:125:PHE:HB2	1:A:129:PHE:CE2	2.51	0.46
1:B:502:VAL:HG13	5:B:771:HOH:O	2.15	0.46
1:A:157:THR:HG21	1:A:179:PHE:CE2	2.51	0.46
1:A:254:ILE:HD12	1:A:257:PRO:HD2	1.97	0.46
1:A:267:ARG:CG	1:A:268:LYS:N	2.78	0.46
1:A:357:VAL:HG12	1:A:358:TYR:N	2.29	0.46
1:B:98:MET:O	1:B:99:GLU:C	2.59	0.46
1:B:234:VAL:O	1:B:234:VAL:HG13	2.16	0.46
1:A:70:VAL:HG23	1:A:74:GLN:CG	2.46	0.46
1:A:226:GLU:O	1:A:229:VAL:HB	2.16	0.46
1:A:329:ILE:HB	1:A:338:ARG:CD	2.45	0.46
1:B:92:LEU:HD23	1:B:275:VAL:HG23	1.98	0.46
1:B:115:ASP:O	1:B:119:MET:HG3	2.15	0.46
1:B:544:ASN:OD1	1:B:547:ARG:NH1	2.48	0.46
1:B:587:HIS:CE1	1:B:591:THR:OG1	2.68	0.46
1:A:135:SER:O	1:A:138:LEU:N	2.48	0.46
1:A:161:PHE:HE1	1:A:171:VAL:O	1.99	0.46
1:A:177:ASP:C	1:A:179:PHE:N	2.72	0.46
1:A:578:GLY:HA2	1:A:586:ILE:HG21	1.98	0.46
1:B:330:GLU:N	1:B:331:PRO:HD3	2.31	0.46
1:A:89:ALA:HB2	1:A:282:LEU:HD23	1.99	0.46
1:A:385:TYR:CE2	1:A:386:MET:HG3	2.51	0.46
1:A:465:ARG:HA	1:A:465:ARG:HD2	1.68	0.46
1:A:544:ASN:HA	1:A:547:ARG:CD	2.45	0.46
1:B:324:TRP:NE1	1:B:579:HIS:HA	2.28	0.46
1:A:83:ASP:O	1:A:84:LYS:C	2.60	0.45
1:A:260:PRO:O	1:A:264:GLU:OE1	2.35	0.45
1:A:296:LYS:O	1:A:300:ARG:HG3	2.16	0.45
1:A:371:ILE:HG22	1:A:421:VAL:HG22	1.97	0.45
1:A:393:LEU:O	1:A:397:VAL:HG13	2.16	0.45
1:B:256:ARG:CB	1:B:257:PRO:HD3	2.45	0.45
1:B:519:SER:O	1:B:520:ASP:C	2.57	0.45
1:A:98:MET:O	1:A:102:LYS:CB	2.64	0.45
1:A:98:MET:O	1:A:102:LYS:HG3	2.15	0.45
1:B:256:ARG:C	1:B:258:ASN:H	2.24	0.45
1:A:70:VAL:H	1:A:70:VAL:HG12	1.50	0.45
1:A:92:LEU:HD23	1:A:279:LEU:CA	2.46	0.45
1:A:273:ASN:OD1	1:A:274:PRO:N	2.49	0.45
1:A:544:ASN:O	1:A:548:VAL:CG2	2.64	0.45
1:A:547:ARG:HA	1:A:559:ILE:CD1	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ASN:HD21	1:B:146:PRO:HG3	1.80	0.45
1:A:119:MET:HG2	1:A:262:TRP:HD1	1.79	0.45
1:A:180:LYS:HB2	1:A:185:GLU:O	2.17	0.45
1:A:367:PHE:CD2	1:A:386:MET:HE2	2.51	0.45
1:A:483:ASP:O	1:A:486:ARG:HB3	2.17	0.45
1:A:548:VAL:O	1:A:549:SER:C	2.58	0.45
1:B:76:LEU:O	1:B:77:LEU:HD12	2.16	0.45
1:B:234:VAL:O	1:B:236:GLY:N	2.44	0.45
1:B:572:MET:HE3	1:B:579:HIS:H	1.78	0.45
1:A:128:GLU:O	1:A:129:PHE:C	2.59	0.45
1:A:204:SER:OG	1:A:218:ARG:HG3	2.16	0.45
1:A:453:ILE:HD13	1:A:493:ARG:HA	1.98	0.45
1:A:493:ARG:HG3	1:A:494:LEU:N	2.17	0.45
1:B:58:ARG:HA	1:B:58:ARG:HD3	1.68	0.45
1:A:96:VAL:CA	1:A:99:GLU:HG3	2.44	0.45
1:A:97:LYS:O	1:A:100:LEU:N	2.49	0.45
1:A:144:LYS:CE	1:A:146:PRO:HD2	2.46	0.45
1:B:237:ASP:O	1:B:238:LEU:C	2.58	0.45
1:B:455:GLY:N	1:B:456:PRO:CD	2.80	0.45
1:B:579:HIS:CG	3:B:1600:F3P:H12	2.51	0.45
1:A:446:LEU:HA	1:A:449:SER:OG	2.17	0.45
1:B:268:LYS:O	1:B:270:PRO:N	2.50	0.45
1:B:269:ARG:O	1:B:270:PRO:C	2.57	0.45
1:A:68:TRP:HZ3	1:A:320:GLU:CD	2.25	0.45
1:A:449:SER:CB	1:A:493:ARG:HD3	2.41	0.45
1:B:270:PRO:O	1:B:272:MET:N	2.42	0.45
1:B:105:ASP:HB3	1:B:108:ARG:HD2	1.99	0.45
1:B:252:TRP:CD1	1:B:252:TRP:N	2.85	0.45
1:B:351:ILE:O	1:B:351:ILE:CG2	2.65	0.45
1:A:140:HIS:O	1:A:141:HIS:C	2.60	0.45
1:A:304:ASN:O	1:A:305:THR:C	2.60	0.45
1:A:507:ARG:O	1:A:507:ARG:HG2	2.16	0.45
1:B:177:ASP:O	1:B:179:PHE:N	2.50	0.45
1:B:208:THR:C	1:B:541:LYS:HD3	2.42	0.45
1:B:224:PHE:CD2	1:B:224:PHE:N	2.85	0.45
1:B:242:ILE:C	1:B:244:TYR:N	2.74	0.45
1:A:70:VAL:HG23	1:A:74:GLN:HB2	1.99	0.44
1:A:222:THR:O	1:A:226:GLU:HG2	2.17	0.44
1:A:364:LEU:HD23	1:A:386:MET:HE1	1.98	0.44
1:A:373:ARG:HH11	1:A:373:ARG:CG	2.27	0.44
1:B:189:SER:O	1:B:191:SER:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ILE:HG12	1:B:568:MET:HA	2.00	0.44
1:A:228:LYS:HB2	1:A:228:LYS:HE3	1.62	0.44
1:A:238:LEU:O	1:A:242:ILE:HB	2.17	0.44
1:B:92:LEU:CD2	1:B:278:GLU:HG2	2.46	0.44
1:B:174:GLU:O	1:B:177:ASP:HB2	2.17	0.44
1:A:235:ASP:HB3	1:A:237:ASP:H	1.83	0.44
1:A:378:SER:O	1:A:380:ASP:N	2.49	0.44
1:A:515:GLN:HA	1:A:518:MET:CE	2.43	0.44
1:B:376:ILE:H	1:B:376:ILE:HG12	1.40	0.44
1:B:443:GLU:OE1	1:B:446:LEU:HB2	2.17	0.44
1:A:175:VAL:C	1:A:177:ASP:H	2.25	0.44
1:B:310:LYS:O	1:B:312:PRO:HD3	2.18	0.44
1:B:559:ILE:O	1:B:563:VAL:HG23	2.16	0.44
1:A:95:LEU:O	1:A:98:MET:SD	2.76	0.44
1:A:223:LYS:HD2	1:A:224:PHE:N	2.32	0.44
1:A:482:HIS:O	1:A:485:VAL:HB	2.17	0.44
1:A:521:TYR:O	1:A:522:ASN:C	2.58	0.44
1:B:60:SER:C	1:B:62:ASN:N	2.75	0.44
1:B:193:ASP:O	1:B:194:THR:C	2.61	0.44
1:B:520:ASP:HB3	1:B:521:TYR:CE2	2.52	0.44
1:A:269:ARG:O	1:A:272:MET:CB	2.64	0.44
1:A:365:GLU:OE2	1:A:365:GLU:HA	2.18	0.44
1:A:433:TRP:HA	1:A:438:HIS:HB3	2.00	0.44
1:B:270:PRO:C	1:B:272:MET:N	2.73	0.44
1:A:116:LEU:HD13	1:A:125:PHE:CD2	2.52	0.44
1:A:125:PHE:O	1:A:129:PHE:CD2	2.71	0.44
1:A:244:TYR:CZ	1:A:253:ARG:HD3	2.52	0.44
1:A:353:ASP:O	1:A:357:VAL:HB	2.18	0.44
1:B:329:ILE:CG2	1:B:334:HIS:HB2	2.48	0.44
1:B:412:VAL:C	1:B:414:PRO:CD	2.90	0.44
1:B:543:MET:O	1:B:543:MET:HG3	2.05	0.44
3:A:600:F3P:C6	3:A:600:F3P:C1	2.74	0.44
1:B:129:PHE:O	1:B:133:LEU:HD12	2.18	0.44
1:B:411:ASN:C	1:B:411:ASN:HD22	2.25	0.44
1:B:512:LYS:C	1:B:515:GLN:NE2	2.76	0.44
4:A:604:BTB:C2	4:A:604:BTB:C5	2.82	0.44
1:B:60:SER:O	1:B:62:ASN:N	2.46	0.44
1:B:176:PHE:CE1	1:B:214:LEU:HD21	2.53	0.44
1:B:181:ASN:N	1:B:187:LYS:HG2	2.33	0.44
1:A:107:ILE:HG12	1:A:156:SER:HB2	2.00	0.43
1:A:259:ALA:HB3	1:A:260:PRO:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ASP:O	1:B:507:ARG:NH2	2.51	0.43
1:B:529:ARG:HA	1:B:529:ARG:HD3	1.89	0.43
1:A:107:ILE:HG23	1:A:111:GLU:OE1	2.18	0.43
1:A:328:ILE:HG12	1:A:565:LEU:HA	2.00	0.43
1:A:365:GLU:CD	1:A:428:MET:HE2	2.43	0.43
1:A:378:SER:O	1:A:379:ILE:C	2.61	0.43
1:A:520:ASP:HB3	1:A:521:TYR:CD2	2.53	0.43
1:A:550:LYS:NZ	5:A:755:HOH:O	2.45	0.43
1:B:61:GLY:O	1:B:62:ASN:C	2.61	0.43
1:B:79:ASP:C	1:B:81:LYS:H	2.25	0.43
1:B:198:LEU:O	1:B:202:GLU:HB2	2.19	0.43
1:B:216:SER:HA	1:B:219:GLU:HG3	2.00	0.43
1:A:465:ARG:HH11	1:A:465:ARG:CG	2.31	0.43
1:B:70:VAL:HG13	1:B:74:GLN:HG3	2.00	0.43
1:B:457:CYS:O	1:B:461:HIS:CD2	2.69	0.43
1:B:496:ASP:HA	1:B:573:TYR:CG	2.53	0.43
1:A:103:GLU:HG2	1:A:109:GLN:HG3	2.01	0.43
1:A:107:ILE:HD11	1:A:156:SER:OG	2.18	0.43
1:A:168:GLY:HA2	1:A:548:VAL:HG12	2.00	0.43
1:B:311:LEU:CD1	1:B:385:TYR:HB2	2.45	0.43
1:B:567:ARG:HA	1:B:570:GLN:HG3	2.01	0.43
1:A:379:ILE:O	1:A:387:GLN:HG2	2.18	0.43
1:A:454:SER:OG	1:A:458:MET:HG3	2.19	0.43
1:A:535:LEU:HA	1:A:535:LEU:HD23	1.77	0.43
1:A:571:LEU:HD23	1:A:572:MET:N	2.33	0.43
1:B:147:PHE:CA	1:B:149:LYS:NZ	2.79	0.43
1:B:181:ASN:ND2	1:B:184:GLY:O	2.52	0.43
1:B:188:GLU:O	1:B:189:SER:C	2.60	0.43
1:B:290:GLN:O	1:B:294:GLU:HG3	2.18	0.43
1:A:477:SER:O	1:A:478:LEU:C	2.58	0.43
1:A:586:ILE:HG22	1:A:587:HIS:N	2.33	0.43
1:A:587:HIS:C	1:A:587:HIS:CD2	2.96	0.43
1:A:189:SER:C	1:A:191:SER:N	2.72	0.43
1:B:147:PHE:HA	1:B:149:LYS:HE2	2.01	0.43
1:A:313:PHE:CZ	1:A:354:ILE:HG13	2.54	0.43
1:A:426:LYS:HG3	1:A:451:GLN:HB3	2.00	0.43
1:A:577:ASP:C	1:A:579:HIS:N	2.77	0.43
1:B:128:GLU:O	1:B:129:PHE:C	2.62	0.43
1:B:155:TYR:HD1	1:B:196:GLY:HA2	1.84	0.43
1:B:485:VAL:O	1:B:489:SER:OG	2.36	0.43
1:B:585:ILE:O	1:B:588:GLN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ASN:HA	1:A:65:PRO:HD3	1.88	0.43
1:A:232:GLY:C	1:A:234:VAL:H	2.25	0.43
1:B:107:ILE:O	1:B:111:GLU:HB2	2.19	0.43
1:B:218:ARG:HH11	1:B:218:ARG:CG	2.32	0.43
1:B:426:LYS:HD3	1:B:426:LYS:HA	1.81	0.43
1:B:525:GLU:O	1:B:529:ARG:HB2	2.18	0.43
1:A:113:ILE:HG22	1:A:114:ASP:N	2.31	0.43
1:A:207:LEU:HG	1:A:541:LYS:HD3	2.00	0.43
1:A:220:PHE:CE1	1:A:224:PHE:HE2	2.36	0.43
1:A:228:LYS:O	1:A:232:GLY:N	2.52	0.43
1:B:95:LEU:HD23	1:B:275:VAL:CG2	2.48	0.43
1:B:165:ARG:HB2	1:B:206:LEU:HD22	2.01	0.43
1:B:535:LEU:HD23	1:B:535:LEU:HA	1.82	0.43
1:A:138:LEU:CD1	1:A:138:LEU:C	2.92	0.42
1:B:95:LEU:O	1:B:98:MET:N	2.46	0.42
1:B:153:ASP:O	1:B:154:LEU:C	2.62	0.42
1:B:220:PHE:CD2	1:B:220:PHE:C	2.97	0.42
1:B:416:LEU:HD12	1:B:416:LEU:HA	1.77	0.42
1:B:572:MET:O	1:B:586:ILE:HD11	2.19	0.42
1:B:592:ARG:NH2	1:B:598:PHE:HE1	2.17	0.42
1:A:311:LEU:HD23	1:A:350:VAL:HG11	2.00	0.42
1:A:442:LEU:HD23	1:A:516:CYS:CB	2.49	0.42
1:A:592:ARG:NH2	1:A:598:PHE:HD2	2.17	0.42
1:B:98:MET:C	1:B:100:LEU:N	2.75	0.42
1:B:412:VAL:C	1:B:414:PRO:HD2	2.44	0.42
1:B:580:GLY:C	1:B:582:GLN:H	2.25	0.42
1:A:95:LEU:C	1:A:97:LYS:H	2.28	0.42
1:A:147:PHE:CE2	1:A:177:ASP:OD1	2.73	0.42
1:A:507:ARG:NH2	1:A:508:GLY:O	2.53	0.42
1:B:115:ASP:O	1:B:116:LEU:C	2.62	0.42
1:B:255:LYS:O	1:B:256:ARG:C	2.61	0.42
1:B:477:SER:HA	1:B:480:LYS:HE2	2.02	0.42
1:A:115:ASP:O	1:A:116:LEU:C	2.63	0.42
1:A:579:HIS:HB3	1:A:580:GLY:H	1.57	0.42
1:B:117:GLN:NE2	1:B:167:HIS:CE1	2.79	0.42
1:B:135:SER:O	1:B:138:LEU:N	2.53	0.42
1:B:165:ARG:HB2	1:B:206:LEU:CD2	2.49	0.42
1:B:182:GLU:HG2	1:B:183:GLU:CG	2.50	0.42
1:B:458:MET:SD	3:B:1600:F3P:H91	2.59	0.42
1:A:177:ASP:O	1:A:179:PHE:N	2.52	0.42
1:A:330:GLU:N	1:A:331:PRO:CD	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:O	1:B:102:LYS:N	2.53	0.42
1:B:181:ASN:ND2	1:B:182:GLU:N	2.67	0.42
1:B:182:GLU:C	1:B:184:GLY:N	2.76	0.42
1:B:189:SER:C	1:B:191:SER:N	2.75	0.42
1:B:329:ILE:H	1:B:329:ILE:HD12	1.84	0.42
1:B:491:VAL:O	1:B:492:LEU:C	2.60	0.42
1:A:311:LEU:HD11	1:A:385:TYR:HB2	2.01	0.42
1:A:373:ARG:HG3	1:A:373:ARG:NH1	2.27	0.42
4:A:604:BTB:H42	4:A:604:BTB:C6	2.46	0.42
1:B:92:LEU:CD2	1:B:275:VAL:HG23	2.49	0.42
1:B:453:ILE:HB	1:B:493:ARG:NH1	2.35	0.42
1:B:580:GLY:O	1:B:582:GLN:N	2.42	0.42
1:A:147:PHE:HA	1:A:148:PRO:HD3	1.82	0.42
1:A:187:LYS:CB	1:A:190:LEU:HD22	2.49	0.42
1:A:220:PHE:O	1:A:223:LYS:HG3	2.19	0.42
1:B:64:ASN:HA	1:B:65:PRO:HD3	1.73	0.42
1:B:180:LYS:HA	1:B:186:PHE:HA	2.02	0.42
1:B:515:GLN:CA	1:B:518:MET:HG3	2.43	0.42
1:B:580:GLY:HA2	1:B:583:HIS:CE1	2.54	0.42
1:A:117:GLN:C	1:A:119:MET:N	2.77	0.42
1:B:317:ARG:HE	1:B:317:ARG:HB3	1.33	0.42
1:B:353:ASP:O	1:B:357:VAL:HB	2.20	0.42
1:B:483:ASP:HB3	1:B:487:TRP:NE1	2.35	0.42
1:A:93:VAL:HA	1:A:279:LEU:HD22	2.02	0.42
1:A:105:ASP:HB3	1:A:108:ARG:HB2	2.02	0.42
1:A:144:LYS:HD3	1:A:146:PRO:HG2	2.02	0.42
1:B:507:ARG:NH2	1:B:508:GLY:O	2.53	0.42
1:B:575:ASN:HD22	1:B:586:ILE:HD11	1.85	0.42
1:A:203:ALA:C	1:A:205:PHE:N	2.77	0.42
1:A:571:LEU:C	1:A:571:LEU:CD2	2.92	0.42
1:B:255:LYS:O	1:B:258:ASN:N	2.45	0.42
1:A:72:PHE:HE2	1:A:595:PHE:CE2	2.38	0.41
1:A:174:GLU:O	1:A:177:ASP:HB2	2.20	0.41
1:A:182:GLU:O	1:A:184:GLY:N	2.53	0.41
1:A:268:LYS:HG3	1:A:269:ARG:N	2.35	0.41
1:A:433:TRP:CA	1:A:438:HIS:HB3	2.50	0.41
1:B:454:SER:O	1:B:455:GLY:C	2.63	0.41
1:A:95:LEU:HB2	1:A:275:VAL:HG11	2.01	0.41
1:A:373:ARG:CG	1:A:373:ARG:NH1	2.83	0.41
1:B:239:LEU:N	1:B:239:LEU:HD23	2.35	0.41
1:B:260:PRO:HD3	1:B:284:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:LEU:HD23	1:B:350:VAL:CG1	2.50	0.41
1:A:224:PHE:O	1:A:225:LEU:C	2.62	0.41
1:A:362:GLU:OE2	1:A:362:GLU:HA	2.18	0.41
1:A:418:GLN:O	1:A:418:GLN:HG3	2.20	0.41
1:A:426:LYS:HA	1:A:426:LYS:HD3	1.60	0.41
1:B:83:ASP:OD2	1:B:83:ASP:N	2.51	0.41
1:B:177:ASP:O	1:B:180:LYS:CG	2.69	0.41
1:B:182:GLU:HG2	1:B:183:GLU:HG2	2.01	0.41
1:B:216:SER:O	1:B:217:ALA:C	2.63	0.41
1:B:333:GLN:H	1:B:333:GLN:HG3	1.34	0.41
1:B:348:ILE:HD13	1:B:454:SER:HB2	2.01	0.41
1:B:482:HIS:ND1	1:B:483:ASP:N	2.67	0.41
1:B:518:MET:O	1:B:522:ASN:CA	2.68	0.41
1:A:220:PHE:CZ	1:A:224:PHE:CE2	3.08	0.41
1:B:165:ARG:CB	1:B:206:LEU:HD23	2.50	0.41
1:B:510:VAL:HG12	1:B:511:PRO:N	2.34	0.41
1:A:96:VAL:HG22	1:A:276:VAL:HG23	2.02	0.41
1:A:583:HIS:ND1	1:A:583:HIS:C	2.78	0.41
1:B:103:GLU:OE1	1:B:105:ASP:N	2.54	0.41
1:B:162:ARG:HH11	1:B:162:ARG:CG	2.33	0.41
1:B:234:VAL:C	1:B:236:GLY:N	2.73	0.41
1:B:255:LYS:HZ3	1:B:255:LYS:N	2.08	0.41
1:B:393:LEU:O	1:B:397:VAL:HG13	2.19	0.41
1:B:482:HIS:ND1	1:B:482:HIS:C	2.79	0.41
1:B:496:ASP:HB2	1:B:573:TYR:CE2	2.56	0.41
1:A:130:LYS:O	1:A:134:SER:HB2	2.20	0.41
1:A:241:ARG:O	1:A:241:ARG:NH2	2.53	0.41
1:B:93:VAL:CG1	1:B:97:LYS:HE2	2.50	0.41
1:B:256:ARG:HB2	1:B:330:GLU:CD	2.46	0.41
1:A:232:GLY:C	1:A:234:VAL:N	2.78	0.41
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.93	0.41
1:A:402:TYR:HD1	1:B:391:LEU:HD23	1.85	0.41
1:B:411:ASN:ND2	1:B:413:ILE:HD13	2.36	0.41
1:A:260:PRO:O	1:A:261:VAL:C	2.62	0.41
1:B:75:SER:O	1:B:76:LEU:C	2.63	0.41
1:A:97:LYS:O	1:A:98:MET:C	2.64	0.41
1:A:166:GLU:HB2	1:A:206:LEU:HD11	2.03	0.41
1:A:186:PHE:CD2	1:A:190:LEU:HD23	2.46	0.41
1:A:205:PHE:CE1	1:A:249:PRO:HG3	2.56	0.41
1:A:263:ILE:CD1	1:A:284:LEU:HD12	2.51	0.41
1:A:496:ASP:OD2	1:A:496:ASP:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ARG:O	1:B:60:SER:O	2.38	0.41
1:B:70:VAL:O	1:B:74:GLN:HG2	2.21	0.41
1:B:92:LEU:HD11	1:B:278:GLU:CG	2.50	0.41
1:B:147:PHE:C	1:B:149:LYS:NZ	2.79	0.41
1:B:299:PHE:HA	1:B:318:LEU:CD2	2.48	0.41
1:A:323:PHE:O	1:A:326:THR:HG23	2.21	0.41
1:B:241:ARG:HG2	1:B:265:TRP:CZ3	2.56	0.41
1:B:267:ARG:HA	1:B:277:LEU:HD11	2.00	0.41
1:B:268:LYS:CD	1:B:270:PRO:HD3	2.47	0.41
1:B:374:TRP:CD2	1:B:417:ARG:HG2	2.55	0.41
1:B:585:ILE:O	1:B:587:HIS:N	2.54	0.41
1:A:113:ILE:CD1	1:A:132:ILE:HG21	2.51	0.40
1:B:124:HIS:ND1	1:B:124:HIS:N	2.69	0.40
1:B:137:TYR:CD1	1:B:142:TYR:HB2	2.56	0.40
1:B:165:ARG:NH2	1:B:211:GLU:OE1	2.49	0.40
1:B:273:ASN:HA	1:B:274:PRO:HD3	1.96	0.40
1:A:74:GLN:OE1	1:A:299:PHE:HD1	2.03	0.40
1:A:79:ASP:C	1:A:82:GLU:OE1	2.64	0.40
1:A:220:PHE:O	1:A:222:THR:N	2.54	0.40
1:A:532:VAL:O	1:A:536:ILE:HG13	2.22	0.40
1:A:535:LEU:HD22	4:A:604:BTB:H71	2.02	0.40
4:A:604:BTB:C1	4:A:604:BTB:H52	2.46	0.40
1:B:457:CYS:O	1:B:458:MET:C	2.62	0.40
1:B:481:TYR:HD1	1:B:481:TYR:HA	1.67	0.40
1:B:512:LYS:O	1:B:513:SER:C	2.64	0.40
1:A:93:VAL:C	1:A:95:LEU:H	2.30	0.40
1:A:137:TYR:HB2	1:A:164:LEU:HD21	2.02	0.40
1:A:153:ASP:OD1	1:A:155:TYR:N	2.55	0.40
1:A:204:SER:O	1:A:218:ARG:NH1	2.53	0.40
4:A:604:BTB:C4	4:A:604:BTB:C5	2.99	0.40
1:B:132:ILE:O	1:B:133:LEU:C	2.61	0.40
1:B:358:TYR:HB3	1:B:359:GLY:H	1.76	0.40
1:A:96:VAL:HG13	1:A:276:VAL:HG22	2.02	0.40
1:A:229:VAL:HA	1:A:239:LEU:HD13	2.03	0.40
1:A:512:LYS:O	1:A:515:GLN:N	2.53	0.40
1:B:59:ARG:NH2	1:B:435:TYR:OH	2.52	0.40
1:B:198:LEU:HD22	1:B:242:ILE:HG12	2.04	0.40
1:B:227:GLU:O	1:B:228:LYS:C	2.64	0.40
1:B:238:LEU:HD12	1:B:238:LEU:HA	1.77	0.40
1:A:175:VAL:CG1	1:A:176:PHE:N	2.85	0.40
1:A:493:ARG:CG	1:A:494:LEU:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:SER:OG	1:B:218:ARG:HB2	2.21	0.40
1:B:486:ARG:NH1	1:B:490:PHE:CE2	2.87	0.40
1:B:540:TRP:NE1	1:B:570:GLN:OE1	2.46	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:737:HOH:O	5:B:707:HOH:O[7_554]	2.12	0.08

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	541/543 (100%)	428 (79%)	78 (14%)	35 (6%)	1	1
1	B	541/543 (100%)	407 (75%)	94 (17%)	40 (7%)	1	1
All	All	1082/1086 (100%)	835 (77%)	172 (16%)	75 (7%)	1	1

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	76	LEU
1	A	181	ASN
1	A	193	ASP
1	A	235	ASP
1	A	502	VAL
1	A	513	SER
1	B	60	SER
1	B	62	ASN
1	B	76	LEU

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Mol	Chain	Res	Type
1	B	140	HIS
1	B	146	PRO
1	B	147	PHE
1	B	150	GLU
1	B	155	TYR
1	B	185	GLU
1	B	359	GLY
1	B	556	LYS
1	B	579	HIS
1	B	582	GLN
1	A	94	THR
1	A	152	ARG
1	A	260	PRO
1	A	359	GLY
1	A	580	GLY
1	A	582	GLN
1	B	59	ARG
1	B	69	ASP
1	B	101	GLU
1	B	178	SER
1	B	190	LEU
1	B	193	ASP
1	B	210	GLY
1	B	231	GLU
1	B	233	GLY
1	B	260	PRO
1	B	358	TYR
1	B	502	VAL
1	B	507	ARG
1	B	584	PRO
1	A	59	ARG
1	A	136	ILE
1	A	178	SER
1	A	221	ALA
1	A	472	LYS
1	A	584	PRO
1	B	156	SER
1	B	162	ARG
1	B	183	GLU
1	B	332	ARG
1	A	195	ARG
1	A	358	TYR

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Mol	Chain	Res	Type
1	A	442	LEU
1	A	504	GLU
1	B	94	THR
1	B	100	LEU
1	B	481	TYR
1	A	176	PHE
1	A	190	LEU
1	A	234	VAL
1	A	522	ASN
1	B	182	GLU
1	B	228	LYS
1	B	514	LEU
1	A	58	ARG
1	A	96	VAL
1	A	224	PHE
1	A	236	GLY
1	A	440	PRO
1	B	93	VAL
1	B	269	ARG
1	A	269	ARG
1	A	274	PRO
1	B	578	GLY
1	A	308	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	491/492 (100%)	337 (69%)	154 (31%)	0	1
1	B	491/492 (100%)	346 (70%)	145 (30%)	0	1
All	All	982/984 (100%)	683 (70%)	299 (30%)	0	1

All (299) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ARG
1	A	59	ARG
1	A	60	SER
1	A	62	ASN
1	A	69	ASP
1	A	70	VAL
1	A	77	LEU
1	A	78	SER
1	A	79	ASP
1	A	81	LYS
1	A	84	LYS
1	A	85	HIS
1	A	88	ARG
1	A	90	SER
1	A	93	VAL
1	A	98	MET
1	A	101	GLU
1	A	103	GLU
1	A	104	THR
1	A	107	ILE
1	A	108	ARG
1	A	111	GLU
1	A	113	ILE
1	A	122	SER
1	A	126	GLN
1	A	127	ASN
1	A	131	GLU
1	A	132	ILE
1	A	134	SER
1	A	138	LEU
1	A	140	HIS
1	A	144	LYS
1	A	147	PHE
1	A	149	LYS
1	A	150	GLU
1	A	151	GLU
1	A	152	ARG
1	A	153	ASP
1	A	157	THR
1	A	165	ARG
1	A	173	GLN
1	A	174	GLU
1	A	180	LYS

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Mol	Chain	Res	Type
1	A	181	ASN
1	A	183	GLU
1	A	186	PHE
1	A	187	LYS
1	A	188	GLU
1	A	189	SER
1	A	190	LEU
1	A	191	SER
1	A	199	GLN
1	A	200	LEU
1	A	201	TYR
1	A	202	GLU
1	A	206	LEU
1	A	207	LEU
1	A	208	THR
1	A	214	LEU
1	A	218	ARG
1	A	222	THR
1	A	223	LYS
1	A	225	LEU
1	A	228	LYS
1	A	229	VAL
1	A	231	GLU
1	A	234	VAL
1	A	238	LEU
1	A	241	ARG
1	A	242	ILE
1	A	254	ILE
1	A	255	LYS
1	A	256	ARG
1	A	261	VAL
1	A	263	ILE
1	A	264	GLU
1	A	268	LYS
1	A	272	MET
1	A	278	GLU
1	A	290	GLN
1	A	296	LYS
1	A	297	GLU
1	A	298	SER
1	A	305	THR
1	A	308	VAL

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Mol	Chain	Res	Type
1	A	309	GLU
1	A	310	LYS
1	A	311	LEU
1	A	317	ARG
1	A	319	VAL
1	A	329	ILE
1	A	333	GLN
1	A	336	SER
1	A	339	ILE
1	A	361	LEU
1	A	362	GLU
1	A	366	GLN
1	A	370	LEU
1	A	376	ILE
1	A	381	GLN
1	A	382	LEU
1	A	384	ASP
1	A	388	LEU
1	A	393	LEU
1	A	397	VAL
1	A	399	ASP
1	A	404	VAL
1	A	405	MET
1	A	406	LYS
1	A	407	GLU
1	A	413	ILE
1	A	417	ARG
1	A	429	VAL
1	A	439	LYS
1	A	442	LEU
1	A	454	SER
1	A	465	ARG
1	A	466	VAL
1	A	469	SER
1	A	470	PHE
1	A	473	GLU
1	A	489	SER
1	A	490	PHE
1	A	493	ARG
1	A	501	SER
1	A	503	GLU
1	A	505	VAL

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Mol	Chain	Res	Type
1	A	506	SER
1	A	507	ARG
1	A	510	VAL
1	A	512	LYS
1	A	513	SER
1	A	519	SER
1	A	520	ASP
1	A	533	LYS
1	A	536	ILE
1	A	543	MET
1	A	544	ASN
1	A	548	VAL
1	A	550	LYS
1	A	552	SER
1	A	556	LYS
1	A	559	ILE
1	A	575	ASN
1	A	579	HIS
1	A	581	THR
1	A	582	GLN
1	A	585	ILE
1	A	586	ILE
1	A	588	GLN
1	A	589	GLN
1	A	590	MET
1	A	591	THR
1	A	592	ARG
1	B	59	ARG
1	B	60	SER
1	B	62	ASN
1	B	66	SER
1	B	72	PHE
1	B	74	GLN
1	B	77	LEU
1	B	78	SER
1	B	81	LYS
1	B	83	ASP
1	B	84	LYS
1	B	86	VAL
1	B	87	ILE
1	B	95	LEU
1	B	97	LYS

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Mol	Chain	Res	Type
1	B	98	MET
1	B	99	GLU
1	B	102	LYS
1	B	107	ILE
1	B	111	GLU
1	B	118	ARG
1	B	119	MET
1	B	121	LEU
1	B	122	SER
1	B	124	HIS
1	B	127	ASN
1	B	130	LYS
1	B	131	GLU
1	B	134	SER
1	B	140	HIS
1	B	147	PHE
1	B	149	LYS
1	B	154	LEU
1	B	159	LEU
1	B	164	LEU
1	B	170	GLN
1	B	171	VAL
1	B	173	GLN
1	B	174	GLU
1	B	178	SER
1	B	180	LYS
1	B	181	ASN
1	B	183	GLU
1	B	187	LYS
1	B	188	GLU
1	B	189	SER
1	B	195	ARG
1	B	199	GLN
1	B	201	TYR
1	B	202	GLU
1	B	207	LEU
1	B	208	THR
1	B	209	GLU
1	B	211	GLU
1	B	215	GLU
1	B	216	SER
1	B	218	ARG

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Mol	Chain	Res	Type
1	B	225	LEU
1	B	228	LYS
1	B	231	GLU
1	B	235	ASP
1	B	239	LEU
1	B	242	ILE
1	B	250	LEU
1	B	253	ARG
1	B	254	ILE
1	B	255	LYS
1	B	256	ARG
1	B	258	ASN
1	B	261	VAL
1	B	264	GLU
1	B	269	ARG
1	B	271	ASP
1	B	272	MET
1	B	276	VAL
1	B	278	GLU
1	B	281	ILE
1	B	290	GLN
1	B	304	ASN
1	B	308	VAL
1	B	309	GLU
1	B	317	ARG
1	B	318	LEU
1	B	319	VAL
1	B	332	ARG
1	B	333	GLN
1	B	336	SER
1	B	361	LEU
1	B	362	GLU
1	B	370	LEU
1	B	371	ILE
1	B	376	ILE
1	B	384	ASP
1	B	393	LEU
1	B	397	VAL
1	B	401	SER
1	B	405	MET
1	B	406	LYS
1	B	413	ILE

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Mol	Chain	Res	Type
1	B	416	LEU
1	B	418	GLN
1	B	426	LYS
1	B	429	VAL
1	B	439	LYS
1	B	441	SER
1	B	443	GLU
1	B	453	ILE
1	B	466	VAL
1	B	470	PHE
1	B	471	THR
1	B	472	LYS
1	B	473	GLU
1	B	480	LYS
1	B	486	ARG
1	B	489	SER
1	B	493	ARG
1	B	496	ASP
1	B	501	SER
1	B	502	VAL
1	B	503	GLU
1	B	507	ARG
1	B	512	LYS
1	B	513	SER
1	B	515	GLN
1	B	518	MET
1	B	519	SER
1	B	529	ARG
1	B	530	LYS
1	B	535	LEU
1	B	542	LYS
1	B	547	ARG
1	B	548	VAL
1	B	550	LYS
1	B	552	SER
1	B	556	LYS
1	B	570	GLN
1	B	571	LEU
1	B	575	ASN
1	B	581	THR
1	B	582	GLN
1	B	583	HIS

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Mol	Chain	Res	Type
1	B	585	ILE
1	B	589	GLN
1	B	591	THR
1	B	596	GLU

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

Mol	Chain	Res	Type
1	A	64	ASN
1	A	71	ASN
1	A	106	GLN
1	A	117	GLN
1	A	124	HIS
1	A	173	GLN
1	A	181	ASN
1	A	230	ASN
1	A	333	GLN
1	A	366	GLN
1	A	381	GLN
1	A	411	ASN
1	A	451	GLN
1	A	461	HIS
1	A	544	ASN
1	A	588	GLN
1	B	74	GLN
1	B	85	HIS
1	B	145	ASN
1	B	167	HIS
1	B	181	ASN
1	B	258	ASN
1	B	288	GLN
1	B	325	ASN
1	B	333	GLN
1	B	345	ASN
1	B	387	GLN
1	B	411	ASN
1	B	461	HIS
1	B	515	GLN
1	B	574	HIS
1	B	575	ASN
1	B	587	HIS
1	B	589	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	BTB	A	604	-	13,13,13	3.77	5 (38%)	7,16,16	0.72	0
3	F3P	B	1600	2	14,19,19	2.02	5 (35%)	20,29,29	1.34	2 (10%)
3	F3P	A	600	2	14,19,19	2.03	6 (42%)	20,29,29	1.29	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTB	A	604	-	-	8/21/21/21	-
3	F3P	B	1600	2	-	2/17/25/25	-
3	F3P	A	600	2	-	2/17/25/25	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	BTB	C2-N	10.39	1.68	1.48
4	A	604	BTB	C5-N	5.05	1.55	1.48
4	A	604	BTB	C7-N	4.69	1.54	1.48
3	A	600	F3P	C10-C3	-3.98	1.42	1.52
3	B	1600	F3P	C10-C3	-3.94	1.42	1.52
4	A	604	BTB	C4-C2	3.67	1.57	1.53
4	A	604	BTB	C1-C2	3.54	1.57	1.53
3	B	1600	F3P	PA-O1A	3.45	1.62	1.50
3	A	600	F3P	PA-O1A	3.42	1.62	1.50
3	A	600	F3P	C9-C7	-2.50	1.43	1.50
3	B	1600	F3P	C9-C7	-2.44	1.43	1.50
3	A	600	F3P	PB-O3B	2.36	1.63	1.54
3	B	1600	F3P	C6-C7	2.34	1.39	1.32
3	A	600	F3P	C6-C7	2.30	1.39	1.32
3	B	1600	F3P	PB-O3B	2.11	1.62	1.54
3	A	600	F3P	PA-O3A	2.04	1.61	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1600	F3P	C3-C2-C1	-3.71	111.36	122.08
3	A	600	F3P	C3-C2-C1	-3.01	113.40	122.08
3	B	1600	F3P	C9-C7-C8	2.34	119.97	114.59
3	A	600	F3P	C9-C7-C8	2.26	119.78	114.59

There are no chirality outliers.

All (12) torsion outliers are listed below:

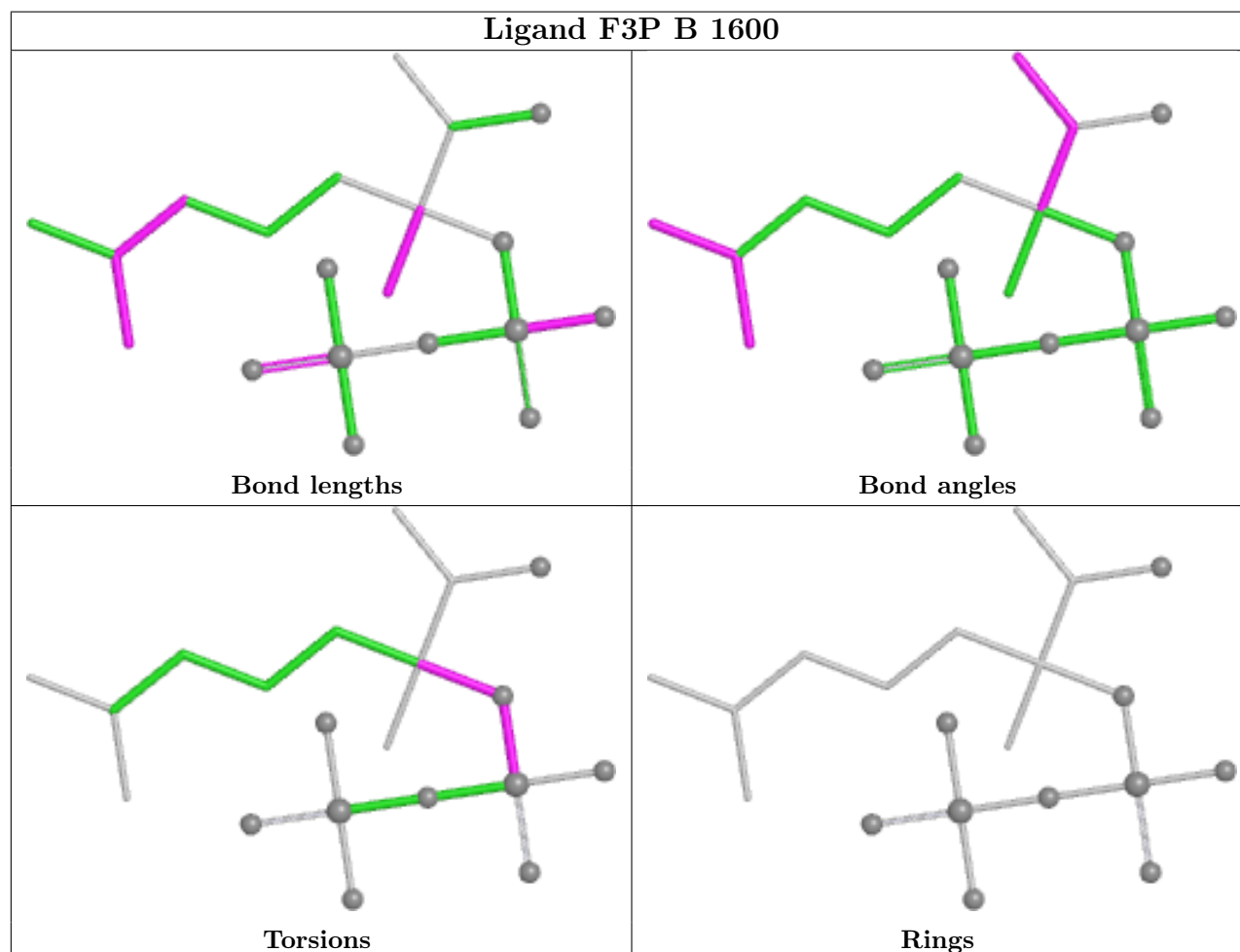
Mol	Chain	Res	Type	Atoms
3	A	600	F3P	PA-O3A-PB-O2B
4	A	604	BTB	O1-C1-C2-C4
4	A	604	BTB	O1-C1-C2-N
4	A	604	BTB	C4-C2-C3-O3
4	A	604	BTB	N-C2-C3-O3
4	A	604	BTB	C1-C2-C4-O4
4	A	604	BTB	N-C2-C4-O4
4	A	604	BTB	C6-C5-N-C2
4	A	604	BTB	N-C5-C6-O6
3	A	600	F3P	PA-O3A-PB-O1B
3	B	1600	F3P	C3-O1-PA-O3A
3	B	1600	F3P	C10-C3-O1-PA

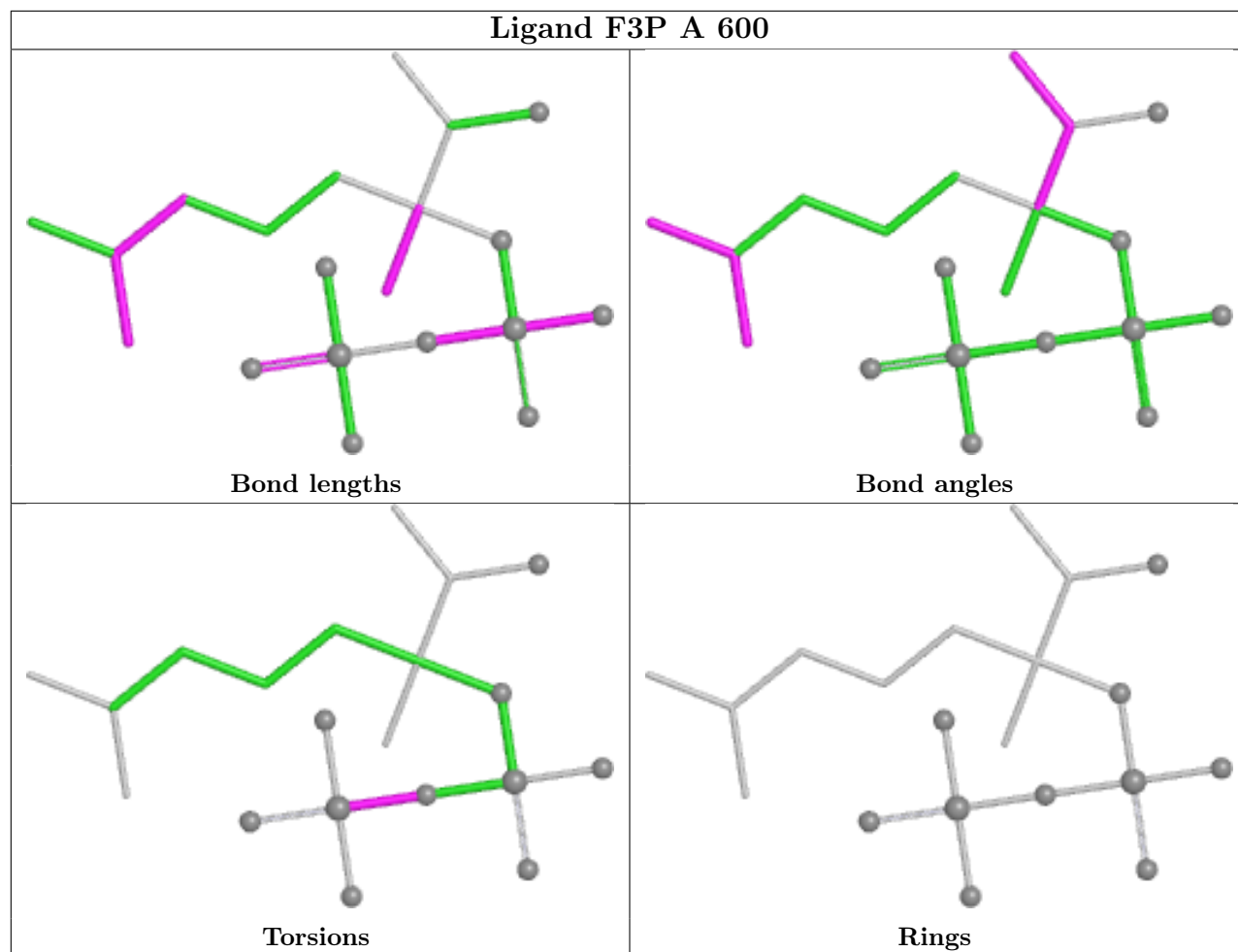
There are no ring outliers.

3 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	BTB	29	0
3	B	1600	F3P	12	0
3	A	600	F3P	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	543/543 (100%)	-1.33	1 (0%) 91 90	24, 52, 97, 100	0
1	B	543/543 (100%)	-1.37	0 100 100	23, 52, 98, 100	0
All	All	1086/1086 (100%)	-1.35	1 (0%) 92 91	23, 52, 98, 100	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	580	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BTB	A	604	14/14	0.99	0.05	84,91,100,100	0
2	MN	A	602	1/1	1.00	0.02	52,52,52,52	0
2	MN	A	603	1/1	1.00	0.01	54,54,54,54	0
2	MN	B	1601	1/1	1.00	0.04	49,49,49,49	0

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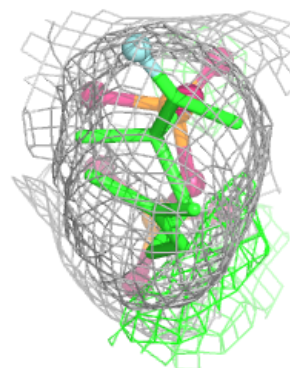
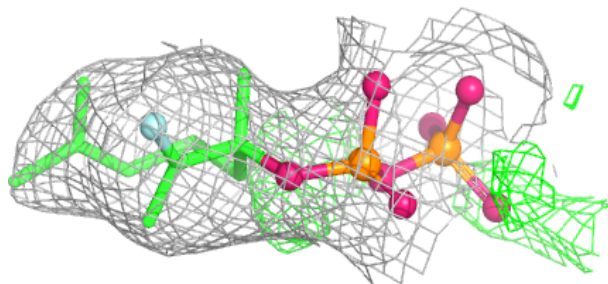
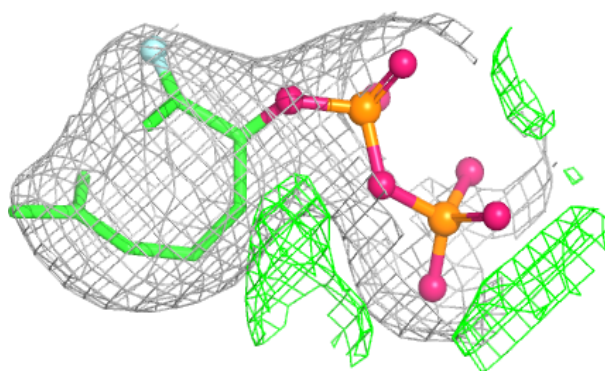
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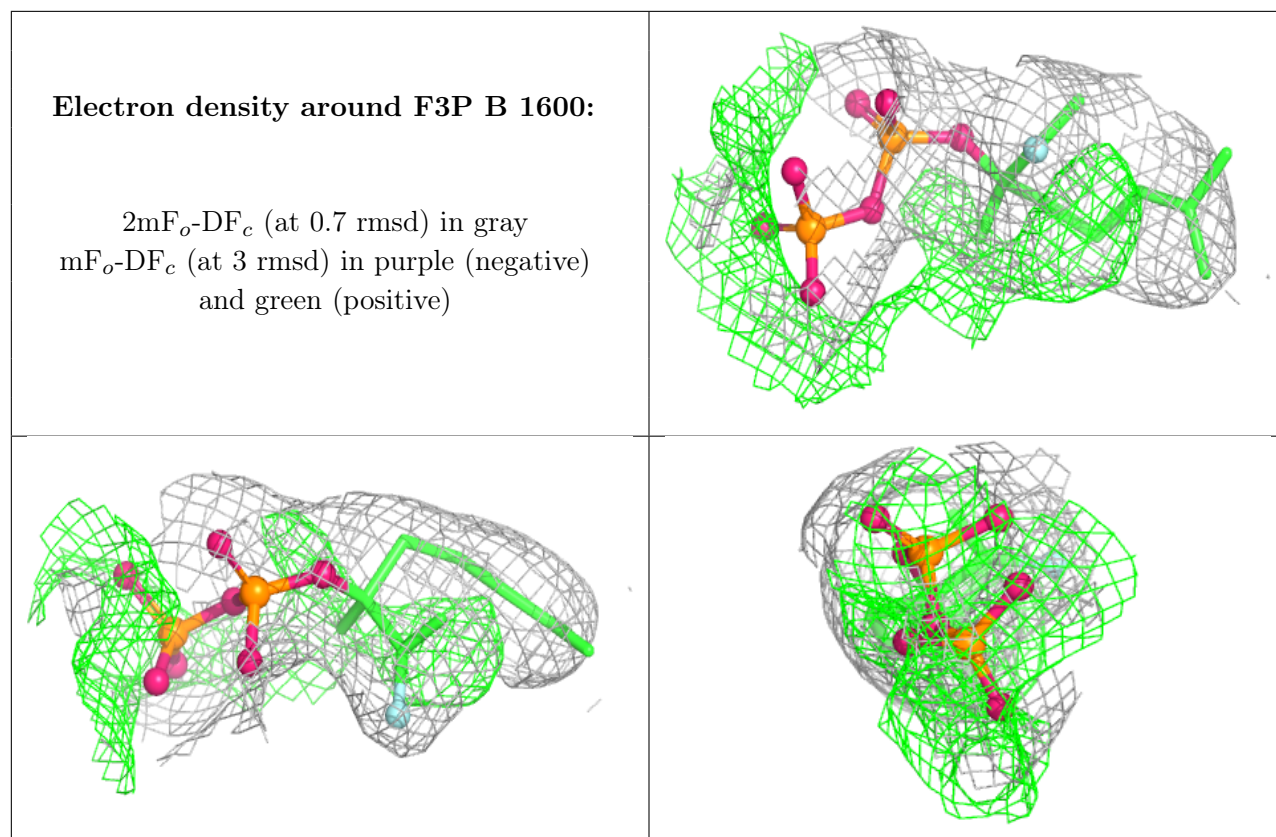
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	B	1602	1/1	1.00	0.04	70,70,70,70	0
2	MN	B	1603	1/1	1.00	0.04	55,55,55,55	0
3	F3P	A	600	20/20	1.00	0.03	45,55,64,67	0
3	F3P	B	1600	20/20	1.00	0.03	45,53,63,66	0
2	MN	A	601	1/1	1.00	0.04	61,61,61,61	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around F3P A 600:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.