



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 12:23 PM EDT

PDB ID : 2ONH
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

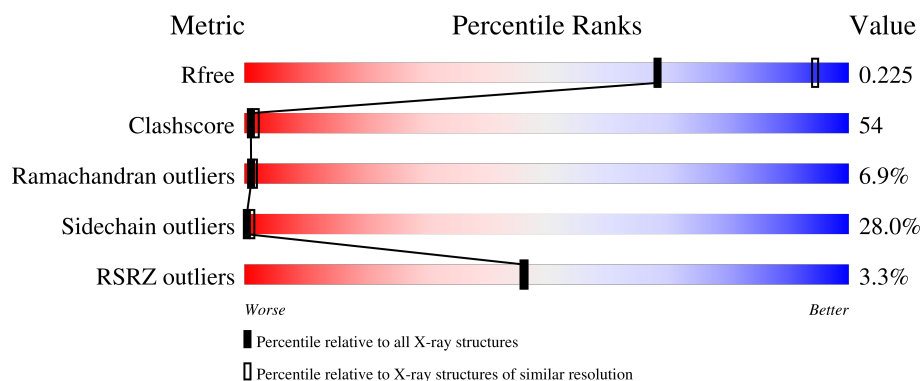
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

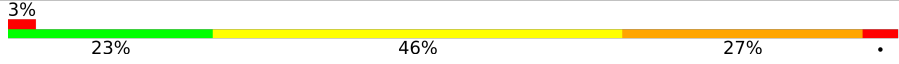
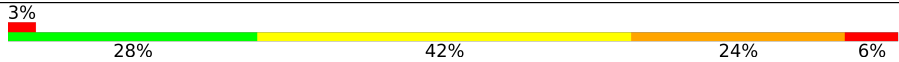
The reported resolution of this entry is 2.70 Å.

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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	
1	B	543	

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	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			

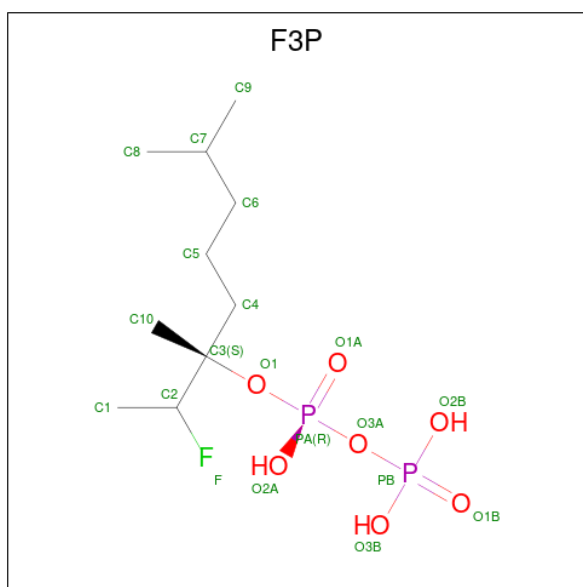
There are 2 discrepancies between the modelled and reference sequences:

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 (three-letter code: MN) (formula: Mn).

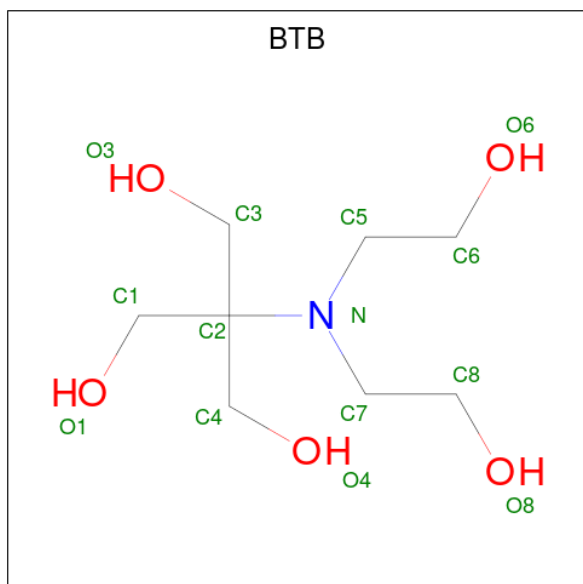
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mn	0	0
			3	3		
2	B	3	Total	Mn	0	0
			3	3		

- Molecule 3 is (1S)-1-[(1S)-1-FLUOROETHYL]-1,5-DIMETHYLHEXYL TRIHYDROGEN DIPHOSPHATE (three-letter code: F3P) (formula: C₁₀H₂₃FO₇P₂).



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 (three-letter code: BTB) (formula: C₈H₁₉NO₅).



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

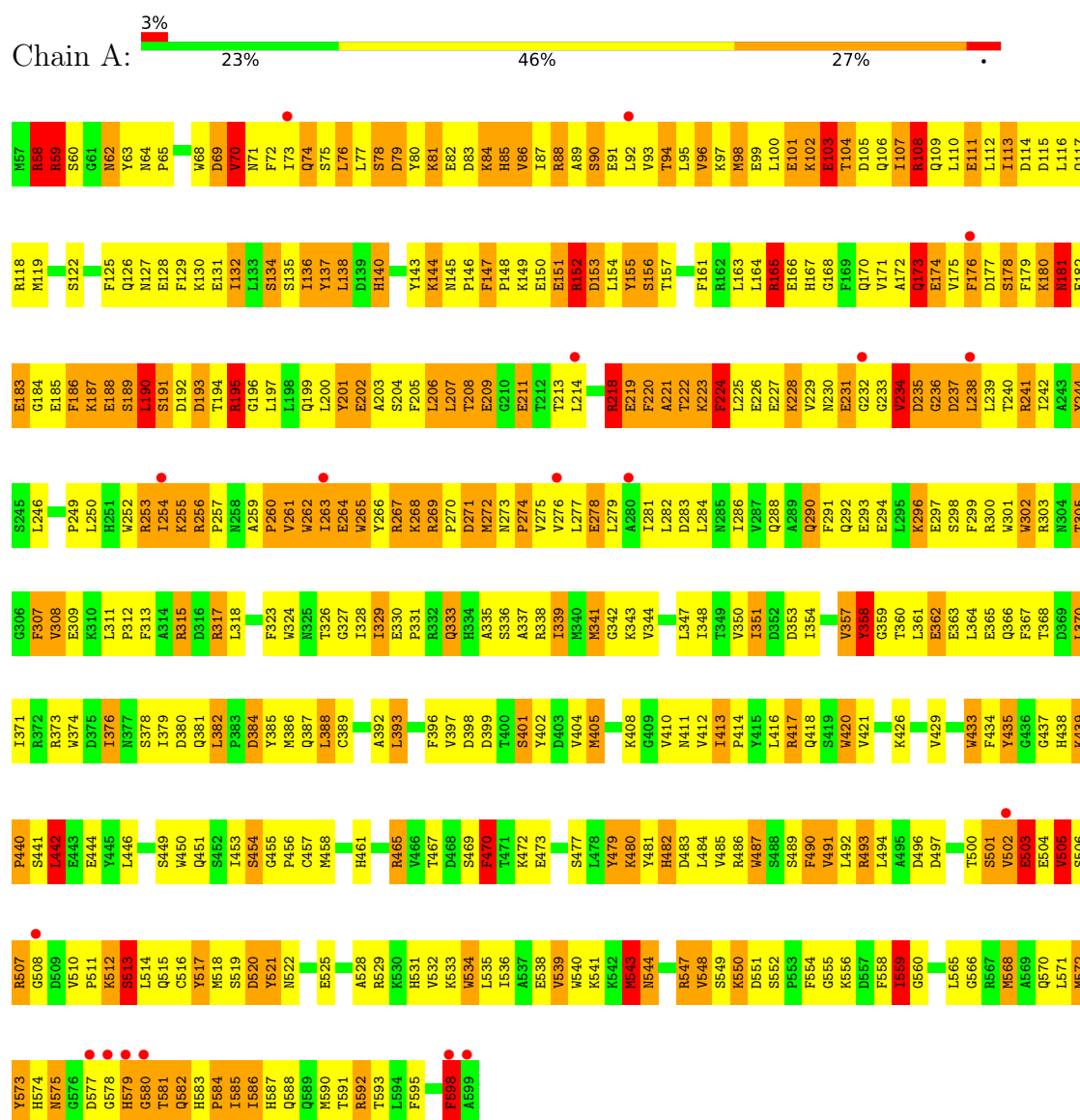
- Molecule 5 is water.

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

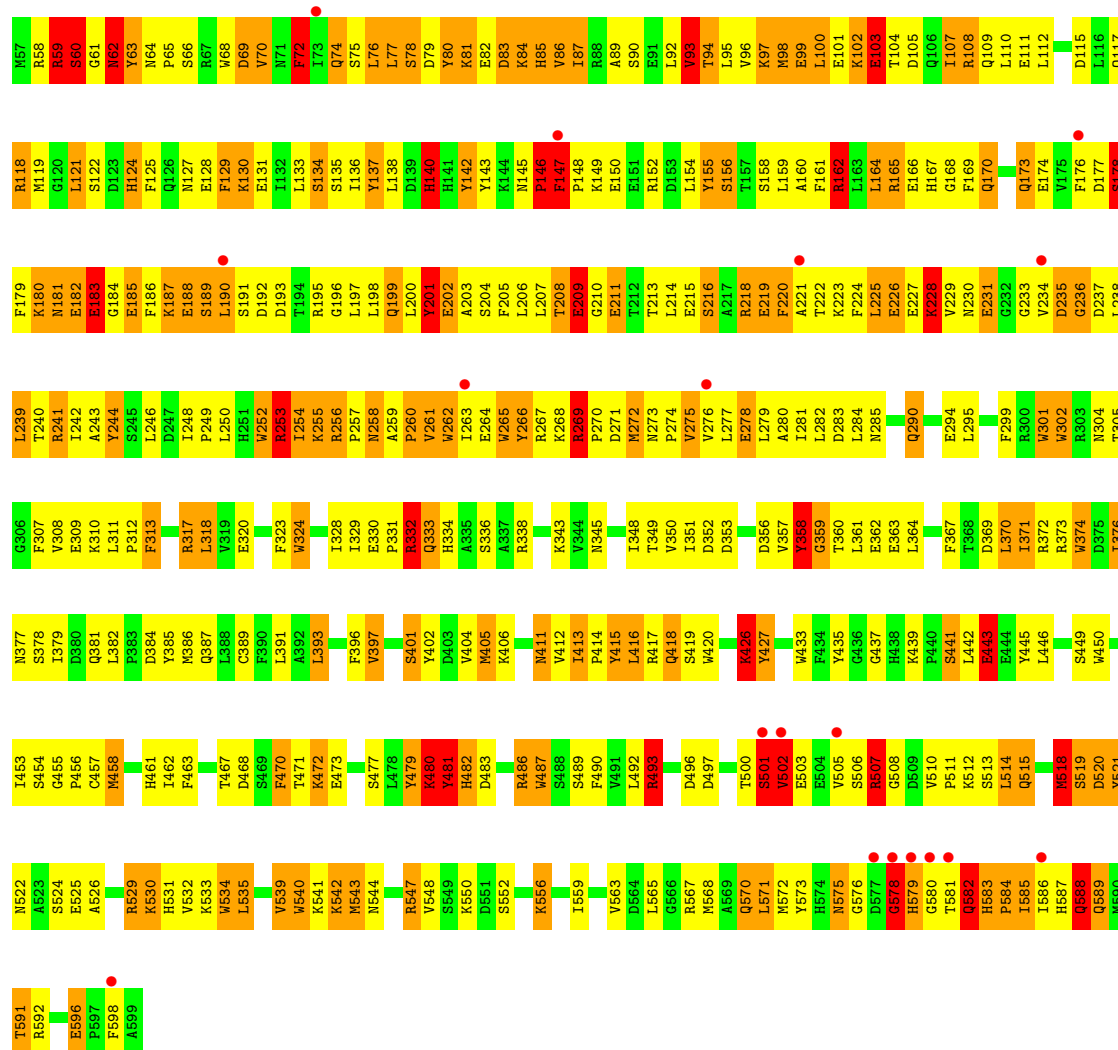
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 46.20 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.70) 89.7 (46.20-2.60)	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 , 0.225	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)	0.35 , 94.6	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	0.94	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: BTB, F3P, 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	1.08	15/4609 (0.3%)	1.48	115/6237 (1.8%)
1	B	1.07	11/4609 (0.2%)	1.49	111/6237 (1.8%)
All	All	1.07	26/9218 (0.3%)	1.48	226/12474 (1.8%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	487	TRP	CG-CD2	-8.29	1.29	1.43
1	B	209	GLU	CG-CD	8.26	1.64	1.51
1	B	219	GLU	CG-CD	7.69	1.63	1.51
1	A	209	GLU	CD-OE2	-7.53	1.17	1.25
1	B	209	GLU	CD-OE1	-7.37	1.17	1.25
1	B	131	GLU	CG-CD	6.63	1.61	1.51
1	A	368	THR	C-O	6.18	1.35	1.23
1	A	209	GLU	CG-CD	6.09	1.61	1.51
1	B	539	VAL	CA-CB	-5.89	1.42	1.54
1	A	108	ARG	NE-CZ	5.86	1.40	1.33
1	A	384	ASP	CB-CG	5.85	1.64	1.51
1	A	420	TRP	CG-CD2	-5.75	1.33	1.43
1	A	368	THR	C-N	5.66	1.47	1.34
1	A	227	GLU	CG-CD	5.62	1.60	1.51
1	A	482	HIS	N-CA	-5.57	1.35	1.46
1	A	374	TRP	CG-CD2	-5.42	1.34	1.43
1	B	404	VAL	CA-CB	-5.36	1.43	1.54
1	B	443	GLU	CG-CD	5.29	1.59	1.51
1	B	450	TRP	CG-CD2	-5.29	1.34	1.43
1	A	351	ILE	CA-CB	-5.23	1.42	1.54
1	B	252	TRP	CG-CD2	-5.18	1.34	1.43
1	A	252	TRP	CG-CD2	-5.17	1.34	1.43
1	A	219	GLU	CG-CD	5.11	1.59	1.51
1	A	218	ARG	NE-CZ	5.09	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	GLU	CB-CG	5.04	1.61	1.52
1	B	108	ARG	NE-CZ	5.03	1.39	1.33

All (226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	266	TYR	CB-CG-CD1	-14.20	112.48	121.00
1	B	358	TYR	CB-CG-CD2	-13.56	112.86	121.00
1	A	266	TYR	CB-CG-CD1	-12.45	113.53	121.00
1	B	420	TRP	CD1-CG-CD2	12.26	116.11	106.30
1	A	374	TRP	CD1-CG-CD2	11.98	115.89	106.30
1	B	426	LYS	CA-CB-CG	-11.38	88.35	113.40
1	B	450	TRP	CD1-CG-CD2	11.29	115.33	106.30
1	A	433	TRP	CD1-CG-CD2	10.63	114.81	106.30
1	A	517	TYR	CB-CG-CD1	-10.48	114.71	121.00
1	A	420	TRP	CD1-CG-CD2	10.48	114.68	106.30
1	A	450	TRP	CD1-CG-CD2	10.39	114.61	106.30
1	B	108	ARG	CA-CB-CG	10.21	135.86	113.40
1	A	470	PHE	CB-CG-CD1	-10.05	113.77	120.80
1	B	80	TYR	CB-CG-CD1	-9.79	115.12	121.00
1	B	63	TYR	CB-CG-CD2	-9.71	115.17	121.00
1	B	543	MET	CG-SD-CE	-9.68	84.72	100.20
1	B	201	TYR	CB-CG-CD1	-9.38	115.37	121.00
1	B	72	PHE	CB-CG-CD1	-9.30	114.29	120.80
1	B	209	GLU	CB-CG-CD	9.12	138.82	114.20
1	B	420	TRP	CG-CD1-NE1	-9.07	101.03	110.10
1	A	244	TYR	CB-CG-CD2	-8.97	115.62	121.00
1	B	307	PHE	CB-CG-CD2	-8.90	114.57	120.80
1	A	534	TRP	CD1-CG-CD2	8.86	113.39	106.30
1	B	540	TRP	CD1-CG-CD2	8.81	113.34	106.30
1	B	433	TRP	CD1-CG-CD2	8.77	113.32	106.30
1	A	265	TRP	CD1-CG-CD2	8.75	113.30	106.30
1	A	68	TRP	CD1-CG-CD2	8.68	113.24	106.30
1	A	487	TRP	CE2-CD2-CE3	8.65	129.08	118.70
1	A	252	TRP	CD1-CG-CD2	8.61	113.19	106.30
1	B	72	PHE	CB-CG-CD2	8.48	126.74	120.80
1	A	487	TRP	CD1-NE1-CE2	-8.31	101.52	109.00
1	A	482	HIS	ND1-CG-CD2	8.23	120.33	108.80
1	A	590	MET	CG-SD-CE	-8.22	87.05	100.20
1	B	374	TRP	CD1-CG-CD2	8.13	112.81	106.30
1	B	481	TYR	CB-CG-CD1	-8.09	116.15	121.00
1	B	142	TYR	CB-CG-CD2	-8.01	116.20	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	TYR	CB-CG-CD2	-7.86	116.28	121.00
1	B	118	ARG	CA-CB-CG	-7.80	96.24	113.40
1	B	265	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	B	324	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	B	534	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	A	487	TRP	CG-CD2-CE3	-7.75	126.93	133.90
1	B	540	TRP	CB-CG-CD1	-7.74	116.94	127.00
1	B	543	MET	CA-CB-CG	-7.71	100.19	113.30
1	A	487	TRP	NE1-CE2-CD2	7.69	114.99	107.30
1	A	521	TYR	CB-CG-CD2	-7.67	116.40	121.00
1	A	367	PHE	CB-CG-CD2	-7.64	115.45	120.80
1	A	108	ARG	CA-CB-CG	7.59	130.10	113.40
1	B	412	VAL	CG1-CB-CG2	-7.56	98.80	110.90
1	B	68	TRP	CD1-CG-CD2	7.53	112.32	106.30
1	B	450	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	B	358	TYR	CD1-CG-CD2	7.37	126.01	117.90
1	B	302	TRP	CD1-CG-CD2	7.33	112.17	106.30
1	B	262	TRP	CD1-CG-CD2	7.31	112.15	106.30
1	B	252	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	A	63	TYR	CB-CG-CD2	-7.25	116.65	121.00
1	B	534	TRP	CB-CG-CD1	-7.22	117.62	127.00
1	B	187	LYS	CA-CB-CG	-7.20	97.56	113.40
1	A	357	VAL	CG1-CB-CG2	-7.19	99.40	110.90
1	A	262	TRP	CD1-CG-CD2	7.16	112.03	106.30
1	B	358	TYR	CG-CD1-CE1	-7.15	115.58	121.30
1	A	450	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	B	415	TYR	CB-CG-CD1	-7.12	116.73	121.00
1	B	542	LYS	CB-CG-CD	-7.08	93.19	111.60
1	B	427	TYR	CB-CG-CD2	-7.06	116.76	121.00
1	B	220	PHE	CB-CG-CD2	7.06	125.74	120.80
1	B	450	TRP	CG-CD1-NE1	-7.06	103.04	110.10
1	A	236	GLY	N-CA-C	-7.04	95.51	113.10
1	A	74	GLN	CA-CB-CG	-7.02	97.96	113.40
1	A	450	TRP	CG-CD1-NE1	-7.00	103.10	110.10
1	B	219	GLU	CA-CB-CG	6.94	128.67	113.40
1	A	374	TRP	CG-CD1-NE1	-6.92	103.18	110.10
1	B	427	TYR	CB-CG-CD1	6.91	125.15	121.00
1	A	598	PHE	CB-CG-CD1	-6.89	115.98	120.80
1	A	278	GLU	CA-CB-CG	-6.85	98.34	113.40
1	B	534	TRP	CG-CD2-CE3	6.82	140.04	133.90
1	A	374	TRP	CE2-CD2-CG	-6.81	101.86	107.30
1	A	420	TRP	CG-CD1-NE1	-6.69	103.41	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	MET	CA-CB-CG	-6.67	101.95	113.30
1	B	324	TRP	CB-CG-CD1	-6.67	118.32	127.00
1	B	540	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	A	450	TRP	CG-CD2-CE3	6.63	139.87	133.90
1	A	491	VAL	CG1-CB-CG2	-6.60	100.33	110.90
1	B	324	TRP	CE2-CD2-CG	-6.57	102.05	107.30
1	A	543	MET	CA-CB-CG	-6.52	102.21	113.30
1	B	143	TYR	CB-CG-CD2	-6.52	117.09	121.00
1	B	129	PHE	CB-CG-CD2	-6.50	116.25	120.80
1	A	433	TRP	CE2-CD2-CG	-6.49	102.11	107.30
1	B	487	TRP	NE1-CE2-CD2	6.47	113.77	107.30
1	A	209	GLU	CB-CG-CD	6.46	131.64	114.20
1	B	301	TRP	CD1-CG-CD2	6.45	111.46	106.30
1	B	420	TRP	CE2-CD2-CG	-6.44	102.14	107.30
1	A	433	TRP	CG-CD1-NE1	-6.42	103.68	110.10
1	B	582	GLN	CA-CB-CG	-6.42	99.28	113.40
1	A	59	ARG	CA-CB-CG	6.41	127.50	113.40
1	B	137	TYR	CB-CG-CD2	-6.39	117.17	121.00
1	A	266	TYR	CB-CG-CD2	6.38	124.83	121.00
1	B	131	GLU	CB-CG-CD	6.38	131.42	114.20
1	A	307	PHE	CB-CG-CD2	-6.36	116.35	120.80
1	A	68	TRP	CE2-CD2-CG	-6.34	102.22	107.30
1	B	236	GLY	N-CA-C	-6.34	97.25	113.10
1	A	480	LYS	CA-CB-CG	6.30	127.27	113.40
1	B	534	TRP	CE2-CD2-CG	-6.30	102.26	107.30
1	A	543	MET	CG-SD-CE	-6.29	90.14	100.20
1	A	505	VAL	CG1-CB-CG2	-6.27	100.87	110.90
1	A	173	GLN	CA-CB-CG	6.25	127.16	113.40
1	B	578	GLY	N-CA-C	-6.22	97.55	113.10
1	B	68	TRP	CE2-CD2-CG	-6.21	102.33	107.30
1	A	324	TRP	CD1-CG-CD2	6.21	111.27	106.30
1	A	211	GLU	CA-CB-CG	-6.21	99.74	113.40
1	A	401	SER	CA-CB-OG	-6.18	94.51	111.20
1	A	137	TYR	CD1-CG-CD2	6.16	124.67	117.90
1	B	493	ARG	CA-CB-CG	-6.16	99.86	113.40
1	A	195	ARG	CA-CB-CG	6.15	126.93	113.40
1	A	224	PHE	CB-CG-CD1	-6.14	116.50	120.80
1	B	244	TYR	CB-CG-CD1	6.14	124.69	121.00
1	A	261	VAL	CG1-CB-CG2	6.14	120.72	110.90
1	A	265	TRP	CG-CD1-NE1	-6.13	103.97	110.10
1	A	503	GLU	CA-CB-CG	6.13	126.89	113.40
1	B	480	LYS	CA-CB-CG	6.12	126.87	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	TRP	CB-CG-CD2	-6.12	118.64	126.60
1	A	165	ARG	CA-CB-CG	-6.10	99.98	113.40
1	A	315	ARG	CB-CG-CD	-6.08	95.80	111.60
1	A	103	GLU	CB-CG-CD	-6.07	97.81	114.20
1	A	265	TRP	CE2-CD2-CG	-6.07	102.45	107.30
1	B	146	PRO	CA-N-CD	-6.05	103.03	111.50
1	B	302	TRP	CE2-CD2-CG	-6.05	102.46	107.30
1	A	80	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	B	433	TRP	CE2-CD2-CG	-6.02	102.48	107.30
1	B	253	ARG	CA-CB-CG	5.98	126.57	113.40
1	A	517	TYR	CB-CG-CD2	5.98	124.59	121.00
1	B	142	TYR	CD1-CG-CD2	5.93	124.42	117.90
1	A	534	TRP	CB-CG-CD1	-5.92	119.31	127.00
1	A	70	VAL	CG1-CB-CG2	5.91	120.36	110.90
1	A	450	TRP	CB-CG-CD1	-5.91	119.32	127.00
1	A	302	TRP	CD1-CG-CD2	5.90	111.02	106.30
1	A	534	TRP	CE2-CD2-CG	-5.88	102.59	107.30
1	B	540	TRP	CG-CD2-CE3	5.88	139.19	133.90
1	A	137	TYR	CB-CG-CD2	-5.86	117.48	121.00
1	A	262	TRP	CE2-CD2-CG	-5.85	102.62	107.30
1	A	358	TYR	CD1-CG-CD2	5.84	124.32	117.90
1	A	396	PHE	CB-CG-CD1	-5.83	116.72	120.80
1	A	219	GLU	CB-CG-CD	5.82	129.92	114.20
1	A	324	TRP	CE2-CD2-CG	-5.82	102.64	107.30
1	A	568	MET	CA-CB-CG	-5.82	103.41	113.30
1	B	540	TRP	CG-CD1-NE1	-5.81	104.29	110.10
1	A	479	TYR	CB-CG-CD1	-5.77	117.54	121.00
1	A	539	VAL	CG1-CB-CG2	-5.76	101.68	110.90
1	A	155	TYR	CG-CD1-CE1	-5.73	116.71	121.30
1	A	420	TRP	CE2-CD2-CG	-5.72	102.72	107.30
1	B	262	TRP	CE2-CD2-CG	-5.72	102.73	107.30
1	A	434	PHE	CB-CG-CD1	-5.69	116.82	120.80
1	A	155	TYR	CB-CG-CD2	-5.67	117.59	121.00
1	B	301	TRP	CB-CG-CD1	-5.67	119.63	127.00
1	B	539	VAL	CG1-CB-CG2	5.65	119.94	110.90
1	B	487	TRP	CE2-CD2-CG	-5.64	102.79	107.30
1	B	219	GLU	CB-CG-CD	5.63	129.41	114.20
1	A	143	TYR	CB-CG-CD2	-5.62	117.62	121.00
1	B	220	PHE	CB-CG-CD1	-5.60	116.88	120.80
1	B	70	VAL	CG1-CB-CG2	5.58	119.84	110.90
1	B	479	TYR	CG-CD2-CE2	-5.58	116.83	121.30
1	B	458	MET	CA-CB-CG	-5.57	103.83	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	588	GLN	CB-CG-CD	5.55	126.04	111.60
1	B	265	TRP	CE2-CD2-CG	-5.54	102.87	107.30
1	B	275	VAL	CG1-CB-CG2	-5.53	102.05	110.90
1	A	170	GLN	CA-CB-CG	5.53	125.57	113.40
1	A	227	GLU	CB-CG-CD	5.53	129.12	114.20
1	A	534	TRP	CG-CD1-NE1	-5.52	104.58	110.10
1	B	301	TRP	CE2-CD2-CG	-5.52	102.88	107.30
1	B	405	MET	CG-SD-CE	-5.50	91.40	100.20
1	B	487	TRP	CD1-CG-CD2	5.50	110.70	106.30
1	A	358	TYR	CB-CG-CD1	-5.49	117.70	121.00
1	A	540	TRP	NE1-CE2-CD2	5.48	112.78	107.30
1	B	374	TRP	CE2-CD2-CG	-5.46	102.94	107.30
1	A	137	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	B	576	GLY	N-CA-C	-5.44	99.50	113.10
1	B	266	TYR	CD1-CG-CD2	5.44	123.88	117.90
1	A	252	TRP	CE2-CD2-CE3	5.44	125.22	118.70
1	A	573	TYR	CD1-CG-CD2	5.43	123.87	117.90
1	A	63	TYR	CD1-CG-CD2	5.43	123.87	117.90
1	B	252	TRP	CE2-CD2-CG	-5.43	102.96	107.30
1	B	93	VAL	CA-CB-CG2	-5.42	102.77	110.90
1	A	252	TRP	CG-CD1-NE1	-5.41	104.69	110.10
1	B	433	TRP	CG-CD1-NE1	-5.39	104.71	110.10
1	B	479	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	B	63	TYR	CD1-CG-CD2	5.32	123.75	117.90
1	A	573	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	B	324	TRP	NE1-CE2-CZ2	-5.29	124.58	130.40
1	A	324	TRP	CB-CG-CD1	-5.25	120.17	127.00
1	A	470	PHE	CB-CG-CD2	5.25	124.47	120.80
1	B	482	HIS	ND1-CG-CD2	5.25	116.15	108.80
1	B	63	TYR	CG-CD1-CE1	-5.24	117.11	121.30
1	A	540	TRP	CE2-CD2-CG	-5.23	103.12	107.30
1	A	80	TYR	CD1-CG-CD2	5.22	123.65	117.90
1	B	142	TYR	CG-CD1-CE1	-5.20	117.14	121.30
1	A	252	TRP	CB-CG-CD2	-5.20	119.85	126.60
1	B	137	TYR	CG-CD1-CE1	-5.18	117.15	121.30
1	B	241	ARG	CA-CB-CG	-5.18	102.01	113.40
1	A	482	HIS	CG-ND1-CE1	-5.16	98.99	105.70
1	B	313	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	A	572	MET	CA-CB-CG	-5.15	104.54	113.30
1	B	80	TYR	CD1-CG-CD2	5.14	123.56	117.90
1	B	396	PHE	CB-CG-CD1	-5.14	117.20	120.80
1	B	85	HIS	ND1-CG-CD2	5.11	115.95	108.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	PHE	CB-CG-CD2	-5.10	117.23	120.80
1	B	479	TYR	CD1-CG-CD2	5.09	123.50	117.90
1	B	518	MET	CB-CG-SD	-5.08	97.15	112.40
1	B	524	SER	CA-CB-OG	-5.08	97.48	111.20
1	A	559	ILE	CB-CG1-CD1	-5.07	99.71	113.90
1	A	137	TYR	CG-CD1-CE1	-5.07	117.25	121.30
1	B	103	GLU	CB-CG-CD	-5.07	100.52	114.20
1	A	170	GLN	CB-CG-CD	5.06	124.76	111.60
1	A	143	TYR	CD1-CG-CD2	5.05	123.45	117.90
1	A	155	TYR	CD1-CG-CD2	5.04	123.45	117.90
1	A	102	LYS	CA-CB-CG	-5.04	102.30	113.40
1	A	358	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	A	252	TRP	CE2-CD2-CG	-5.04	103.27	107.30
1	A	291	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	A	324	TRP	NE1-CE2-CD2	5.03	112.33	107.30
1	A	86	VAL	CG1-CB-CG2	5.03	118.94	110.90
1	B	501	SER	CA-CB-OG	-5.01	97.66	111.20
1	A	420	TRP	CB-CG-CD2	-5.01	120.09	126.60
1	B	266	TYR	CG-CD2-CE2	-5.01	117.29	121.30
1	B	521	TYR	CB-CG-CD1	-5.01	118.00	121.00
1	A	435	TYR	CB-CG-CD1	-5.01	118.00	121.00
1	B	301	TRP	CG-CD2-CE3	5.00	138.40	133.90

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	466	0
1	B	4497	0	4353	459	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	58	0	0	4	1
5	B	53	0	0	3	1
All	All	9165	0	8761	961	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 54.

All (961) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:515:GLN:HA	1:A:518:MET:HE2	1.62	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:147:PHE:HA	1:B:149:LYS:HZ1	1.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:255:LYS:H	1:B:255:LYS:HZ3	1.30	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:301:TRP:CD2	1:B:343:LYS:HG2	2.25	0.71
1:B:181:ASN:C	1:B:181:ASN:HD22	1.93	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:283:ASP:CG	1:B:332:ARG:HH22	1.95	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: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:103:GLU:CD	1:B:104:THR:H	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:543:MET:O	1:A:543:MET:HG3	1.92	0.67
1:A:181:ASN:C	1:A:181:ASN:HD22	1.96	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:A:149:LYS:C	1:A:151:GLU:H	2.00	0.64
1:B:222:THR:O	1:B:226:GLU:HB2	1.96	0.64
1:A:333:GLN:HE21	1:A:333:GLN:N	1.84	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:105:ASP:OD1	1:B:107:ILE:HG22	1.98	0.63
1:B:435:TYR:C	1:B:437:GLY:H	2.01	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:255:LYS:H	1:B:255:LYS:HZ2	1.45	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: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: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: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
1:B:413:ILE:HG12	1:B:414:PRO:CD	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:LYS:O	1:B:481:TYR:HB2	2.00	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:A:197:LEU:HD21	1:A:224:PHE:CD2	2.37	0.60
1:A:100:LEU:HD13	1:A:112:LEU:HD23	1.82	0.60
1:A:376:ILE:O	1:A:376:ILE:HG13	2.00	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:235:ASP:C	1:B:237:ASP:H	2.06	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:A:106:GLN:O	1:A:109:GLN:HB2	2.01	0.59
1:B:103:GLU:CD	1:B:104:THR:N	2.54	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: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:A:571:LEU:HD23	1:A:571:LEU:C	2.23	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:146:PRO:C	1:B:148:PRO:HD3	2.23	0.58
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
1:B:69:ASP:CG	1:B:70:VAL:N	2.57	0.58
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:72:PHE:C	1:B:72:PHE:CD2	2.77	0.58
1:A:315:ARG:HB3	1:A:317:ARG:CD	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:534:TRP:O	1:A:538:GLU:HG2	2.04	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: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:479:TYR:C	1:B:481:TYR:N	2.54	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
1:A:153:ASP:OD1	1:A:156:SER:N	2.38	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: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:162:ARG:HG2	1:B:162:ARG:HH11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:VAL:O	1:B:235:ASP:HB2	2.04	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:60:SER:C	1:B:62:ASN:H	2.09	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:182:GLU:C	1:B:184:GLY:H	2.08	0.55
1:B:457:CYS:O	1:B:461:HIS:HD2	1.89	0.55
1:A:105:ASP:OD1	1:A:105:ASP:C	2.43	0.55
1:A:256:ARG:CB	1:A:257:PRO:HD3	2.35	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:435:TYR:C	1:A:437:GLY:H	2.09	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:487:TRP:HA	1:B:487:TRP:CE3	2.42	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:72:PHE:C	1:B:72:PHE:HD2	2.10	0.55
1:B:501:SER:O	1:B:505:VAL:HG22	2.06	0.55
1:A:137:TYR:HD1	1:A:164:LEU:HD13	1.71	0.55
1:A:259:ALA:O	1:A:260:PRO:C	2.43	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:493:ARG:HG3	1:A:494:LEU:N	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:SER:C	1:A:380:ASP:N	2.57	0.54
1:B:222:THR:O	1:B:223:LYS:C	2.45	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:177:ASP:C	1:B:179:PHE:H	2.11	0.54
1:B:205:PHE:CE1	1:B:249:PRO:HG3	2.42	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: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
1:A:559:ILE:HD12	1:A:559:ILE:O	2.08	0.54
1:B:70:VAL:O	1:B:74:GLN:N	2.40	0.54
1:B:267:ARG:HA	1:B:277:LEU:HD13	1.90	0.54
1:B:571:LEU:C	1:B:571:LEU:HD12	2.29	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:290:GLN:HA	1:B:290:GLN:OE1	2.08	0.53
1:B:311:LEU:HG	1:B:313:PHE:CE2	2.43	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: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:A:79:ASP:HA	1:A:81:LYS:CE	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:145:ASN:CG	1:B:146:PRO:HD3	2.29	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: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:453:ILE:O	1:A:454:SER:CB	2.57	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:B:181:ASN:C	1:B:181:ASN:ND2	2.62	0.53
1:B:220:PHE:HD2	1:B:221:ALA:N	2.07	0.53
1:B:310:LYS:C	1:B:312:PRO:HD3	2.29	0.53
1:B:369:ASP:OD1	1:B:372:ARG:NH1	2.42	0.53
1:A:189:SER:O	1:A:190:LEU:C	2.48	0.53
1:A:255:LYS:HB2	1:A:330:GLU:OE2	2.08	0.53
1:A:555:GLY:O	1:A:559:ILE:HG23	2.09	0.53
1:B:83:ASP:C	1:B:85:HIS:H	2.12	0.53
1:B:189:SER:C	1:B:191:SER:H	2.12	0.53
1:B:311:LEU:HG	1:B:313:PHE:CZ	2.43	0.53
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:117:GLN:HE22	1:B:167:HIS:CE1	2.17	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
1:A:202:GLU:CD	1:A:250:LEU:HG	2.29	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: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:146:PRO:O	1:B:147:PHE:HB2	2.09	0.52
1:B:283:ASP:OD2	1:B:332:ARG:NH2	2.43	0.52
1:A:149:LYS:C	1:A:151:GLU:N	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:83:ASP:O	1:A:87:ILE:HG13	2.10	0.52
1:A:218:ARG:HG3	1:A:218:ARG:NH1	2.05	0.52
1:A:479:TYR:C	1:A:481:TYR:N	2.60	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
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:78:SER:HG	1:B:80:TYR:HD2	1.58	0.51
1:B:164:LEU:O	1:B:169:PHE:HB2	2.10	0.51
1:B:234:VAL:C	1:B:236:GLY:H	2.13	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: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:B:228:LYS:HE2	1:B:234:VAL:HG11	1.93	0.51
1:B:331:PRO:HB3	1:B:333:GLN:HE21	1.75	0.51
1:A:299:PHE:HA	1:A:318:LEU:CD2	2.40	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:98:MET:HA	1:A:101:GLU:CD	2.31	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:A:441:SER:O	1:A:442:LEU:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:547:ARG:HG3	1:B:548:VAL:N	2.26	0.50
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:B:227:GLU:C	1:B:229:VAL:N	2.65	0.50
1:B:70:VAL:CG1	1:B:74:GLN:HG3	2.42	0.50
1:B:418:GLN:O	1:B:419:SER:C	2.48	0.50
1:A:95:LEU:C	1:A:97:LYS:N	2.63	0.50
1:A:182:GLU:C	1:A:184:GLY:H	2.15	0.50
1:A:194:THR:HG21	1:A:234:VAL:HG22	1.92	0.50
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:181:ASN:C	1:A:181:ASN:ND2	2.65	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:435:TYR:C	1:B:437:GLY:N	2.65	0.50
1:A:378:SER:C	1:A:380:ASP:H	2.15	0.50
1:B:161:PHE:CD2	1:B:203:ALA:HB1	2.43	0.50
1:A:442:LEU:HD23	1:A:517:TYR:N	2.26	0.50
1:A:177:ASP:C	1:A:179:PHE:H	2.15	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:B:487:TRP:HA	1:B:487:TRP:HE3	1.77	0.49
1:A:222:THR:CG2	1:A:223:LYS:N	2.75	0.49
1:B:63:TYR:HD1	1:B:581:THR:HG23	1.78	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:182:GLU:C	1:A:184:GLY:N	2.65	0.49
1:B:268:LYS:HD3	1:B:268:LYS:C	2.32	0.49
1:B:531:HIS:O	1:B:532:VAL:C	2.49	0.49
1:B:585:ILE:O	1:B:586:ILE:C	2.48	0.49
1:A:299:PHE:CD1	1:A:303:ARG:HD2	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:59:ARG:O	1:B:60:SER:C	2.51	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:B:135:SER:O	1:B:136:ILE:C	2.51	0.49
1:B:479:TYR:C	1:B:481:TYR:H	2.12	0.49
1:A:220:PHE:CE1	1:A:224:PHE:CE2	3.01	0.49
1:A:401:SER:HB2	1:A:413:ILE:HG22	1.95	0.49
1:A:220:PHE:C	1:A:222:THR:H	2.15	0.49
1:B:147:PHE:O	1:B:149:LYS:HD2	2.13	0.49
1:B:190:LEU:C	1:B:192:ASP:H	2.15	0.49
1:B:377:ASN:C	1:B:379:ILE:N	2.66	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:254:ILE:H	1:B:254:ILE:CD1	2.16	0.48
1:A:93:VAL:C	1:A:95:LEU:N	2.65	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:B:370:LEU:HD22	1:B:382:LEU:HD11	1.94	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: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:A:579:HIS:O	1:A:580:GLY:C	2.52	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:109:GLN:O	1:A:110:LEU:C	2.51	0.48
1:A:135:SER:O	1:A:136:ILE:C	2.52	0.48
1:A:145:ASN:HB3	1:A:146:PRO:HD3	1.96	0.48
1:B:295:LEU:O	1:B:295:LEU:HD12	2.13	0.48
1:B:541:LYS:HE2	5:B:788:HOH:O	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:492:LEU:HD22	1:B:565:LEU:HD11	1.95	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:109:GLN:O	1:B:110:LEU:C	2.51	0.48
1:B:237:ASP:C	1:B:241:ARG:HE	2.16	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: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:85:HIS:O	1:A:86:VAL:C	2.50	0.47
1:A:157:THR:HG21	1:A:179:PHE:HE2	1.79	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:B:363:GLU:HB3	1:B:386:MET:HE3	1.95	0.47
1:A:208:THR:C	1:A:541:LYS:HD2	2.33	0.47
1:B:79:ASP:C	1:B:81:LYS:N	2.66	0.47
1:B:301:TRP:CG	1:B:343:LYS:HG2	2.49	0.47
1:A:188:GLU:H	1:A:188:GLU:HG3	1.35	0.47
1:B:263:ILE:HG22	1:B:263:ILE:O	2.12	0.47
1:A:496:ASP:HA	1:A:573:TYR:CG	2.48	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:B:348:ILE:O	1:B:349:THR:C	2.52	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:235:ASP:C	1:B:237:ASP:N	2.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:MET:O	1:A:272:MET:HE3	2.15	0.47
1:A:410:VAL:HG21	1:A:470:PHE:CE1	2.50	0.47
1:A:479:TYR:C	1:A:481:TYR:H	2.09	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: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: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:A:70:VAL:HG23	1:A:74:GLN:HG3	1.97	0.47
1:A:144:LYS:HE2	1:A:146:PRO:HD2	1.96	0.47
1:A:512:LYS:O	1:A:513:SER:C	2.53	0.47
1:B:259:ALA:HB3	1:B:260:PRO:CD	2.45	0.47
1:B:520:ASP:HB3	1:B:521:TYR:CD2	2.50	0.47
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:462:ILE:O	1:B:463:PHE:C	2.53	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:240:THR:C	1:B:242:ILE:H	2.17	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:341:MET:O	1:A:342:GLY:C	2.54	0.46
1:A:438:HIS:CD2	1:A:439:LYS:H	2.33	0.46
1:A:513:SER:O	1:A:514:LEU:C	2.53	0.46
1:B:147:PHE:HA	1:B:149:LYS:CE	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:517:TYR:CD2	1:A:517:TYR:C	2.89	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:493:ARG:CG	1:A:494:LEU:N	2.79	0.46
1:A:511:PRO:HB3	1:A:515:GLN:CD	2.36	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: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:458:MET:HE2	1:B:565:LEU:HD13	1.98	0.45
1:A:98:MET:O	1:A:102:LYS:HG3	2.15	0.45
1:A:98:MET:O	1:A:102:LYS:CB	2.64	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
1:B:145:ASN:HD21	1:B:146:PRO:HG3	1.80	0.45
1:A:113:ILE:HG22	1:A:114:ASP:N	2.31	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:483:ASP:O	1:A:486:ARG:HB3	2.17	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:A:190:LEU:O	1:A:191:SER:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:259:ALA:O	1:B:260:PRO:C	2.55	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:587:HIS:ND1	1:B:587:HIS:C	2.69	0.45
1:A:284:LEU:C	1:A:284:LEU:HD23	2.36	0.45
1:A:449:SER:CB	1:A:493:ARG:HD3	2.41	0.45
1:A:491:VAL:O	1:A:492:LEU:C	2.54	0.45
1:B:103:GLU:CD	1:B:108:ARG:HD3	2.38	0.45
1:B:270:PRO:O	1:B:272:MET:N	2.42	0.45
1:B:270:PRO:C	1:B:272:MET:H	2.18	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:B:385:TYR:OH	1:B:386:MET:HE3	2.17	0.45
1:A:207:LEU:C	1:A:207:LEU:HD23	2.37	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:201:TYR:CD2	1:B:201:TYR:C	2.90	0.45
1:B:224:PHE:CD2	1:B:224:PHE:N	2.85	0.45
1:A:70:VAL:HG23	1:A:74:GLN:HB2	1.99	0.44
1:A:201:TYR:CD2	1:A:201:TYR:C	2.91	0.44
1:A:222:THR:O	1:A:226:GLU:HG2	2.17	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
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:203:ALA:C	1:A:205:PHE:H	2.20	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:B:93:VAL:C	1:B:95:LEU:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:520:ASP:HB3	1:B:521:TYR:CE2	2.52	0.44
1:A:209:GLU:CD	5:A:739:HOH:O	2.47	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:412:VAL:C	1:A:414:PRO:HD2	2.38	0.44
1:A:433:TRP:HA	1:A:438:HIS:HB3	2.00	0.44
1:B:332:ARG:C	1:B:338:ARG:HH22	2.21	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:224:PHE:O	1:B:225:LEU:C	2.56	0.44
1:B:329:ILE:CG2	1:B:334:HIS:HB2	2.48	0.44
1:B:543:MET:O	1:B:543:MET:HG3	2.05	0.44
1:A:220:PHE:C	1:A:222:THR:N	2.71	0.44
1:A:264:GLU:O	1:A:265:TRP:C	2.56	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
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:69:ASP:OD1	1:B:69:ASP:C	2.55	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:69:ASP:OD2	1:A:69:ASP:C	2.56	0.43
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
1:B:248:ILE:O	1:B:249:PRO:C	2.56	0.43
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:144:LYS:HZ3	1:A:146:PRO:HD2	1.83	0.43
1:A:328:ILE:HG12	1:A:565:LEU:HA	2.00	0.43
1:A:520:ASP:HB3	1:A:521:TYR:CD2	2.53	0.43
1:A:577:ASP:C	1:A:579:HIS:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:227:GLU:C	1:B:229:VAL:H	2.21	0.43
1:A:268:LYS:O	1:A:269:ARG:C	2.57	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:445:TYR:CD2	1:B:445:TYR:C	2.92	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:A:584:PRO:O	1:A:585:ILE:C	2.56	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:290:GLN:O	1:B:294:GLU:HG3	2.18	0.43
1:A:558:PHE:C	1:A:560:GLY:N	2.69	0.43
1:A:586:ILE:HG22	1:A:587:HIS:N	2.33	0.43
1:B:147:PHE:CA	1:B:149:LYS:HZ1	2.26	0.43
1:B:147:PHE:HA	1:B:149:LYS:HE2	2.01	0.43
1:B:377:ASN:C	1:B:379:ILE:H	2.21	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:B:155:TYR:HD1	1:B:196:GLY:HA2	1.84	0.43
1:B:585:ILE:O	1:B:588:GLN:N	2.52	0.43
1:A:64:ASN:HA	1:A:65:PRO:HD3	1.88	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:LEU:HD23	1:B:535:LEU:HA	1.82	0.43
1:A:93:VAL:O	1:A:94:THR:C	2.58	0.42
1:A:193:ASP:O	1:A:194:THR:C	2.57	0.42
1:B:95:LEU:O	1:B:98:MET:N	2.46	0.42
1:B:100:LEU:C	1:B:102:LYS:H	2.22	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:435:TYR:C	1:A:437:GLY:N	2.73	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:240:THR:C	1:B:242:ILE:N	2.72	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:177:ASP:C	1:B:179:PHE:N	2.72	0.42
1:B:268:LYS:O	1:B:269:ARG:C	2.57	0.42
1:B:323:PHE:O	1:B:324:TRP:C	2.57	0.42
1:B:477:SER:HA	1:B:480:LYS:HE2	2.02	0.42
1:A:531:HIS:O	1:A:532:VAL:C	2.57	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:B:585:ILE:C	1:B:587:HIS:N	2.70	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
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:329:ILE:H	1:B:329:ILE:HD12	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ASN:HA	1:B:65:PRO:HD3	1.73	0.42
1:B:83:ASP:C	1:B:85:HIS:N	2.73	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:189:SER:C	1:A:191:SER:N	2.72	0.42
1:B:93:VAL:O	1:B:94:THR:C	2.56	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:75:SER:O	1:A:76:LEU:C	2.57	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:117:GLN:C	1:A:119:MET:H	2.24	0.42
1:A:144:LYS:HD3	1:A:146:PRO:HG2	2.02	0.42
1:B:441:SER:O	1:B:442:LEU:C	2.58	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:B:238:LEU:O	1:B:239:LEU:C	2.58	0.42
1:B:255:LYS:O	1:B:258:ASN:N	2.45	0.42
1:B:415:TYR:HH	1:B:472:LYS:HD3	1.84	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:177:ASP:C	1:A:179:PHE:N	2.72	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: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:A:484:LEU:O	1:A:485:VAL:C	2.58	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
1:B:311:LEU:HD23	1:B:350:VAL:CG1	2.50	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:95:LEU:O	1:A:96:VAL:C	2.58	0.41
1:A:220:PHE:CZ	1:A:224:PHE:CE2	3.08	0.41
1:B:98:MET:O	1:B:99:GLU:C	2.59	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:B:571:LEU:HD12	1:B:571:LEU:O	2.20	0.41
1:A:96:VAL:HG22	1:A:276:VAL:HG23	2.02	0.41
1:A:405:MET:HE1	1:B:387:GLN:HB3	2.01	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:393:LEU:O	1:B:397:VAL:HG13	2.19	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: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:B:234:VAL:C	1:B:236:GLY:N	2.73	0.41
1:A:83:ASP:O	1:A:84:LYS:C	2.60	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: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:256:ARG:C	1:B:258:ASN:H	2.24	0.41
1:B:299:PHE:HA	1:B:318:LEU:CD2	2.48	0.41
1:B:519:SER:O	1:B:520:ASP:C	2.57	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:A:548:VAL:O	1:A:549:SER:C	2.58	0.40
1:B:124:HIS:ND1	1:B:124:HIS:N	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:270:PRO:C	1:B:272:MET:N	2.73	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:128:GLU:O	1:A:129:PHE:C	2.59	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:481:TYR:HD1	1:B:481:TYR:HA	1.67	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: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:237:ASP:O	1:B:238:LEU:C	2.58	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:B:204:SER:OG	1:B:218:ARG:HB2	2.21	0.40
1:B:269:ARG:O	1:B:270:PRO:C	2.57	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	2
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	349 (71%)	142 (29%)	0	1
1	B	491/492 (100%)	358 (73%)	133 (27%)	0	1
All	All	982/984 (100%)	707 (72%)	275 (28%)	0	1

All (275) 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	98	MET

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Mol	Chain	Res	Type
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	150	GLU
1	A	151	GLU
1	A	152	ARG
1	A	153	ASP
1	A	156	SER
1	A	165	ARG
1	A	173	GLN
1	A	174	GLU
1	A	180	LYS
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	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

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Mol	Chain	Res	Type
1	A	222	THR
1	A	223	LYS
1	A	228	LYS
1	A	231	GLU
1	A	234	VAL
1	A	237	ASP
1	A	238	LEU
1	A	241	ARG
1	A	253	ARG
1	A	254	ILE
1	A	255	LYS
1	A	256	ARG
1	A	263	ILE
1	A	264	GLU
1	A	267	ARG
1	A	268	LYS
1	A	271	ASP
1	A	272	MET
1	A	278	GLU
1	A	290	GLN
1	A	293	GLU
1	A	296	LYS
1	A	297	GLU
1	A	298	SER
1	A	305	THR
1	A	308	VAL
1	A	309	GLU
1	A	317	ARG
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

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Mol	Chain	Res	Type
1	A	399	ASP
1	A	405	MET
1	A	413	ILE
1	A	417	ARG
1	A	429	VAL
1	A	439	LYS
1	A	442	LEU
1	A	444	GLU
1	A	454	SER
1	A	465	ARG
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
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	543	MET
1	A	544	ASN
1	A	547	ARG
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	585	ILE
1	A	586	ILE
1	A	588	GLN
1	A	591	THR
1	A	592	ARG

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Mol	Chain	Res	Type
1	A	598	PHE
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	97	LYS
1	B	98	MET
1	B	99	GLU
1	B	102	LYS
1	B	103	GLU
1	B	107	ILE
1	B	118	ARG
1	B	121	LEU
1	B	122	SER
1	B	124	HIS
1	B	127	ASN
1	B	130	LYS
1	B	134	SER
1	B	140	HIS
1	B	147	PHE
1	B	154	LEU
1	B	159	LEU
1	B	162	ARG
1	B	164	LEU
1	B	165	ARG
1	B	170	GLN
1	B	173	GLN
1	B	178	SER
1	B	180	LYS
1	B	181	ASN
1	B	183	GLU
1	B	188	GLU
1	B	189	SER

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Mol	Chain	Res	Type
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	216	SER
1	B	218	ARG
1	B	225	LEU
1	B	226	GLU
1	B	228	LYS
1	B	231	GLU
1	B	235	ASP
1	B	239	LEU
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	269	ARG
1	B	271	ASP
1	B	272	MET
1	B	278	GLU
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	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

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Mol	Chain	Res	Type
1	B	393	LEU
1	B	397	VAL
1	B	401	SER
1	B	405	MET
1	B	406	LYS
1	B	411	ASN
1	B	413	ILE
1	B	416	LEU
1	B	418	GLN
1	B	426	LYS
1	B	427	TYR
1	B	439	LYS
1	B	441	SER
1	B	443	GLU
1	B	468	ASP
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	501	SER
1	B	502	VAL
1	B	503	GLU
1	B	507	ARG
1	B	513	SER
1	B	515	GLN
1	B	518	MET
1	B	519	SER
1	B	520	ASP
1	B	529	ARG
1	B	530	LYS
1	B	535	LEU
1	B	542	LYS
1	B	547	ARG
1	B	550	LYS
1	B	552	SER
1	B	556	LYS
1	B	570	GLN
1	B	571	LEU

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Mol	Chain	Res	Type
1	B	575	ASN
1	B	582	GLN
1	B	583	HIS
1	B	585	ILE
1	B	588	GLN
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 (32) 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	126	GLN
1	A	173	GLN
1	A	181	ASN
1	A	230	ASN
1	A	333	GLN
1	A	411	ASN
1	A	461	HIS
1	A	544	ASN
1	B	74	GLN
1	B	85	HIS
1	B	117	GLN
1	B	145	ASN
1	B	167	HIS
1	B	170	GLN
1	B	181	ASN
1	B	288	GLN
1	B	325	ASN
1	B	333	GLN
1	B	345	ASN
1	B	387	GLN
1	B	394	ASN
1	B	411	ASN
1	B	461	HIS
1	B	515	GLN
1	B	575	ASN

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Mol	Chain	Res	Type
1	B	587	HIS
1	B	589	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	F3P	A	600	2	16,19,19	2.18	4 (25%)	20,29,29	2.63	4 (20%)
4	BTB	A	604	-	13,13,13	3.62	5 (38%)	7,16,16	0.69	0
3	F3P	B	1600	2	16,19,19	2.24	4 (25%)	20,29,29	2.56	4 (20%)

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
3	F3P	A	600	2	-	7/19/25/25	-
4	BTB	A	604	-	-	8/21/21/21	-
3	F3P	B	1600	2	-	5/19/25/25	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	BTB	C2-N	10.21	1.68	1.48
3	B	1600	F3P	C1-C2	-5.73	1.39	1.50
4	A	604	BTB	C5-N	4.91	1.55	1.48
3	A	600	F3P	C1-C2	-4.90	1.41	1.50
4	A	604	BTB	C7-N	4.56	1.54	1.48
3	A	600	F3P	C10-C3	-4.24	1.42	1.52
3	B	1600	F3P	C10-C3	-4.20	1.42	1.52
3	B	1600	F3P	PA-O1A	3.35	1.62	1.50
3	A	600	F3P	PA-O1A	3.32	1.62	1.50
4	A	604	BTB	C4-C2	3.12	1.57	1.53
4	A	604	BTB	C1-C2	3.01	1.57	1.53
3	A	600	F3P	PB-O3B	2.26	1.63	1.54
3	B	1600	F3P	PB-O3B	2.03	1.62	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	F3P	F-C2-C1	10.35	125.19	108.18
3	B	1600	F3P	F-C2-C1	9.91	124.48	108.18
3	A	600	F3P	PA-O3A-PB	-3.12	122.12	132.83
3	B	1600	F3P	PA-O3A-PB	-2.94	122.74	132.83
3	B	1600	F3P	C5-C6-C7	2.41	127.36	115.98
3	A	600	F3P	C5-C6-C7	2.32	126.89	115.98
3	B	1600	F3P	C9-C7-C8	2.05	119.97	110.51
3	A	600	F3P	C9-C7-C8	2.01	119.78	110.51

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	F3P	C1-C2-C3-C4
3	A	600	F3P	C1-C2-C3-C10
3	A	600	F3P	PA-O3A-PB-O2B
4	A	604	BTB	O1-C1-C2-C4

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Mol	Chain	Res	Type	Atoms
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	C4-C5-C6-C7
3	B	1600	F3P	C5-C6-C7-C9
3	A	600	F3P	C5-C6-C7-C9
3	A	600	F3P	PA-O3A-PB-O1B
3	B	1600	F3P	C3-O1-PA-O3A
3	B	1600	F3P	C10-C3-O1-PA
3	A	600	F3P	C3-C4-C5-C6
3	B	1600	F3P	C3-C4-C5-C6
3	B	1600	F3P	C1-C2-C3-C10

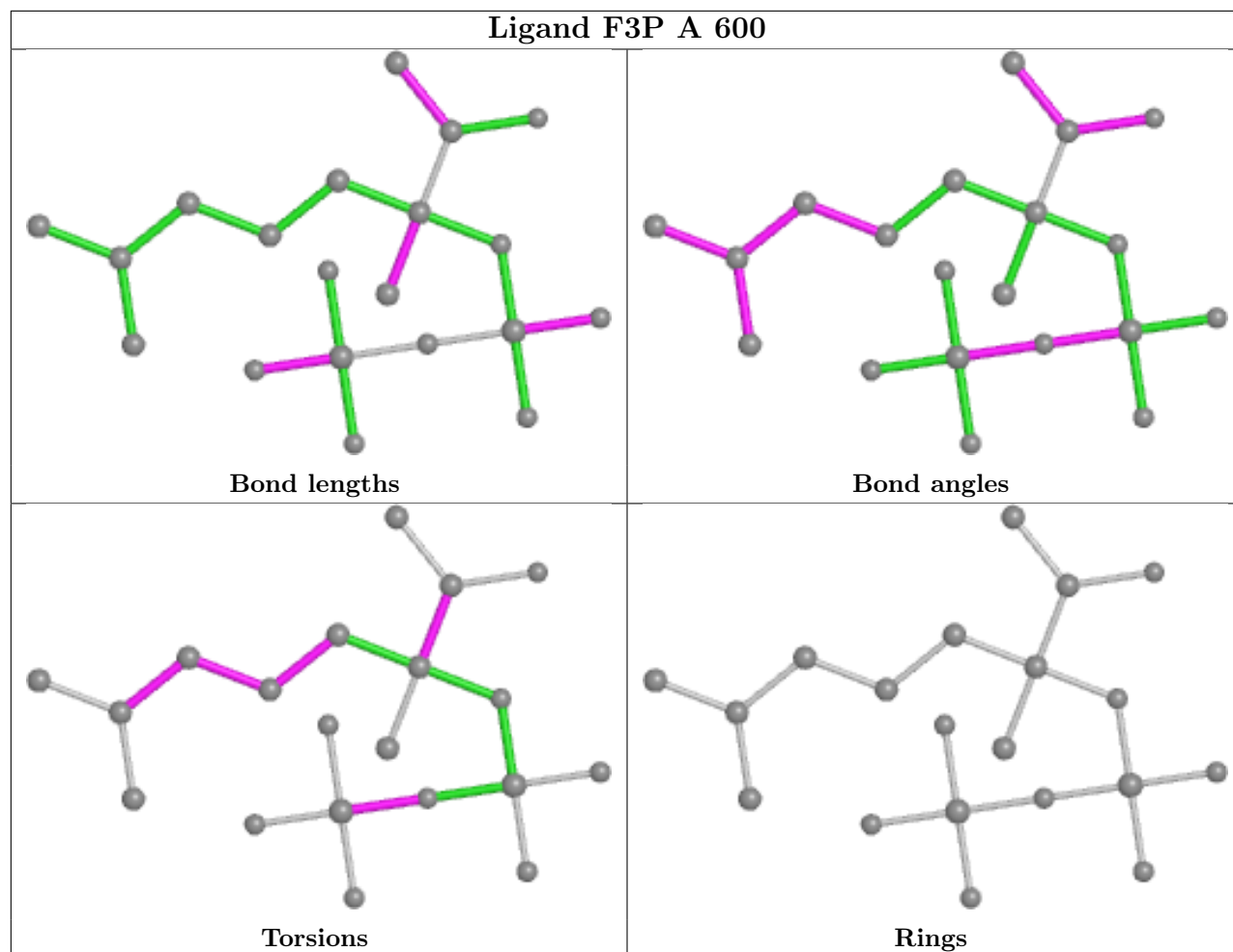
There are no ring outliers.

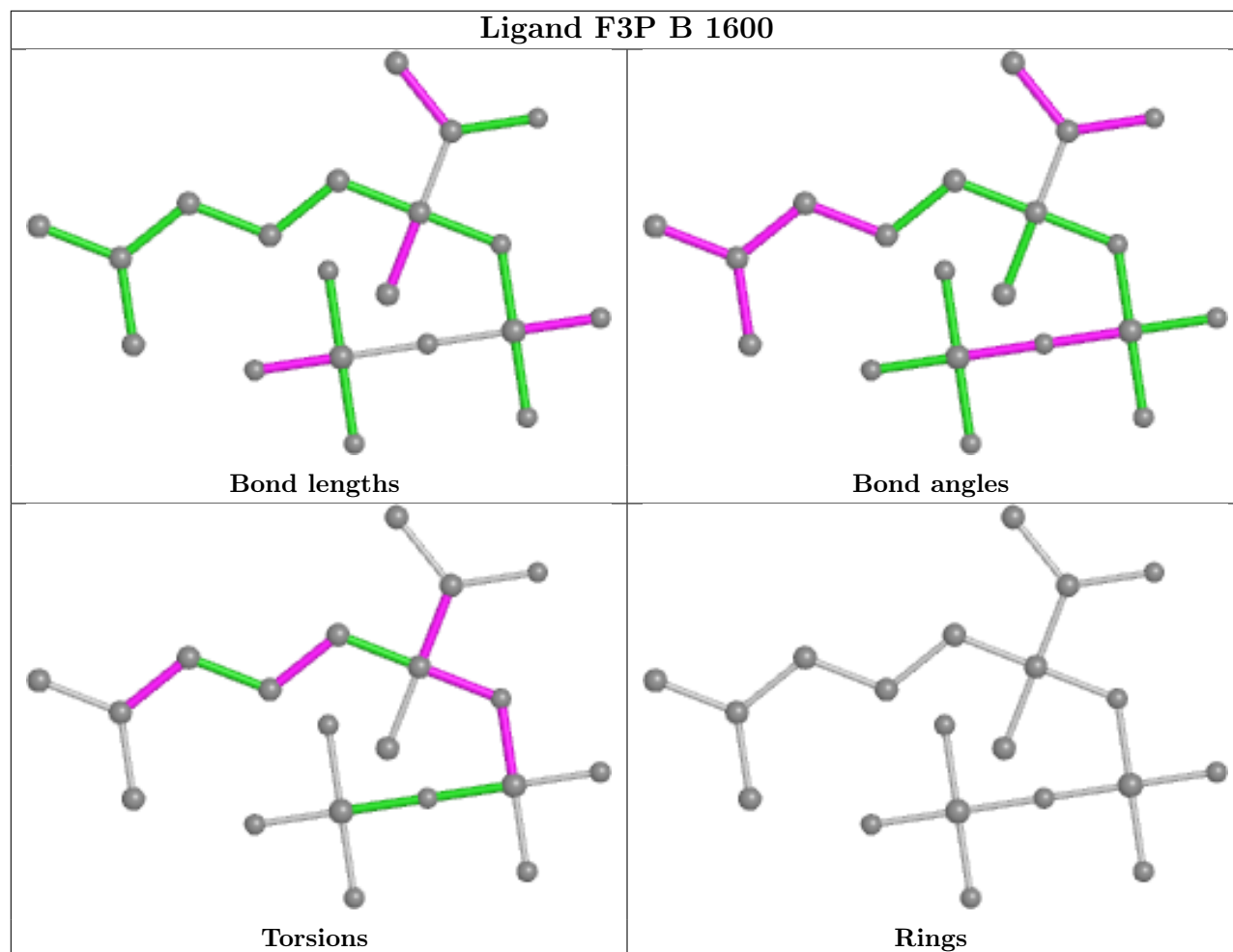
3 monomers are involved in 48 short contacts:

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

Ligand F3P A 600





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	543/543 (100%)	0.21	18 (3%)	46	46	24, 52, 97, 100	0
1	B	543/543 (100%)	0.22	18 (3%)	46	46	23, 52, 98, 100	0
All	All	1086/1086 (100%)	0.21	36 (3%)	46	46	23, 52, 98, 100	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	579	HIS	8.1
1	A	580	GLY	6.5
1	A	577	ASP	5.8
1	A	578	GLY	5.2
1	B	581	THR	4.8
1	B	579	HIS	4.6
1	B	598	PHE	4.4
1	A	598	PHE	3.6
1	B	578	GLY	3.6
1	B	73	ILE	3.6
1	B	502	VAL	3.5
1	B	234	VAL	3.3
1	B	577	ASP	3.2
1	B	147	PHE	2.9
1	B	580	GLY	2.9
1	B	190	LEU	2.9
1	A	92	LEU	2.8
1	B	263	ILE	2.6
1	A	502	VAL	2.5
1	B	176	PHE	2.5
1	B	505	VAL	2.4
1	A	263	ILE	2.4
1	A	508	GLY	2.3
1	A	238	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	254	ILE	2.2
1	A	232	GLY	2.2
1	B	501	SER	2.2
1	B	221	ALA	2.2
1	B	586	ILE	2.1
1	A	280	ALA	2.1
1	A	599	ALA	2.1
1	A	176	PHE	2.1
1	A	214	LEU	2.0
1	B	276	VAL	2.0
1	A	73	ILE	2.0
1	A	276	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

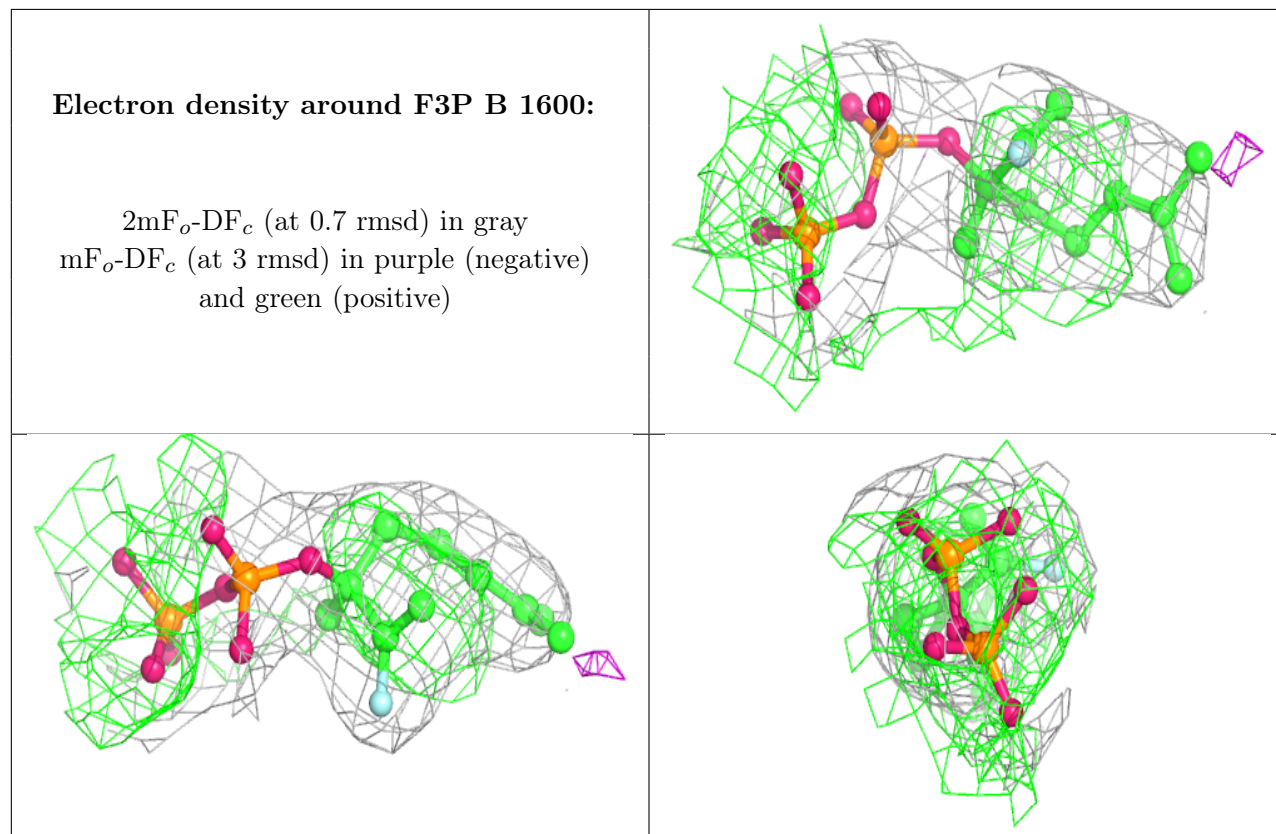
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
4	BTB	A	604	14/14	0.83	0.42	84,91,100,100	0
3	F3P	B	1600	20/20	0.92	0.26	45,53,63,66	0
2	MN	B	1602	1/1	0.94	0.30	70,70,70,70	0
3	F3P	A	600	20/20	0.94	0.24	45,55,64,67	0
2	MN	A	602	1/1	0.97	0.28	52,52,52,52	0
2	MN	B	1603	1/1	0.98	0.26	55,55,55,55	0
2	MN	A	603	1/1	0.98	0.23	54,54,54,54	0
2	MN	B	1601	1/1	0.98	0.30	49,49,49,49	0
2	MN	A	601	1/1	0.98	0.32	61,61,61,61	0

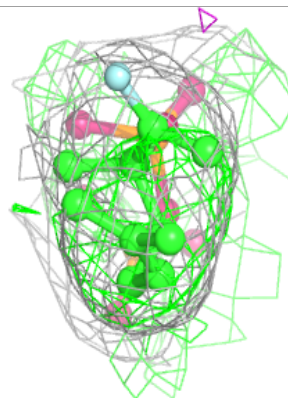
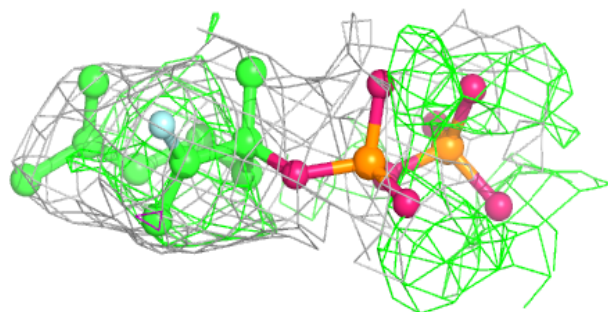
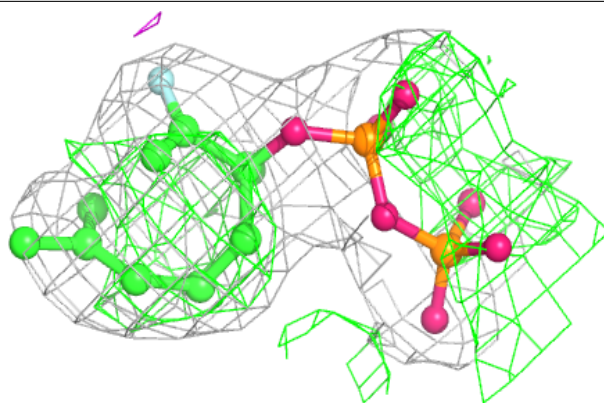
The following is a graphical depiction of the model fit to experimental electron density of all

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.