



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 04:45 PM EDT

PDB ID : 2ONG
Title : Crystal Structure of of limonene synthase with 2-fluorogeranyl diphosphate (FGPP).
Authors : Hyatt, D.C.; Youn, B.; Croteau, R.; Kang, C.
Deposited on : 2007-01-23
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

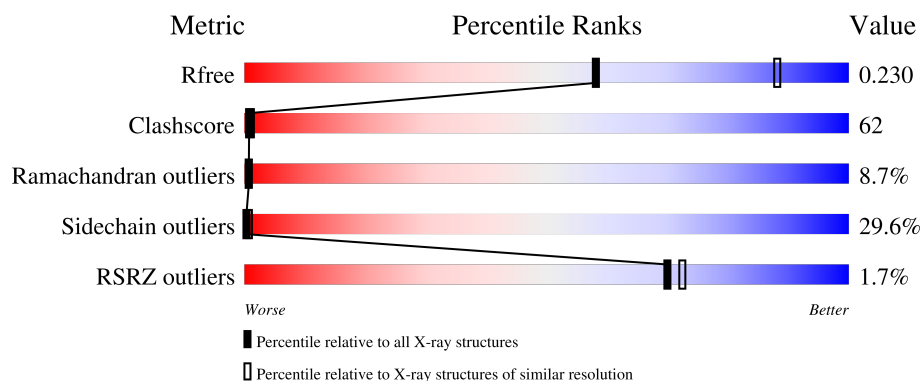
1 Overall quality at a glance

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	<div> <div>2%</div> <div>19% 47% 29% 6%</div> </div>
1	B	543	<div> <div>%</div> <div>20% 45% 30% 5%</div> </div>

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	FPG	A	600	-	-	X	-
3	FPG	B	1600	-	-	X	-
4	BTB	A	605	-	-	X	-
4	BTB	B	1604	-	-	X	-
4	BTB	B	1605	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9181 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
			4495	2871	761	843	20			
1	B	543	Total	C	N	O	S	0	0	0
			4491	2870	758	843	20			

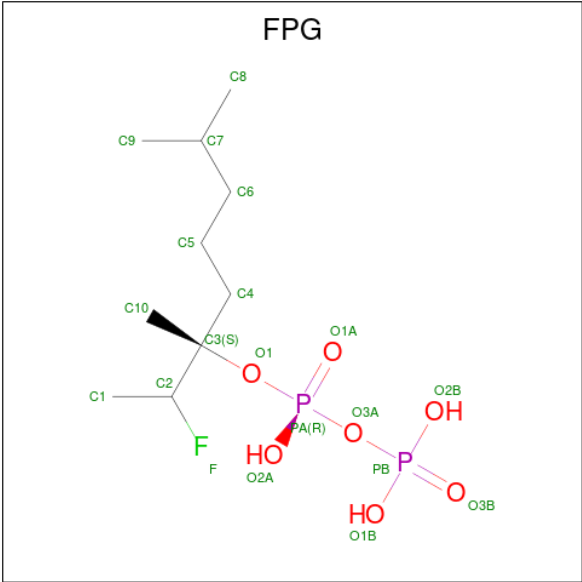
There are 2 discrepancies between the modelled and reference sequences:

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).

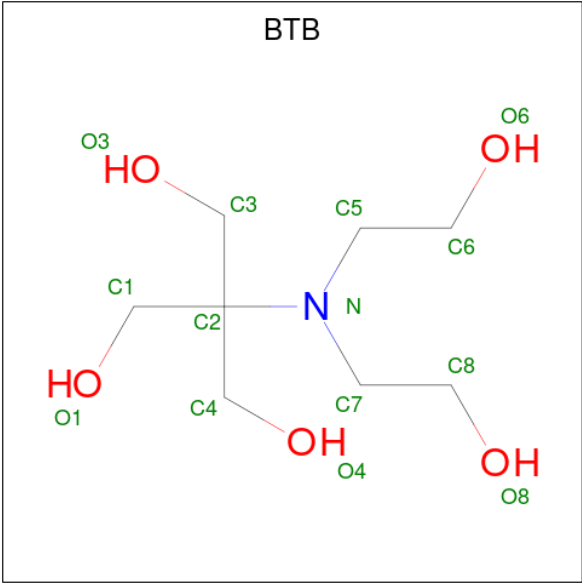
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mn	0	0
			3	3		
2	B	3	Total	Mn	0	0
			3	3		

- Molecule 3 is (1S)-1-[(1R)-1-FLUOROETHYL]-1,5-DIMETHYLHEXYL TRIHYDROGEN DIPHOSPHATE (three-letter code: FPG) (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		

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

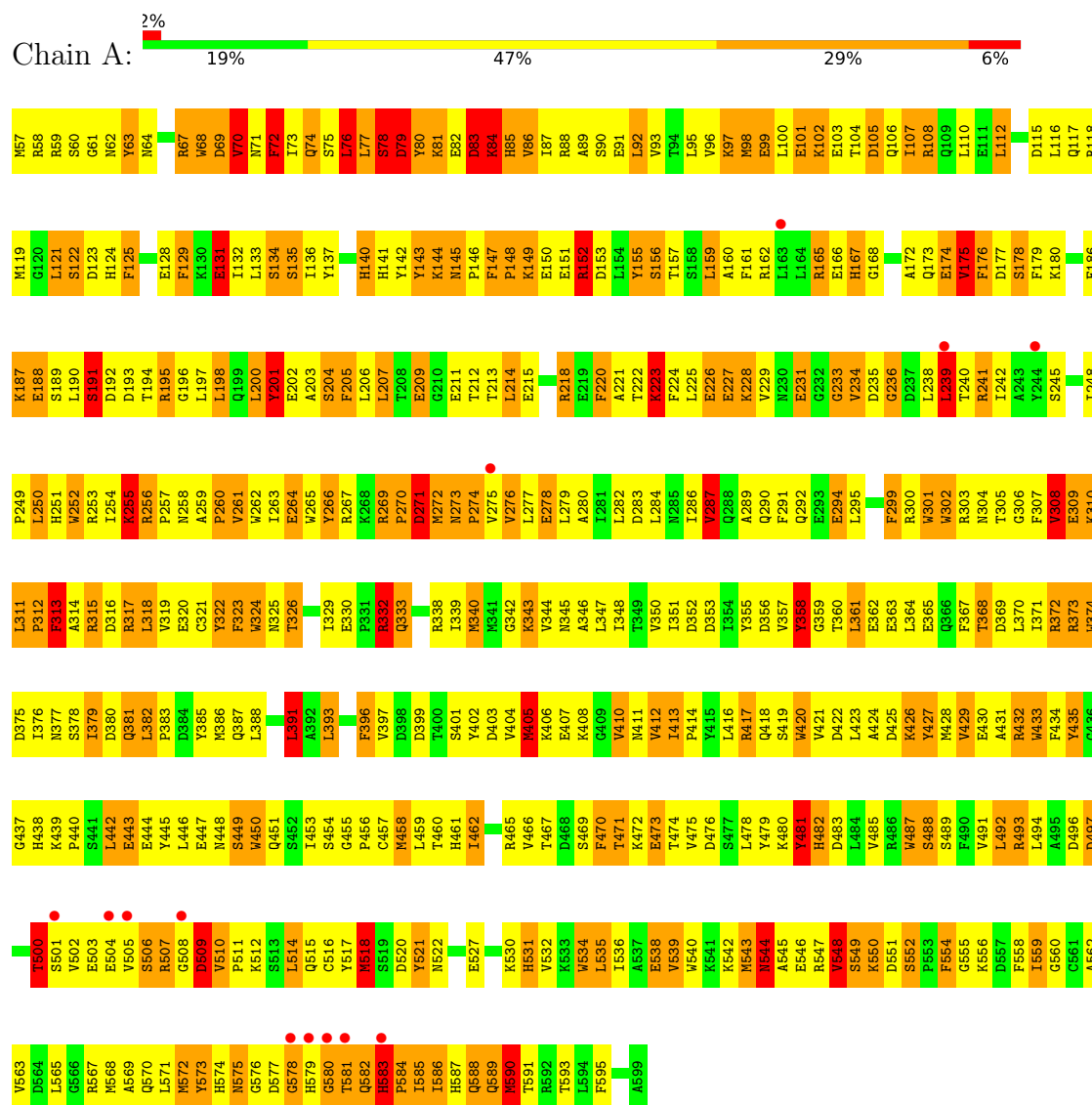
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total	O	0	0
			39	39		
5	B	54	Total	O	0	0
			54	54		

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



G560	G561	A562	V563	D564	L565	G566	S567	M568	A569	Q570	L571	M572	S573	H574	N575	G576	D577	G578	H579	G580	T581	Q582	H583	P584	I585	I586	H587	Q588	Q589	M590	T591	R592	K593	T593	L594	F595	E596	P597	F598	A599																			
L494	A495	D496	D497	L498	G499	T500	S501	V502	E503	E504	L505	S506	G507	M508	D509	V510	P511	K512	L513	L514	Q515	C516	Y517	M518	S519	D520	A526	E527	A528	R529	K530	H531	W534	L535	I536	A537	W540	K541	M542	M543	N544	A545	E546	R547	V548	S549	K550	D551	S552	P553	F554	G555	K556	D557	L558	L559			
W434	Y435	G436	G437	H438	L439	P440	S441	L442	E443	E444	Y445	L446	E447	M448	S449	W450	Q451	S452	T453	S454	P455	C457	M458	L459	T460	H461	L462	F463	F464	R465	V466	D467	D468	S469	F470	T471	K472	E473	T474	V475	D476	S477	L478	Y479	K480	Y481	H482	D483	L484	V485	R486	W487	S488	S489	F490	V491	L492	R493	
I371	R372	K373	W374	D375	L376	K377	S378	L379	D380	Q381	L382	P383	D384	Y385	K386	Q387	L388	L391	A392	L393	N394	N395	F396	V397	D398	D399	T400	S401	L402	K406	E407	K408	G409	V410	N411	I412	I413	P414	Y415	L416	R417	Q418	S419	V420	Y421	D422	L423	A424	D425	K426	Y427	M428	V429	E430	A431	R432	W433		
V308	E309	K310	L311	P312	F313	A314	R315	D316	R317	L318	V319	E320	C321	T322	F323	W324	N325	T326	T329	K332	Q333	Q334	A335	S336	P337	R338	L339	V339	K340	G342	K343	V344	L345	L347	I348	V349	V350	I351	D352	D353	I354	V357	E362	E363	L364	K365	M366	F367	T368	D369	L370								
D247	I248	P249	L250	P251	W252	R253	L254	K255	R256	P257	W258	F259	P260	W261	W262	I263	W265	W266	R267	K268	R269	P270	D271	W272	R273	P274	W275	V276	L277	E278	L279	A280	I281	L282	D283	L284	W285	L286	V287	Q288	A289	Q290	F291	Q292	E293	E294	L295	K296	F299	K300	W301	K302	R303	I304	T305	G306	F307		
E185	E188	E189	L190	S191	D192	D193	D194	R195	G196	Q199	L200	Y201	E202	A203	S204	F205	L206	L207	T208	E209	G210	E211	T212	T213	L214	E215	S216	A217	R218	E219	F220	A221	T222	K223	F224	L225	E226	E227	K228	V229	W230	E231	G232	G233	V234	D235	G236	D237	L238	L239	T240	R241	L242	A243	Y244	E245	L246		
Q117	R118	M119	G120	S121	L121	D123	H124	L125	Q126	N127	E128	F129	K130	E131	I132	Y137	L138	D139	H140	H141	Y142	Y143	K144	N145	P146	F147	P148	K149	V150	E151	R152	D153	L154	Y155	S156	T157	S158	L159	A160	F161	R162	L163	L164	R165	F169	E174	V176	Q177	S178	F179	K180	N181	E182	G306	F307				
M57	R58	R59	S60	G61	M62	Y63	M64	P65	S66	R67	W68	F69	D70	W71	F72	I73	Q74	S75	L76	L77	S78	D79	Y80	K81	E82	K83	P84	H85	V86	I87	R88	A89	S90	E91	L92	V93	T94	L95	V96	K97	M98	E99	L100	E101	A102	E103	T104	D105	Q106	I107	R108	Q109	L110	E111	L112	I113	D114	E115	L116

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	200.48Å 200.48Å 123.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 27.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.70) 93.0 (27.90-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.61Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.208 , 0.241 0.221 , 0.230	Depositor DCC
R_{free} test set	3503 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 120.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.478 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9181	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BTB, FPG, 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	0.91	9/4607 (0.2%)	1.67	129/6234 (2.1%)
1	B	0.89	4/4603 (0.1%)	1.62	108/6230 (1.7%)
All	All	0.90	13/9210 (0.1%)	1.65	237/12464 (1.9%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	THR	C-O	8.06	1.38	1.23
1	A	131	GLU	CG-CD	7.48	1.63	1.51
1	B	368	THR	C-O	6.90	1.36	1.23
1	A	487	TRP	CG-CD2	-6.30	1.32	1.43
1	A	433	TRP	CG-CD2	-6.29	1.32	1.43
1	A	209	GLU	CG-CD	6.14	1.61	1.51
1	B	131	GLU	CG-CD	5.71	1.60	1.51
1	B	209	GLU	CG-CD	5.50	1.60	1.51
1	A	374	TRP	CG-CD2	-5.36	1.34	1.43
1	B	252	TRP	CG-CD2	-5.26	1.34	1.43
1	A	262	TRP	CG-CD2	-5.13	1.34	1.43
1	A	68	TRP	CG-CD2	-5.05	1.35	1.43
1	A	252	TRP	CG-CD2	-5.03	1.35	1.43

All (237) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	TYR	N-CA-C	-11.62	79.63	111.00
1	B	266	TYR	CB-CG-CD1	-11.53	114.08	121.00
1	A	266	TYR	CB-CG-CD1	-10.92	114.45	121.00
1	A	433	TRP	CD1-CG-CD2	10.65	114.82	106.30
1	A	143	TYR	CB-CG-CD1	-10.62	114.62	121.00
1	B	324	TRP	CD1-CG-CD2	10.34	114.57	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	358	TYR	CB-CG-CD2	-10.26	114.85	121.00
1	A	356	ASP	CB-CG-OD2	-10.24	109.08	118.30
1	B	481	TYR	CB-CG-CD2	-10.06	114.97	121.00
1	B	420	TRP	CD1-CG-CD2	9.96	114.27	106.30
1	B	63	TYR	CB-CG-CD2	-9.96	115.02	121.00
1	A	581	THR	N-CA-C	-9.44	85.52	111.00
1	A	590	MET	CG-SD-CE	-9.21	85.46	100.20
1	A	420	TRP	CD1-CG-CD2	9.18	113.64	106.30
1	B	209	GLU	N-CA-C	-9.10	86.43	111.00
1	A	356	ASP	CB-CG-OD1	9.09	126.48	118.30
1	A	302	TRP	CD1-CG-CD2	9.07	113.56	106.30
1	A	583	HIS	N-CA-C	8.98	135.26	111.00
1	A	534	TRP	CD1-CG-CD2	8.82	113.35	106.30
1	B	265	TRP	CD1-CG-CD2	8.78	113.32	106.30
1	A	573	TYR	CB-CG-CD1	-8.77	115.74	121.00
1	A	481	TYR	CA-CB-CG	-8.76	96.75	113.40
1	A	324	TRP	CD1-CG-CD2	8.68	113.25	106.30
1	A	551	ASP	N-CA-C	-8.52	88.00	111.00
1	B	72	PHE	CB-CG-CD2	-8.48	114.86	120.80
1	A	313	PHE	C-N-CA	8.41	142.72	121.70
1	B	479	TYR	CB-CG-CD2	-8.38	115.97	121.00
1	A	548	VAL	CG1-CB-CG2	-8.25	97.69	110.90
1	B	137	TYR	CB-CG-CD2	-8.19	116.09	121.00
1	B	302	TRP	CB-CG-CD1	-8.11	116.45	127.00
1	A	262	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	B	263	ILE	CA-CB-CG2	-8.04	94.83	110.90
1	A	481	TYR	CB-CG-CD2	-8.04	116.18	121.00
1	B	68	TRP	CD1-CG-CD2	8.01	112.71	106.30
1	A	374	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	B	341	MET	CG-SD-CE	-7.99	87.42	100.20
1	B	549	SER	C-N-CA	7.94	141.54	121.70
1	A	68	TRP	CD1-CG-CD2	7.91	112.63	106.30
1	B	450	TRP	CD1-CG-CD2	7.87	112.60	106.30
1	A	167	HIS	CA-CB-CG	-7.86	100.24	113.60
1	A	543	MET	CG-SD-CE	-7.80	87.72	100.20
1	B	340	MET	CG-SD-CE	-7.73	87.83	100.20
1	B	534	TRP	CG-CD2-CE3	7.72	140.85	133.90
1	A	479	TYR	CB-CG-CD1	-7.70	116.38	121.00
1	A	265	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	B	475	VAL	CG1-CB-CG2	-7.67	98.62	110.90
1	A	450	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	A	531	HIS	CA-CB-CG	-7.64	100.60	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	534	TRP	CB-CG-CD1	-7.64	117.07	127.00
1	A	302	TRP	CB-CG-CD1	-7.62	117.10	127.00
1	A	287	VAL	CA-CB-CG1	-7.50	99.64	110.90
1	B	464	PHE	CB-CG-CD1	-7.39	115.62	120.80
1	B	129	PHE	CB-CG-CD2	-7.38	115.63	120.80
1	B	302	TRP	CG-CD2-CE3	7.36	140.53	133.90
1	A	480	LYS	N-CA-C	-7.31	91.25	111.00
1	A	534	TRP	CB-CG-CD1	-7.31	117.49	127.00
1	B	433	TRP	CD1-CG-CD2	7.28	112.12	106.30
1	A	142	TYR	CB-CG-CD1	-7.27	116.64	121.00
1	B	209	GLU	CB-CG-CD	7.06	133.26	114.20
1	B	302	TRP	NE1-CE2-CZ2	-7.04	122.66	130.40
1	A	518	MET	CB-CG-SD	-7.03	91.31	112.40
1	A	410	VAL	N-CA-C	7.01	129.93	111.00
1	B	211	GLU	N-CA-C	6.93	129.72	111.00
1	A	313	PHE	N-CA-C	-6.93	92.29	111.00
1	A	195	ARG	N-CA-C	-6.90	92.38	111.00
1	B	302	TRP	CD1-CG-CD2	6.87	111.79	106.30
1	A	544	ASN	CA-CB-CG	-6.83	98.37	113.40
1	A	155	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	B	420	TRP	CG-CD1-NE1	-6.81	103.29	110.10
1	B	572	MET	CG-SD-CE	-6.78	89.36	100.20
1	B	324	TRP	CE2-CD2-CG	-6.77	101.89	107.30
1	A	580	GLY	N-CA-C	-6.74	96.25	113.10
1	B	540	TRP	CD1-CG-CD2	6.71	111.67	106.30
1	A	487	TRP	CD1-NE1-CE2	-6.71	102.96	109.00
1	B	324	TRP	CG-CD1-NE1	-6.71	103.39	110.10
1	A	487	TRP	NE1-CE2-CD2	6.71	114.01	107.30
1	B	262	TRP	CD1-CG-CD2	6.66	111.63	106.30
1	A	433	TRP	CG-CD1-NE1	-6.66	103.44	110.10
1	B	385	TYR	CB-CG-CD1	-6.65	117.01	121.00
1	A	534	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	A	302	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	B	63	TYR	CB-CG-CD1	6.62	124.97	121.00
1	A	302	TRP	CG-CD2-CE3	6.61	139.85	133.90
1	A	450	TRP	CE2-CD2-CG	-6.61	102.02	107.30
1	A	252	TRP	NE1-CE2-CD2	6.58	113.88	107.30
1	A	209	GLU	CB-CG-CD	6.57	131.94	114.20
1	B	311	LEU	N-CA-C	-6.57	93.27	111.00
1	B	71	ASN	CA-CB-CG	-6.56	98.97	113.40
1	A	521	TYR	CA-CB-CG	-6.54	100.98	113.40
1	B	302	TRP	CE2-CD2-CG	-6.54	102.07	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	GLU	CB-CG-CD	6.53	131.84	114.20
1	A	301	TRP	CB-CG-CD1	-6.53	118.52	127.00
1	A	586	ILE	N-CA-C	-6.52	93.40	111.00
1	B	420	TRP	CE2-CD2-CG	-6.52	102.09	107.30
1	A	129	PHE	CB-CG-CD1	-6.50	116.25	120.80
1	B	301	TRP	CD1-CG-CD2	6.50	111.50	106.30
1	B	85	HIS	CA-CB-CG	-6.44	102.65	113.60
1	B	487	TRP	CD1-CG-CD2	6.38	111.41	106.30
1	A	405	MET	CG-SD-CE	-6.38	89.99	100.20
1	A	85	HIS	CA-CB-CG	-6.36	102.79	113.60
1	B	450	TRP	CE2-CD2-CG	-6.35	102.22	107.30
1	B	534	TRP	CD1-CG-CD2	6.27	111.32	106.30
1	A	482	HIS	CA-CB-CG	-6.26	102.95	113.60
1	B	598	PHE	C-N-CA	6.26	137.35	121.70
1	A	63	TYR	N-CA-C	-6.23	94.17	111.00
1	B	396	PHE	CB-CG-CD1	-6.23	116.44	120.80
1	B	265	TRP	CG-CD1-NE1	-6.22	103.88	110.10
1	B	415	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	A	433	TRP	CE2-CD2-CG	-6.20	102.34	107.30
1	A	420	TRP	CE2-CD2-CG	-6.20	102.34	107.30
1	B	68	TRP	CE2-CD2-CG	-6.18	102.36	107.30
1	A	72	PHE	CB-CG-CD1	-6.16	116.49	120.80
1	A	322	TYR	CB-CG-CD1	-6.15	117.31	121.00
1	B	263	ILE	CA-CB-CG1	6.14	122.68	111.00
1	A	534	TRP	NE1-CE2-CZ2	-6.11	123.68	130.40
1	A	262	TRP	CE2-CD2-CG	-6.11	102.41	107.30
1	A	142	TYR	CD1-CG-CD2	6.10	124.61	117.90
1	B	334	HIS	CA-CB-CG	-6.10	103.23	113.60
1	B	339	ILE	CA-CB-CG2	-6.10	98.70	110.90
1	B	445	TYR	CB-CG-CD1	-6.10	117.34	121.00
1	B	265	TRP	CE2-CD2-CG	-6.10	102.42	107.30
1	A	205	PHE	CA-CB-CG	-6.09	99.29	113.90
1	B	97	LYS	N-CA-C	-6.08	94.59	111.00
1	B	238	LEU	N-CA-C	-6.07	94.62	111.00
1	B	380	ASP	CA-CB-CG	-6.07	100.06	113.40
1	A	301	TRP	NE1-CE2-CZ2	-6.04	123.76	130.40
1	B	534	TRP	CE2-CD2-CG	-6.01	102.49	107.30
1	A	487	TRP	CE2-CD2-CE3	5.99	125.88	118.70
1	A	175	VAL	CA-CB-CG2	-5.96	101.95	110.90
1	A	420	TRP	CG-CD1-NE1	-5.96	104.14	110.10
1	A	480	LYS	C-N-CA	5.94	136.55	121.70
1	B	468	ASP	C-N-CA	-5.94	106.85	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	422	ASP	CA-CB-CG	5.92	126.43	113.40
1	A	68	TRP	CE2-CD2-CG	-5.91	102.58	107.30
1	B	543	MET	CG-SD-CE	-5.90	90.76	100.20
1	B	517	TYR	CB-CG-CD1	-5.90	117.46	121.00
1	A	538	GLU	C-N-CA	-5.85	107.08	121.70
1	A	265	TRP	CE2-CD2-CG	-5.83	102.64	107.30
1	A	148	PRO	C-N-CA	5.81	136.22	121.70
1	A	324	TRP	CG-CD1-NE1	-5.81	104.29	110.10
1	B	301	TRP	CE2-CD2-CG	-5.81	102.66	107.30
1	A	358	TYR	CD1-CG-CD2	5.79	124.27	117.90
1	A	252	TRP	CD1-NE1-CE2	-5.78	103.79	109.00
1	B	421	VAL	CG1-CB-CG2	-5.73	101.73	110.90
1	B	72	PHE	CB-CG-CD1	5.70	124.79	120.80
1	B	223	LYS	C-N-CA	-5.69	107.46	121.70
1	A	487	TRP	CG-CD2-CE3	-5.68	128.79	133.90
1	B	244	TYR	C-N-CA	-5.67	107.52	121.70
1	A	223	LYS	C-N-CA	-5.66	107.56	121.70
1	B	464	PHE	CD1-CG-CD2	5.65	125.64	118.30
1	B	201	TYR	CB-CG-CD1	-5.64	117.61	121.00
1	B	207	LEU	N-CA-C	5.64	126.22	111.00
1	B	262	TRP	CE2-CD2-CG	-5.62	102.80	107.30
1	A	324	TRP	CE2-CD2-CG	-5.61	102.81	107.30
1	B	534	TRP	NE1-CE2-CZ2	-5.61	124.22	130.40
1	A	80	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	A	458	MET	CG-SD-CE	5.60	109.16	100.20
1	B	374	TRP	NE1-CE2-CD2	5.60	112.90	107.30
1	A	482	HIS	ND1-CG-CD2	5.60	116.64	108.80
1	A	410	VAL	CB-CA-C	-5.58	100.79	111.40
1	A	302	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	A	374	TRP	CE2-CD2-CG	-5.56	102.86	107.30
1	A	301	TRP	CG-CD2-CE3	5.53	138.87	133.90
1	B	318	LEU	C-N-CA	-5.52	107.90	121.70
1	B	470	PHE	CB-CG-CD1	-5.51	116.94	120.80
1	B	342	GLY	N-CA-C	-5.50	99.35	113.10
1	B	450	TRP	CG-CD2-CE3	5.50	138.85	133.90
1	A	201	TYR	CB-CG-CD1	-5.49	117.71	121.00
1	A	358	TYR	CB-CG-CD1	-5.49	117.71	121.00
1	A	420	TRP	CA-CB-CG	-5.47	103.31	113.70
1	A	299	PHE	CB-CG-CD1	-5.46	116.97	120.80
1	A	155	TYR	CD1-CG-CD2	5.45	123.89	117.90
1	B	252	TRP	CD1-CG-CD2	5.44	110.66	106.30
1	A	105	ASP	CA-CB-CG	-5.44	101.43	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	374	TRP	CD1-CG-CD2	5.43	110.64	106.30
1	B	68	TRP	CA-CB-CG	-5.43	103.39	113.70
1	B	480	LYS	N-CA-C	-5.42	96.35	111.00
1	A	323	PHE	CB-CG-CD2	-5.42	117.00	120.80
1	B	590	MET	CG-SD-CE	-5.42	91.53	100.20
1	B	435	TYR	CB-CG-CD2	-5.41	117.75	121.00
1	A	554	PHE	CB-CG-CD2	-5.41	117.01	120.80
1	B	195	ARG	N-CA-C	-5.38	96.46	111.00
1	A	576	GLY	C-N-CA	5.38	135.14	121.70
1	A	585	ILE	CA-CB-CG1	-5.38	100.78	111.00
1	B	387	GLN	N-CA-C	-5.38	96.49	111.00
1	A	86	VAL	CA-CB-CG2	-5.36	102.85	110.90
1	A	99	GLU	N-CA-C	-5.36	96.53	111.00
1	B	209	GLU	N-CA-CB	5.36	120.25	110.60
1	A	308	VAL	CG1-CB-CG2	5.36	119.47	110.90
1	A	439	LYS	N-CA-C	-5.36	96.53	111.00
1	A	583	HIS	N-CA-CB	-5.32	101.02	110.60
1	A	302	TRP	NE1-CE2-CZ2	-5.29	124.58	130.40
1	A	80	TYR	N-CA-C	-5.29	96.71	111.00
1	B	107	ILE	CA-CB-CG1	-5.29	100.95	111.00
1	A	271	ASP	CA-CB-CG	5.28	125.01	113.40
1	A	265	TRP	CG-CD1-NE1	-5.28	104.83	110.10
1	B	307	PHE	CB-CG-CD2	-5.28	117.11	120.80
1	A	250	LEU	C-N-CA	-5.27	108.52	121.70
1	B	188	GLU	CB-CG-CD	5.26	128.40	114.20
1	B	262	TRP	NE1-CE2-CD2	5.25	112.55	107.30
1	A	582	GLN	CB-CG-CD	5.25	125.24	111.60
1	B	479	TYR	CG-CD2-CE2	-5.25	117.10	121.30
1	B	450	TRP	CB-CG-CD1	-5.24	120.19	127.00
1	A	201	TYR	CG-CD1-CE1	-5.24	117.11	121.30
1	A	396	PHE	C-N-CA	-5.23	108.62	121.70
1	B	439	LYS	N-CA-C	-5.21	96.93	111.00
1	B	318	LEU	N-CA-C	5.21	125.07	111.00
1	A	534	TRP	NE1-CE2-CD2	5.20	112.50	107.30
1	A	307	PHE	CB-CG-CD2	-5.18	117.17	120.80
1	A	485	VAL	C-N-CA	-5.18	108.74	121.70
1	B	142	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	A	175	VAL	CA-CB-CG1	5.16	118.64	110.90
1	A	340	MET	C-N-CA	-5.16	108.81	121.70
1	A	248	ILE	CA-CB-CG2	-5.15	100.59	110.90
1	A	534	TRP	CG-CD1-NE1	-5.14	104.96	110.10
1	A	407	GLU	N-CA-C	5.14	124.89	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	79	ASP	CA-CB-CG	5.14	124.71	113.40
1	B	487	TRP	CE2-CD2-CG	-5.12	103.20	107.30
1	A	176	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	B	123	ASP	N-CA-C	5.12	124.82	111.00
1	B	169	PHE	N-CA-C	-5.11	97.20	111.00
1	A	143	TYR	CA-CB-CG	5.10	123.09	113.40
1	B	94	THR	C-N-CA	-5.09	108.98	121.70
1	B	131	GLU	CB-CG-CD	5.09	127.93	114.20
1	B	143	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	A	85	HIS	ND1-CG-CD2	5.08	115.92	108.80
1	B	450	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	B	146	PRO	C-N-CA	5.07	134.38	121.70
1	B	487	TRP	NE1-CE2-CD2	5.05	112.35	107.30
1	A	374	TRP	NE1-CE2-CD2	5.04	112.34	107.30
1	B	433	TRP	CE2-CD2-CG	-5.04	103.27	107.30
1	A	316	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	220	PHE	CA-CB-CG	5.02	125.95	113.90
1	A	391	LEU	C-N-CA	-5.02	109.16	121.70
1	A	540	TRP	NE1-CE2-CD2	5.02	112.32	107.30
1	A	342	GLY	N-CA-C	-5.01	100.59	113.10
1	A	352	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4495	0	4346	544	0
1	B	4491	0	4342	495	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	20	0	18	9	0
3	B	20	0	18	13	0
4	A	28	0	38	22	0
4	B	28	0	38	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	39	0	0	1	0
5	B	54	0	0	2	0
All	All	9181	0	8800	1101	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 62.

All (1101) 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:B:1604:BTB:N	4:B:1604:BTB:C2	1.68	1.56
4:B:1605:BTB:N	4:B:1605:BTB:C2	1.69	1.51
4:A:605:BTB:N	4:A:605:BTB:C2	1.71	1.49
1:B:579:HIS:CD2	3:B:1600:FPG:H92	1.67	1.28
4:B:1605:BTB:C7	4:B:1605:BTB:H32	1.72	1.19
4:B:1605:BTB:H32	4:B:1605:BTB:H71	1.24	1.18
4:B:1604:BTB:N	4:B:1604:BTB:C1	2.10	1.14
4:B:1604:BTB:C7	4:B:1604:BTB:H42	1.78	1.12
1:B:218:ARG:HG3	1:B:218:ARG:HH11	1.14	1.11
1:B:302:TRP:HB2	1:B:318:LEU:HD13	1.28	1.11
4:B:1605:BTB:N	4:B:1605:BTB:C3	2.12	1.10
4:A:605:BTB:N	4:A:605:BTB:C3	2.19	1.05
4:B:1604:BTB:H32	4:B:1604:BTB:C5	1.86	1.05
1:A:324:TRP:HE1	1:A:579:HIS:HB2	1.19	1.03
1:B:579:HIS:HD2	3:B:1600:FPG:H92	1.24	1.02
1:B:254:ILE:HD12	1:B:254:ILE:H	1.25	1.01
4:B:1604:BTB:H42	4:B:1604:BTB:H72	1.02	1.01
1:A:315:ARG:HB2	1:A:317:ARG:HE	1.25	1.01
4:B:1604:BTB:N	4:B:1604:BTB:C3	2.25	0.99
1:B:411:ASN:ND2	1:B:413:ILE:HG23	1.78	0.98
4:B:1605:BTB:N	4:B:1605:BTB:C1	2.25	0.98
4:B:1604:BTB:H72	4:B:1604:BTB:C4	1.93	0.98
4:B:1604:BTB:H32	4:B:1604:BTB:H52	1.45	0.97
1:A:315:ARG:HH21	3:A:600:FPG:H102	1.27	0.97
4:A:605:BTB:H42	4:A:605:BTB:C5	1.95	0.97
1:B:211:GLU:HG2	1:B:214:LEU:HD12	1.46	0.97
1:A:282:LEU:HG	1:A:286:ILE:HD11	1.44	0.96
1:B:145:ASN:HD22	1:B:146:PRO:HD3	1.28	0.96
4:B:1604:BTB:N	4:B:1604:BTB:H12	1.81	0.95
1:A:311:LEU:HD12	1:A:385:TYR:HB2	1.46	0.95
1:A:333:GLN:H	1:A:333:GLN:HE21	1.01	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:605:BTB:C1	4:A:605:BTB:H71	1.97	0.94
1:B:502:VAL:HG13	1:B:503:GLU:H	1.31	0.94
3:B:1600:FPG:C2	3:B:1600:FPG:H62	1.96	0.93
1:B:59:ARG:HG3	1:B:59:ARG:HH11	1.34	0.93
1:A:376:ILE:HD11	1:A:391:LEU:HD12	1.49	0.92
4:A:605:BTB:N	4:A:605:BTB:C4	2.33	0.91
4:B:1605:BTB:C7	4:B:1605:BTB:C3	2.48	0.90
1:A:256:ARG:HG2	1:A:256:ARG:HH11	1.37	0.90
4:A:605:BTB:N	4:A:605:BTB:C1	2.34	0.89
1:A:333:GLN:HE21	1:A:333:GLN:N	1.70	0.89
1:A:403:ASP:HA	1:A:406:LYS:HE3	1.54	0.89
1:A:585:ILE:HG13	1:A:588:GLN:HB2	1.55	0.89
1:B:583:HIS:HB2	1:B:586:ILE:HB	1.55	0.88
4:A:605:BTB:H71	4:A:605:BTB:H12	1.56	0.87
4:B:1605:BTB:N	4:B:1605:BTB:C4	2.37	0.87
1:A:465:ARG:HH11	1:A:465:ARG:HG3	1.36	0.87
1:B:95:LEU:HD11	1:B:275:VAL:HG21	1.56	0.87
1:B:575:ASN:HD22	1:B:586:ILE:HD11	1.40	0.87
4:A:605:BTB:C1	4:A:605:BTB:C7	2.54	0.86
4:B:1604:BTB:N	4:B:1604:BTB:C4	2.39	0.85
4:B:1604:BTB:C7	4:B:1604:BTB:C4	2.52	0.85
4:A:605:BTB:H42	4:A:605:BTB:H52	1.58	0.85
1:A:471:THR:HG23	1:A:474:THR:H	1.42	0.85
4:B:1605:BTB:H71	4:B:1605:BTB:C3	2.03	0.84
1:A:324:TRP:NE1	1:A:579:HIS:HB2	1.92	0.84
4:A:605:BTB:H12	4:A:605:BTB:C7	2.07	0.84
1:A:402:TYR:HD1	1:B:391:LEU:HD23	1.42	0.84
1:B:165:ARG:HB3	1:B:206:LEU:HD23	1.58	0.84
1:B:514:LEU:O	1:B:518:MET:HG2	1.78	0.83
1:B:371:ILE:HD13	1:B:372:ARG:N	1.93	0.83
1:A:456:PRO:O	1:A:460:THR:HG23	1.79	0.83
1:B:579:HIS:CD2	3:B:1600:FPG:C9	2.58	0.82
1:A:504:GLU:O	1:A:509:ASP:HB2	1.79	0.82
1:B:554:PHE:HB2	1:B:559:ILE:HG22	1.62	0.81
3:B:1600:FPG:H62	3:B:1600:FPG:C1	2.11	0.81
4:A:605:BTB:H62	4:A:605:BTB:O3	1.81	0.81
4:A:605:BTB:N	4:A:605:BTB:H32	1.96	0.80
1:A:510:VAL:HG23	1:A:511:PRO:HD2	1.63	0.80
1:B:302:TRP:CB	1:B:318:LEU:HD13	2.11	0.80
1:A:68:TRP:HB3	1:A:73:ILE:HD11	1.63	0.80
1:B:493:ARG:HG3	1:B:494:LEU:N	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLU:O	1:A:177:ASP:HB2	1.83	0.79
1:A:493:ARG:HG2	1:A:493:ARG:HH11	1.47	0.79
1:A:256:ARG:HG2	1:A:256:ARG:NH1	1.95	0.79
3:B:1600:FPG:H62	3:B:1600:FPG:H103	1.62	0.79
1:B:241:ARG:HH21	1:B:244:TYR:HD2	1.27	0.79
1:A:340:MET:O	1:A:344:VAL:HG23	1.83	0.79
1:A:177:ASP:O	1:A:180:LYS:HG3	1.82	0.79
1:A:315:ARG:NH2	3:A:600:FPG:H102	1.97	0.79
1:B:119:MET:HG3	1:B:262:TRP:HD1	1.48	0.79
4:B:1605:BTB:N	4:B:1605:BTB:H32	1.86	0.79
1:B:401:SER:HB3	1:B:413:ILE:HG22	1.64	0.78
1:B:458:MET:O	1:B:462:ILE:HG13	1.81	0.78
1:A:70:VAL:O	1:A:74:GLN:HG2	1.82	0.78
1:A:370:LEU:HD13	1:A:382:LEU:HD21	1.66	0.78
1:B:527:GLU:HA	1:B:530:LYS:HZ2	1.48	0.78
1:B:145:ASN:ND2	1:B:146:PRO:HD3	1.98	0.78
1:A:78:SER:HB2	1:A:81:LYS:HG3	1.65	0.78
1:A:283:ASP:HA	1:A:286:ILE:HD12	1.65	0.78
1:A:501:SER:HA	1:A:512:LYS:HG3	1.63	0.78
1:A:453:ILE:HG12	1:A:492:LEU:HG	1.66	0.77
1:A:136:ILE:O	1:A:140:HIS:HB2	1.83	0.77
1:B:577:ASP:HB2	1:B:582:GLN:HB3	1.66	0.77
1:A:578:GLY:C	1:A:580:GLY:H	1.86	0.77
1:B:73:ILE:HG21	1:B:299:PHE:CD2	2.20	0.77
1:A:493:ARG:HD3	1:A:493:ARG:C	2.05	0.77
1:A:483:ASP:HB3	1:A:487:TRP:CZ3	2.20	0.76
1:B:92:LEU:HD22	1:B:278:GLU:HG2	1.66	0.76
1:A:256:ARG:HH11	1:A:256:ARG:CG	1.98	0.76
1:A:465:ARG:HG3	1:A:465:ARG:NH1	1.96	0.76
1:A:98:MET:O	1:A:102:LYS:HB2	1.86	0.76
1:A:320:GLU:HG3	1:A:590:MET:HE1	1.68	0.76
4:B:1605:BTB:C7	4:B:1605:BTB:H12	2.16	0.76
1:A:413:ILE:HG12	1:A:414:PRO:HD3	1.68	0.76
1:B:145:ASN:ND2	1:B:145:ASN:H	1.83	0.75
1:B:411:ASN:HD21	1:B:413:ILE:HG23	1.52	0.75
3:B:1600:FPG:H62	3:B:1600:FPG:C10	2.16	0.75
1:A:201:TYR:HB2	1:A:221:ALA:HB1	1.67	0.75
1:A:173:GLN:HE22	1:A:211:GLU:C	1.90	0.75
1:A:449:SER:HB2	1:A:493:ARG:HH11	1.51	0.74
1:B:165:ARG:HB3	1:B:206:LEU:CD2	2.17	0.74
1:B:315:ARG:HD3	1:B:353:ASP:OD2	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ASP:O	1:A:197:LEU:HB2	1.88	0.74
1:B:218:ARG:HG3	1:B:218:ARG:NH1	1.94	0.74
4:B:1605:BTB:N	4:B:1605:BTB:H12	2.01	0.74
4:B:1604:BTB:C5	4:B:1604:BTB:C3	2.65	0.74
1:B:401:SER:CB	1:B:413:ILE:HG22	2.18	0.74
1:B:554:PHE:HB3	1:B:558:PHE:HD2	1.51	0.73
1:A:238:LEU:HG	1:A:242:ILE:HD11	1.68	0.73
1:B:483:ASP:HB3	1:B:487:TRP:NE1	2.03	0.73
1:A:345:ASN:HB3	3:A:600:FPG:C9	2.18	0.73
1:B:323:PHE:CD2	1:B:590:MET:HG2	2.23	0.73
1:B:514:LEU:HD11	1:B:529:ARG:HA	1.69	0.73
1:A:273:ASN:HD21	1:A:275:VAL:HG23	1.53	0.73
1:B:103:GLU:HB3	1:B:109:GLN:HG3	1.70	0.73
1:A:514:LEU:H	1:A:514:LEU:HD12	1.52	0.73
1:B:73:ILE:HG21	1:B:299:PHE:CG	2.24	0.73
1:A:102:LYS:HE2	1:A:102:LYS:HA	1.70	0.73
1:B:89:ALA:HA	1:B:92:LEU:HD12	1.71	0.73
1:B:510:VAL:HG12	1:B:511:PRO:HD2	1.69	0.73
1:B:116:LEU:HD23	1:B:121:LEU:HD12	1.71	0.73
1:B:148:PRO:HB3	1:B:178:SER:OG	1.89	0.73
1:A:315:ARG:HH11	1:A:353:ASP:CG	1.91	0.72
1:A:442:LEU:HD22	1:A:516:CYS:HB2	1.69	0.72
1:B:484:LEU:HD23	1:B:554:PHE:CD2	2.24	0.72
1:A:333:GLN:H	1:A:333:GLN:NE2	1.83	0.72
1:A:459:LEU:HD13	1:A:565:LEU:HD22	1.71	0.72
1:B:59:ARG:HG3	1:B:59:ARG:NH1	1.94	0.72
1:A:201:TYR:HB2	1:A:221:ALA:CB	2.20	0.71
1:A:222:THR:O	1:A:226:GLU:HB2	1.90	0.71
1:A:259:ALA:O	1:A:263:ILE:HG12	1.91	0.71
1:B:302:TRP:HB2	1:B:318:LEU:CD1	2.15	0.71
1:B:254:ILE:HD12	1:B:254:ILE:N	2.03	0.71
1:A:496:ASP:O	1:A:500:THR:HG23	1.90	0.71
4:B:1605:BTB:C2	4:B:1605:BTB:C7	2.69	0.70
4:B:1604:BTB:N	4:B:1604:BTB:H32	2.00	0.70
1:A:144:LYS:HG3	1:A:146:PRO:HD2	1.73	0.70
1:A:188:GLU:CD	1:A:188:GLU:H	1.94	0.70
1:B:242:ILE:HG22	1:B:243:ALA:N	2.06	0.70
1:A:131:GLU:HG3	1:A:132:ILE:N	2.05	0.70
1:A:544:ASN:O	1:A:548:VAL:HG23	1.91	0.70
1:A:577:ASP:HB3	1:A:582:GLN:H	1.56	0.70
1:B:317:ARG:HH21	1:B:581:THR:HA	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ARG:HH11	1:A:162:ARG:HG2	1.56	0.69
1:B:218:ARG:HH11	1:B:218:ARG:CG	1.99	0.69
1:A:67:ARG:HD3	1:A:587:HIS:CD2	2.27	0.69
1:B:530:LYS:HZ2	1:B:530:LYS:HB3	1.58	0.69
1:A:229:VAL:HG13	1:A:239:LEU:HD13	1.73	0.69
1:A:548:VAL:O	1:A:549:SER:HB3	1.93	0.69
1:B:97:LYS:HD3	1:B:128:GLU:OE1	1.93	0.69
1:B:177:ASP:OD2	1:B:180:LYS:HE3	1.92	0.69
1:B:221:ALA:O	1:B:225:LEU:HB2	1.93	0.69
1:A:345:ASN:HB3	3:A:600:FPG:H93	1.74	0.69
1:B:183:GLU:HB2	1:B:185:GLU:HG3	1.75	0.69
1:A:174:GLU:H	1:A:174:GLU:CD	1.97	0.69
1:A:577:ASP:OD1	1:A:584:PRO:HD3	1.92	0.69
1:B:433:TRP:CE3	1:B:440:PRO:HG3	2.27	0.69
4:B:1604:BTB:C2	4:B:1604:BTB:C7	2.71	0.69
1:A:115:ASP:O	1:A:119:MET:HG3	1.94	0.68
1:A:500:THR:OG1	1:A:501:SER:N	2.21	0.68
1:B:581:THR:HG23	1:B:582:GLN:N	2.08	0.68
1:B:80:TYR:HA	1:B:85:HIS:CD2	2.27	0.68
1:B:231:GLU:O	1:B:234:VAL:HG23	1.94	0.68
1:A:161:PHE:HD2	1:A:203:ALA:HB1	1.58	0.68
1:A:315:ARG:HD3	1:A:353:ASP:OD2	1.93	0.68
1:B:211:GLU:CG	1:B:214:LEU:HD12	2.23	0.68
1:B:269:ARG:O	1:B:272:MET:HB3	1.94	0.68
1:B:579:HIS:HD2	3:B:1600:FPG:C9	2.02	0.68
1:A:317:ARG:HH11	1:A:317:ARG:HB3	1.58	0.68
1:A:302:TRP:HB2	1:A:318:LEU:HG	1.76	0.67
1:B:93:VAL:HG13	1:B:94:THR:H	1.59	0.67
3:B:1600:FPG:H103	3:B:1600:FPG:C6	2.22	0.67
1:B:527:GLU:HA	1:B:530:LYS:NZ	2.09	0.67
1:B:272:MET:HE1	1:B:277:LEU:HB2	1.77	0.67
4:B:1605:BTB:H12	4:B:1605:BTB:H72	1.76	0.67
1:A:494:LEU:HD13	1:A:535:LEU:HB3	1.76	0.67
1:B:209:GLU:O	1:B:210:GLY:C	2.31	0.67
1:B:137:TYR:CD1	1:B:142:TYR:HB2	2.29	0.67
1:B:222:THR:O	1:B:226:GLU:HG2	1.93	0.67
1:A:145:ASN:ND2	1:A:174:GLU:HG3	2.10	0.67
1:A:294:GLU:HB3	1:A:339:ILE:CD1	2.24	0.67
1:B:116:LEU:CD2	1:B:121:LEU:HD12	2.25	0.67
1:B:554:PHE:CB	1:B:559:ILE:HG22	2.23	0.67
1:A:238:LEU:O	1:A:242:ILE:HG12	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:GLU:O	1:B:231:GLU:HG2	1.95	0.67
1:A:144:LYS:HG3	1:A:146:PRO:CD	2.25	0.66
1:B:86:VAL:HA	1:B:286:ILE:HD13	1.77	0.66
1:B:502:VAL:HG13	1:B:503:GLU:N	2.08	0.66
1:A:497:ASP:O	1:A:501:SER:HB2	1.95	0.66
1:A:95:LEU:HB2	1:A:275:VAL:HG11	1.78	0.66
1:B:290:GLN:O	1:B:294:GLU:HG3	1.95	0.66
1:B:337:ALA:O	1:B:341:MET:HB2	1.96	0.66
1:B:93:VAL:HG13	1:B:94:THR:N	2.10	0.66
1:A:153:ASP:HB3	1:A:156:SER:HB3	1.78	0.66
1:A:401:SER:HB2	1:A:413:ILE:HG22	1.78	0.66
1:A:136:ILE:HG23	1:A:140:HIS:HD2	1.61	0.65
1:A:413:ILE:O	1:A:417:ARG:HB2	1.96	0.65
1:B:586:ILE:HD13	1:B:589:GLN:HE21	1.61	0.65
1:A:289:ALA:O	1:A:292:GLN:HB2	1.96	0.65
1:A:150:GLU:C	1:A:152:ARG:H	2.00	0.65
1:A:67:ARG:HD2	1:A:583:HIS:CE1	2.32	0.65
1:A:202:GLU:OE2	1:A:250:LEU:HG	1.96	0.65
1:A:282:LEU:HG	1:A:286:ILE:CD1	2.25	0.65
1:B:571:LEU:C	1:B:571:LEU:HD23	2.17	0.65
1:A:401:SER:CB	1:A:413:ILE:HG22	2.27	0.65
1:A:149:LYS:C	1:A:151:GLU:H	1.99	0.65
1:B:121:LEU:HD21	1:B:280:ALA:HA	1.77	0.65
1:B:581:THR:HG23	1:B:582:GLN:H	1.61	0.65
1:A:198:LEU:HA	1:A:225:LEU:HD21	1.79	0.65
1:B:534:TRP:O	1:B:537:ALA:HB3	1.97	0.65
1:A:402:TYR:CD1	1:B:391:LEU:HD23	2.29	0.64
1:B:73:ILE:O	1:B:76:LEU:HD22	1.97	0.64
1:B:164:LEU:HB3	1:B:169:PHE:HB2	1.77	0.64
1:B:316:ASP:O	1:B:317:ARG:HD3	1.96	0.64
4:B:1605:BTB:H12	4:B:1605:BTB:H52	1.79	0.64
1:A:179:PHE:HB3	1:A:190:LEU:HD11	1.79	0.64
1:B:442:LEU:HG	1:B:442:LEU:O	1.98	0.64
1:A:152:ARG:HG3	1:A:152:ARG:HH11	1.62	0.64
1:B:243:ALA:HA	1:B:246:LEU:HB2	1.78	0.64
1:B:284:LEU:HD22	1:B:598:PHE:HB2	1.79	0.64
1:A:204:SER:O	1:A:207:LEU:HD22	1.97	0.64
1:A:433:TRP:CE3	1:A:440:PRO:HG3	2.32	0.64
1:A:510:VAL:HG23	1:A:511:PRO:CD	2.27	0.64
1:B:592:ARG:HG3	1:B:592:ARG:HH11	1.63	0.64
1:A:121:LEU:HD11	1:A:280:ALA:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ILE:HD12	1:B:110:LEU:HD12	1.80	0.64
1:B:484:LEU:HD23	1:B:554:PHE:HD2	1.63	0.64
1:A:105:ASP:HB3	1:A:108:ARG:HB2	1.78	0.64
4:A:605:BTB:C2	4:A:605:BTB:C7	2.73	0.63
4:B:1605:BTB:C1	4:B:1605:BTB:C5	2.76	0.63
3:B:1600:FPG:C2	3:B:1600:FPG:C6	2.70	0.63
1:A:67:ARG:HD3	1:A:587:HIS:HD2	1.62	0.63
1:B:512:LYS:H	1:B:515:GLN:NE2	1.97	0.63
1:A:462:ILE:O	1:A:466:VAL:HG22	1.99	0.63
4:A:605:BTB:H71	4:A:605:BTB:O1	1.98	0.63
1:B:75:SER:O	1:B:77:LEU:N	2.31	0.63
1:B:82:GLU:O	1:B:84:LYS:HD2	1.98	0.63
1:B:236:GLY:O	1:B:239:LEU:HB2	1.98	0.63
1:A:162:ARG:HG2	1:A:162:ARG:NH1	2.11	0.63
1:A:228:LYS:HZ1	1:A:234:VAL:H	1.47	0.63
1:B:95:LEU:CD1	1:B:275:VAL:HG21	2.26	0.63
1:B:475:VAL:O	1:B:478:LEU:HB3	1.98	0.63
4:B:1605:BTB:H12	4:B:1605:BTB:C5	2.28	0.63
1:B:257:PRO:HA	1:B:593:THR:HG21	1.81	0.63
1:B:547:ARG:HA	1:B:559:ILE:HD13	1.81	0.63
1:B:209:GLU:O	1:B:211:GLU:N	2.32	0.62
1:B:251:HIS:O	1:B:567:ARG:NH1	2.31	0.62
1:B:256:ARG:HB3	1:B:257:PRO:HD3	1.80	0.62
1:A:78:SER:HB2	1:A:81:LYS:CG	2.28	0.62
1:B:336:SER:HA	1:B:339:ILE:HG12	1.81	0.62
1:B:583:HIS:CB	1:B:586:ILE:HB	2.27	0.62
1:A:108:ARG:HB2	1:A:108:ARG:CZ	2.29	0.62
1:A:177:ASP:HA	1:A:180:LYS:HD2	1.80	0.62
1:B:504:GLU:O	1:B:509:ASP:HB2	1.99	0.62
1:B:266:TYR:CE2	1:B:272:MET:HE1	2.34	0.62
1:B:311:LEU:HD21	1:B:354:ILE:HD11	1.81	0.62
1:B:137:TYR:CE2	1:B:143:TYR:HB3	2.34	0.62
1:B:208:THR:HG21	1:B:545:ALA:HB2	1.82	0.62
1:B:281:ILE:HG23	1:B:598:PHE:HD2	1.64	0.62
1:B:70:VAL:HG23	1:B:74:GLN:HG3	1.80	0.62
1:A:361:LEU:HD12	1:A:435:TYR:HB3	1.79	0.62
1:B:483:ASP:HB3	1:B:487:TRP:HE1	1.65	0.62
1:B:72:PHE:CD1	1:B:72:PHE:C	2.73	0.62
1:B:76:LEU:HD23	1:B:77:LEU:H	1.65	0.62
1:B:446:LEU:HD12	1:B:490:PHE:HE1	1.65	0.62
1:B:586:ILE:HA	1:B:589:GLN:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:GLN:O	1:A:574:HIS:HB2	2.00	0.61
1:B:575:ASN:ND2	1:B:586:ILE:HD11	2.12	0.61
1:B:544:ASN:HA	1:B:547:ARG:HH11	1.65	0.61
1:A:188:GLU:O	1:A:191:SER:HB3	2.00	0.61
1:B:311:LEU:HG	1:B:313:PHE:CZ	2.35	0.61
1:A:347:LEU:O	1:A:351:ILE:HG13	2.01	0.61
1:B:201:TYR:HB2	1:B:221:ALA:CB	2.31	0.61
1:B:87:ILE:O	1:B:91:GLU:HG3	1.99	0.61
1:B:310:LYS:C	1:B:312:PRO:HD3	2.21	0.61
1:B:315:ARG:HD3	1:B:315:ARG:H	1.64	0.61
4:A:605:BTB:N	4:A:605:BTB:H12	2.13	0.61
1:A:311:LEU:N	1:A:312:PRO:HD3	2.14	0.61
1:A:105:ASP:HB3	1:A:108:ARG:CB	2.32	0.60
1:A:368:THR:O	1:A:371:ILE:HB	2.01	0.60
1:B:411:ASN:HD22	1:B:413:ILE:HG23	1.64	0.60
1:A:228:LYS:NZ	1:A:234:VAL:H	2.00	0.60
1:A:256:ARG:HB3	1:A:257:PRO:HD3	1.81	0.60
1:A:577:ASP:HB2	1:A:584:PRO:CD	2.31	0.60
1:B:63:TYR:CZ	1:B:315:ARG:HD2	2.37	0.60
1:B:530:LYS:HB3	1:B:530:LYS:NZ	2.16	0.60
1:B:547:ARG:HB2	1:B:559:ILE:CD1	2.31	0.60
1:B:555:GLY:O	1:B:559:ILE:HG23	2.01	0.60
1:A:175:VAL:HG12	1:A:176:PHE:CD1	2.36	0.60
1:A:323:PHE:O	1:A:326:THR:HB	2.02	0.60
1:B:383:PRO:HD2	1:B:386:MET:HE1	1.83	0.60
1:A:92:LEU:HA	1:A:95:LEU:HG	1.82	0.60
1:A:493:ARG:HG2	1:A:493:ARG:NH1	2.16	0.60
1:A:96:VAL:HA	1:A:99:GLU:HG3	1.81	0.60
1:B:103:GLU:CD	1:B:104:THR:H	2.05	0.60
1:B:72:PHE:C	1:B:72:PHE:HD1	2.05	0.60
1:A:531:HIS:O	1:A:534:TRP:HB3	2.01	0.59
1:B:79:ASP:O	1:B:82:GLU:HG3	2.02	0.59
1:B:95:LEU:HD11	1:B:275:VAL:HG11	1.84	0.59
1:B:159:LEU:HD23	1:B:199:GLN:CD	2.22	0.59
1:B:209:GLU:H	1:B:541:LYS:HD2	1.67	0.59
1:B:571:LEU:HD23	1:B:572:MET:N	2.18	0.59
1:A:345:ASN:HA	1:A:348:ILE:HD12	1.85	0.59
1:A:555:GLY:O	1:A:559:ILE:HG23	2.02	0.59
1:B:145:ASN:HD22	1:B:145:ASN:H	1.50	0.59
1:B:296:LYS:O	1:B:299:PHE:HB3	2.03	0.59
1:A:559:ILE:HG13	1:A:560:GLY:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1605:BTB:N	4:B:1605:BTB:H42	2.17	0.59
1:A:278:GLU:HG3	1:A:279:LEU:N	2.17	0.59
1:B:83:ASP:C	1:B:85:HIS:N	2.55	0.59
1:B:128:GLU:O	1:B:132:ILE:HD12	2.03	0.59
1:B:350:VAL:HG12	1:B:351:ILE:N	2.18	0.59
1:B:77:LEU:HG	1:B:296:LYS:NZ	2.18	0.58
1:A:168:GLY:HA2	1:A:548:VAL:CG1	2.33	0.58
1:A:378:SER:HB3	1:A:381:GLN:OE1	2.02	0.58
1:B:456:PRO:HD3	1:B:489:SER:OG	2.03	0.58
1:B:93:VAL:HG22	1:B:97:LYS:HE2	1.84	0.58
1:B:312:PRO:O	1:B:314:ALA:N	2.36	0.58
1:A:121:LEU:HB3	1:A:125:PHE:HE2	1.68	0.58
1:A:266:TYR:O	1:A:269:ARG:HB3	2.02	0.58
1:A:547:ARG:C	1:A:549:SER:H	2.06	0.58
1:B:459:LEU:HD12	1:B:462:ILE:HD12	1.85	0.58
1:A:79:ASP:N	1:A:81:LYS:HG3	2.19	0.58
1:A:345:ASN:CB	3:A:600:FPG:H93	2.33	0.58
4:A:605:BTB:N	4:A:605:BTB:H42	2.13	0.58
1:A:173:GLN:NE2	1:A:213:THR:N	2.51	0.58
1:A:194:THR:HA	1:A:197:LEU:HB2	1.84	0.58
1:B:61:GLY:O	1:B:62:ASN:HB2	2.02	0.58
1:A:87:ILE:O	1:A:91:GLU:HG3	2.02	0.58
1:A:577:ASP:OD2	1:A:582:GLN:HB2	2.03	0.58
1:B:70:VAL:O	1:B:74:GLN:HG3	2.03	0.58
1:B:315:ARG:NH1	1:B:349:THR:HG23	2.19	0.58
1:B:314:ALA:HA	1:B:353:ASP:OD2	2.03	0.58
1:B:75:SER:O	1:B:77:LEU:HD12	2.03	0.58
1:B:320:GLU:HB3	1:B:579:HIS:O	2.04	0.58
1:B:471:THR:O	1:B:472:LYS:C	2.42	0.58
1:B:103:GLU:OE1	1:B:103:GLU:HA	2.04	0.57
1:B:159:LEU:HD23	1:B:199:GLN:OE1	2.04	0.57
1:B:492:LEU:HA	1:B:569:ALA:HB1	1.86	0.57
1:A:168:GLY:HA2	1:A:548:VAL:HG13	1.85	0.57
1:B:282:LEU:HG	1:B:286:ILE:HD11	1.86	0.57
1:B:582:GLN:HG2	1:B:584:PRO:HD3	1.85	0.57
1:A:179:PHE:C	1:A:187:LYS:HD3	2.25	0.57
1:B:585:ILE:O	1:B:585:ILE:HG13	2.05	0.57
1:B:114:ASP:O	1:B:118:ARG:HG2	2.02	0.57
1:B:128:GLU:OE2	1:B:128:GLU:N	2.38	0.57
1:A:311:LEU:HG	1:A:313:PHE:CZ	2.40	0.57
1:B:592:ARG:HH11	1:B:592:ARG:CG	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:VAL:HA	1:A:89:ALA:HB3	1.85	0.57
1:A:315:ARG:NH2	3:A:600:FPG:O2A	2.38	0.57
1:A:449:SER:HB2	1:A:493:ARG:NH1	2.18	0.57
1:A:577:ASP:HB2	1:A:584:PRO:HD2	1.86	0.57
1:B:254:ILE:HG12	1:B:568:MET:HA	1.85	0.57
1:B:544:ASN:O	1:B:547:ARG:HG2	2.03	0.57
1:A:86:VAL:HG23	1:A:286:ILE:HG21	1.85	0.57
1:A:554:PHE:HB3	1:A:558:PHE:HD2	1.69	0.57
1:B:93:VAL:HG22	1:B:97:LYS:HG3	1.86	0.57
4:B:1605:BTB:C7	4:B:1605:BTB:C1	2.79	0.57
1:A:90:SER:O	1:A:93:VAL:HG12	2.04	0.57
1:A:166:GLU:C	1:A:168:GLY:H	2.07	0.57
1:A:190:LEU:O	1:A:192:ASP:N	2.37	0.57
1:A:212:THR:O	1:A:213:THR:C	2.39	0.57
1:B:59:ARG:HH11	1:B:59:ARG:CG	2.11	0.57
1:A:103:GLU:CD	1:A:105:ASP:H	2.08	0.57
1:A:453:ILE:O	1:A:453:ILE:HG13	2.03	0.57
1:A:493:ARG:HD3	1:A:493:ARG:O	2.04	0.57
1:A:527:GLU:OE1	1:A:527:GLU:HA	2.04	0.57
1:A:70:VAL:HG12	1:A:74:GLN:NE2	2.19	0.56
1:A:106:GLN:HG2	1:A:136:ILE:HG12	1.86	0.56
1:A:325:ASN:HB3	1:A:338:ARG:HG3	1.87	0.56
1:B:116:LEU:HD13	1:B:125:PHE:CD1	2.40	0.56
1:B:371:ILE:HG12	1:B:421:VAL:HG22	1.86	0.56
1:A:204:SER:HB2	1:A:218:ARG:NH1	2.20	0.56
1:A:209:GLU:OE1	5:A:700:HOH:O	2.18	0.56
1:A:311:LEU:HD21	1:A:350:VAL:CG1	2.35	0.56
1:A:324:TRP:CZ2	1:A:572:MET:HG2	2.38	0.56
1:A:379:ILE:HD13	1:A:387:GLN:HG2	1.86	0.56
1:A:413:ILE:HG12	1:A:414:PRO:CD	2.35	0.56
1:B:301:TRP:HZ2	1:B:347:LEU:HD21	1.70	0.56
1:B:515:GLN:HA	1:B:518:MET:HG3	1.86	0.56
1:A:207:LEU:H	1:A:207:LEU:CD2	2.19	0.56
1:A:279:LEU:HD12	1:A:279:LEU:O	2.06	0.56
1:A:100:LEU:HD12	1:A:112:LEU:HD12	1.86	0.56
1:B:87:ILE:HA	1:B:90:SER:OG	2.06	0.56
1:B:493:ARG:O	1:B:496:ASP:N	2.38	0.56
1:A:317:ARG:HB3	1:A:317:ARG:NH1	2.20	0.56
1:B:323:PHE:O	1:B:326:THR:HB	2.06	0.56
1:A:266:TYR:CE2	1:A:272:MET:HG2	2.40	0.56
1:A:274:PRO:O	1:A:275:VAL:C	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:GLY:O	1:A:459:LEU:HB2	2.05	0.56
1:B:344:VAL:HG12	1:B:348:ILE:CD1	2.36	0.56
1:A:559:ILE:HD12	1:A:559:ILE:O	2.05	0.56
1:B:317:ARG:HD2	1:B:320:GLU:OE2	2.06	0.56
1:A:376:ILE:O	1:A:379:ILE:HB	2.05	0.55
1:A:192:ASP:O	1:A:194:THR:HG23	2.07	0.55
1:A:290:GLN:NE2	1:A:294:GLU:HG2	2.21	0.55
1:A:500:THR:HG1	1:A:501:SER:H	1.53	0.55
1:A:571:LEU:HD23	1:A:571:LEU:C	2.26	0.55
1:B:299:PHE:HA	1:B:318:LEU:HD22	1.87	0.55
1:A:95:LEU:O	1:A:99:GLU:HG2	2.06	0.55
1:A:116:LEU:HD13	1:A:125:PHE:CD2	2.41	0.55
1:A:573:TYR:HE1	1:A:578:GLY:HA2	1.70	0.55
1:B:92:LEU:HD13	1:B:279:LEU:HA	1.89	0.55
1:B:428:MET:HG3	1:B:432:ARG:HE	1.72	0.55
1:A:367:PHE:HB2	1:A:386:MET:SD	2.47	0.55
1:A:547:ARG:HB2	1:A:559:ILE:HD13	1.88	0.55
1:B:83:ASP:O	1:B:85:HIS:N	2.40	0.55
1:B:116:LEU:HD22	1:B:125:PHE:CE1	2.41	0.55
1:B:211:GLU:HG2	1:B:214:LEU:CD1	2.26	0.55
1:B:267:ARG:HH22	1:B:599:ALA:HA	1.71	0.55
1:A:194:THR:HA	1:A:197:LEU:CB	2.37	0.55
1:A:318:LEU:HD13	1:A:318:LEU:O	2.07	0.55
1:A:405:MET:HE1	1:B:387:GLN:C	2.26	0.55
1:B:360:THR:HG23	1:B:363:GLU:OE1	2.07	0.55
1:B:559:ILE:O	1:B:559:ILE:HD12	2.06	0.55
1:A:151:GLU:O	1:A:152:ARG:O	2.23	0.55
1:B:309:GLU:HG3	1:B:310:LYS:HG2	1.87	0.55
1:B:547:ARG:HB2	1:B:559:ILE:HD11	1.87	0.55
1:A:205:PHE:CZ	1:A:249:PRO:HG3	2.42	0.54
1:A:294:GLU:HB3	1:A:339:ILE:HD11	1.88	0.54
1:A:465:ARG:HH11	1:A:465:ARG:CG	2.11	0.54
1:A:100:LEU:CD1	1:A:112:LEU:HD12	2.37	0.54
1:A:405:MET:CE	1:B:388:LEU:HA	2.37	0.54
1:B:204:SER:O	1:B:207:LEU:HD13	2.07	0.54
1:B:216:SER:HA	1:B:219:GLU:CD	2.28	0.54
1:A:521:TYR:CD2	1:A:521:TYR:N	2.75	0.54
1:B:93:VAL:CG1	1:B:94:THR:H	2.20	0.54
1:B:370:LEU:O	1:B:374:TRP:N	2.41	0.54
1:A:161:PHE:CZ	1:A:165:ARG:NE	2.74	0.54
1:B:77:LEU:HG	1:B:296:LYS:CE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASP:OD1	1:A:269:ARG:NH2	2.40	0.54
1:B:95:LEU:HA	1:B:98:MET:HB2	1.89	0.54
1:A:223:LYS:HD3	1:A:224:PHE:CZ	2.43	0.54
1:B:299:PHE:HE1	1:B:303:ARG:HD2	1.73	0.54
4:B:1604:BTB:C5	4:B:1604:BTB:H12	2.36	0.54
1:B:86:VAL:HG23	1:B:286:ILE:HD13	1.89	0.54
1:A:302:TRP:HB2	1:A:318:LEU:CG	2.38	0.54
1:A:361:LEU:HD12	1:A:435:TYR:CB	2.37	0.54
1:B:575:ASN:HB2	1:B:584:PRO:HG2	1.90	0.54
1:B:588:GLN:O	1:B:592:ARG:HB2	2.08	0.54
4:B:1604:BTB:H12	4:B:1604:BTB:C6	2.38	0.54
1:A:212:THR:O	1:A:215:GLU:N	2.41	0.54
1:A:315:ARG:NH1	1:A:353:ASP:CG	2.61	0.54
1:B:176:PHE:HA	1:B:179:PHE:CE2	2.42	0.54
1:B:540:TRP:O	1:B:543:MET:HB3	2.08	0.54
1:B:544:ASN:HD22	1:B:547:ARG:NH1	2.06	0.54
1:B:546:GLU:O	1:B:549:SER:HB3	2.08	0.54
1:B:587:HIS:ND1	1:B:587:HIS:C	2.60	0.54
1:A:77:LEU:O	1:A:78:SER:O	2.25	0.53
1:A:319:VAL:HG12	1:A:590:MET:CE	2.37	0.53
1:A:363:GLU:HG2	1:A:383:PRO:HG3	1.89	0.53
1:B:456:PRO:O	1:B:460:THR:HG23	2.07	0.53
1:A:172:ALA:HB1	1:A:174:GLU:HG2	1.89	0.53
1:A:70:VAL:O	1:A:72:PHE:N	2.42	0.53
1:A:559:ILE:O	1:A:562:ALA:HB3	2.09	0.53
1:B:453:ILE:HG23	1:B:453:ILE:O	2.07	0.53
1:A:264:GLU:HB2	1:A:267:ARG:CZ	2.36	0.53
1:A:423:LEU:HD12	1:A:423:LEU:O	2.08	0.53
1:A:426:LYS:N	1:A:426:LYS:HD3	2.22	0.53
1:B:223:LYS:HB3	1:B:223:LYS:HZ2	1.73	0.53
1:B:426:LYS:O	1:B:429:VAL:HG23	2.08	0.53
1:B:516:CYS:O	1:B:520:ASP:HB2	2.08	0.53
1:B:95:LEU:HD11	1:B:275:VAL:CG2	2.35	0.53
1:B:416:LEU:HD22	1:B:461:HIS:CE1	2.43	0.53
1:A:446:LEU:HA	1:A:449:SER:OG	2.09	0.53
1:A:256:ARG:HB2	1:A:330:GLU:OE2	2.08	0.53
1:B:77:LEU:HG	1:B:296:LYS:HE2	1.90	0.53
1:A:329:ILE:HB	1:A:338:ARG:HD3	1.91	0.53
1:B:174:GLU:CD	1:B:174:GLU:H	2.10	0.53
1:B:329:ILE:HG21	1:B:334:HIS:HB2	1.90	0.53
1:B:543:MET:O	1:B:543:MET:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:HD13	1:A:277:LEU:C	2.29	0.53
1:A:302:TRP:HB2	1:A:318:LEU:CD2	2.39	0.53
1:B:494:LEU:O	1:B:498:LEU:HB2	2.09	0.53
1:A:306:GLY:HA2	1:A:308:VAL:HG23	1.91	0.53
1:B:259:ALA:O	1:B:260:PRO:C	2.45	0.53
1:A:82:GLU:N	1:A:82:GLU:OE1	2.42	0.52
1:A:177:ASP:OD2	1:A:180:LYS:HD2	2.08	0.52
1:A:283:ASP:O	1:A:286:ILE:N	2.42	0.52
1:B:188:GLU:H	1:B:188:GLU:CD	2.12	0.52
1:A:102:LYS:HA	1:A:102:LYS:CE	2.35	0.52
1:A:155:TYR:HB2	1:A:196:GLY:CA	2.39	0.52
1:B:299:PHE:CE1	1:B:303:ARG:HD2	2.44	0.52
1:A:152:ARG:NH1	1:A:178:SER:OG	2.43	0.52
1:A:241:ARG:NH2	1:A:245:SER:OG	2.42	0.52
1:A:417:ARG:O	1:A:421:VAL:HG23	2.09	0.52
1:A:155:TYR:HA	1:A:196:GLY:HA2	1.90	0.52
1:A:273:ASN:HD21	1:A:275:VAL:CG2	2.22	0.52
1:A:587:HIS:O	1:A:591:THR:HG23	2.10	0.52
1:B:103:GLU:OE2	1:B:105:ASP:N	2.43	0.52
1:A:302:TRP:CB	1:A:318:LEU:HG	2.38	0.52
1:A:505:VAL:HG23	1:A:506:SER:N	2.23	0.52
1:A:456:PRO:HD3	1:A:489:SER:OG	2.09	0.52
1:B:97:LYS:O	1:B:100:LEU:N	2.42	0.52
1:B:201:TYR:HB2	1:B:221:ALA:HB3	1.92	0.52
1:B:207:LEU:H	1:B:207:LEU:HD22	1.74	0.52
1:B:282:LEU:HG	1:B:286:ILE:CD1	2.39	0.52
1:B:376:ILE:HA	1:B:379:ILE:HB	1.92	0.52
1:A:95:LEU:HD12	1:A:275:VAL:HG13	1.91	0.52
1:A:274:PRO:C	1:A:276:VAL:N	2.62	0.52
1:A:547:ARG:CB	1:A:559:ILE:HD13	2.39	0.52
1:B:502:VAL:CG1	1:B:503:GLU:H	2.14	0.52
1:A:145:ASN:N	1:A:146:PRO:HD2	2.25	0.52
4:A:605:BTB:C5	4:A:605:BTB:C4	2.72	0.52
1:B:87:ILE:O	1:B:88:ARG:C	2.48	0.52
1:A:283:ASP:CG	1:A:332:ARG:HH22	2.13	0.52
1:A:491:VAL:O	1:A:492:LEU:C	2.47	0.52
1:B:578:GLY:O	1:B:580:GLY:N	2.42	0.52
1:A:252:TRP:HB3	1:A:570:GLN:NE2	2.26	0.52
1:A:270:PRO:O	1:A:271:ASP:C	2.48	0.52
1:B:78:SER:O	1:B:81:LYS:HG2	2.10	0.52
1:B:267:ARG:NH2	1:B:599:ALA:HA	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ASN:OD1	1:B:377:ASN:N	2.42	0.52
1:A:69:ASP:OD2	1:A:69:ASP:C	2.47	0.51
1:A:378:SER:O	1:A:379:ILE:C	2.47	0.51
1:B:283:ASP:CG	1:B:332:ARG:HH22	2.13	0.51
1:A:128:GLU:O	1:A:129:PHE:C	2.44	0.51
1:A:144:LYS:HG3	1:A:146:PRO:CG	2.41	0.51
1:A:547:ARG:HD2	1:A:563:VAL:HG21	1.92	0.51
1:A:75:SER:O	1:A:77:LEU:N	2.44	0.51
1:A:276:VAL:O	1:A:277:LEU:C	2.48	0.51
1:A:369:ASP:HA	1:A:372:ARG:HB2	1.92	0.51
1:A:442:LEU:HD12	1:A:446:LEU:HG	1.92	0.51
1:A:547:ARG:HB2	1:A:559:ILE:CD1	2.40	0.51
1:B:484:LEU:HD12	1:B:484:LEU:O	2.10	0.51
1:A:269:ARG:HG3	1:A:270:PRO:HD2	1.92	0.51
1:A:273:ASN:ND2	1:A:275:VAL:HG23	2.23	0.51
1:A:433:TRP:HA	1:A:438:HIS:HB3	1.93	0.51
1:B:426:LYS:HA	1:B:429:VAL:CG2	2.40	0.51
1:B:546:GLU:HA	1:B:549:SER:HB2	1.93	0.51
1:A:304:ASN:O	1:B:406:LYS:HE3	2.10	0.51
1:A:311:LEU:HD21	1:A:350:VAL:HG13	1.93	0.51
1:B:334:HIS:HB3	1:B:337:ALA:HB3	1.91	0.51
1:A:401:SER:HB3	1:A:412:VAL:HG23	1.91	0.51
1:B:119:MET:HG3	1:B:262:TRP:CD1	2.36	0.51
1:A:224:PHE:O	1:A:225:LEU:C	2.47	0.51
1:A:370:LEU:HD13	1:A:382:LEU:CD2	2.39	0.51
1:A:393:LEU:HD21	1:A:420:TRP:CE2	2.46	0.51
1:A:80:TYR:HA	1:A:85:HIS:CD2	2.45	0.51
1:A:81:LYS:H	1:A:81:LYS:CD	2.22	0.51
1:A:175:VAL:HG12	1:A:176:PHE:CE1	2.46	0.51
1:A:473:GLU:O	1:A:474:THR:C	2.47	0.51
1:B:116:LEU:HD13	1:B:125:PHE:CG	2.46	0.51
1:A:144:LYS:HE2	1:A:146:PRO:HD2	1.93	0.51
1:B:232:GLY:HA2	1:B:239:LEU:CD2	2.40	0.51
1:B:264:GLU:HB3	1:B:267:ARG:NH1	2.25	0.51
1:A:70:VAL:C	1:A:74:GLN:HG2	2.32	0.50
1:A:110:LEU:HD21	1:A:136:ILE:CD1	2.41	0.50
1:A:128:GLU:OE2	1:A:128:GLU:N	2.44	0.50
1:A:472:LYS:HD3	1:A:476:ASP:OD2	2.10	0.50
1:B:75:SER:OG	1:B:76:LEU:N	2.44	0.50
1:B:201:TYR:HB2	1:B:221:ALA:HB1	1.92	0.50
1:B:207:LEU:H	1:B:207:LEU:CD2	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:GLY:O	1:B:310:LYS:HG3	2.11	0.50
4:B:1604:BTB:C2	4:B:1604:BTB:C5	2.85	0.50
1:A:97:LYS:O	1:A:100:LEU:HB3	2.10	0.50
1:A:180:LYS:NZ	1:A:213:THR:HG23	2.26	0.50
1:A:535:LEU:O	1:A:539:VAL:HG13	2.11	0.50
1:B:433:TRP:CZ3	1:B:440:PRO:HG3	2.46	0.50
1:A:229:VAL:HA	1:A:239:LEU:CD2	2.40	0.50
1:A:493:ARG:O	1:A:494:LEU:C	2.49	0.50
1:B:191:SER:HA	1:B:224:PHE:CD2	2.47	0.50
1:B:371:ILE:CD1	1:B:372:ARG:N	2.72	0.50
1:A:370:LEU:HG	1:A:375:ASP:HB3	1.93	0.50
1:A:388:LEU:HG	1:B:402:TYR:OH	2.11	0.50
1:B:413:ILE:O	1:B:417:ARG:HB2	2.12	0.50
1:A:98:MET:C	1:A:100:LEU:N	2.59	0.50
1:B:410:VAL:HG22	1:B:411:ASN:N	2.26	0.50
1:A:121:LEU:HB3	1:A:125:PHE:CE2	2.47	0.50
1:B:281:ILE:HG23	1:B:598:PHE:CD2	2.46	0.50
1:B:513:SER:O	1:B:514:LEU:C	2.49	0.50
1:A:123:ASP:CG	1:A:332:ARG:HD2	2.31	0.50
1:B:93:VAL:CG1	1:B:94:THR:N	2.75	0.50
1:B:95:LEU:CG	1:B:275:VAL:HG21	2.41	0.50
1:A:301:TRP:CZ3	1:A:346:ALA:HB3	2.47	0.50
1:A:431:ALA:O	1:A:432:ARG:C	2.50	0.50
1:A:493:ARG:C	1:A:493:ARG:CD	2.78	0.50
1:B:190:LEU:C	1:B:192:ASP:N	2.65	0.50
1:B:301:TRP:CG	1:B:343:LYS:HD3	2.47	0.50
1:A:254:ILE:O	1:A:254:ILE:HG23	2.12	0.50
1:B:132:ILE:HG22	1:B:132:ILE:O	2.12	0.50
1:B:158:SER:HB3	1:B:200:LEU:HA	1.92	0.50
1:B:242:ILE:HG23	1:B:246:LEU:HD12	1.92	0.50
1:B:457:CYS:O	1:B:461:HIS:CD2	2.64	0.50
1:B:89:ALA:CA	1:B:92:LEU:HD12	2.42	0.49
1:B:223:LYS:HG2	1:B:224:PHE:CD1	2.47	0.49
1:B:238:LEU:HD23	1:B:239:LEU:N	2.27	0.49
1:A:97:LYS:HE3	1:A:128:GLU:OE1	2.12	0.49
1:A:578:GLY:C	1:A:580:GLY:N	2.58	0.49
1:A:514:LEU:O	1:A:518:MET:HG3	2.13	0.49
1:B:318:LEU:HA	1:B:321:CYS:HB2	1.94	0.49
1:B:581:THR:CG2	1:B:582:GLN:H	2.25	0.49
1:B:581:THR:CG2	1:B:582:GLN:N	2.75	0.49
1:A:201:TYR:C	1:A:201:TYR:CD2	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:ILE:HD13	1:B:589:GLN:NE2	2.27	0.49
1:A:79:ASP:C	1:A:81:LYS:H	2.15	0.49
1:A:405:MET:HE2	1:B:388:LEU:HA	1.95	0.49
1:A:422:ASP:O	1:A:423:LEU:C	2.50	0.49
1:A:543:MET:O	1:A:547:ARG:HG2	2.12	0.49
1:A:144:LYS:HG3	1:A:146:PRO:HG2	1.94	0.49
1:A:179:PHE:O	1:A:187:LYS:HB2	2.12	0.49
1:B:344:VAL:HG12	1:B:348:ILE:HD13	1.94	0.49
1:B:377:ASN:C	1:B:379:ILE:H	2.16	0.49
1:A:375:ASP:OD1	1:A:378:SER:OG	2.23	0.49
1:B:428:MET:O	1:B:429:VAL:C	2.50	0.49
1:B:482:HIS:CD2	1:B:554:PHE:HE2	2.31	0.49
1:A:110:LEU:HD21	1:A:136:ILE:HD12	1.93	0.49
1:A:514:LEU:HD12	1:A:514:LEU:N	2.24	0.49
1:B:315:ARG:H	1:B:315:ARG:CD	2.25	0.49
1:B:497:ASP:CG	1:B:512:LYS:HB3	2.32	0.49
1:B:83:ASP:O	1:B:84:LYS:C	2.51	0.49
1:B:323:PHE:CE1	1:B:326:THR:HG21	2.48	0.49
1:B:471:THR:H	1:B:474:THR:HG23	1.77	0.49
1:B:592:ARG:CG	1:B:592:ARG:NH1	2.75	0.49
1:A:165:ARG:HB3	1:A:206:LEU:CD2	2.42	0.49
1:A:172:ALA:HB1	1:A:174:GLU:OE1	2.13	0.49
1:B:429:VAL:HG12	5:B:778:HOH:O	2.13	0.49
1:A:207:LEU:N	1:A:207:LEU:HD23	2.27	0.48
1:B:112:LEU:HD13	1:B:116:LEU:HG	1.95	0.48
1:B:241:ARG:HH22	1:B:250:LEU:HD13	1.78	0.48
1:A:107:ILE:HG12	1:A:156:SER:HB2	1.94	0.48
1:A:309:GLU:HG3	1:A:310:LYS:N	2.27	0.48
1:B:61:GLY:HA3	1:B:63:TYR:CE2	2.47	0.48
1:B:232:GLY:HA2	1:B:239:LEU:HD21	1.94	0.48
1:B:294:GLU:HG2	1:B:339:ILE:HD11	1.95	0.48
1:B:535:LEU:HD21	4:B:1604:BTB:H12	1.94	0.48
1:A:101:GLU:OE2	1:A:132:ILE:HD11	2.13	0.48
1:A:345:ASN:CB	3:A:600:FPG:C9	2.90	0.48
1:B:576:GLY:C	1:B:578:GLY:H	2.14	0.48
1:B:583:HIS:CA	1:B:586:ILE:HB	2.43	0.48
1:A:89:ALA:HA	1:A:92:LEU:HD12	1.95	0.48
1:A:123:ASP:CG	1:A:332:ARG:HH11	2.16	0.48
1:A:136:ILE:HG23	1:A:140:HIS:CD2	2.45	0.48
1:A:190:LEU:HB2	1:A:220:PHE:HZ	1.79	0.48
1:A:241:ARG:HH21	1:A:245:SER:CB	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ILE:CG2	1:A:380:ASP:N	2.77	0.48
1:A:408:LYS:HE2	1:A:467:THR:O	2.14	0.48
1:A:426:LYS:HA	1:A:429:VAL:HG23	1.94	0.48
1:B:367:PHE:O	1:B:368:THR:C	2.51	0.48
1:A:89:ALA:HA	1:A:282:LEU:HD23	1.95	0.48
1:A:119:MET:HB3	1:A:263:ILE:HD13	1.95	0.48
1:A:260:PRO:O	1:A:261:VAL:C	2.51	0.48
1:A:374:TRP:CE3	1:A:417:ARG:HG3	2.48	0.48
1:B:145:ASN:HD22	1:B:146:PRO:CD	2.13	0.48
1:B:311:LEU:HG	1:B:313:PHE:CE2	2.49	0.48
1:B:428:MET:O	1:B:431:ALA:N	2.46	0.48
1:A:282:LEU:O	1:A:286:ILE:HG13	2.12	0.48
1:B:202:GLU:CD	1:B:250:LEU:HD22	2.33	0.48
1:A:98:MET:O	1:A:98:MET:HG2	2.13	0.48
1:A:559:ILE:HD12	1:A:559:ILE:C	2.34	0.48
1:B:202:GLU:OE2	1:B:250:LEU:HD22	2.14	0.48
1:B:329:ILE:CG2	1:B:334:HIS:HB2	2.43	0.48
1:B:369:ASP:O	1:B:372:ARG:HB3	2.13	0.48
1:A:530:LYS:O	1:A:531:HIS:C	2.47	0.48
1:A:70:VAL:CG1	1:A:303:ARG:HD3	2.43	0.48
1:A:117:GLN:HG2	1:A:129:PHE:CE1	2.49	0.48
1:A:287:VAL:O	1:A:290:GLN:HB3	2.13	0.48
1:A:442:LEU:CD1	1:A:446:LEU:HG	2.44	0.48
1:B:103:GLU:HB3	1:B:109:GLN:CG	2.43	0.48
1:B:302:TRP:CZ3	1:B:307:PHE:HD2	2.31	0.48
1:B:492:LEU:HA	1:B:569:ALA:CB	2.44	0.48
1:B:576:GLY:O	1:B:578:GLY:N	2.30	0.48
1:A:404:VAL:CG1	1:A:410:VAL:HG23	2.44	0.48
1:A:428:MET:HG3	1:A:432:ARG:HE	1.79	0.48
1:A:460:THR:HG21	1:A:481:TYR:HE1	1.78	0.48
1:B:112:LEU:HD22	1:B:112:LEU:HA	1.77	0.48
1:B:155:TYR:HB2	1:B:196:GLY:HA2	1.94	0.48
1:B:368:THR:O	1:B:371:ILE:HD13	2.13	0.48
1:B:458:MET:HE2	1:B:565:LEU:HD22	1.96	0.48
1:A:70:VAL:HG12	1:A:74:GLN:CD	2.34	0.47
1:A:391:LEU:HD23	1:B:402:TYR:HD1	1.79	0.47
1:A:585:ILE:O	1:A:585:ILE:HG23	2.14	0.47
1:A:220:PHE:CE1	1:A:224:PHE:HE2	2.33	0.47
1:B:261:VAL:HG22	1:B:262:TRP:N	2.29	0.47
1:B:526:ALA:O	1:B:530:LYS:N	2.41	0.47
3:B:1600:FPG:H103	3:B:1600:FPG:C7	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LYS:NZ	1:A:146:PRO:HG2	2.29	0.47
1:A:317:ARG:O	1:A:318:LEU:C	2.52	0.47
1:A:344:VAL:O	1:A:348:ILE:HG13	2.14	0.47
1:A:550:LYS:HG2	1:A:552:SER:HA	1.95	0.47
1:B:115:ASP:CG	1:B:269:ARG:HH12	2.17	0.47
1:B:190:LEU:O	1:B:192:ASP:N	2.48	0.47
1:B:194:THR:C	1:B:196:GLY:N	2.62	0.47
1:B:256:ARG:HD3	1:B:291:PHE:HZ	1.80	0.47
1:B:272:MET:CE	1:B:277:LEU:HB2	2.43	0.47
4:B:1605:BTB:C2	4:B:1605:BTB:C5	2.86	0.47
1:A:283:ASP:CA	1:A:286:ILE:HD12	2.41	0.47
1:A:435:TYR:C	1:A:437:GLY:H	2.17	0.47
4:A:604:BTB:H62	4:A:604:BTB:C4	2.45	0.47
4:A:604:BTB:H62	4:A:604:BTB:H41	1.96	0.47
1:B:73:ILE:HG21	1:B:299:PHE:CE2	2.49	0.47
1:B:369:ASP:OD2	1:B:372:ARG:NH2	2.47	0.47
1:B:530:LYS:O	1:B:531:HIS:C	2.50	0.47
1:A:75:SER:O	1:A:76:LEU:C	2.53	0.47
1:B:86:VAL:HA	1:B:286:ILE:CD1	2.43	0.47
1:B:299:PHE:O	1:B:302:TRP:N	2.48	0.47
1:A:454:SER:O	1:A:457:CYS:N	2.47	0.47
1:B:506:SER:C	1:B:508:GLY:H	2.18	0.47
1:B:551:ASP:O	1:B:552:SER:C	2.52	0.47
1:A:198:LEU:CA	1:A:225:LEU:HD21	2.43	0.47
1:B:343:LYS:O	1:B:347:LEU:HG	2.14	0.47
1:B:442:LEU:HB3	1:B:520:ASP:OD1	2.15	0.47
1:B:462:ILE:O	1:B:466:VAL:HG22	2.14	0.47
1:B:585:ILE:C	1:B:587:HIS:N	2.67	0.47
1:A:145:ASN:HB3	1:A:146:PRO:HD3	1.95	0.47
1:A:420:TRP:HA	1:A:420:TRP:CE3	2.50	0.47
1:A:501:SER:O	1:A:505:VAL:HG22	2.14	0.47
1:A:503:GLU:HA	1:A:506:SER:HB2	1.97	0.47
1:B:182:GLU:H	1:B:182:GLU:HG3	1.31	0.47
1:B:510:VAL:HG12	1:B:511:PRO:CD	2.42	0.47
1:A:68:TRP:HZ3	1:A:320:GLU:OE2	1.97	0.47
1:A:110:LEU:HB3	1:A:159:LEU:HD13	1.97	0.47
1:A:492:LEU:HA	1:A:569:ALA:CB	2.44	0.47
1:B:103:GLU:CD	1:B:104:THR:N	2.68	0.47
1:B:371:ILE:HD13	1:B:372:ARG:H	1.76	0.47
3:B:1600:FPG:H51	3:B:1600:FPG:H81	1.50	0.47
1:A:89:ALA:O	1:A:92:LEU:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LYS:C	1:A:151:GLU:N	2.68	0.47
1:B:161:PHE:HD2	1:B:203:ALA:HB1	1.79	0.47
1:B:259:ALA:N	1:B:260:PRO:HD2	2.30	0.47
1:B:588:GLN:HA	1:B:591:THR:HG22	1.96	0.47
1:A:294:GLU:HB2	1:A:322:TYR:CE1	2.50	0.46
1:B:84:LYS:HD2	1:B:85:HIS:H	1.80	0.46
1:B:254:ILE:HG13	1:B:567:ARG:HB3	1.97	0.46
1:B:512:LYS:HG2	1:B:515:GLN:HE22	1.80	0.46
1:A:135:SER:O	1:A:136:ILE:C	2.53	0.46
1:B:241:ARG:NH2	1:B:245:SER:OG	2.48	0.46
1:B:457:CYS:O	1:B:461:HIS:HD2	1.97	0.46
1:B:515:GLN:HA	1:B:518:MET:CG	2.46	0.46
1:A:362:GLU:OE2	1:A:362:GLU:HA	2.15	0.46
1:A:502:VAL:O	1:A:505:VAL:HG22	2.16	0.46
4:B:1605:BTB:C1	4:B:1605:BTB:H52	2.44	0.46
1:A:291:PHE:O	1:A:292:GLN:C	2.54	0.46
1:A:324:TRP:CE2	1:A:572:MET:HG2	2.51	0.46
1:A:374:TRP:CZ3	1:A:417:ARG:HG3	2.50	0.46
1:B:82:GLU:O	1:B:85:HIS:HB2	2.16	0.46
1:A:313:PHE:HB3	1:A:358:TYR:CD1	2.51	0.46
1:A:201:TYR:HD2	1:A:202:GLU:HG2	1.81	0.46
1:A:276:VAL:O	1:A:279:LEU:N	2.49	0.46
1:A:283:ASP:O	1:A:284:LEU:C	2.53	0.46
1:A:488:SER:HB2	1:A:562:ALA:O	2.16	0.46
1:A:543:MET:O	1:A:543:MET:HG3	2.14	0.46
1:B:121:LEU:O	1:B:123:ASP:N	2.49	0.46
1:B:181:ASN:C	1:B:181:ASN:OD1	2.51	0.46
1:B:294:GLU:HA	1:B:339:ILE:HD12	1.97	0.46
1:B:556:LYS:HE3	5:B:790:HOH:O	2.15	0.46
1:A:85:HIS:O	1:A:88:ARG:HB3	2.14	0.46
1:A:207:LEU:CD2	1:A:207:LEU:N	2.77	0.46
1:A:301:TRP:CD2	1:A:343:LYS:HB3	2.51	0.46
1:A:369:ASP:OD2	1:A:373:ARG:NH1	2.49	0.46
1:A:501:SER:OG	1:A:512:LYS:HG3	2.16	0.46
1:B:85:HIS:O	1:B:282:LEU:HD21	2.16	0.46
1:B:176:PHE:CD2	1:B:200:LEU:HD12	2.51	0.46
1:B:255:LYS:H	1:B:255:LYS:HG2	1.19	0.46
1:A:471:THR:O	1:A:475:VAL:HG23	2.15	0.46
1:B:442:LEU:HD13	1:B:517:TYR:CA	2.46	0.46
1:A:63:TYR:CG	1:A:315:ARG:HB3	2.51	0.45
1:A:83:ASP:O	1:A:85:HIS:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASP:O	1:A:84:LYS:C	2.55	0.45
1:A:93:VAL:CG2	1:A:124:HIS:HB3	2.46	0.45
1:A:103:GLU:OE1	1:A:104:THR:N	2.34	0.45
1:A:149:LYS:HA	1:A:152:ARG:NH2	2.31	0.45
1:B:181:ASN:N	1:B:185:GLU:O	2.47	0.45
1:B:205:PHE:CZ	1:B:249:PRO:HG3	2.51	0.45
1:B:439:LYS:HD2	1:B:439:LYS:HA	1.66	0.45
1:B:518:MET:HG2	1:B:518:MET:H	1.56	0.45
1:A:145:ASN:HA	1:A:172:ALA:CB	2.46	0.45
1:B:269:ARG:HG2	1:B:271:ASP:OD2	2.16	0.45
1:B:415:TYR:OH	1:B:472:LYS:HD2	2.15	0.45
1:A:311:LEU:O	1:A:311:LEU:HD23	2.16	0.45
1:A:315:ARG:HB2	1:A:317:ARG:NE	2.10	0.45
1:A:481:TYR:HD1	1:A:481:TYR:HA	1.50	0.45
1:B:547:ARG:CA	1:B:559:ILE:HD13	2.47	0.45
1:A:173:GLN:NE2	1:A:211:GLU:C	2.65	0.45
1:A:204:SER:C	1:A:206:LEU:N	2.69	0.45
1:A:229:VAL:HA	1:A:239:LEU:HD21	1.98	0.45
1:A:258:ASN:O	1:A:259:ALA:C	2.55	0.45
1:A:416:LEU:HD22	1:A:461:HIS:CE1	2.52	0.45
1:A:442:LEU:HD23	1:A:517:TYR:HA	1.99	0.45
1:B:365:GLU:OE2	1:B:428:MET:HE1	2.16	0.45
1:A:373:ARG:O	1:A:374:TRP:C	2.54	0.45
1:A:379:ILE:CD1	1:A:387:GLN:HG2	2.47	0.45
1:B:94:THR:O	1:B:98:MET:HB2	2.16	0.45
1:B:302:TRP:O	1:B:305:THR:OG1	2.34	0.45
1:A:69:ASP:OD2	1:A:72:PHE:N	2.49	0.45
1:A:457:CYS:O	1:A:461:HIS:HD2	2.00	0.45
1:A:482:HIS:CG	1:A:554:PHE:HE2	2.35	0.45
1:A:544:ASN:O	1:A:545:ALA:C	2.55	0.45
1:B:139:ASP:C	1:B:141:HIS:H	2.20	0.45
1:B:272:MET:HE3	1:B:277:LEU:HG	1.99	0.45
1:B:325:ASN:CG	1:B:341:MET:HB3	2.37	0.45
1:B:329:ILE:HD13	1:B:337:ALA:CB	2.47	0.45
1:A:211:GLU:OE2	1:A:214:LEU:HD23	2.17	0.45
1:A:377:ASN:C	1:A:379:ILE:H	2.19	0.45
1:A:501:SER:CA	1:A:512:LYS:HG3	2.40	0.45
1:B:84:LYS:HD2	1:B:85:HIS:N	2.31	0.45
1:B:248:ILE:O	1:B:253:ARG:NH1	2.49	0.45
1:B:432:ARG:O	1:B:436:GLY:N	2.46	0.45
1:B:470:PHE:CD2	1:B:470:PHE:N	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:SER:O	1:B:480:LYS:HG2	2.16	0.45
1:B:415:TYR:CZ	1:B:475:VAL:HG11	2.52	0.45
1:A:478:LEU:HA	1:A:482:HIS:HB2	1.99	0.45
1:A:496:ASP:HB2	1:A:573:TYR:CE2	2.52	0.45
1:A:559:ILE:HD12	1:A:563:VAL:HG23	1.98	0.45
1:B:154:LEU:HD11	1:B:200:LEU:HD13	1.99	0.45
1:B:277:LEU:HD13	1:B:277:LEU:C	2.38	0.45
1:B:281:ILE:HG23	1:B:598:PHE:HB3	1.99	0.45
1:B:425:ASP:O	1:B:429:VAL:HG22	2.17	0.45
1:A:145:ASN:HD22	1:A:145:ASN:C	2.21	0.44
1:A:238:LEU:O	1:A:239:LEU:C	2.54	0.44
1:A:259:ALA:O	1:A:260:PRO:C	2.55	0.44
1:A:411:ASN:OD1	1:A:413:ILE:HG23	2.17	0.44
1:A:585:ILE:C	1:A:587:HIS:N	2.60	0.44
4:A:605:BTB:H62	4:A:605:BTB:HO3	1.79	0.44
1:B:179:PHE:HB3	1:B:190:LEU:HD11	1.99	0.44
1:A:107:ILE:CG1	1:A:156:SER:HB2	2.47	0.44
1:A:145:ASN:HA	1:A:172:ALA:HB2	1.99	0.44
1:A:332:ARG:HG2	1:A:333:GLN:N	2.32	0.44
1:A:344:VAL:HG22	1:A:396:PHE:CZ	2.51	0.44
1:A:510:VAL:HG23	1:A:511:PRO:N	2.33	0.44
1:A:534:TRP:CE3	1:A:535:LEU:HD13	2.52	0.44
1:B:155:TYR:CD1	1:B:199:GLN:HG2	2.52	0.44
1:A:60:SER:O	1:A:62:ASN:N	2.50	0.44
1:A:145:ASN:N	1:A:146:PRO:CD	2.79	0.44
1:A:152:ARG:HH11	1:A:152:ARG:CG	2.28	0.44
1:A:301:TRP:HZ3	1:A:346:ALA:CB	2.30	0.44
1:A:323:PHE:CE1	1:A:326:THR:HG21	2.52	0.44
1:A:496:ASP:HA	1:A:573:TYR:CD2	2.52	0.44
1:B:97:LYS:C	1:B:101:GLU:CD	2.76	0.44
1:B:146:PRO:HB2	1:B:147:PHE:H	1.51	0.44
1:B:218:ARG:NH1	1:B:218:ARG:CG	2.67	0.44
1:B:229:VAL:HG23	1:B:242:ILE:HG21	2.00	0.44
1:B:294:GLU:HB3	1:B:339:ILE:HD13	1.99	0.44
1:B:411:ASN:ND2	1:B:413:ILE:H	2.15	0.44
1:A:63:TYR:CE1	1:A:315:ARG:HD2	2.52	0.44
1:A:227:GLU:O	1:A:231:GLU:HG3	2.17	0.44
1:A:442:LEU:HD12	1:A:446:LEU:CG	2.47	0.44
1:B:238:LEU:HD23	1:B:239:LEU:HD12	2.00	0.44
1:B:458:MET:HE1	1:B:565:LEU:HD13	2.00	0.44
1:A:442:LEU:HD12	1:A:446:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:VAL:O	1:A:536:ILE:HG13	2.17	0.44
1:B:137:TYR:CZ	1:B:143:TYR:HB3	2.53	0.44
1:B:222:THR:HG23	1:B:226:GLU:OE2	2.18	0.44
1:B:264:GLU:H	1:B:264:GLU:HG3	1.54	0.44
1:B:139:ASP:O	1:B:141:HIS:N	2.51	0.44
1:B:141:HIS:O	1:B:143:TYR:N	2.51	0.44
1:B:158:SER:HB2	1:B:199:GLN:HB3	2.00	0.44
1:B:311:LEU:HD11	1:B:385:TYR:O	2.18	0.44
1:B:329:ILE:HD13	1:B:337:ALA:HB1	2.00	0.44
1:B:558:PHE:O	1:B:559:ILE:C	2.55	0.44
1:B:570:GLN:O	1:B:574:HIS:HB2	2.16	0.44
1:A:83:ASP:O	1:A:87:ILE:HG12	2.18	0.44
1:A:98:MET:O	1:A:99:GLU:C	2.52	0.44
1:A:152:ARG:HB2	1:A:157:THR:OG1	2.18	0.44
1:A:301:TRP:O	1:A:305:THR:HG23	2.18	0.44
1:A:370:LEU:HD21	1:A:375:ASP:O	2.17	0.44
1:A:402:TYR:CE1	1:B:392:ALA:HB2	2.53	0.44
1:B:310:LYS:O	1:B:312:PRO:HD3	2.18	0.44
1:B:341:MET:HE3	1:B:458:MET:HA	2.00	0.44
1:B:397:VAL:O	1:B:401:SER:HB2	2.18	0.44
1:B:449:SER:OG	1:B:493:ARG:HG2	2.18	0.44
1:B:416:LEU:HD22	1:B:461:HIS:ND1	2.32	0.44
1:B:484:LEU:HB2	1:B:546:GLU:HG2	2.00	0.44
1:A:98:MET:O	1:A:102:LYS:N	2.49	0.43
1:A:165:ARG:HB3	1:A:206:LEU:HD23	1.99	0.43
1:A:204:SER:C	1:A:206:LEU:H	2.21	0.43
1:B:63:TYR:CE1	1:B:315:ARG:HD2	2.52	0.43
1:B:288:GLN:O	1:B:291:PHE:HB2	2.18	0.43
1:B:340:MET:O	1:B:344:VAL:HG23	2.17	0.43
1:A:266:TYR:HE2	1:A:277:LEU:HB2	1.83	0.43
1:A:320:GLU:HA	1:A:590:MET:HE3	2.00	0.43
1:B:447:GLU:O	1:B:447:GLU:HG3	2.18	0.43
1:B:535:LEU:HD23	1:B:535:LEU:HA	1.80	0.43
1:A:60:SER:C	1:A:62:ASN:H	2.21	0.43
1:A:187:LYS:HB3	1:A:190:LEU:HG	2.01	0.43
1:B:588:GLN:HA	1:B:591:THR:CG2	2.48	0.43
1:A:586:ILE:O	1:A:590:MET:HB2	2.18	0.43
1:B:261:VAL:O	1:B:262:TRP:C	2.55	0.43
1:B:386:MET:HB3	1:B:386:MET:HE2	1.56	0.43
1:B:453:ILE:HG23	1:B:492:LEU:HD23	1.99	0.43
1:A:76:LEU:HD21	1:A:595:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LEU:N	1:A:312:PRO:CD	2.82	0.43
1:B:86:VAL:HA	1:B:89:ALA:HB3	2.00	0.43
1:A:140:HIS:O	1:A:141:HIS:C	2.56	0.43
1:A:577:ASP:O	1:A:578:GLY:O	2.37	0.43
1:A:579:HIS:O	1:A:579:HIS:CG	2.71	0.43
1:B:423:LEU:HD22	1:B:423:LEU:O	2.19	0.43
1:B:518:MET:O	1:B:519:SER:C	2.53	0.43
1:A:147:PHE:CE2	1:A:149:LYS:HD3	2.53	0.43
1:A:236:GLY:O	1:A:240:THR:HG23	2.19	0.43
1:A:418:GLN:HG2	1:A:422:ASP:OD1	2.18	0.43
1:A:431:ALA:O	1:A:434:PHE:N	2.52	0.43
1:A:487:TRP:NE1	1:A:542:LYS:HD3	2.33	0.43
1:A:550:LYS:HB2	1:A:550:LYS:HE3	1.44	0.43
1:B:86:VAL:CA	1:B:286:ILE:HD13	2.46	0.43
1:B:89:ALA:CA	1:B:282:LEU:HD23	2.49	0.43
1:B:145:ASN:ND2	1:B:145:ASN:N	2.60	0.43
1:B:500:THR:HG22	1:B:501:SER:N	2.32	0.43
1:A:173:GLN:HE21	1:A:213:THR:CB	2.31	0.43
1:B:176:PHE:HA	1:B:179:PHE:HE2	1.83	0.43
1:B:242:ILE:CG2	1:B:243:ALA:N	2.72	0.43
1:B:493:ARG:O	1:B:494:LEU:C	2.55	0.43
1:A:256:ARG:HB2	1:A:330:GLU:CD	2.39	0.43
1:A:317:ARG:HD2	1:A:579:HIS:CE1	2.54	0.43
1:B:86:VAL:O	1:B:89:ALA:HB3	2.19	0.43
1:B:86:VAL:O	1:B:90:SER:N	2.41	0.43
1:B:162:ARG:NH1	1:B:250:LEU:HD23	2.33	0.43
1:A:144:LYS:CG	1:A:146:PRO:HG2	2.49	0.43
1:A:207:LEU:H	1:A:207:LEU:HD23	1.83	0.43
1:A:266:TYR:O	1:A:272:MET:HG3	2.19	0.43
1:A:283:ASP:OD2	1:A:332:ARG:NH2	2.52	0.43
1:A:393:LEU:HD21	1:A:420:TRP:CD2	2.54	0.43
1:B:188:GLU:CD	1:B:188:GLU:N	2.72	0.43
4:B:1605:BTB:H61	4:B:1605:BTB:O4	2.19	0.43
1:A:205:PHE:HD1	1:A:252:TRP:CZ2	2.37	0.42
1:A:544:ASN:ND2	1:A:547:ARG:HH11	2.17	0.42
1:B:454:SER:O	1:B:455:GLY:C	2.57	0.42
1:A:79:ASP:N	1:A:79:ASP:OD2	2.52	0.42
1:A:273:ASN:OD1	1:A:275:VAL:N	2.51	0.42
1:A:575:ASN:OD1	1:A:575:ASN:N	2.51	0.42
1:B:344:VAL:HG22	1:B:396:PHE:CZ	2.54	0.42
1:B:558:PHE:C	1:B:560:GLY:N	2.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:HD22	1:A:242:ILE:HG23	2.01	0.42
1:A:348:ILE:HG22	3:A:600:FPG:H13	2.00	0.42
1:A:404:VAL:HG12	1:A:410:VAL:HG23	1.99	0.42
1:A:449:SER:O	1:A:451:GLN:N	2.52	0.42
1:A:503:GLU:O	1:A:504:GLU:C	2.55	0.42
1:B:69:ASP:OD1	1:B:72:PHE:N	2.51	0.42
1:B:369:ASP:O	1:B:372:ARG:N	2.52	0.42
1:B:484:LEU:HD11	1:B:562:ALA:CB	2.49	0.42
1:A:152:ARG:NH2	1:A:178:SER:HB3	2.34	0.42
1:A:482:HIS:CG	1:A:554:PHE:CE2	3.07	0.42
1:A:493:ARG:HD3	1:A:497:ASP:HB2	2.00	0.42
1:A:568:MET:O	1:A:572:MET:HB2	2.18	0.42
1:B:241:ARG:NH2	1:B:245:SER:CB	2.82	0.42
1:B:378:SER:C	1:B:380:ASP:N	2.73	0.42
1:B:454:SER:O	1:B:457:CYS:N	2.53	0.42
1:B:548:VAL:O	1:B:548:VAL:CG1	2.67	0.42
1:A:133:LEU:O	1:A:134:SER:C	2.57	0.42
1:A:470:PHE:CD1	1:A:470:PHE:N	2.85	0.42
1:B:190:LEU:C	1:B:192:ASP:H	2.22	0.42
1:B:549:SER:OG	1:B:550:LYS:N	2.52	0.42
1:A:118:ARG:NH1	1:A:255:LYS:HE3	2.35	0.42
1:A:150:GLU:C	1:A:152:ARG:N	2.70	0.42
1:A:231:GLU:OE2	1:A:233:GLY:HA2	2.19	0.42
1:A:152:ARG:NH1	1:A:175:VAL:O	2.52	0.42
1:A:166:GLU:C	1:A:168:GLY:N	2.72	0.42
1:A:449:SER:HA	1:A:493:ARG:HH12	1.85	0.42
1:A:589:GLN:H	1:A:589:GLN:HG2	1.50	0.42
1:B:70:VAL:HG22	1:B:71:ASN:N	2.34	0.42
1:B:413:ILE:HG12	1:B:414:PRO:HD3	2.02	0.42
1:A:144:LYS:CE	1:A:146:PRO:HG2	2.50	0.42
1:A:260:PRO:O	1:A:263:ILE:N	2.52	0.42
1:A:290:GLN:O	1:A:291:PHE:C	2.56	0.42
1:A:360:THR:O	1:A:364:LEU:HB2	2.19	0.42
1:A:445:TYR:C	1:A:447:GLU:N	2.72	0.42
3:A:600:FPG:H81	3:A:600:FPG:H51	1.54	0.42
1:B:146:PRO:C	1:B:148:PRO:HD2	2.40	0.42
1:B:194:THR:O	1:B:195:ARG:C	2.54	0.42
1:B:350:VAL:O	1:B:353:ASP:N	2.53	0.42
1:B:586:ILE:HA	1:B:589:GLN:HE21	1.85	0.42
1:A:173:GLN:HE21	1:A:213:THR:HB	1.85	0.42
1:A:425:ASP:O	1:A:428:MET:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:TRP:CZ2	1:B:347:LEU:HD21	2.51	0.42
1:B:510:VAL:CG1	1:B:511:PRO:HD2	2.45	0.42
1:A:165:ARG:NH2	1:A:211:GLU:OE2	2.53	0.42
1:A:190:LEU:C	1:A:192:ASP:N	2.73	0.42
1:A:458:MET:O	1:A:462:ILE:HG13	2.19	0.42
1:B:103:GLU:OE1	1:B:103:GLU:CA	2.68	0.42
4:B:1604:BTB:H52	4:B:1604:BTB:H81	1.67	0.42
1:A:433:TRP:CZ3	1:A:440:PRO:HG3	2.55	0.41
1:A:550:LYS:O	1:A:550:LYS:HG3	2.20	0.41
1:B:253:ARG:O	1:B:254:ILE:C	2.58	0.41
1:B:424:ALA:O	1:B:427:TYR:HB2	2.20	0.41
1:B:429:VAL:HG21	1:B:448:ASN:HD21	1.85	0.41
1:B:212:THR:O	1:B:213:THR:C	2.59	0.41
1:A:70:VAL:HA	1:A:299:PHE:CE1	2.56	0.41
1:A:112:LEU:HD13	1:A:116:LEU:HG	2.02	0.41
1:A:423:LEU:HD11	1:A:427:TYR:CE2	2.55	0.41
1:B:83:ASP:C	1:B:85:HIS:H	2.24	0.41
1:B:294:GLU:HG2	1:B:339:ILE:CD1	2.50	0.41
1:B:484:LEU:HD11	1:B:562:ALA:HB3	2.03	0.41
1:A:180:LYS:HZ1	1:A:213:THR:HG23	1.84	0.41
4:A:605:BTB:H42	4:A:605:BTB:C6	2.50	0.41
1:B:68:TRP:HZ3	1:B:320:GLU:OE2	2.03	0.41
1:B:374:TRP:HE1	1:B:394:ASN:HD22	1.68	0.41
1:B:580:GLY:O	1:B:581:THR:HB	2.20	0.41
1:B:595:PHE:O	1:B:597:PRO:HD3	2.19	0.41
1:A:201:TYR:O	1:A:204:SER:OG	2.39	0.41
1:A:253:ARG:NH1	1:A:253:ARG:HG3	2.35	0.41
1:A:311:LEU:HG	1:A:313:PHE:CE2	2.56	0.41
1:A:329:ILE:HD11	1:A:462:ILE:HD13	2.03	0.41
1:A:351:ILE:O	1:A:355:TYR:HD2	2.01	0.41
1:A:432:ARG:O	1:A:433:TRP:C	2.58	0.41
1:A:433:TRP:CD1	1:A:438:HIS:CD2	3.08	0.41
1:A:518:MET:HG3	1:A:518:MET:H	1.68	0.41
1:A:93:VAL:O	1:A:97:LYS:HB2	2.20	0.41
1:A:238:LEU:O	1:A:240:THR:N	2.54	0.41
1:A:241:ARG:HH21	1:A:245:SER:HB2	1.84	0.41
1:A:424:ALA:O	1:A:427:TYR:HB2	2.20	0.41
1:B:200:LEU:O	1:B:201:TYR:C	2.57	0.41
1:B:235:ASP:HB3	1:B:236:GLY:H	1.62	0.41
1:B:373:ARG:HB2	1:B:373:ARG:CZ	2.51	0.41
1:B:586:ILE:CA	1:B:589:GLN:HG3	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ALA:CA	1:A:282:LEU:HD23	2.51	0.41
1:A:93:VAL:HG22	1:A:97:LYS:HD2	2.01	0.41
1:A:259:ALA:C	1:A:263:ILE:HG12	2.40	0.41
1:A:413:ILE:N	1:A:414:PRO:CD	2.84	0.41
1:A:418:GLN:O	1:A:419:SER:C	2.58	0.41
1:A:442:LEU:HD23	1:A:517:TYR:CA	2.51	0.41
1:A:442:LEU:HD23	1:A:517:TYR:N	2.36	0.41
1:A:548:VAL:O	1:A:549:SER:CB	2.62	0.41
1:B:220:PHE:CZ	1:B:224:PHE:HE2	2.39	0.41
1:B:228:LYS:HG3	1:B:234:VAL:HG11	2.02	0.41
1:B:508:GLY:O	1:B:509:ASP:HB2	2.19	0.41
1:A:110:LEU:HD11	1:A:160:ALA:HB2	2.02	0.41
1:A:116:LEU:HD22	1:A:121:LEU:HD23	2.03	0.41
1:A:123:ASP:OD2	1:A:332:ARG:NH1	2.48	0.41
1:A:123:ASP:HB2	1:A:332:ARG:NH1	2.35	0.41
1:A:214:LEU:HD12	1:A:214:LEU:HA	1.71	0.41
1:A:233:GLY:HA3	1:A:239:LEU:HD23	2.03	0.41
1:B:177:ASP:O	1:B:179:PHE:N	2.54	0.41
1:B:200:LEU:HD23	1:B:221:ALA:HB2	2.01	0.41
1:B:205:PHE:CE2	1:B:249:PRO:HG3	2.56	0.41
1:B:465:ARG:HA	1:B:465:ARG:HD2	1.62	0.41
1:A:70:VAL:C	1:A:72:PHE:N	2.74	0.41
1:A:117:GLN:HE21	1:A:129:PHE:HE1	1.67	0.41
1:A:145:ASN:ND2	1:A:145:ASN:C	2.73	0.41
1:A:162:ARG:HD3	1:A:202:GLU:O	2.21	0.41
1:A:200:LEU:C	1:A:202:GLU:N	2.73	0.41
1:A:238:LEU:HD12	1:A:238:LEU:HA	1.84	0.41
1:A:507:ARG:NH1	1:A:508:GLY:O	2.54	0.41
1:A:546:GLU:OE1	1:A:550:LYS:HD2	2.21	0.41
1:B:113:ILE:HG23	1:B:129:PHE:CE1	2.56	0.41
1:B:176:PHE:HA	1:B:179:PHE:CD2	2.56	0.41
1:B:188:GLU:OE2	1:B:189:SER:N	2.52	0.41
1:B:228:LYS:HD3	1:B:228:LYS:HA	1.62	0.41
1:B:304:ASN:O	1:B:305:THR:C	2.59	0.41
1:B:341:MET:CE	1:B:458:MET:HG2	2.51	0.41
1:B:382:LEU:HB3	1:B:386:MET:HE1	2.03	0.41
1:B:395:ASN:O	1:B:399:ASP:N	2.51	0.41
1:B:453:ILE:O	1:B:454:SER:CB	2.69	0.41
1:B:493:ARG:O	1:B:496:ASP:HB3	2.20	0.41
1:B:517:TYR:CD2	1:B:517:TYR:C	2.95	0.41
1:B:550:LYS:H	1:B:550:LYS:HG3	1.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ASP:HA	1:A:81:LYS:HD2	2.03	0.41
1:A:155:TYR:CA	1:A:196:GLY:HA2	2.51	0.41
1:A:201:TYR:HB2	1:A:221:ALA:HB3	2.00	0.41
1:A:251:HIS:O	1:A:567:ARG:NE	2.45	0.41
1:A:274:PRO:O	1:A:276:VAL:N	2.54	0.41
1:A:443:GLU:O	1:A:444:GLU:C	2.56	0.41
1:B:309:GLU:CG	1:B:310:LYS:HG2	2.50	0.41
1:B:317:ARG:HG3	1:B:580:GLY:HA3	2.03	0.41
1:A:421:VAL:O	1:A:422:ASP:C	2.58	0.40
4:A:604:BTB:H11	4:A:604:BTB:H71	1.86	0.40
1:B:188:GLU:C	1:B:190:LEU:N	2.74	0.40
1:B:323:PHE:HE1	1:B:326:THR:HG21	1.86	0.40
1:B:361:LEU:O	1:B:365:GLU:HG2	2.21	0.40
1:A:193:ASP:OD2	1:A:193:ASP:C	2.59	0.40
1:A:205:PHE:HE1	1:A:252:TRP:CH2	2.39	0.40
1:A:269:ARG:HG3	1:A:270:PRO:CD	2.51	0.40
1:A:314:ALA:HB1	1:A:350:VAL:HG22	2.04	0.40
1:A:435:TYR:HD2	1:A:435:TYR:HA	1.76	0.40
1:B:81:LYS:HG2	1:B:81:LYS:H	1.56	0.40
1:B:146:PRO:O	1:B:147:PHE:HB2	2.21	0.40
1:B:377:ASN:C	1:B:379:ILE:N	2.75	0.40
1:B:455:GLY:O	1:B:458:MET:HB2	2.21	0.40
1:B:488:SER:O	1:B:489:SER:C	2.58	0.40
1:A:70:VAL:O	1:A:74:GLN:N	2.54	0.40
1:A:79:ASP:CA	1:A:81:LYS:HD2	2.52	0.40
1:B:145:ASN:N	1:B:146:PRO:CD	2.84	0.40
1:B:147:PHE:N	1:B:148:PRO:HD2	2.36	0.40
1:B:313:PHE:CE1	1:B:354:ILE:HG13	2.57	0.40
1:B:360:THR:OG1	1:B:363:GLU:HB2	2.21	0.40
1:B:411:ASN:HD22	1:B:413:ILE:H	1.69	0.40
1:B:413:ILE:N	1:B:414:PRO:CD	2.84	0.40
1:A:81:LYS:CD	1:A:81:LYS:N	2.84	0.40
1:A:311:LEU:HD21	1:A:350:VAL:HG11	2.03	0.40
1:A:425:ASP:O	1:A:428:MET:N	2.55	0.40
1:A:430:GLU:HG2	1:A:510:VAL:HG11	2.03	0.40
1:A:549:SER:OG	1:A:550:LYS:N	2.53	0.40
1:A:589:GLN:HE21	1:A:589:GLN:HB3	1.75	0.40
1:B:491:VAL:O	1:B:492:LEU:C	2.57	0.40
3:B:1600:FPG:H102	3:B:1600:FPG:H11	1.84	0.40
1:A:134:SER:O	1:A:137:TYR:HB3	2.21	0.40
1:A:173:GLN:HE22	1:A:212:THR:N	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:VAL:HA	1:A:239:LEU:HD22	2.04	0.40
1:A:547:ARG:C	1:A:549:SER:N	2.73	0.40
1:B:346:ALA:O	1:B:347:LEU:C	2.58	0.40
1:B:547:ARG:HG3	1:B:548:VAL:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	541/543 (100%)	400 (74%)	93 (17%)	48 (9%)	1	1
1	B	541/543 (100%)	409 (76%)	86 (16%)	46 (8%)	1	1
All	All	1082/1086 (100%)	809 (75%)	179 (16%)	94 (9%)	1	1

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	78	SER
1	A	83	ASP
1	A	125	PHE
1	A	152	ARG
1	A	191	SER
1	A	235	ASP
1	A	272	MET
1	A	357	VAL
1	A	358	TYR
1	A	381	GLN
1	A	500	THR
1	A	520	ASP
1	A	578	GLY

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Mol	Chain	Res	Type
1	A	584	PRO
1	B	76	LEU
1	B	83	ASP
1	B	146	PRO
1	B	147	PHE
1	B	150	GLU
1	B	210	GLY
1	B	211	GLU
1	B	235	ASP
1	B	313	PHE
1	B	437	GLY
1	B	502	VAL
1	B	577	ASP
1	B	579	HIS
1	B	581	THR
1	B	584	PRO
1	A	61	GLY
1	A	71	ASN
1	A	122	SER
1	A	174	GLU
1	A	178	SER
1	A	255	LYS
1	A	270	PRO
1	A	312	PRO
1	A	432	ARG
1	A	481	TYR
1	A	509	ASP
1	A	549	SER
1	B	77	LEU
1	B	122	SER
1	B	142	TYR
1	B	178	SER
1	B	271	ASP
1	B	272	MET
1	B	312	PRO
1	B	357	VAL
1	B	438	HIS
1	B	455	GLY
1	B	500	THR
1	B	549	SER
1	B	578	GLY
1	A	79	ASP

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Mol	Chain	Res	Type
1	A	332	ARG
1	A	359	GLY
1	A	450	TRP
1	B	140	HIS
1	B	148	PRO
1	B	174	GLU
1	B	191	SER
1	B	193	ASP
1	B	481	TYR
1	A	70	VAL
1	A	84	LYS
1	A	135	SER
1	A	236	GLY
1	B	139	ASP
1	B	208	THR
1	B	270	PRO
1	B	374	TRP
1	B	454	SER
1	B	501	SER
1	A	140	HIS
1	A	167	HIS
1	A	239	LEU
1	A	274	PRO
1	A	308	VAL
1	A	449	SER
1	A	581	THR
1	A	583	HIS
1	B	151	GLU
1	B	149	LYS
1	B	376	ILE
1	A	148	PRO
1	A	233	GLY
1	A	234	VAL
1	A	276	VAL
1	B	232	GLY
1	B	508	GLY
1	B	260	PRO
1	A	260	PRO

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	490/492 (100%)	352 (72%)	138 (28%)	0	1
1	B	490/492 (100%)	338 (69%)	152 (31%)	0	0
All	All	980/984 (100%)	690 (70%)	290 (30%)	0	1

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	MET
1	A	58	ARG
1	A	59	ARG
1	A	64	ASN
1	A	67	ARG
1	A	69	ASP
1	A	70	VAL
1	A	72	PHE
1	A	74	GLN
1	A	76	LEU
1	A	77	LEU
1	A	78	SER
1	A	79	ASP
1	A	81	LYS
1	A	83	ASP
1	A	84	LYS
1	A	92	LEU
1	A	97	LYS
1	A	98	MET
1	A	101	GLU
1	A	102	LYS
1	A	107	ILE
1	A	108	ARG
1	A	112	LEU
1	A	121	LEU
1	A	122	SER
1	A	131	GLU

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Mol	Chain	Res	Type
1	A	134	SER
1	A	143	TYR
1	A	144	LYS
1	A	145	ASN
1	A	147	PHE
1	A	149	LYS
1	A	152	ARG
1	A	156	SER
1	A	159	LEU
1	A	165	ARG
1	A	175	VAL
1	A	186	PHE
1	A	187	LYS
1	A	188	GLU
1	A	189	SER
1	A	191	SER
1	A	195	ARG
1	A	198	LEU
1	A	200	LEU
1	A	201	TYR
1	A	204	SER
1	A	207	LEU
1	A	214	LEU
1	A	218	ARG
1	A	223	LYS
1	A	226	GLU
1	A	227	GLU
1	A	228	LYS
1	A	231	GLU
1	A	239	LEU
1	A	241	ARG
1	A	255	LYS
1	A	256	ARG
1	A	261	VAL
1	A	264	GLU
1	A	269	ARG
1	A	271	ASP
1	A	273	ASN
1	A	278	GLU
1	A	287	VAL
1	A	294	GLU
1	A	295	LEU

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Mol	Chain	Res	Type
1	A	300	ARG
1	A	308	VAL
1	A	309	GLU
1	A	310	LYS
1	A	311	LEU
1	A	313	PHE
1	A	315	ARG
1	A	317	ARG
1	A	318	LEU
1	A	321	CYS
1	A	326	THR
1	A	332	ARG
1	A	333	GLN
1	A	343	LYS
1	A	361	LEU
1	A	365	GLU
1	A	372	ARG
1	A	373	ARG
1	A	379	ILE
1	A	382	LEU
1	A	391	LEU
1	A	393	LEU
1	A	397	VAL
1	A	399	ASP
1	A	405	MET
1	A	412	VAL
1	A	413	ILE
1	A	417	ARG
1	A	426	LYS
1	A	427	TYR
1	A	429	VAL
1	A	435	TYR
1	A	442	LEU
1	A	443	GLU
1	A	448	ASN
1	A	462	ILE
1	A	469	SER
1	A	470	PHE
1	A	471	THR
1	A	473	GLU
1	A	488	SER
1	A	492	LEU

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Mol	Chain	Res	Type
1	A	493	ARG
1	A	497	ASP
1	A	500	THR
1	A	506	SER
1	A	507	ARG
1	A	509	ASP
1	A	510	VAL
1	A	514	LEU
1	A	515	GLN
1	A	518	MET
1	A	522	ASN
1	A	535	LEU
1	A	538	GLU
1	A	539	VAL
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	572	MET
1	A	575	ASN
1	A	583	HIS
1	A	588	GLN
1	A	589	GLN
1	A	590	MET
1	A	593	THR
1	B	57	MET
1	B	58	ARG
1	B	59	ARG
1	B	64	ASN
1	B	66	SER
1	B	67	ARG
1	B	69	ASP
1	B	70	VAL
1	B	72	PHE
1	B	73	ILE
1	B	75	SER
1	B	76	LEU
1	B	77	LEU
1	B	81	LYS
1	B	83	ASP

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Mol	Chain	Res	Type
1	B	84	LYS
1	B	88	ARG
1	B	92	LEU
1	B	94	THR
1	B	95	LEU
1	B	99	GLU
1	B	103	GLU
1	B	107	ILE
1	B	112	LEU
1	B	118	ARG
1	B	119	MET
1	B	122	SER
1	B	123	ASP
1	B	124	HIS
1	B	127	ASN
1	B	131	GLU
1	B	145	ASN
1	B	147	PHE
1	B	150	GLU
1	B	152	ARG
1	B	156	SER
1	B	163	LEU
1	B	165	ARG
1	B	174	GLU
1	B	178	SER
1	B	182	GLU
1	B	185	GLU
1	B	188	GLU
1	B	189	SER
1	B	192	ASP
1	B	199	GLN
1	B	200	LEU
1	B	201	TYR
1	B	202	GLU
1	B	206	LEU
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	219	GLU
1	B	223	LYS
1	B	225	LEU
1	B	226	GLU
1	B	227	GLU
1	B	228	LYS
1	B	229	VAL
1	B	231	GLU
1	B	237	ASP
1	B	238	LEU
1	B	240	THR
1	B	241	ARG
1	B	242	ILE
1	B	245	SER
1	B	250	LEU
1	B	253	ARG
1	B	254	ILE
1	B	255	LYS
1	B	256	ARG
1	B	261	VAL
1	B	264	GLU
1	B	274	PRO
1	B	275	VAL
1	B	278	GLU
1	B	293	GLU
1	B	308	VAL
1	B	309	GLU
1	B	310	LYS
1	B	315	ARG
1	B	319	VAL
1	B	321	CYS
1	B	326	THR
1	B	332	ARG
1	B	336	SER
1	B	357	VAL
1	B	361	LEU
1	B	362	GLU
1	B	367	PHE
1	B	371	ILE
1	B	376	ILE
1	B	378	SER
1	B	381	GLN

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Mol	Chain	Res	Type
1	B	382	LEU
1	B	394	ASN
1	B	401	SER
1	B	406	LYS
1	B	408	LYS
1	B	412	VAL
1	B	413	ILE
1	B	417	ARG
1	B	419	SER
1	B	423	LEU
1	B	426	LYS
1	B	429	VAL
1	B	444	GLU
1	B	446	LEU
1	B	449	SER
1	B	451	GLN
1	B	453	ILE
1	B	454	SER
1	B	459	LEU
1	B	468	ASP
1	B	469	SER
1	B	470	PHE
1	B	471	THR
1	B	474	THR
1	B	477	SER
1	B	486	ARG
1	B	490	PHE
1	B	498	LEU
1	B	501	SER
1	B	503	GLU
1	B	506	SER
1	B	513	SER
1	B	514	LEU
1	B	515	GLN
1	B	518	MET
1	B	529	ARG
1	B	530	LYS
1	B	540	TRP
1	B	547	ARG
1	B	548	VAL
1	B	550	LYS
1	B	551	ASP

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Mol	Chain	Res	Type
1	B	552	SER
1	B	556	LYS
1	B	559	ILE
1	B	563	VAL
1	B	570	GLN
1	B	585	ILE
1	B	587	HIS
1	B	588	GLN
1	B	589	GLN
1	B	592	ARG
1	B	593	THR

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	85	HIS
1	A	117	GLN
1	A	140	HIS
1	A	145	ASN
1	A	173	GLN
1	A	258	ASN
1	A	288	GLN
1	A	290	GLN
1	A	333	GLN
1	A	334	HIS
1	A	345	ASN
1	A	438	HIS
1	A	461	HIS
1	A	544	ASN
1	A	587	HIS
1	B	106	GLN
1	B	140	HIS
1	B	145	ASN
1	B	290	GLN
1	B	345	ASN
1	B	381	GLN
1	B	395	ASN
1	B	411	ASN
1	B	451	GLN
1	B	461	HIS
1	B	482	HIS
1	B	515	GLN

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Mol	Chain	Res	Type
1	B	544	ASN
1	B	574	HIS
1	B	575	ASN
1	B	579	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	BTB	B	1604	-	13,13,13	4.34	6 (46%)	7,16,16	1.07	1 (14%)
3	FPG	B	1600	2	16,19,19	1.82	3 (18%)	20,29,29	2.54	4 (20%)
4	BTB	B	1605	-	13,13,13	4.11	6 (46%)	7,16,16	1.04	1 (14%)
4	BTB	A	604	-	13,13,13	1.89	4 (30%)	7,16,16	0.57	0
3	FPG	A	600	2	16,19,19	1.88	4 (25%)	20,29,29	2.13	4 (20%)
4	BTB	A	605	-	13,13,13	4.35	5 (38%)	7,16,16	1.13	1 (14%)

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	B	1604	-	-	10/21/21/21	-
3	FPG	B	1600	2	-	7/19/25/25	-
4	BTB	B	1605	-	-	8/21/21/21	-
4	BTB	A	604	-	-	2/21/21/21	-
3	FPG	A	600	2	-	8/19/25/25	-
4	BTB	A	605	-	-	9/21/21/21	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	BTB	C2-N	11.49	1.71	1.48
4	B	1605	BTB	C2-N	10.46	1.69	1.48
4	B	1604	BTB	C2-N	10.25	1.68	1.48
4	B	1604	BTB	C5-N	7.72	1.59	1.48
4	A	605	BTB	C5-N	7.58	1.59	1.48
4	B	1605	BTB	C5-N	6.30	1.57	1.48
4	B	1604	BTB	C7-N	5.98	1.56	1.48
4	B	1605	BTB	C7-N	5.36	1.55	1.48
4	B	1604	BTB	C4-C2	4.97	1.60	1.53
4	A	604	BTB	C2-N	4.70	1.57	1.48
4	A	605	BTB	C4-C2	4.39	1.59	1.53
4	B	1605	BTB	C4-C2	3.99	1.58	1.53
4	B	1605	BTB	C1-C2	3.94	1.58	1.53
4	A	605	BTB	C7-N	3.87	1.53	1.48
3	A	600	FPG	C1-C2	-3.73	1.43	1.50
4	A	605	BTB	C1-C2	3.67	1.58	1.53
3	B	1600	FPG	C1-C2	-3.59	1.43	1.50
3	B	1600	FPG	PB-O3B	3.34	1.61	1.50
3	A	600	FPG	PB-O3B	3.31	1.61	1.50
4	A	604	BTB	C5-N	3.20	1.52	1.48
4	B	1604	BTB	C1-C2	2.92	1.57	1.53
3	B	1600	FPG	PA-O1A	2.89	1.61	1.50
3	A	600	FPG	PA-O1A	2.82	1.60	1.50
4	B	1605	BTB	C3-C2	2.63	1.57	1.53
4	B	1604	BTB	C3-C2	2.62	1.56	1.53
3	A	600	FPG	C4-C3	2.38	1.58	1.52
4	A	604	BTB	C1-C2	2.12	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	BTB	C3-C2	2.04	1.56	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1600	FPG	F-C2-C1	8.32	121.86	108.18
3	A	600	FPG	F-C2-C1	7.14	119.92	108.18
3	B	1600	FPG	O1-C3-C10	-4.70	86.95	107.58
3	B	1600	FPG	PA-O3A-PB	-3.89	119.46	132.83
3	A	600	FPG	PA-O3A-PB	-3.38	121.22	132.83
4	A	605	BTB	C6-C5-N	2.61	121.79	111.59
4	B	1605	BTB	C6-C5-N	2.47	121.24	111.59
3	A	600	FPG	O1B-PB-O3A	2.13	111.78	104.64
3	A	600	FPG	PA-O1-C3	-2.08	123.80	128.06
3	B	1600	FPG	O1B-PB-O3A	2.07	111.58	104.64
4	B	1604	BTB	C6-C5-N	2.07	119.66	111.59

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	FPG	C1-C2-C3-C10
3	A	600	FPG	C1-C2-C3-C4
3	A	600	FPG	C2-C3-C4-C5
3	B	1600	FPG	C1-C2-C3-C10
3	B	1600	FPG	C1-C2-C3-C4
3	B	1600	FPG	C3-C4-C5-C6
4	A	604	BTB	N-C5-C6-O6
4	A	605	BTB	O1-C1-C2-C4
4	A	605	BTB	O1-C1-C2-N
4	A	605	BTB	C4-C2-C3-O3
4	A	605	BTB	N-C2-C3-O3
4	A	605	BTB	C1-C2-C4-O4
4	A	605	BTB	N-C2-C4-O4
4	A	605	BTB	C6-C5-N-C2
4	B	1604	BTB	O1-C1-C2-C4
4	B	1604	BTB	O1-C1-C2-N
4	B	1604	BTB	C4-C2-C3-O3
4	B	1604	BTB	N-C2-C3-O3
4	B	1604	BTB	C1-C2-C4-O4
4	B	1604	BTB	N-C2-C4-O4
4	B	1604	BTB	C6-C5-N-C2

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Mol	Chain	Res	Type	Atoms
4	B	1604	BTB	C8-C7-N-C5
4	B	1605	BTB	O1-C1-C2-C4
4	B	1605	BTB	O1-C1-C2-N
4	B	1605	BTB	C4-C2-C3-O3
4	B	1605	BTB	N-C2-C3-O3
4	B	1605	BTB	C1-C2-C4-O4
4	B	1605	BTB	N-C2-C4-O4
4	B	1605	BTB	C6-C5-N-C2
4	B	1605	BTB	N-C7-C8-O8
3	A	600	FPG	C4-C5-C6-C7
3	B	1600	FPG	C4-C5-C6-C7
4	A	605	BTB	N-C5-C6-O6
4	A	605	BTB	N-C7-C8-O8
4	B	1604	BTB	N-C7-C8-O8
3	A	600	FPG	C5-C6-C7-C8
3	B	1600	FPG	C5-C6-C7-C8
3	A	600	FPG	O1-C3-C4-C5
4	A	604	BTB	C6-C5-N-C2
4	B	1604	BTB	C4-C2-N-C7
3	B	1600	FPG	PA-O3A-PB-O3B
3	B	1600	FPG	C3-O1-PA-O3A
3	A	600	FPG	C10-C3-C4-C5
3	A	600	FPG	C3-C4-C5-C6

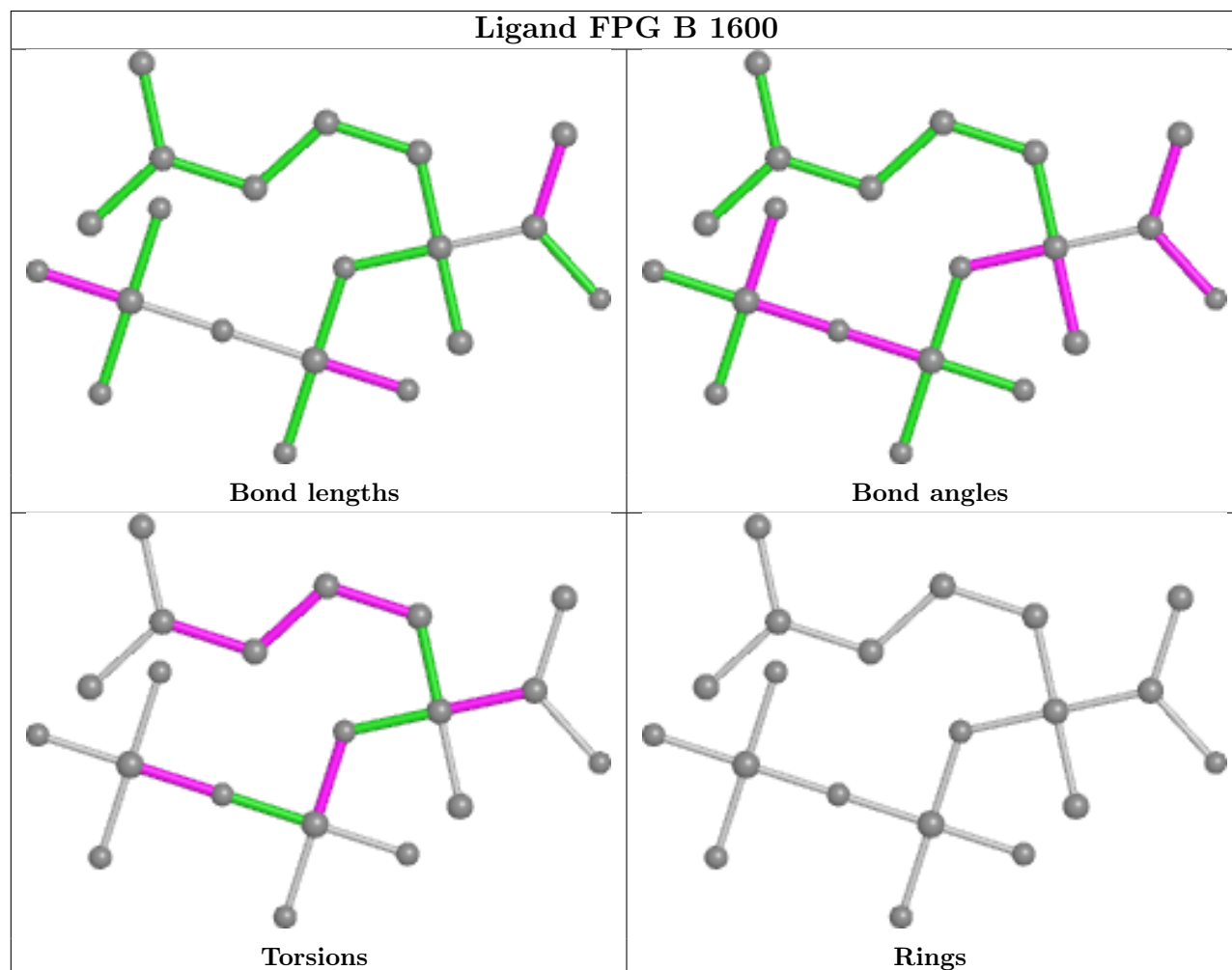
There are no ring outliers.

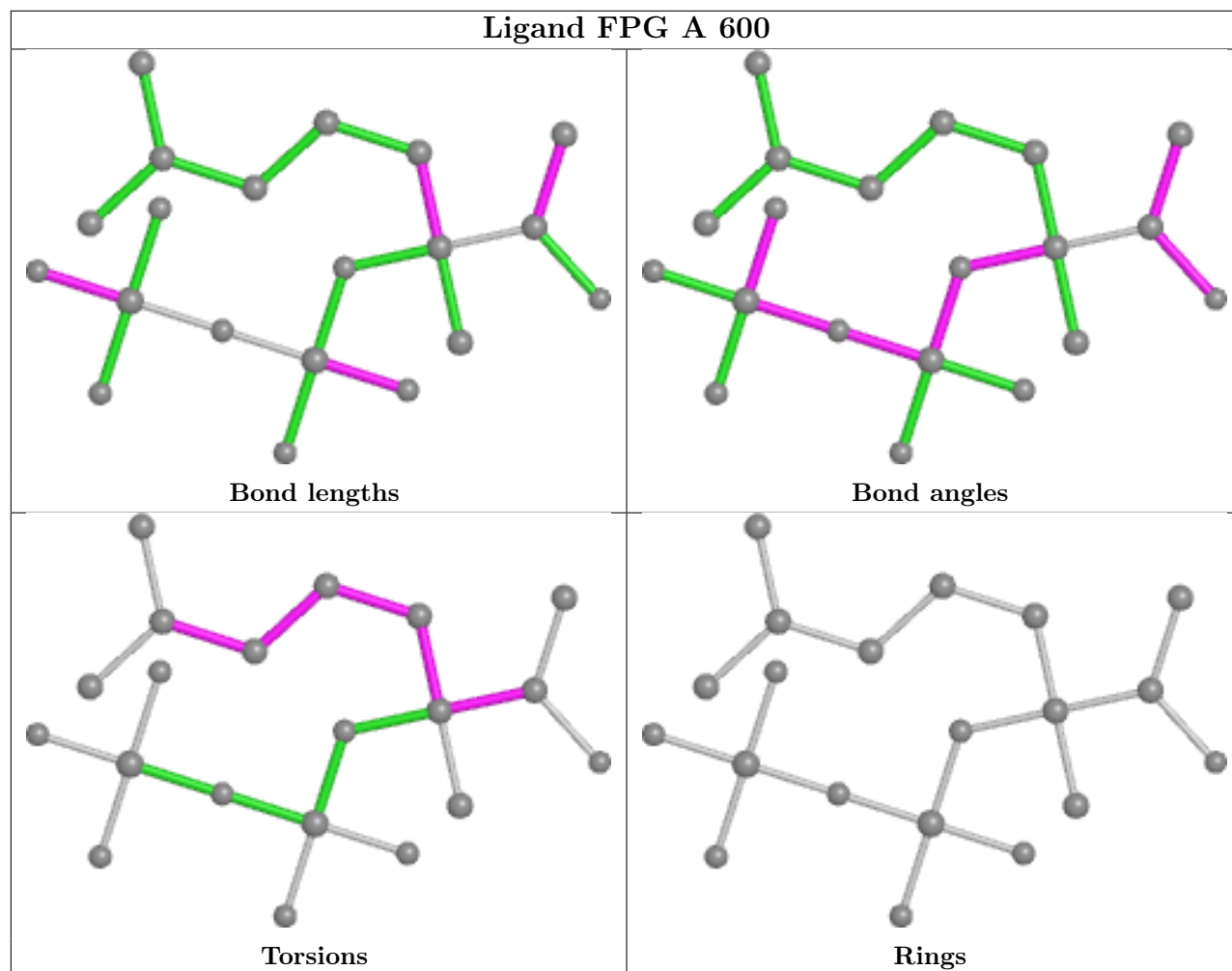
6 monomers are involved in 84 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1604	BTB	19	0
3	B	1600	FPG	13	0
4	B	1605	BTB	21	0
4	A	604	BTB	3	0
3	A	600	FPG	9	0
4	A	605	BTB	19	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%)	0.07	13 (2%) 59 60	18, 46, 94, 100	0
1	B	543/543 (100%)	0.04	6 (1%) 80 82	16, 46, 96, 100	0
All	All	1086/1086 (100%)	0.05	19 (1%) 70 72	16, 46, 95, 100	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	579	HIS	6.5
1	B	579	HIS	6.3
1	B	505	VAL	4.9
1	B	580	GLY	4.3
1	B	504	GLU	4.1
1	A	239	LEU	4.0
1	A	578	GLY	3.7
1	A	505	VAL	3.5
1	A	580	GLY	3.4
1	A	501	SER	3.0
1	A	504	GLU	2.9
1	A	581	THR	2.8
1	B	89	ALA	2.5
1	A	583	HIS	2.3
1	A	163	LEU	2.3
1	A	508	GLY	2.2
1	B	201	TYR	2.1
1	A	244	TYR	2.1
1	A	275	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

There are no monosaccharides in this entry.

6.4 Ligands

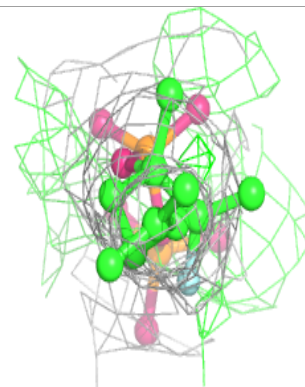
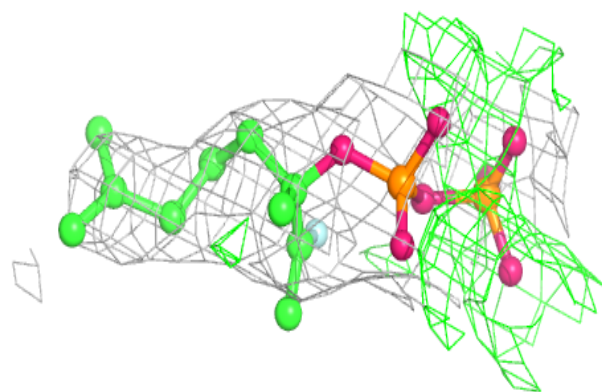
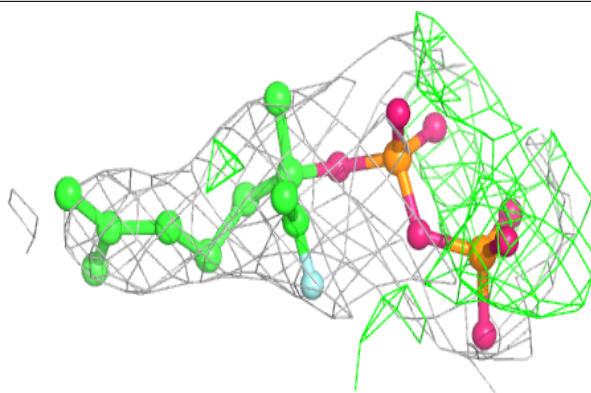
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	BTB	B	1604	14/14	0.66	0.33	67,89,100,100	0
4	BTB	A	604	14/14	0.82	0.50	83,90,96,100	0
4	BTB	A	605	14/14	0.83	0.23	98,100,100,100	0
4	BTB	B	1605	14/14	0.87	0.20	93,100,100,100	0
3	FPG	A	600	20/20	0.97	0.26	54,69,76,82	0
3	FPG	B	1600	20/20	0.97	0.27	44,71,100,100	0
2	MN	A	602	1/1	0.97	0.27	41,41,41,41	0
2	MN	A	601	1/1	0.98	0.26	52,52,52,52	0
2	MN	B	1602	1/1	0.98	0.24	49,49,49,49	0
2	MN	B	1601	1/1	0.99	0.25	52,52,52,52	0
2	MN	B	1603	1/1	0.99	0.25	44,44,44,44	0
2	MN	A	603	1/1	1.00	0.26	43,43,43,43	0

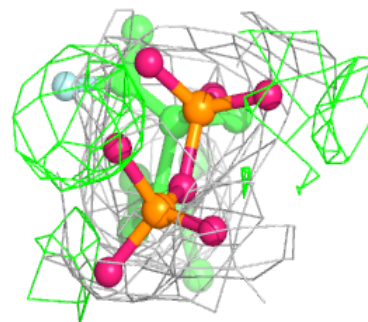
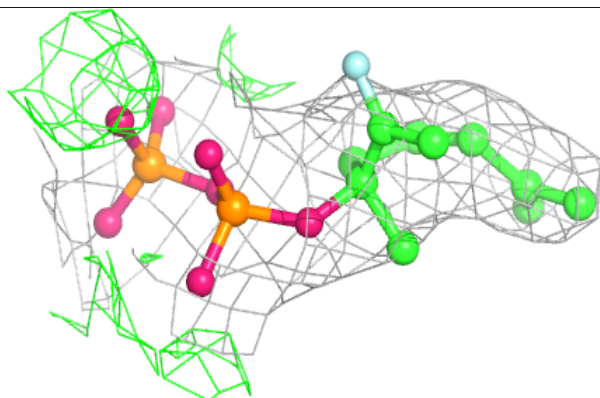
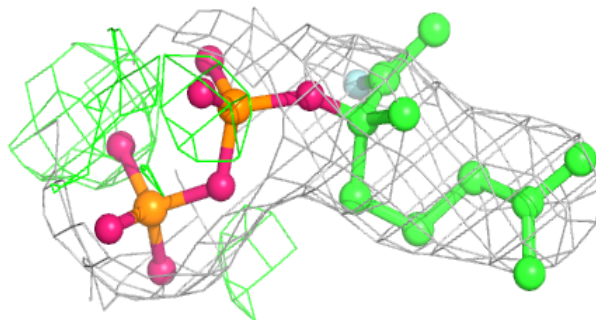
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FPG 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)

**Electron density around FPG B 1600:**

$2mF_o-DF_c$ (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.