



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:43 PM UTC

PDB ID : 8H75 / pdb_00008h75
Title : FGFR2 in complex with YJ001
Authors : Yan, X.E.; Yun, C.H.
Deposited on : 2022-10-19
Resolution : 3.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

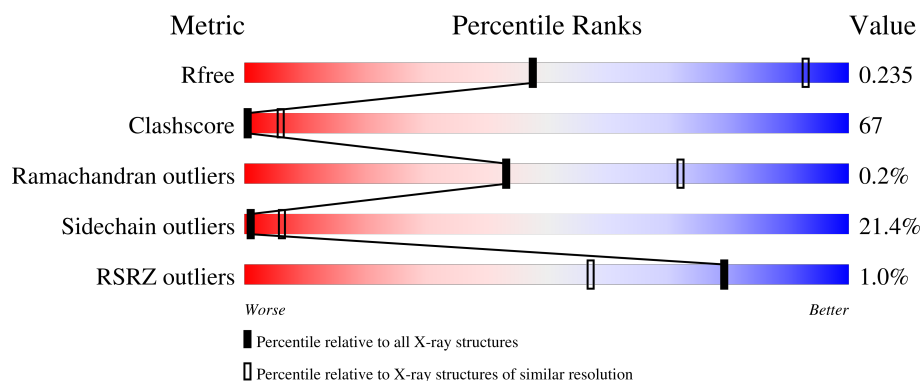
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1029 (3.90-3.62)
Clashscore	190562	1061 (3.90-3.62)
Ramachandran outliers	187476	1014 (3.90-3.62)
Sidechain outliers	187428	1009 (3.90-3.62)
RSRZ outliers	180081	1028 (3.90-3.62)

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	312	
1	B	312	
1	C	312	
1	D	312	

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
1	PTR	A	656	-	-	X	-
3	CL	A	1002	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8793 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.

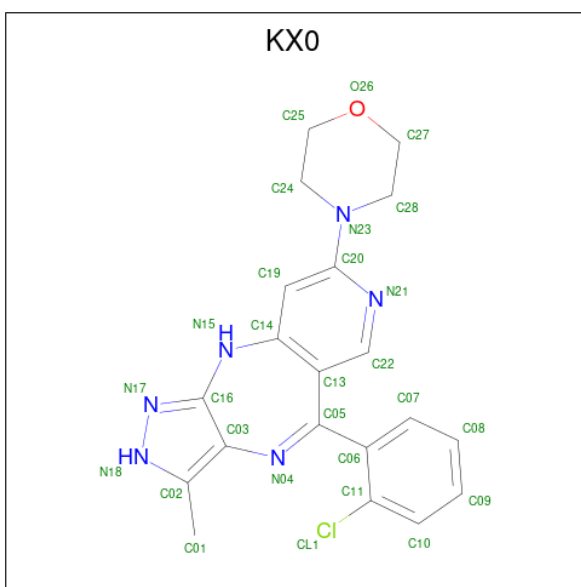
- Molecule 1 is a protein called Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	P	S	0	0	0
			2207	1403	374	410	1	19			
1	B	283	Total	C	N	O	P	S	0	0	0
			2203	1403	371	408	1	20			
1	C	275	Total	C	N	O	P	S	0	0	0
			2087	1326	364	378		19			
1	D	277	Total	C	N	O	P	S	0	0	0
			2157	1378	363	396		20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	457	GLY	-	expression tag	UNP P21802
A	458	HIS	-	expression tag	UNP P21802
B	457	GLY	-	expression tag	UNP P21802
B	458	HIS	-	expression tag	UNP P21802
C	457	GLY	-	expression tag	UNP P21802
C	458	HIS	-	expression tag	UNP P21802
D	457	GLY	-	expression tag	UNP P21802
D	458	HIS	-	expression tag	UNP P21802

- Molecule 2 is Tinengotinib (CCD ID: KX0) (formula: C₂₀H₁₉ClN₆O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			28	20	1	6	1		
2	B	1	Total	C	Cl	N	O	0	0
			28	20	1	6	1		
2	C	1	Total	C	Cl	N	O	0	0
			28	20	1	6	1		
2	D	1	Total	C	Cl	N	O	0	0
			28	20	1	6	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

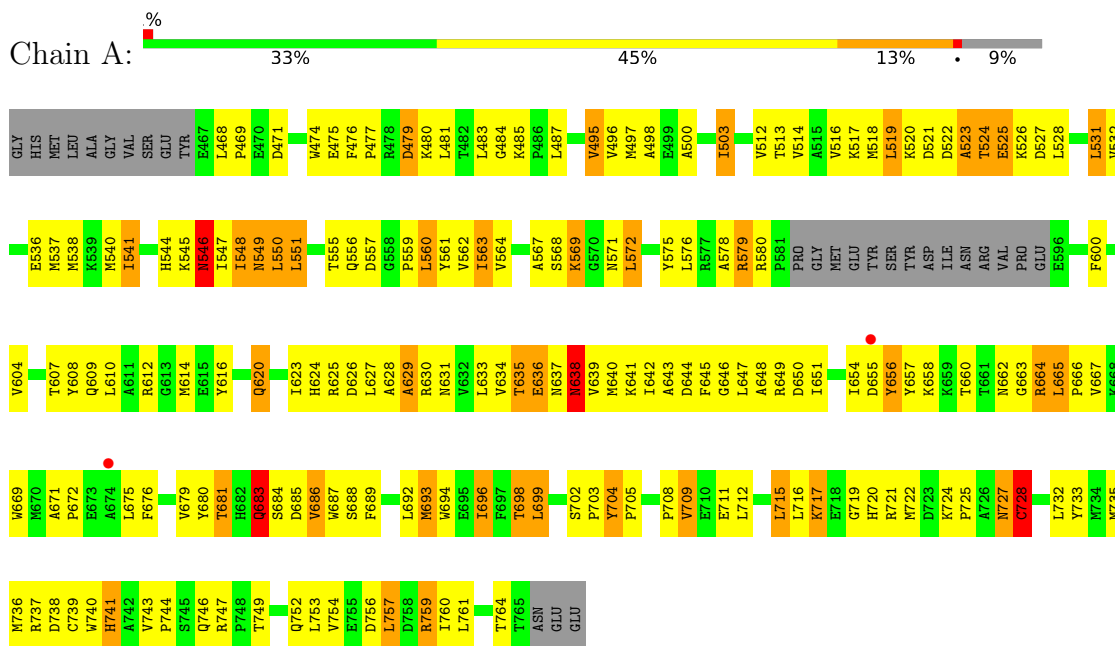
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	6	Total	O	0	0
			6	6		
4	C	6	Total	O	0	0
			6	6		
4	D	10	Total	O	0	0
			10	10		

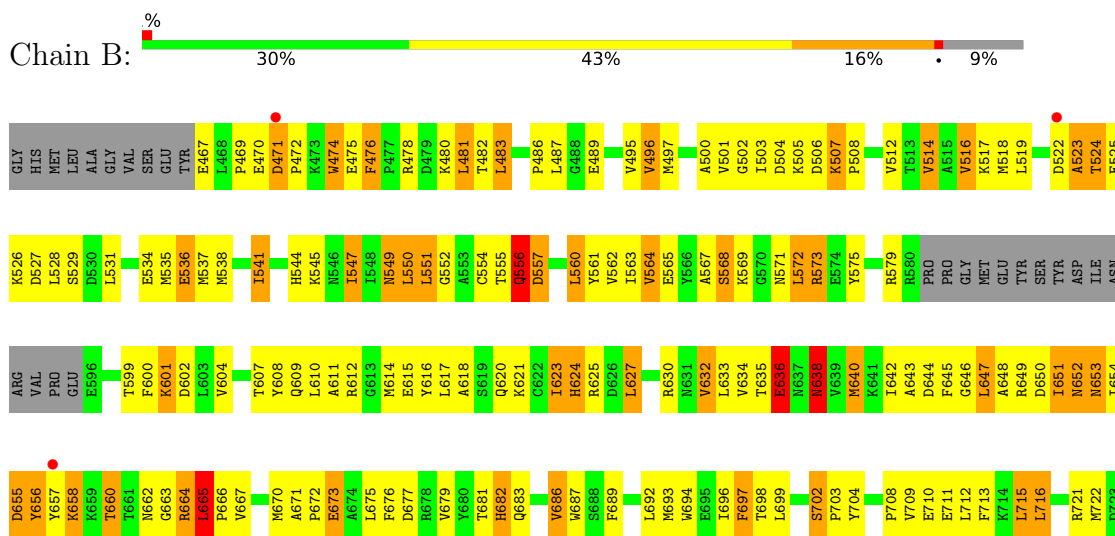
3 Residue-property plots

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: Fibroblast growth factor receptor 2

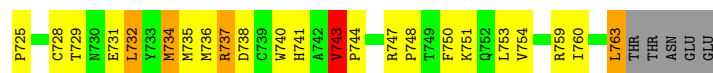
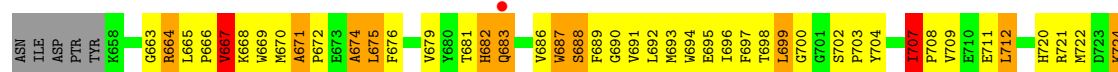
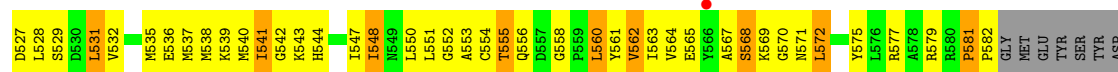


• Molecule 1: Fibroblast growth factor receptor 2

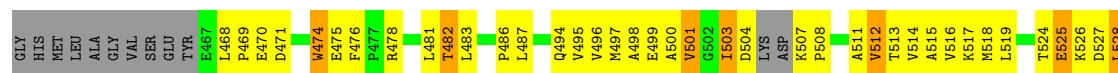




• Molecule 1: Fibroblast growth factor receptor 2



• Molecule 1: Fibroblast growth factor receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.02Å 198.59Å 67.20Å 90.00° 92.94° 90.00°	Depositor
Resolution (Å)	27.80 – 3.75 27.80 – 3.75	Depositor EDS
% Data completeness (in resolution range)	70.6 (27.80-3.75) 90.2 (27.80-3.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 3.76Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.214 , 0.238 0.226 , 0.235	Depositor DCC
R_{free} test set	562 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	53.6	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8793	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: CL, KX0, PTR

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	0.87	0/2235	1.22	31/3028 (1.0%)
1	B	0.92	1/2230 (0.0%)	1.30	31/3015 (1.0%)
1	C	0.84	0/2126	1.32	41/2878 (1.4%)
1	D	0.87	0/2200	1.19	22/2973 (0.7%)
All	All	0.88	1/8791 (0.0%)	1.26	125/11894 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	632	VAL	C-O	-5.24	1.18	1.24

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	652	ASN	N-CA-C	10.21	122.41	111.28
1	C	568	SER	N-CA-C	9.92	122.17	111.36
1	C	556	GLN	N-CA-C	9.91	122.08	111.28
1	D	651	ILE	N-CA-C	9.18	119.99	110.72
1	C	555	THR	N-CA-C	8.86	123.05	108.08
1	B	638	ASN	N-CA-C	8.84	123.89	111.52
1	B	502	GLY	N-CA-C	8.63	123.09	112.73
1	A	572	LEU	N-CA-C	8.58	120.63	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	638	ASN	N-CA-C	8.42	123.10	111.74
1	C	664	ARG	N-CA-C	8.21	122.12	112.93
1	C	676	PHE	N-CA-C	8.11	119.90	111.14
1	A	485	LYS	CA-C-N	8.02	128.04	119.78
1	A	485	LYS	C-N-CA	8.02	128.04	119.78
1	C	743	VAL	CA-C-N	7.94	127.87	119.05
1	C	743	VAL	C-N-CA	7.94	127.87	119.05
1	B	664	ARG	N-CA-C	7.89	119.88	111.28
1	A	638	ASN	N-CA-C	7.66	122.08	111.74
1	D	638	ASN	N-CA-C	7.63	122.04	111.74
1	C	474	TRP	N-CA-C	7.63	119.67	111.36
1	A	579	ARG	N-CA-C	7.48	122.13	112.26
1	C	507	LYS	CA-C-N	7.25	127.09	119.05
1	C	507	LYS	C-N-CA	7.25	127.09	119.05
1	B	471	ASP	CA-C-N	-7.17	111.09	119.05
1	B	471	ASP	C-N-CA	-7.17	111.09	119.05
1	D	624	HIS	N-CA-C	7.17	118.88	111.14
1	D	726	ALA	N-CA-C	7.16	118.73	111.07
1	A	728	CYS	N-CA-C	7.14	120.58	110.23
1	B	697	PHE	N-CA-C	7.00	118.99	111.36
1	C	555	THR	CB-CA-C	-6.97	108.54	116.63
1	D	724	LYS	CA-C-N	6.95	126.87	119.85
1	D	724	LYS	C-N-CA	6.95	126.87	119.85
1	D	641	LYS	N-CA-C	6.94	119.72	108.34
1	D	568	SER	N-CA-C	6.86	119.63	111.33
1	C	624	HIS	N-CA-C	6.81	118.70	111.28
1	D	507	LYS	CA-C-N	6.80	126.95	119.87
1	D	507	LYS	C-N-CA	6.80	126.95	119.87
1	C	702	SER	CA-C-N	6.77	126.69	119.85
1	C	702	SER	C-N-CA	6.77	126.69	119.85
1	C	674	ALA	N-CA-C	6.76	118.73	111.36
1	B	643	ALA	N-CA-C	6.75	117.18	108.34
1	C	646	GLY	N-CA-C	6.52	120.56	112.73
1	C	492	PHE	N-CA-C	6.51	118.17	111.14
1	D	658	LYS	N-CA-C	6.43	119.11	108.49
1	B	665	LEU	N-CA-C	6.42	118.57	108.55
1	C	581	PRO	N-CA-C	6.42	118.53	110.70
1	D	546	ASN	N-CA-C	6.41	119.22	111.40
1	B	522	ASP	N-CA-C	-6.40	100.36	109.96
1	A	746	GLN	N-CA-C	6.26	119.39	111.69
1	A	541	ILE	N-CA-C	6.23	116.97	110.62
1	C	614	MET	N-CA-C	-6.23	104.49	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	658	LYS	N-CA-C	6.22	120.35	110.70
1	B	636	GLU	N-CA-C	-6.21	100.64	109.96
1	A	471	ASP	N-CA-C	-6.15	98.87	109.15
1	A	636	GLU	N-CA-C	-6.04	101.47	110.23
1	C	712	LEU	N-CA-C	6.01	117.83	111.28
1	A	522	ASP	N-CA-C	-5.96	99.02	108.73
1	B	660	THR	N-CA-C	5.94	118.84	110.23
1	A	635	THR	N-CA-C	5.87	118.11	110.53
1	B	541	ILE	N-CA-C	5.86	116.60	110.62
1	C	688	SER	N-CA-C	-5.83	104.93	111.28
1	A	569	LYS	N-CA-C	5.81	117.69	111.36
1	C	558	GLY	CA-C-N	5.79	125.70	119.85
1	C	558	GLY	C-N-CA	5.79	125.70	119.85
1	A	471	ASP	CA-C-N	5.79	125.47	119.05
1	A	471	ASP	C-N-CA	5.79	125.47	119.05
1	D	727	ASN	N-CA-C	5.76	117.64	111.36
1	A	683	GLN	N-CA-C	-5.76	105.09	111.71
1	A	665	LEU	CA-C-N	-5.75	114.01	119.76
1	A	665	LEU	C-N-CA	-5.75	114.01	119.76
1	A	704	TYR	CA-C-N	5.72	125.66	119.76
1	A	704	TYR	C-N-CA	5.72	125.66	119.76
1	C	471	ASP	CA-C-N	5.72	125.40	119.05
1	C	471	ASP	C-N-CA	5.72	125.40	119.05
1	B	516	VAL	CB-CA-C	-5.71	103.07	110.84
1	C	554	CYS	N-CA-C	5.71	117.50	111.28
1	C	618	ALA	N-CA-C	-5.69	102.48	110.50
1	D	719	GLY	N-CA-C	5.66	124.27	115.72
1	C	541	ILE	N-CA-C	5.64	118.10	111.05
1	B	523	ALA	N-CA-C	5.61	117.79	108.99
1	C	643	ALA	N-CA-C	5.61	115.68	108.34
1	A	604	VAL	CB-CA-C	-5.60	104.49	112.22
1	B	556	GLN	N-CA-C	5.60	117.39	111.28
1	B	552	GLY	N-CA-C	5.60	121.52	110.83
1	C	707	ILE	CA-C-N	5.59	125.50	119.85
1	C	707	ILE	C-N-CA	5.59	125.50	119.85
1	C	645	PHE	N-CA-C	5.59	121.09	113.37
1	A	688	SER	N-CA-C	-5.56	105.30	111.36
1	B	557	ASP	N-CA-C	5.56	118.28	109.50
1	D	702	SER	CA-C-N	5.55	125.75	120.31
1	D	702	SER	C-N-CA	5.55	125.75	120.31
1	C	667	VAL	N-CA-C	5.54	116.32	110.72
1	A	546	ASN	N-CA-C	5.51	119.99	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	714	LYS	N-CA-C	5.50	117.27	111.28
1	B	551	LEU	N-CA-C	5.49	117.26	111.28
1	A	709	VAL	CB-CA-C	-5.46	104.77	112.14
1	B	704	TYR	CA-C-N	-5.46	114.34	119.85
1	B	704	TYR	C-N-CA	-5.46	114.34	119.85
1	A	629	ALA	N-CA-C	5.45	117.22	111.28
1	A	702	SER	CA-C-N	5.44	125.34	119.85
1	A	702	SER	C-N-CA	5.44	125.34	119.85
1	C	671	ALA	CA-C-N	5.43	125.08	119.05
1	C	671	ALA	C-N-CA	5.43	125.08	119.05
1	D	643	ALA	N-CA-C	5.42	115.27	108.45
1	B	702	SER	CA-C-N	-5.40	114.77	120.66
1	B	702	SER	C-N-CA	-5.40	114.77	120.66
1	D	569	LYS	N-CA-C	5.36	119.80	113.16
1	B	640	MET	N-CA-C	5.34	117.92	109.96
1	B	474	TRP	N-CA-C	5.31	117.15	111.36
1	B	505	LYS	N-CA-C	-5.28	105.52	111.28
1	C	513	THR	N-CA-C	5.24	118.04	110.28
1	C	483	LEU	N-CA-C	5.23	116.98	111.28
1	B	572	LEU	N-CA-C	5.21	116.96	111.28
1	D	747	ARG	CA-C-N	5.21	125.13	119.76
1	D	747	ARG	C-N-CA	5.21	125.13	119.76
1	B	677	ASP	CA-C-N	5.20	131.94	123.93
1	B	677	ASP	C-N-CA	5.20	131.94	123.93
1	A	483	LEU	N-CA-C	5.17	117.38	110.35
1	A	764	THR	N-CA-C	5.13	116.87	111.28
1	C	485	LYS	CA-C-N	5.09	125.00	119.76
1	C	485	LYS	C-N-CA	5.09	125.00	119.76
1	A	551	LEU	N-CA-C	-5.07	107.16	113.55
1	B	632	VAL	N-CA-C	-5.07	100.59	107.99
1	D	474	TRP	N-CA-C	5.07	116.88	111.36
1	A	523	ALA	N-CA-C	5.05	116.65	108.41
1	C	540	MET	N-CA-C	5.02	117.64	111.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	656	PTR	Mainchain

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	2207	0	2142	306	0
1	B	2203	0	2155	319	0
1	C	2087	0	2045	296	0
1	D	2157	0	2121	280	0
2	A	28	0	0	4	0
2	B	28	0	0	2	0
2	C	28	0	0	2	0
2	D	28	0	0	2	0
3	A	1	0	0	6	0
4	A	4	0	0	0	0
4	B	6	0	0	1	0
4	C	6	0	0	0	0
4	D	10	0	0	0	0
All	All	8793	0	8463	1160	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 67.

All (1160) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:606:CYS:SG	1:D:640:MET:HE2	1.46	1.55
1:B:686:VAL:HG12	1:B:750:PHE:CE1	1.55	1.39
1:D:474:TRP:CD1	1:D:539:LYS:HE2	1.57	1.39
1:C:667:VAL:HG21	1:C:709:VAL:CG1	1.54	1.34
1:A:735:MET:HE1	1:A:757:LEU:CD2	1.65	1.27
1:C:469:PRO:HD3	1:D:469:PRO:CB	1.66	1.25
3:A:1002:CL:CL	1:B:744:PRO:HG2	1.73	1.25
1:A:744:PRO:HG2	3:A:1002:CL:CL	1.73	1.24
1:B:568:SER:OG	1:B:636:GLU:HB2	1.38	1.23
1:D:621:LYS:HE3	1:D:651:ILE:CG2	1.68	1.22
1:C:667:VAL:CG2	1:C:709:VAL:HG13	1.71	1.21
1:D:487:LEU:CD2	1:D:497:MET:HB2	1.72	1.20
1:B:610:LEU:HD21	1:B:632:VAL:CG1	1.72	1.19
1:B:634:VAL:HG22	1:B:640:MET:CE	1.73	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:LYS:CG	1:C:501:VAL:HG22	1.74	1.18
1:C:469:PRO:CD	1:D:469:PRO:HB2	1.72	1.18
1:B:624:HIS:O	1:B:648:ALA:HB2	1.44	1.17
1:B:634:VAL:HG22	1:B:640:MET:HE1	1.22	1.17
1:B:537:MET:HA	1:B:537:MET:HE3	1.27	1.17
1:D:667:VAL:HG21	1:D:709:VAL:CG1	1.74	1.16
1:C:694:TRP:NE1	1:C:725:PRO:HG3	1.61	1.14
1:B:524:THR:HG22	1:D:664:ARG:HA	1.14	1.14
1:B:623:ILE:O	1:B:648:ALA:HB1	1.46	1.14
1:D:474:TRP:CD1	1:D:539:LYS:CE	2.31	1.14
1:D:667:VAL:HG21	1:D:709:VAL:HG11	1.21	1.13
1:B:623:ILE:HG12	1:B:651:ILE:HD11	1.14	1.13
1:C:686:VAL:HG21	1:C:747:ARG:HB3	1.21	1.12
1:D:478:ARG:CB	1:D:556:GLN:HE21	1.62	1.12
1:D:621:LYS:HE3	1:D:651:ILE:HG21	1.16	1.11
1:B:524:THR:CG2	1:D:664:ARG:HA	1.81	1.10
1:A:704:TYR:CE1	1:A:722:MET:HE3	1.86	1.10
1:B:610:LEU:HD21	1:B:632:VAL:HG11	1.34	1.10
1:B:623:ILE:HG13	1:B:651:ILE:HG13	1.33	1.10
1:C:581:PRO:CG	1:C:582:PRO:HD3	1.81	1.10
1:A:704:TYR:CD1	1:A:722:MET:CE	2.35	1.10
1:D:606:CYS:SG	1:D:640:MET:CE	2.40	1.09
1:C:480:LYS:HG3	1:C:501:VAL:CG2	1.81	1.09
1:B:686:VAL:HG12	1:B:750:PHE:CD1	1.88	1.09
1:D:621:LYS:CE	1:D:651:ILE:HG22	1.83	1.09
1:D:610:LEU:CD1	1:D:692:LEU:HD21	1.84	1.08
1:D:474:TRP:NE1	1:D:539:LYS:HG2	1.67	1.08
1:A:735:MET:HE1	1:A:757:LEU:HD23	1.14	1.08
1:D:487:LEU:HD21	1:D:497:MET:CB	1.83	1.07
1:B:601:LYS:HD3	1:B:761:LEU:CD1	1.84	1.07
1:D:634:VAL:HG23	1:D:640:MET:SD	1.94	1.07
1:A:709:VAL:HG11	1:C:523:ALA:HB3	1.37	1.07
1:D:575:TYR:HE1	1:D:579:ARG:CZ	1.66	1.07
1:D:621:LYS:CE	1:D:651:ILE:CG2	2.32	1.07
1:C:581:PRO:HG2	1:C:582:PRO:HD3	1.08	1.06
1:D:683:GLN:O	1:D:686:VAL:HG13	1.56	1.06
1:B:634:VAL:CG2	1:B:640:MET:HE1	1.86	1.05
1:D:534:GLU:HB2	1:D:646:GLY:HA2	1.07	1.05
1:D:572:LEU:HD13	1:D:640:MET:HE3	1.39	1.05
1:D:760:ILE:O	1:D:764:THR:HG23	1.56	1.05
1:B:735:MET:HE3	1:B:753:LEU:HD22	1.33	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:PTR:HD2	1:B:743:VAL:HG23	1.35	1.04
1:C:667:VAL:HG21	1:C:709:VAL:HG13	1.08	1.03
1:D:534:GLU:HB2	1:D:646:GLY:CA	1.89	1.03
1:C:672:PRO:HD3	1:C:687:TRP:CD1	1.93	1.03
1:D:495:VAL:HG12	1:D:517:LYS:CA	1.89	1.03
1:D:732:LEU:HD21	1:D:760:ILE:CD1	1.87	1.02
1:C:544:HIS:CD2	1:C:616:TYR:CB	2.42	1.02
1:D:610:LEU:HD12	1:D:692:LEU:HD21	1.38	1.02
1:A:704:TYR:CD1	1:A:722:MET:HE3	1.93	1.01
1:A:650:ASP:O	1:A:651:ILE:HD13	1.60	1.01
1:B:475:GLU:CD	1:B:556:GLN:HG2	1.86	1.01
1:D:575:TYR:HE1	1:D:579:ARG:NH1	1.57	1.01
1:C:581:PRO:HG2	1:C:582:PRO:CD	1.91	1.01
1:D:500:ALA:CB	1:D:503:ILE:HD11	1.91	1.01
1:B:662:ASN:O	1:D:525:GLU:HB3	1.59	1.00
1:B:752:GLN:HB3	4:B:1101:HOH:O	1.57	1.00
1:C:535:MET:HG3	1:C:562:VAL:CG2	1.91	1.00
1:D:526:LYS:HE3	1:D:664:ARG:HD2	1.43	1.00
1:D:495:VAL:HG12	1:D:517:LYS:HA	1.02	1.00
1:D:704:TYR:CD1	1:D:722:MET:SD	2.54	1.00
1:B:624:HIS:C	1:B:648:ALA:HB2	1.86	1.00
1:C:686:VAL:HG21	1:C:747:ARG:CB	1.92	0.99
1:B:686:VAL:CG1	1:B:750:PHE:CE1	2.46	0.99
1:B:623:ILE:HG12	1:B:651:ILE:CD1	1.91	0.99
1:D:575:TYR:CE1	1:D:579:ARG:CZ	2.45	0.99
1:A:709:VAL:HG11	1:C:523:ALA:CB	1.92	0.99
1:C:667:VAL:CG2	1:C:709:VAL:CG1	2.34	0.99
1:B:623:ILE:HG13	1:B:651:ILE:CG1	1.91	0.98
1:A:735:MET:SD	1:A:757:LEU:HD21	2.04	0.98
1:C:480:LYS:CG	1:C:501:VAL:CG2	2.40	0.98
1:B:476:PHE:HE2	1:B:503:ILE:CG1	1.76	0.98
1:C:664:ARG:H	1:C:664:ARG:HD3	1.27	0.97
1:C:480:LYS:HG3	1:C:501:VAL:HG22	0.97	0.97
1:A:744:PRO:CG	3:A:1002:CL:CL	2.50	0.96
1:D:673:GLU:CG	1:D:747:ARG:HH22	1.76	0.96
1:C:704:TYR:H	1:C:722:MET:HE2	1.29	0.96
1:B:556:GLN:HE21	1:B:556:GLN:HA	1.30	0.96
1:B:476:PHE:HE2	1:B:503:ILE:HG13	1.30	0.95
1:B:710:GLU:OE2	1:D:519:LEU:HD12	1.64	0.95
1:D:683:GLN:OE1	1:D:747:ARG:HB2	1.65	0.95
1:C:694:TRP:CD1	1:C:725:PRO:CG	2.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:VAL:O	1:A:536:GLU:HG2	1.67	0.94
1:A:735:MET:CE	1:A:757:LEU:CD2	2.44	0.94
1:B:569:LYS:HE3	1:B:638:ASN:OD1	1.67	0.94
1:C:480:LYS:HD2	1:C:501:VAL:HG21	1.48	0.94
1:B:614:MET:SD	1:B:627:LEU:CD2	2.56	0.93
1:C:469:PRO:HD3	1:D:469:PRO:HB2	0.95	0.93
1:B:601:LYS:HE3	1:B:764:THR:C	1.94	0.93
1:B:667:VAL:HG13	1:B:675:LEU:HD21	1.50	0.93
1:A:495:VAL:HG23	1:A:517:LYS:HG2	1.47	0.93
1:D:534:GLU:CB	1:D:646:GLY:HA2	1.98	0.93
1:D:732:LEU:HD21	1:D:760:ILE:HD13	1.48	0.93
1:C:694:TRP:NE1	1:C:725:PRO:CG	2.31	0.93
1:D:495:VAL:CG1	1:D:517:LYS:HG2	1.97	0.93
1:A:571:ASN:HD22	2:A:1001:KX0:C08	1.81	0.93
1:A:628:ALA:CB	1:A:630:ARG:HH12	1.80	0.93
1:C:480:LYS:HD2	1:C:501:VAL:CG2	1.99	0.92
1:A:651:ILE:HG23	1:A:654:ILE:O	1.68	0.92
1:D:621:LYS:HE2	1:D:651:ILE:HG22	1.49	0.92
1:B:519:LEU:HD21	1:B:528:LEU:HA	1.52	0.92
1:A:572:LEU:HD21	1:A:696:ILE:HD11	1.51	0.92
1:C:686:VAL:CG2	1:C:747:ARG:HD3	1.98	0.91
1:A:735:MET:CE	1:A:757:LEU:HD23	1.99	0.91
1:B:623:ILE:CG1	1:B:651:ILE:HD11	1.99	0.91
1:C:486:PRO:HA	1:C:496:VAL:HG12	1.53	0.91
1:B:475:GLU:CD	1:B:556:GLN:CG	2.43	0.91
1:A:572:LEU:HD21	1:A:696:ILE:CD1	2.00	0.91
1:B:663:GLY:CA	1:D:526:LYS:HB2	2.01	0.90
1:A:572:LEU:CD2	1:A:696:ILE:HD11	2.01	0.90
1:D:541:ILE:CG2	1:D:616:TYR:HE2	1.83	0.90
1:B:535:MET:HE1	1:B:560:LEU:HD21	1.50	0.90
1:D:495:VAL:CG1	1:D:517:LYS:HA	1.97	0.90
1:B:544:HIS:HD2	1:B:616:TYR:CG	1.88	0.90
1:A:575:TYR:HE1	1:A:579:ARG:NE	1.69	0.89
1:B:610:LEU:CD2	1:B:632:VAL:CG1	2.51	0.89
1:C:683:GLN:HE21	1:C:683:GLN:HA	1.38	0.89
1:B:470:GLU:HB3	1:B:556:GLN:OE1	1.72	0.89
1:C:672:PRO:CD	1:C:687:TRP:CD1	2.56	0.89
1:B:610:LEU:CD2	1:B:632:VAL:HG11	2.03	0.89
1:C:687:TRP:HH2	1:C:704:TYR:HH	0.95	0.88
1:A:624:HIS:HA	1:A:648:ALA:HB2	1.53	0.88
1:D:541:ILE:HG22	1:D:616:TYR:HE2	1.39	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:LYS:HB2	1:B:601:LYS:NZ	1.84	0.88
1:B:575:TYR:HD2	1:B:634:VAL:HG21	1.39	0.88
1:A:698:THR:HG22	1:A:725:PRO:HB3	1.55	0.88
1:B:525:GLU:CB	1:D:663:GLY:HA2	2.04	0.88
1:B:535:MET:CE	1:B:560:LEU:HD21	2.03	0.88
1:A:524:THR:HG22	1:A:527:ASP:H	1.36	0.87
1:D:715:LEU:HB3	1:D:720:HIS:HB3	1.54	0.87
1:D:637:ASN:O	1:D:637:ASN:ND2	2.07	0.87
1:A:631:ASN:O	1:A:643:ALA:HB3	1.75	0.87
1:A:704:TYR:HD1	1:A:722:MET:CE	1.85	0.87
1:C:614:MET:HE3	1:C:614:MET:HA	1.55	0.87
1:D:500:ALA:HB1	1:D:503:ILE:HD11	1.57	0.87
1:B:524:THR:HG22	1:D:664:ARG:CA	2.03	0.87
1:C:569:LYS:HB2	1:C:634:VAL:HG11	1.55	0.86
1:A:497:MET:HE3	1:A:513:THR:HG21	1.55	0.86
1:D:683:GLN:HA	1:D:686:VAL:CG1	2.05	0.86
1:A:497:MET:HE3	1:A:513:THR:CG2	2.04	0.86
1:C:535:MET:HG3	1:C:562:VAL:HG21	1.57	0.86
1:A:575:TYR:CD2	1:A:634:VAL:HG11	2.10	0.86
1:D:724:LYS:NZ	1:D:724:LYS:O	2.08	0.86
1:B:554:CYS:HB2	1:B:561:TYR:HB2	1.57	0.86
1:B:686:VAL:HG12	1:B:750:PHE:HE1	1.39	0.86
1:C:507:LYS:N	1:C:508:PRO:HD3	1.89	0.86
1:A:560:LEU:HD21	1:A:562:VAL:HG23	1.57	0.85
1:C:575:TYR:HE1	1:C:579:ARG:CZ	1.89	0.85
1:B:573:ARG:HG2	1:B:573:ARG:HH21	1.39	0.85
1:B:663:GLY:HA3	1:D:526:LYS:HB2	1.55	0.85
1:B:575:TYR:CD2	1:B:634:VAL:HG21	2.10	0.85
1:C:548:ILE:HG13	1:C:565:GLU:HG3	1.58	0.85
1:D:495:VAL:HG11	1:D:517:LYS:HG2	1.57	0.84
1:A:614:MET:HE3	1:A:614:MET:HA	1.57	0.84
1:A:531:LEU:HD12	1:A:531:LEU:O	1.76	0.84
1:D:481:LEU:HD12	1:D:500:ALA:HB2	1.60	0.83
1:B:601:LYS:CD	1:B:761:LEU:HD11	2.07	0.83
1:D:673:GLU:HG3	1:D:747:ARG:HH22	1.42	0.83
1:B:560:LEU:HD11	1:B:562:VAL:HG23	1.60	0.83
1:D:635:THR:HG23	1:D:641:LYS:HG3	1.60	0.83
1:D:474:TRP:HD1	1:D:539:LYS:HE2	1.07	0.83
1:B:483:LEU:H	1:B:483:LEU:HD13	1.42	0.83
1:D:531:LEU:O	1:D:531:LEU:HD22	1.78	0.83
1:A:628:ALA:CB	1:A:630:ARG:NH1	2.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:ILE:CG1	1:B:651:ILE:CG1	2.57	0.82
3:A:1002:CL:CL	1:B:744:PRO:CG	2.62	0.82
1:D:487:LEU:HD21	1:D:497:MET:HB2	0.87	0.82
1:B:549:ASN:ND2	1:B:565:GLU:CB	2.43	0.82
1:B:617:LEU:HD12	1:B:617:LEU:O	1.79	0.82
1:C:737:ARG:HH21	1:C:737:ARG:HG3	1.42	0.82
1:D:478:ARG:CB	1:D:556:GLN:NE2	2.43	0.82
1:C:686:VAL:HG23	1:C:747:ARG:HD3	1.60	0.82
1:B:480:LYS:HG3	1:B:501:VAL:HB	1.60	0.82
1:C:535:MET:HG3	1:C:562:VAL:HG22	1.60	0.82
1:C:480:LYS:CD	1:C:501:VAL:CG2	2.58	0.82
1:C:694:TRP:CD1	1:C:725:PRO:HG3	2.11	0.82
1:D:692:LEU:HD12	1:D:692:LEU:O	1.80	0.81
1:C:575:TYR:CE1	1:C:579:ARG:HD2	2.15	0.81
1:C:603:LEU:HD21	1:C:699:LEU:CD1	2.10	0.81
1:D:474:TRP:HE1	1:D:539:LYS:HG2	1.45	0.81
1:A:664:ARG:HA	1:C:524:THR:CG2	2.11	0.81
1:D:568:SER:HB2	1:D:636:GLU:HG2	1.61	0.81
1:A:704:TYR:H	1:A:722:MET:CE	1.94	0.81
1:B:601:LYS:CD	1:B:761:LEU:CD1	2.59	0.81
1:B:735:MET:CE	1:B:753:LEU:HD22	2.09	0.81
1:C:575:TYR:HE1	1:C:579:ARG:NE	1.79	0.81
1:A:761:LEU:HD12	1:A:761:LEU:O	1.81	0.81
1:D:631:ASN:O	1:D:643:ALA:HB3	1.79	0.81
1:D:732:LEU:CD2	1:D:760:ILE:CD1	2.58	0.81
1:A:475:GLU:OE2	1:A:556:GLN:HG3	1.81	0.80
1:A:663:GLY:C	1:A:664:ARG:HD3	2.05	0.80
1:D:635:THR:CG2	1:D:641:LYS:HG3	2.12	0.80
1:C:694:TRP:CD2	1:C:722:MET:SD	2.75	0.80
1:C:743:VAL:HG12	1:C:744:PRO:HD2	1.62	0.80
1:D:704:TYR:HD1	1:D:722:MET:SD	2.00	0.80
1:C:569:LYS:HB2	1:C:634:VAL:CG1	2.12	0.80
1:A:607:THR:HG22	1:A:757:LEU:CD1	2.12	0.80
1:B:476:PHE:CE2	1:B:503:ILE:CG1	2.64	0.79
1:B:610:LEU:HD21	1:B:632:VAL:HG13	1.60	0.79
1:C:478:ARG:CZ	1:C:561:TYR:OH	2.31	0.79
1:B:476:PHE:CE2	1:B:503:ILE:HG13	2.18	0.79
1:D:474:TRP:CE2	1:D:539:LYS:HG2	2.17	0.79
1:B:537:MET:HE3	1:B:537:MET:CA	2.10	0.78
1:B:544:HIS:HD2	1:B:616:TYR:CD2	2.02	0.78
1:C:537:MET:HE3	1:C:537:MET:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:LEU:HD11	1:B:632:VAL:HG11	1.63	0.78
1:C:474:TRP:NE1	1:C:539:LYS:HG2	1.98	0.78
1:B:523:ALA:O	1:D:666:PRO:HA	1.83	0.78
1:C:720:HIS:O	1:C:721:ARG:NH1	2.17	0.78
1:A:623:ILE:O	1:A:648:ALA:HB1	1.84	0.77
1:A:664:ARG:HD3	1:A:664:ARG:N	1.98	0.77
1:B:531:LEU:HD11	1:B:560:LEU:HD11	1.65	0.77
1:B:537:MET:HA	1:B:537:MET:CE	2.11	0.77
1:A:692:LEU:HD12	1:A:692:LEU:O	1.84	0.77
1:B:712:LEU:HD12	1:B:712:LEU:O	1.84	0.77
1:A:656:PTR:HD2	1:B:743:VAL:CG2	2.15	0.77
1:A:717:LYS:O	1:B:658:LYS:HD3	1.85	0.77
1:B:623:ILE:CG1	1:B:651:ILE:CD1	2.61	0.77
1:A:495:VAL:CG2	1:A:517:LYS:HG2	2.14	0.76
1:A:698:THR:HG22	1:A:725:PRO:CB	2.14	0.76
1:C:763:LEU:HD13	1:C:763:LEU:O	1.86	0.76
1:D:667:VAL:CG2	1:D:709:VAL:CG1	2.61	0.76
1:A:479:ASP:N	1:A:479:ASP:OD1	2.19	0.76
1:B:573:ARG:HG2	1:B:573:ARG:NH2	1.98	0.76
1:C:732:LEU:HD22	1:C:732:LEU:H	1.51	0.76
1:B:623:ILE:CG1	1:B:651:ILE:HG13	2.13	0.76
1:D:610:LEU:HD13	1:D:692:LEU:HD21	1.68	0.76
1:B:662:ASN:CB	1:D:525:GLU:HG2	2.15	0.76
1:D:683:GLN:O	1:D:686:VAL:CG1	2.32	0.76
1:D:704:TYR:CE1	1:D:722:MET:SD	2.79	0.76
1:B:544:HIS:CD2	1:B:616:TYR:CB	2.68	0.76
1:C:552:GLY:O	1:C:563:ILE:HB	1.84	0.76
3:A:1002:CL:CL	1:B:745:SER:OG	2.42	0.75
1:C:664:ARG:H	1:C:664:ARG:CD	1.99	0.75
1:B:739:CYS:O	1:B:747:ARG:HD3	1.86	0.75
1:D:552:GLY:O	1:D:563:ILE:HB	1.85	0.75
1:C:698:THR:HG22	1:C:725:PRO:HB3	1.67	0.75
1:B:572:LEU:HD12	1:B:572:LEU:O	1.86	0.75
1:C:478:ARG:NH2	1:C:561:TYR:CE2	2.55	0.75
1:D:634:VAL:CG2	1:D:640:MET:SD	2.73	0.75
1:B:544:HIS:CD2	1:B:616:TYR:CG	2.73	0.75
1:D:720:HIS:ND1	1:D:720:HIS:O	2.18	0.75
1:B:624:HIS:HA	1:B:648:ALA:CB	2.17	0.75
1:D:575:TYR:CE1	1:D:579:ARG:NH1	2.48	0.75
1:A:519:LEU:HD12	1:A:523:ALA:HB2	1.68	0.75
1:B:692:LEU:HD12	1:B:692:LEU:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:TYR:CE1	1:C:579:ARG:CD	2.69	0.74
1:A:516:VAL:HG11	1:A:561:TYR:HB3	1.68	0.74
1:A:541:ILE:CD1	1:A:645:PHE:CE2	2.69	0.74
1:B:483:LEU:HD13	1:B:483:LEU:N	2.02	0.74
1:B:481:LEU:C	1:B:481:LEU:HD23	2.13	0.74
1:C:614:MET:HA	1:C:614:MET:CE	2.07	0.74
1:C:737:ARG:HG3	1:C:737:ARG:NH2	1.98	0.74
1:A:519:LEU:HD11	1:A:523:ALA:HB1	1.68	0.74
1:B:624:HIS:CA	1:B:648:ALA:HB2	2.18	0.74
1:B:686:VAL:CG1	1:B:750:PHE:CD1	2.70	0.74
1:C:704:TYR:N	1:C:722:MET:HE2	2.02	0.74
1:D:667:VAL:CG2	1:D:709:VAL:HG11	2.10	0.74
1:A:559:PRO:HG3	1:C:708:PRO:HG3	1.70	0.74
1:B:504:ASP:HB2	1:B:507:LYS:HA	1.68	0.74
1:C:630:ARG:HG3	1:C:630:ARG:HH11	1.53	0.74
1:C:635:THR:O	1:C:636:GLU:C	2.27	0.73
1:B:663:GLY:HA2	1:D:526:LYS:CB	2.18	0.73
1:C:600:PHE:CE2	1:C:729:THR:OG1	2.41	0.73
1:D:661:THR:HA	1:D:678:ARG:CB	2.17	0.73
1:C:622:CYS:O	1:C:682:HIS:NE2	2.21	0.73
1:A:614:MET:HE3	1:A:614:MET:CA	2.17	0.73
1:B:623:ILE:O	1:B:648:ALA:CB	2.32	0.73
1:C:724:LYS:N	1:C:724:LYS:HD2	2.04	0.73
1:A:560:LEU:HD13	1:A:560:LEU:O	1.89	0.73
1:A:580:ARG:HE	1:A:699:LEU:CB	2.02	0.73
1:A:628:ALA:HB3	1:A:630:ARG:NH1	2.04	0.73
1:B:535:MET:HE1	1:B:560:LEU:CD2	2.19	0.73
1:C:575:TYR:CE1	1:C:579:ARG:CZ	2.72	0.73
1:D:516:VAL:HG22	1:D:563:ILE:HD13	1.70	0.73
1:B:614:MET:SD	1:B:627:LEU:HD21	2.29	0.73
1:B:662:ASN:O	1:D:525:GLU:CB	2.36	0.72
1:C:522:ASP:OD1	1:C:522:ASP:N	2.22	0.72
1:C:538:MET:SD	1:C:550:LEU:HD13	2.29	0.72
1:D:568:SER:HB2	1:D:636:GLU:CG	2.19	0.72
1:A:662:ASN:HB2	1:C:525:GLU:CB	2.20	0.72
1:A:503:ILE:O	1:A:503:ILE:HD12	1.90	0.72
1:C:478:ARG:CZ	1:C:561:TYR:CZ	2.72	0.72
1:D:741:HIS:HB2	1:D:747:ARG:HG2	1.71	0.72
1:A:503:ILE:CG2	1:A:512:VAL:CG2	2.68	0.72
1:B:531:LEU:HD13	1:B:531:LEU:O	1.90	0.72
1:B:727:ASN:N	1:B:727:ASN:HD22	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:621:LYS:O	1:C:651:ILE:N	2.23	0.72
1:A:555:THR:HG22	1:A:555:THR:O	1.90	0.72
1:B:663:GLY:CA	1:D:526:LYS:CB	2.67	0.72
1:B:653:ASN:OD1	1:B:653:ASN:N	2.21	0.71
1:D:546:ASN:OD1	1:D:609:GLN:HB3	1.90	0.71
1:D:673:GLU:HG2	1:D:747:ARG:HH22	1.55	0.71
1:A:567:ALA:HB1	1:A:635:THR:HA	1.71	0.71
1:D:495:VAL:CG1	1:D:517:LYS:CG	2.67	0.71
1:C:581:PRO:CB	1:C:582:PRO:HD3	2.20	0.71
1:D:474:TRP:NE1	1:D:539:LYS:CG	2.51	0.71
1:B:550:LEU:HD13	1:B:550:LEU:O	1.90	0.71
1:B:531:LEU:HD13	1:B:531:LEU:C	2.15	0.71
1:B:610:LEU:CD2	1:B:632:VAL:HG13	2.19	0.71
1:B:550:LEU:C	1:B:550:LEU:HD22	2.14	0.71
1:B:568:SER:CB	1:B:636:GLU:HB2	2.20	0.71
1:B:615:GLU:OE1	1:B:754:VAL:HG21	1.90	0.71
1:B:556:GLN:HE21	1:B:556:GLN:CA	2.00	0.71
1:B:651:ILE:HG23	1:B:655:ASP:HA	1.73	0.71
1:A:476:PHE:CZ	1:A:500:ALA:HB1	2.25	0.71
1:D:495:VAL:HG11	1:D:517:LYS:CG	2.21	0.71
1:B:476:PHE:HE1	1:B:480:LYS:HB3	1.54	0.71
1:D:541:ILE:CG2	1:D:616:TYR:CE2	2.71	0.71
1:A:560:LEU:HD21	1:A:562:VAL:CG2	2.21	0.71
1:A:560:LEU:C	1:A:560:LEU:HD22	2.15	0.71
1:B:476:PHE:CE2	1:B:503:ILE:HG12	2.26	0.70
1:B:549:ASN:ND2	1:B:549:ASN:H	1.84	0.70
1:B:471:ASP:HB2	1:B:474:TRP:HB2	1.70	0.70
1:B:623:ILE:O	1:B:623:ILE:HD12	1.90	0.70
1:C:667:VAL:HG21	1:C:709:VAL:HG12	1.69	0.70
1:C:688:SER:O	1:C:691:VAL:HG12	1.92	0.70
1:D:541:ILE:HG22	1:D:616:TYR:CE2	2.26	0.70
1:A:541:ILE:HD13	1:A:645:PHE:CE2	2.25	0.70
1:C:575:TYR:HE1	1:C:579:ARG:CD	2.04	0.70
1:A:572:LEU:O	1:A:572:LEU:HD12	1.90	0.70
1:B:489:GLU:O	1:B:489:GLU:HG3	1.92	0.70
1:D:547:ILE:HG21	1:D:617:LEU:HD11	1.73	0.70
1:A:712:LEU:HD12	1:A:712:LEU:O	1.91	0.70
1:B:556:GLN:HA	1:B:556:GLN:NE2	2.06	0.69
1:C:694:TRP:HE1	1:C:725:PRO:HD3	1.57	0.69
1:A:572:LEU:HD21	1:A:696:ILE:CG1	2.22	0.69
1:A:689:PHE:HE2	1:A:753:LEU:HD13	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:VAL:HG22	1:B:640:MET:SD	2.32	0.69
1:A:614:MET:SD	1:A:627:LEU:HD11	2.33	0.69
1:C:694:TRP:NE1	1:C:725:PRO:HD3	2.07	0.69
1:B:624:HIS:HA	1:B:648:ALA:HB2	1.74	0.69
1:B:721:ARG:HG2	1:B:721:ARG:HH11	1.56	0.69
1:C:694:TRP:NE1	1:C:725:PRO:CD	2.55	0.69
1:A:614:MET:SD	1:A:627:LEU:CD1	2.80	0.69
1:A:667:VAL:HG23	1:C:523:ALA:O	1.92	0.69
1:A:681:THR:H	1:A:684:SER:HB3	1.58	0.69
1:A:683:GLN:HA	1:A:683:GLN:HE21	1.58	0.69
1:B:614:MET:SD	1:B:627:LEU:HD22	2.32	0.69
1:B:687:TRP:HZ3	1:B:721:ARG:HH21	1.37	0.69
1:D:572:LEU:HD13	1:D:640:MET:CE	2.20	0.69
1:C:687:TRP:CH2	1:C:704:TYR:OH	2.39	0.69
1:D:526:LYS:HE3	1:D:664:ARG:CD	2.21	0.69
1:C:519:LEU:HD11	1:C:528:LEU:HG	1.73	0.68
1:A:656:PTR:HD1	1:A:658:LYS:H	1.58	0.68
1:A:546:ASN:N	1:A:546:ASN:HD22	1.92	0.68
1:C:542:GLY:C	1:C:543:LYS:HD2	2.18	0.68
1:B:506:ASP:H	1:B:508:PRO:HD3	1.57	0.68
1:A:735:MET:CE	1:A:757:LEU:HD21	2.18	0.68
1:B:601:LYS:HD2	1:B:761:LEU:HD11	1.75	0.68
1:C:535:MET:CG	1:C:562:VAL:CG2	2.68	0.68
1:B:614:MET:HB3	1:B:750:PHE:CE2	2.29	0.68
1:C:560:LEU:HD13	1:C:560:LEU:O	1.94	0.68
1:C:732:LEU:HD22	1:C:732:LEU:N	2.08	0.68
1:A:519:LEU:CD1	1:A:523:ALA:HB1	2.24	0.68
1:A:575:TYR:CE1	1:A:579:ARG:NE	2.59	0.67
1:A:698:THR:HG22	1:A:725:PRO:CG	2.23	0.67
1:C:480:LYS:CD	1:C:501:VAL:HG21	2.21	0.67
1:A:541:ILE:HD13	1:A:645:PHE:HE2	1.59	0.67
1:B:610:LEU:CD1	1:B:632:VAL:HG11	2.24	0.67
1:B:761:LEU:HD12	1:B:761:LEU:O	1.94	0.67
1:D:514:VAL:HG21	1:D:563:ILE:HG23	1.77	0.67
1:D:693:MET:CE	1:D:736:MET:HB2	2.24	0.67
1:A:575:TYR:HE1	1:A:579:ARG:HE	1.40	0.67
1:C:694:TRP:CD1	1:C:725:PRO:CD	2.77	0.67
1:C:694:TRP:HE1	1:C:725:PRO:CD	2.07	0.67
1:D:482:THR:O	1:D:498:ALA:HB1	1.93	0.67
1:A:759:ARG:CG	1:A:760:ILE:N	2.57	0.67
1:C:732:LEU:H	1:C:732:LEU:CD2	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:LEU:CD1	1:A:692:LEU:HD21	2.24	0.67
1:C:694:TRP:CE2	1:C:725:PRO:HG3	2.30	0.67
1:A:537:MET:O	1:A:541:ILE:HG13	1.95	0.67
1:A:683:GLN:HA	1:A:683:GLN:NE2	2.08	0.67
1:B:531:LEU:CD1	1:B:560:LEU:HD11	2.24	0.67
1:A:519:LEU:HD12	1:A:523:ALA:CB	2.25	0.67
1:D:531:LEU:HD22	1:D:531:LEU:C	2.17	0.67
1:A:503:ILE:HG22	1:A:512:VAL:CG2	2.25	0.67
1:A:541:ILE:O	1:A:616:TYR:CE2	2.48	0.66
1:A:704:TYR:H	1:A:722:MET:HE2	1.58	0.66
1:C:647:LEU:N	1:C:647:LEU:HD23	2.09	0.66
1:D:673:GLU:CG	1:D:747:ARG:NH2	2.55	0.66
1:A:704:TYR:H	1:A:722:MET:HE1	1.60	0.66
1:A:503:ILE:CG2	1:A:512:VAL:HG21	2.25	0.66
1:A:625:ARG:HH12	1:A:665:LEU:HD11	1.61	0.66
1:A:671:ALA:HB1	1:A:672:PRO:HD2	1.78	0.66
1:C:694:TRP:CD1	1:C:725:PRO:HD3	2.30	0.65
1:D:500:ALA:C	1:D:503:ILE:HD11	2.21	0.65
1:A:656:PTR:HB2	1:B:743:VAL:CG2	2.26	0.65
1:A:719:GLY:HA2	1:A:721:ARG:HH12	1.60	0.65
1:D:621:LYS:HE2	1:D:651:ILE:CG2	2.17	0.65
1:A:575:TYR:HD2	1:A:634:VAL:HG11	1.60	0.65
1:A:495:VAL:CG2	1:A:517:LYS:CG	2.74	0.65
1:C:469:PRO:HD3	1:D:469:PRO:CG	2.25	0.65
1:C:536:GLU:OE1	1:C:536:GLU:HA	1.95	0.65
1:C:475:GLU:HA	1:C:553:ALA:O	1.96	0.65
1:D:571:ASN:N	1:D:571:ASN:OD1	2.27	0.65
1:A:571:ASN:HB2	1:A:630:ARG:O	1.96	0.65
1:B:572:LEU:HD21	1:B:696:ILE:HG12	1.77	0.65
1:C:600:PHE:CZ	1:C:729:THR:OG1	2.49	0.65
1:A:476:PHE:HZ	1:A:500:ALA:HB1	1.61	0.65
1:A:519:LEU:CD1	1:A:523:ALA:CB	2.75	0.65
1:A:724:LYS:O	1:A:724:LYS:HD3	1.97	0.65
1:D:500:ALA:HB3	1:D:503:ILE:HD11	1.77	0.65
1:D:694:TRP:CZ3	1:D:703:PRO:HA	2.32	0.65
1:A:704:TYR:HD1	1:A:722:MET:HE1	1.61	0.64
1:D:470:GLU:HB2	1:D:475:GLU:HG3	1.77	0.64
1:B:467:GLU:OE2	1:D:713:PHE:CD1	2.50	0.64
1:D:568:SER:CB	1:D:636:GLU:HG2	2.27	0.64
1:D:732:LEU:CD2	1:D:760:ILE:HD11	2.26	0.64
1:B:663:GLY:HA2	1:D:526:LYS:H	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:LEU:HG	1:C:481:LEU:O	1.97	0.64
1:A:759:ARG:CG	1:A:759:ARG:HH21	2.11	0.64
1:C:581:PRO:CG	1:C:582:PRO:CD	2.65	0.64
1:A:568:SER:HB2	1:A:636:GLU:HB2	1.78	0.64
1:A:665:LEU:O	1:C:524:THR:HA	1.97	0.64
1:C:575:TYR:CE1	1:C:579:ARG:NH1	2.66	0.64
1:A:651:ILE:CG2	1:A:655:ASP:HA	2.27	0.63
1:D:749:THR:CG2	1:D:750:PHE:N	2.61	0.63
1:C:712:LEU:HD12	1:C:712:LEU:O	1.98	0.63
1:A:739:CYS:SG	1:A:753:LEU:HD11	2.39	0.63
1:C:467:GLU:O	1:D:469:PRO:HG3	1.98	0.63
1:C:720:HIS:ND1	1:C:721:ARG:N	2.46	0.63
1:A:689:PHE:CE2	1:A:753:LEU:CD1	2.81	0.63
1:B:687:TRP:CH2	1:B:721:ARG:NH2	2.67	0.63
1:A:572:LEU:HD21	1:A:696:ILE:HG12	1.81	0.63
1:A:689:PHE:CE2	1:A:753:LEU:HD13	2.34	0.63
1:D:621:LYS:CE	1:D:651:ILE:HG21	2.04	0.63
1:D:624:HIS:HE1	1:D:644:ASP:O	1.81	0.63
1:B:655:ASP:OD1	1:B:655:ASP:N	2.32	0.63
1:C:537:MET:HG2	1:C:648:ALA:HB3	1.81	0.63
1:A:704:TYR:CD1	1:A:722:MET:HE2	2.34	0.63
1:C:537:MET:HE3	1:C:537:MET:HA	1.80	0.63
1:D:474:TRP:CD1	1:D:539:LYS:HE3	2.31	0.63
1:C:548:ILE:HG22	1:C:645:PHE:HE1	1.64	0.62
1:B:544:HIS:HB3	1:B:547:ILE:HG23	1.81	0.62
1:B:608:TYR:HA	1:B:757:LEU:HD13	1.81	0.62
1:B:614:MET:CA	1:B:614:MET:HE3	2.29	0.62
1:D:673:GLU:HG3	1:D:747:ARG:NH2	2.14	0.62
1:A:516:VAL:CG1	1:A:561:TYR:HB3	2.29	0.62
1:B:623:ILE:CD1	1:B:649:ARG:O	2.47	0.62
1:B:663:GLY:HA3	1:D:526:LYS:CB	2.29	0.62
1:A:612:ARG:HA	1:A:754:VAL:HG21	1.81	0.62
1:C:478:ARG:NH2	1:C:561:TYR:HE2	1.97	0.62
1:C:610:LEU:HD13	1:C:692:LEU:HD21	1.81	0.62
1:B:721:ARG:HH11	1:B:721:ARG:CG	2.12	0.62
1:C:628:ALA:HB2	1:C:669:TRP:CD1	2.34	0.62
1:A:683:GLN:HE21	1:A:683:GLN:CA	2.13	0.62
1:B:656:PTR:HE1	1:B:656:PTR:O2P	2.00	0.62
1:B:686:VAL:CG1	1:B:750:PHE:HE1	2.03	0.62
1:D:500:ALA:C	1:D:503:ILE:CD1	2.73	0.62
1:A:512:VAL:HG23	1:A:512:VAL:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:MET:HE3	1:B:614:MET:HA	1.82	0.62
1:A:563:ILE:HD13	1:A:563:ILE:H	1.65	0.62
1:B:475:GLU:CD	1:B:556:GLN:CB	2.73	0.62
1:C:686:VAL:CG2	1:C:747:ARG:CD	2.75	0.62
1:C:478:ARG:NH2	1:C:561:TYR:OH	2.33	0.61
1:D:545:LYS:HE3	1:D:639:VAL:HG11	1.82	0.61
1:A:610:LEU:HD12	1:A:692:LEU:HD21	1.81	0.61
1:A:627:LEU:C	1:A:627:LEU:HD23	2.23	0.61
1:D:673:GLU:OE2	1:D:684:SER:HB2	1.98	0.61
1:D:743:VAL:CG1	1:D:744:PRO:HD2	2.29	0.61
1:B:474:TRP:HA	1:B:474:TRP:CE3	2.36	0.61
1:B:651:ILE:HG22	1:B:651:ILE:O	2.01	0.61
1:B:698:THR:HG23	1:B:698:THR:O	1.99	0.61
1:A:525:GLU:OE2	1:A:525:GLU:HA	1.99	0.61
1:C:485:LYS:CB	1:C:486:PRO:HD2	2.30	0.61
1:C:667:VAL:HG23	1:C:709:VAL:HG13	1.75	0.61
1:A:580:ARG:HE	1:A:699:LEU:HB2	1.63	0.61
1:A:623:ILE:O	1:A:648:ALA:CB	2.49	0.61
1:C:729:THR:HB	1:C:732:LEU:HD23	1.81	0.61
1:D:614:MET:SD	1:D:627:LEU:HD21	2.40	0.61
1:A:524:THR:HG22	1:A:527:ASP:N	2.12	0.61
1:B:531:LEU:CD1	1:B:560:LEU:CD1	2.77	0.61
1:B:573:ARG:HH21	1:B:573:ARG:CG	2.11	0.61
1:C:683:GLN:HA	1:C:683:GLN:NE2	2.13	0.61
1:A:503:ILE:HG23	1:A:512:VAL:HG21	1.82	0.61
1:B:544:HIS:CD2	1:B:616:TYR:HB2	2.35	0.61
1:A:580:ARG:HE	1:A:699:LEU:HB3	1.64	0.61
1:A:647:LEU:HD11	1:A:664:ARG:O	2.00	0.61
1:D:673:GLU:HG2	1:D:747:ARG:NH2	2.16	0.61
1:A:563:ILE:HD13	1:A:563:ILE:N	2.15	0.61
1:A:560:LEU:CD2	1:A:562:VAL:HG23	2.29	0.60
1:D:623:ILE:HG13	1:D:623:ILE:O	2.01	0.60
1:A:651:ILE:HG22	1:A:651:ILE:O	2.00	0.60
1:B:735:MET:HE1	1:B:757:LEU:HG	1.84	0.60
1:A:497:MET:HE3	1:A:513:THR:HG23	1.82	0.60
1:A:568:SER:CB	1:A:636:GLU:HB2	2.30	0.60
1:C:469:PRO:CG	1:D:469:PRO:HB2	2.30	0.60
1:B:683:GLN:OE1	1:B:683:GLN:HA	2.02	0.60
1:C:683:GLN:HE21	1:C:683:GLN:CA	2.09	0.60
1:B:735:MET:HE3	1:B:753:LEU:CD2	2.21	0.60
1:B:610:LEU:HD13	1:B:632:VAL:HG21	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:LEU:HD21	1:B:624:HIS:HB2	1.84	0.60
1:A:514:VAL:HG11	1:A:563:ILE:HB	1.84	0.60
1:B:534:GLU:HA	1:B:646:GLY:HA2	1.83	0.60
1:B:697:PHE:CZ	1:B:732:LEU:HD23	2.37	0.60
1:B:675:LEU:HD22	1:B:713:PHE:CE2	2.37	0.59
1:C:575:TYR:CD1	1:C:579:ARG:HD2	2.36	0.59
1:D:632:VAL:HG12	1:D:632:VAL:O	2.00	0.59
1:A:724:LYS:HB3	1:A:733:TYR:CG	2.36	0.59
1:B:623:ILE:HD11	1:B:649:ARG:O	2.02	0.59
1:B:663:GLY:HA2	1:D:526:LYS:HB2	1.79	0.59
1:C:672:PRO:HD3	1:C:687:TRP:NE1	2.16	0.59
1:D:624:HIS:CE1	1:D:644:ASP:O	2.55	0.59
1:B:665:LEU:HB2	1:B:670:MET:SD	2.42	0.59
1:A:624:HIS:HA	1:A:648:ALA:CB	2.30	0.59
1:A:628:ALA:HB1	1:A:630:ARG:NH1	2.15	0.59
1:A:689:PHE:CD2	1:A:753:LEU:CD1	2.85	0.59
1:A:698:THR:CG2	1:A:725:PRO:HB3	2.30	0.59
1:B:624:HIS:O	1:B:648:ALA:CB	2.37	0.59
1:A:531:LEU:HD12	1:A:531:LEU:C	2.23	0.59
1:C:743:VAL:CG1	1:C:744:PRO:HD2	2.32	0.59
1:A:626:ASP:HB2	1:A:647:LEU:HD12	1.83	0.59
1:C:507:LYS:N	1:C:508:PRO:CD	2.62	0.59
1:C:568:SER:CB	1:C:636:GLU:CB	2.80	0.59
1:B:601:LYS:HB2	1:B:601:LYS:HZ2	1.64	0.59
1:C:547:ILE:O	1:C:547:ILE:HG13	2.02	0.59
1:D:495:VAL:HA	1:D:516:VAL:O	2.02	0.59
1:A:625:ARG:NH1	1:A:665:LEU:HD11	2.18	0.58
1:A:704:TYR:HE1	1:A:722:MET:HE3	1.63	0.58
1:B:504:ASP:HB2	1:B:508:PRO:HD2	1.84	0.58
1:B:664:ARG:O	1:B:665:LEU:HD23	2.02	0.58
1:A:572:LEU:HB2	1:A:640:MET:HE1	1.85	0.58
1:A:607:THR:CG2	1:A:757:LEU:HD11	2.33	0.58
1:A:694:TRP:NE1	1:A:725:PRO:HG3	2.17	0.58
1:C:635:THR:HB	1:C:639:VAL:HB	1.86	0.58
1:D:570:GLY:O	1:D:634:VAL:HG12	2.03	0.58
1:B:471:ASP:O	1:B:472:PRO:C	2.46	0.58
1:D:694:TRP:CE3	1:D:703:PRO:HA	2.39	0.58
1:D:708:PRO:HD2	1:D:711:GLU:HB3	1.84	0.58
1:A:698:THR:O	1:A:698:THR:OG1	2.14	0.58
1:A:761:LEU:HD12	1:A:761:LEU:C	2.28	0.58
1:C:612:ARG:O	1:C:615:GLU:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:704:TYR:HD1	1:D:704:TYR:N	2.02	0.58
1:A:516:VAL:HG22	1:A:563:ILE:HG22	1.85	0.58
1:A:575:TYR:HE1	1:A:579:ARG:CZ	2.15	0.58
1:A:614:MET:SD	1:A:627:LEU:HD12	2.43	0.58
1:A:634:VAL:HG13	1:A:634:VAL:O	2.04	0.58
1:D:501:VAL:HA	1:D:511:ALA:HA	1.86	0.58
1:D:624:HIS:NE2	1:D:643:ALA:O	2.35	0.58
1:D:672:PRO:CG	1:D:687:TRP:CH2	2.86	0.58
1:D:732:LEU:HD22	1:D:760:ILE:HD11	1.85	0.58
1:B:504:ASP:HB2	1:B:507:LYS:CA	2.33	0.57
1:B:514:VAL:HG21	1:B:563:ILE:HG23	1.85	0.57
1:D:710:GLU:OE1	1:D:710:GLU:N	2.30	0.57
1:D:667:VAL:HG21	1:D:709:VAL:HG13	1.82	0.57
1:D:692:LEU:HD12	1:D:692:LEU:C	2.28	0.57
1:B:601:LYS:HD3	1:B:761:LEU:HD13	1.82	0.57
1:C:614:MET:CB	1:C:750:PHE:CE1	2.86	0.57
1:C:729:THR:HB	1:C:732:LEU:CD2	2.33	0.57
1:B:475:GLU:CD	1:B:556:GLN:HB2	2.29	0.57
1:B:620:GLN:OE1	1:B:620:GLN:HA	2.04	0.57
1:D:541:ILE:HG23	1:D:616:TYR:CE2	2.40	0.57
1:D:672:PRO:HD3	1:D:687:TRP:CZ2	2.39	0.57
1:A:555:THR:O	1:A:555:THR:CG2	2.52	0.57
1:A:647:LEU:HD21	1:A:664:ARG:HG2	1.86	0.57
1:A:699:LEU:N	1:A:699:LEU:HD13	2.19	0.57
1:B:526:LYS:H	1:D:664:ARG:H	1.53	0.57
1:C:670:MET:SD	1:C:675:LEU:HG	2.44	0.57
1:A:600:PHE:HE2	1:A:727:ASN:O	1.87	0.57
1:C:614:MET:HB3	1:C:750:PHE:CE1	2.39	0.57
1:A:689:PHE:CD2	1:A:753:LEU:HD12	2.40	0.57
1:B:507:LYS:N	1:B:508:PRO:CD	2.68	0.57
1:B:712:LEU:HD12	1:B:712:LEU:C	2.26	0.57
1:B:665:LEU:HB3	1:B:666:PRO:HD2	1.87	0.57
1:C:535:MET:SD	1:C:562:VAL:CG2	2.93	0.57
1:A:607:THR:CG2	1:A:757:LEU:CD1	2.83	0.57
1:C:535:MET:CG	1:C:562:VAL:HG22	2.31	0.57
1:C:694:TRP:CD1	1:C:725:PRO:HG2	2.39	0.57
1:C:694:TRP:CG	1:C:722:MET:SD	2.98	0.57
1:A:481:LEU:HD11	1:A:498:ALA:HB1	1.86	0.56
1:B:624:HIS:CA	1:B:648:ALA:CB	2.80	0.56
2:D:1001:KX0:C07	2:D:1001:KX0:C22	2.82	0.56
1:B:475:GLU:OE1	1:B:556:GLN:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:HIS:C	1:B:624:HIS:HD1	2.11	0.56
1:B:630:ARG:NH2	1:B:666:PRO:HG3	2.19	0.56
1:C:568:SER:HB3	1:C:636:GLU:CA	2.35	0.56
1:D:487:LEU:CD2	1:D:497:MET:CB	2.62	0.56
1:D:498:ALA:O	1:D:514:VAL:N	2.38	0.56
1:D:704:TYR:CD1	1:D:704:TYR:N	2.73	0.56
1:B:617:LEU:HD12	1:B:617:LEU:C	2.29	0.56
1:D:470:GLU:O	1:D:470:GLU:HG3	2.05	0.56
1:D:514:VAL:CG2	1:D:563:ILE:HG23	2.35	0.56
1:C:630:ARG:HG3	1:C:630:ARG:NH1	2.21	0.56
1:C:635:THR:CB	1:C:639:VAL:O	2.54	0.56
1:C:668:LYS:NZ	1:C:707:ILE:O	2.31	0.56
1:C:692:LEU:O	1:C:692:LEU:HD12	2.04	0.56
1:B:531:LEU:HD12	1:B:560:LEU:CD1	2.35	0.56
2:B:1001:KX0:N04	2:B:1001:KX0:CL1	2.76	0.56
1:A:575:TYR:O	1:A:578:ALA:HB3	2.06	0.56
1:B:693:MET:HE1	1:B:735:MET:HG2	1.88	0.56
2:D:1001:KX0:N04	2:D:1001:KX0:CL1	2.76	0.56
1:C:516:VAL:HG12	1:C:563:ILE:HG12	1.87	0.56
1:C:703:PRO:CB	1:C:722:MET:HE1	2.36	0.56
1:C:737:ARG:HH21	1:C:737:ARG:CG	2.13	0.56
1:A:759:ARG:HG3	1:A:760:ILE:N	2.21	0.56
1:B:486:PRO:HA	1:B:496:VAL:HA	1.88	0.56
1:B:560:LEU:C	1:B:560:LEU:HD13	2.30	0.56
1:D:575:TYR:CE1	1:D:579:ARG:HD2	2.41	0.56
1:D:760:ILE:O	1:D:764:THR:CG2	2.44	0.56
1:A:735:MET:HA	1:A:738:ASP:HB2	1.88	0.55
1:C:537:MET:HA	1:C:537:MET:CE	2.35	0.55
1:B:478:ARG:NE	1:B:557:ASP:O	2.39	0.55
1:B:624:HIS:C	1:B:648:ALA:CB	2.72	0.55
1:B:652:ASN:C	1:B:653:ASN:OD1	2.49	0.55
1:B:699:LEU:HD22	1:B:699:LEU:N	2.21	0.55
1:B:712:LEU:HD11	1:B:716:LEU:HG	1.88	0.55
1:C:531:LEU:HD13	1:C:531:LEU:O	2.06	0.55
1:A:614:MET:HA	1:A:614:MET:CE	2.31	0.55
1:D:672:PRO:HG2	1:D:687:TRP:CH2	2.42	0.55
1:B:698:THR:HB	1:B:725:PRO:HB3	1.88	0.55
1:C:603:LEU:HD21	1:C:699:LEU:HD11	1.86	0.55
1:C:614:MET:HE3	1:C:614:MET:CA	2.31	0.55
1:C:687:TRP:CZ2	1:C:704:TYR:OH	2.57	0.55
1:A:628:ALA:HB3	1:A:630:ARG:HH12	1.61	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:537:MET:HE3	1:C:537:MET:CA	2.37	0.55
2:A:1001:KX0:N04	2:A:1001:KX0:CL1	2.77	0.55
1:D:672:PRO:HD3	1:D:687:TRP:CE2	2.41	0.55
1:D:683:GLN:CA	1:D:686:VAL:CG1	2.80	0.55
1:A:759:ARG:HG3	1:A:759:ARG:NH2	2.22	0.55
1:D:614:MET:SD	1:D:627:LEU:CD2	2.95	0.55
1:B:486:PRO:HB3	1:B:496:VAL:HG22	1.88	0.55
1:C:610:LEU:HD12	1:C:696:ILE:HD11	1.88	0.55
1:D:687:TRP:CD1	1:D:687:TRP:C	2.84	0.55
1:A:476:PHE:CD2	1:A:503:ILE:HD13	2.42	0.55
1:A:687:TRP:CD1	1:A:687:TRP:C	2.85	0.55
1:C:724:LYS:HD2	1:C:724:LYS:H	1.71	0.55
2:C:1001:KX0:C22	2:C:1001:KX0:C07	2.85	0.55
1:D:712:LEU:O	1:D:712:LEU:HD12	2.07	0.55
1:D:749:THR:HG22	1:D:751:LYS:H	1.72	0.55
1:B:694:TRP:CD2	1:B:722:MET:HE1	2.42	0.54
1:B:616:TYR:CD1	1:B:616:TYR:C	2.85	0.54
1:C:612:ARG:HA	1:C:754:VAL:HG21	1.89	0.54
1:C:708:PRO:HG2	1:C:711:GLU:HB3	1.89	0.54
1:D:476:PHE:HB3	1:D:554:CYS:SG	2.47	0.54
1:D:610:LEU:N	1:D:610:LEU:HD23	2.21	0.54
1:D:627:LEU:HD12	1:D:692:LEU:HD22	1.88	0.54
1:B:610:LEU:HD12	1:B:696:ILE:HD11	1.90	0.54
1:D:499:GLU:HA	1:D:513:THR:HA	1.89	0.54
1:D:546:ASN:O	1:D:641:LYS:HA	2.07	0.54
1:B:675:LEU:HD22	1:B:713:PHE:HE2	1.72	0.54
1:B:687:TRP:C	1:B:687:TRP:CD1	2.85	0.54
1:C:478:ARG:CZ	1:C:561:TYR:CE2	2.91	0.54
1:C:686:VAL:O	1:C:690:GLY:N	2.34	0.54
1:D:575:TYR:CE1	1:D:579:ARG:NE	2.74	0.54
1:B:673:GLU:OE2	1:B:744:PRO:HB3	2.07	0.54
1:C:478:ARG:NH2	1:C:561:TYR:CZ	2.76	0.54
1:A:656:PTR:O	1:A:657:TYR:HB3	2.08	0.54
1:C:622:CYS:HA	1:C:650:ASP:HA	1.88	0.54
1:B:600:PHE:CD1	1:B:600:PHE:C	2.85	0.54
1:C:476:PHE:HZ	1:C:501:VAL:O	1.90	0.54
1:B:715:LEU:CD2	1:B:715:LEU:H	2.21	0.54
1:A:568:SER:HB2	1:A:636:GLU:CB	2.37	0.54
1:A:568:SER:OG	1:A:636:GLU:HB2	2.07	0.54
1:B:651:ILE:HD13	1:B:656:PTR:HB3	1.89	0.54
1:A:468:LEU:HB3	1:A:469:PRO:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:720:HIS:O	1:C:721:ARG:HG2	2.08	0.53
2:A:1001:KX0:C22	2:A:1001:KX0:C07	2.86	0.53
1:B:617:LEU:HD22	1:B:645:PHE:HE1	1.74	0.53
1:D:694:TRP:CD1	1:D:736:MET:HE1	2.43	0.53
1:A:647:LEU:HD13	1:A:665:LEU:HG	1.90	0.53
1:D:495:VAL:CB	1:D:516:VAL:O	2.56	0.53
1:D:512:VAL:HG23	1:D:514:VAL:HG13	1.90	0.53
1:D:689:PHE:CE2	1:D:753:LEU:HD13	2.43	0.53
1:A:477:PRO:HG2	1:A:480:LYS:HG2	1.91	0.53
1:A:759:ARG:HH21	1:A:759:ARG:HB2	1.73	0.53
1:B:617:LEU:HD22	1:B:645:PHE:CE1	2.43	0.53
1:C:600:PHE:HE2	1:C:729:THR:OG1	1.91	0.53
1:A:474:TRP:CE3	1:A:474:TRP:HA	2.43	0.53
1:A:541:ILE:O	1:A:616:TYR:HE2	1.90	0.53
1:A:669:TRP:CZ2	1:A:703:PRO:HG3	2.42	0.53
1:B:654:ILE:HG23	1:B:654:ILE:O	2.07	0.53
1:C:560:LEU:HD13	1:C:560:LEU:C	2.33	0.53
1:C:722:MET:HB3	1:C:740:TRP:CH2	2.44	0.53
1:A:608:TYR:CE1	1:A:612:ARG:HG3	2.44	0.53
1:B:500:ALA:HB1	1:B:503:ILE:HG13	1.90	0.53
1:D:487:LEU:CD1	1:D:515:ALA:HB1	2.38	0.53
1:A:671:ALA:HB1	1:A:672:PRO:CD	2.38	0.53
1:A:683:GLN:NE2	1:A:683:GLN:CA	2.72	0.53
1:C:636:GLU:O	1:C:637:ASN:ND2	2.42	0.53
1:D:683:GLN:C	1:D:686:VAL:HG13	2.31	0.53
1:D:699:LEU:HD23	1:D:699:LEU:N	2.23	0.53
1:B:601:LYS:O	1:B:602:ASP:C	2.51	0.53
1:B:694:TRP:CE2	1:B:722:MET:HE3	2.43	0.53
1:C:567:ALA:HB3	1:C:633:LEU:HD22	1.89	0.53
1:C:675:LEU:HD23	1:C:675:LEU:O	2.09	0.53
1:A:559:PRO:HG3	1:C:708:PRO:CG	2.38	0.53
1:B:531:LEU:HD11	1:B:560:LEU:CD1	2.36	0.53
1:B:486:PRO:CA	1:B:496:VAL:HG22	2.39	0.53
1:B:694:TRP:CD2	1:B:722:MET:CE	2.92	0.53
1:D:575:TYR:CZ	1:D:579:ARG:CZ	2.91	0.53
1:A:607:THR:HG22	1:A:757:LEU:HD12	1.89	0.52
1:B:708:PRO:HG2	1:B:711:GLU:HB3	1.90	0.52
1:D:624:HIS:ND1	1:D:624:HIS:O	2.42	0.52
1:C:543:LYS:N	1:C:543:LYS:CD	2.73	0.52
1:C:623:ILE:HG22	1:C:682:HIS:CD2	2.44	0.52
1:B:614:MET:CB	1:B:750:PHE:CE2	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:575:TYR:OH	1:D:579:ARG:CZ	2.57	0.52
1:D:625:ARG:HH21	1:D:662:ASN:ND2	2.07	0.52
1:A:545:LYS:HE3	1:A:639:VAL:HG13	1.92	0.52
1:A:711:GLU:HG2	1:A:711:GLU:O	2.09	0.52
1:C:572:LEU:HD23	1:C:629:ALA:HB1	1.91	0.52
1:D:724:LYS:HB2	1:D:733:TYR:CG	2.45	0.52
1:A:664:ARG:HA	1:C:524:THR:HG22	1.91	0.52
1:B:474:TRP:HA	1:B:474:TRP:HE3	1.73	0.52
1:C:571:ASN:HB2	1:C:630:ARG:O	2.10	0.52
1:B:623:ILE:HD13	1:B:625:ARG:CG	2.39	0.52
1:A:544:HIS:H	1:A:549:ASN:HD22	1.57	0.52
1:C:544:HIS:NE2	1:C:616:TYR:CB	2.72	0.52
1:A:608:TYR:HE1	1:A:612:ARG:HG3	1.72	0.52
1:A:664:ARG:HA	1:C:524:THR:HG21	1.91	0.52
1:A:704:TYR:N	1:A:722:MET:HE1	2.24	0.52
1:A:546:ASN:O	1:A:641:LYS:HA	2.09	0.52
1:A:571:ASN:ND2	2:A:1001:KX0:C08	2.63	0.52
1:B:601:LYS:HD3	1:B:761:LEU:HD12	1.85	0.52
1:B:518:MET:HE2	1:B:561:TYR:CE1	2.45	0.51
1:C:568:SER:HB2	1:C:636:GLU:CB	2.40	0.51
1:C:688:SER:O	1:C:691:VAL:CG1	2.58	0.51
1:D:569:LYS:HB2	1:D:634:VAL:HG13	1.91	0.51
1:B:471:ASP:CB	1:B:474:TRP:HB2	2.39	0.51
2:B:1001:KX0:C07	2:B:1001:KX0:C22	2.85	0.51
1:B:481:LEU:HD12	1:B:563:ILE:HD11	1.91	0.51
1:A:496:VAL:HG23	1:A:496:VAL:O	2.10	0.51
1:A:538:MET:HB2	1:A:550:LEU:HD22	1.92	0.51
1:A:693:MET:HE2	1:A:736:MET:HG3	1.91	0.51
1:C:672:PRO:CG	1:C:687:TRP:NE1	2.74	0.51
1:C:686:VAL:CG2	1:C:747:ARG:HB3	2.15	0.51
1:B:663:GLY:HA2	1:D:526:LYS:N	2.26	0.51
1:D:699:LEU:N	1:D:699:LEU:CD2	2.73	0.51
1:B:623:ILE:HD13	1:B:625:ARG:HG3	1.93	0.51
1:D:683:GLN:HA	1:D:686:VAL:HG12	1.89	0.51
1:B:697:PHE:CE1	1:B:732:LEU:HD23	2.46	0.51
1:D:568:SER:CB	1:D:636:GLU:CG	2.85	0.51
1:D:737:ARG:NH1	1:D:737:ARG:HG3	2.26	0.51
1:A:759:ARG:HG2	1:A:760:ILE:H	1.76	0.51
1:C:601:LYS:NZ	1:C:601:LYS:HB3	2.26	0.51
1:D:737:ARG:HG3	1:D:737:ARG:HH11	1.76	0.51
1:B:569:LYS:HB2	1:B:634:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:THR:HG22	1:A:526:LYS:N	2.27	0.50
1:B:721:ARG:CG	1:B:721:ARG:NH1	2.73	0.50
1:A:699:LEU:HD13	1:A:699:LEU:H	1.76	0.50
1:B:470:GLU:OE1	1:B:472:PRO:HD3	2.11	0.50
1:C:575:TYR:CD1	1:C:579:ARG:NH1	2.78	0.50
1:A:721:ARG:HH11	1:A:721:ARG:HG2	1.77	0.50
1:C:665:LEU:HB2	1:C:670:MET:HE3	1.93	0.50
1:B:544:HIS:CD2	1:B:616:TYR:CD2	2.92	0.50
1:D:495:VAL:CA	1:D:516:VAL:O	2.58	0.50
1:D:514:VAL:HG21	1:D:563:ILE:CG2	2.41	0.50
1:B:741:HIS:HB2	1:B:747:ARG:HG2	1.93	0.50
1:C:537:MET:HE3	1:C:537:MET:C	2.36	0.50
1:D:500:ALA:O	1:D:503:ILE:HD13	2.12	0.50
1:B:487:LEU:HD21	1:B:497:MET:HB2	1.94	0.50
1:C:469:PRO:CD	1:D:469:PRO:CB	2.51	0.50
1:C:623:ILE:HG13	1:C:625:ARG:HG2	1.93	0.50
1:A:572:LEU:CD1	1:A:576:LEU:HG	2.42	0.50
1:A:759:ARG:HH21	1:A:759:ARG:CB	2.24	0.50
1:D:559:PRO:HG2	1:D:561:TYR:CE1	2.47	0.50
1:A:546:ASN:OD1	1:A:609:GLN:HB3	2.12	0.49
1:C:623:ILE:HG12	1:C:623:ILE:O	2.11	0.49
1:C:695:GLU:O	1:C:700:GLY:N	2.38	0.49
1:A:572:LEU:HD11	1:A:576:LEU:HG	1.94	0.49
1:D:600:PHE:CD1	1:D:600:PHE:C	2.89	0.49
1:C:531:LEU:CD1	1:C:531:LEU:C	2.85	0.49
1:B:531:LEU:HD11	1:B:562:VAL:CG2	2.42	0.49
1:B:541:ILE:HG21	1:B:547:ILE:CD1	2.42	0.49
1:B:638:ASN:OD1	1:B:638:ASN:N	2.44	0.49
1:D:621:LYS:HG2	1:D:652:ASN:HA	1.95	0.49
1:B:504:ASP:HB2	1:B:507:LYS:H	1.78	0.49
1:B:689:PHE:CD1	1:B:692:LEU:HD23	2.48	0.49
1:D:657:TYR:HA	1:D:679:VAL:HB	1.94	0.49
1:D:743:VAL:HG12	1:D:744:PRO:HD2	1.95	0.49
1:B:478:ARG:NE	1:B:554:CYS:HB3	2.28	0.49
1:B:519:LEU:HD21	1:B:528:LEU:CA	2.35	0.49
1:C:496:VAL:HG23	1:C:516:VAL:HG22	1.95	0.49
1:C:625:ARG:O	1:C:665:LEU:HD13	2.12	0.49
1:C:694:TRP:CZ3	1:C:703:PRO:HA	2.48	0.49
1:A:656:PTR:O	1:A:680:TYR:O	2.30	0.49
1:C:635:THR:N	1:C:639:VAL:O	2.46	0.49
1:D:495:VAL:HB	1:D:516:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:683:GLN:HA	1:D:686:VAL:HG11	1.92	0.49
1:A:756:ASP:O	1:A:759:ARG:HG2	2.13	0.49
1:B:495:VAL:HG22	1:B:517:LYS:HG3	1.95	0.49
1:B:724:LYS:HB2	1:B:733:TYR:CG	2.48	0.49
1:C:667:VAL:CG2	1:C:709:VAL:HG11	2.36	0.49
1:C:734:MET:O	1:C:735:MET:C	2.54	0.49
1:D:621:LYS:CG	1:D:651:ILE:HG22	2.43	0.49
1:D:724:LYS:HZ2	1:D:724:LYS:CB	2.26	0.49
1:B:560:LEU:CD1	1:B:562:VAL:HG23	2.37	0.49
1:A:496:VAL:HG22	1:A:518:MET:HE3	1.95	0.48
1:A:536:GLU:HA	1:A:536:GLU:OE1	2.12	0.48
1:B:634:VAL:HG21	1:B:640:MET:HE1	1.86	0.48
1:C:622:CYS:O	1:C:682:HIS:CD2	2.65	0.48
1:C:665:LEU:HB2	1:C:670:MET:CE	2.42	0.48
1:C:731:GLU:OE1	1:C:760:ILE:HD11	2.12	0.48
1:A:541:ILE:HD11	1:A:645:PHE:CD2	2.48	0.48
1:A:544:HIS:H	1:A:549:ASN:ND2	2.11	0.48
1:A:627:LEU:C	1:A:627:LEU:CD2	2.86	0.48
1:A:629:ALA:HB2	1:A:692:LEU:CD1	2.43	0.48
1:A:672:PRO:HD3	1:A:687:TRP:CD2	2.48	0.48
1:D:743:VAL:HG13	1:D:744:PRO:HD2	1.96	0.48
1:B:575:TYR:HE1	1:B:579:ARG:CZ	2.27	0.48
1:C:675:LEU:C	1:C:675:LEU:CD2	2.85	0.48
1:D:572:LEU:HD21	1:D:696:ILE:HG12	1.94	0.48
1:D:715:LEU:HD13	1:D:715:LEU:N	2.28	0.48
1:A:481:LEU:HD11	1:A:498:ALA:CB	2.42	0.48
1:A:538:MET:HB3	1:A:550:LEU:HB2	1.95	0.48
1:A:610:LEU:HD13	1:A:692:LEU:HD21	1.95	0.48
1:C:477:PRO:HG2	1:C:480:LYS:HB2	1.95	0.48
1:D:474:TRP:NE1	1:D:539:LYS:CE	2.73	0.48
1:D:535:MET:HE3	1:D:539:LYS:NZ	2.28	0.48
1:D:635:THR:HG21	1:D:641:LYS:HE3	1.95	0.48
1:A:651:ILE:HG21	1:A:655:ASP:HA	1.94	0.48
1:A:680:TYR:CE1	1:A:685:ASP:OD1	2.67	0.48
1:B:504:ASP:HB2	1:B:507:LYS:N	2.29	0.48
1:A:646:GLY:O	1:A:649:ARG:NH1	2.46	0.48
1:C:672:PRO:CD	1:C:687:TRP:NE1	2.75	0.48
1:D:550:LEU:C	1:D:550:LEU:HD12	2.39	0.48
1:B:575:TYR:HE1	1:B:579:ARG:NH1	2.10	0.48
1:C:630:ARG:NH1	1:C:630:ARG:CG	2.73	0.48
1:D:694:TRP:HZ3	1:D:703:PRO:HA	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:ARG:HH21	1:A:759:ARG:HG3	1.75	0.48
1:A:528:LEU:HD12	1:A:528:LEU:O	2.14	0.48
1:B:486:PRO:HA	1:B:496:VAL:HG22	1.96	0.48
1:B:623:ILE:HD13	1:B:625:ARG:HD2	1.95	0.48
1:C:470:GLU:O	1:C:470:GLU:HG3	2.12	0.48
1:A:487:LEU:HD11	1:A:497:MET:HB2	1.95	0.48
1:B:572:LEU:HD12	1:B:572:LEU:C	2.39	0.48
1:C:481:LEU:HD11	1:C:498:ALA:CB	2.44	0.48
1:B:527:ASP:OD1	1:B:527:ASP:O	2.32	0.47
1:B:531:LEU:HD11	1:B:562:VAL:HG23	1.96	0.47
1:C:672:PRO:HD3	1:C:687:TRP:CG	2.46	0.47
1:C:720:HIS:C	1:C:721:ARG:HG2	2.39	0.47
1:D:560:LEU:C	1:D:560:LEU:HD13	2.38	0.47
1:A:625:ARG:HH12	1:A:665:LEU:CD1	2.26	0.47
1:C:535:MET:CG	1:C:562:VAL:HG21	2.37	0.47
1:D:601:LYS:H	1:D:601:LYS:HG2	1.47	0.47
1:C:474:TRP:HE3	1:C:552:GLY:HA2	1.79	0.47
1:D:503:ILE:CD1	1:D:503:ILE:N	2.78	0.47
1:D:555:THR:O	1:D:555:THR:OG1	2.30	0.47
1:D:689:PHE:HE2	1:D:753:LEU:HD13	1.79	0.47
1:B:610:LEU:CD1	1:B:632:VAL:HG21	2.43	0.47
1:C:572:LEU:O	1:C:572:LEU:HG	2.13	0.47
1:C:686:VAL:CG2	1:C:747:ARG:CB	2.80	0.47
1:C:519:LEU:HD22	1:C:523:ALA:HB2	1.96	0.47
1:C:548:ILE:HD12	1:C:641:LYS:HD2	1.95	0.47
1:D:543:LYS:NZ	1:D:549:ASN:HD21	2.13	0.47
1:B:481:LEU:HD23	1:B:481:LEU:O	2.14	0.47
1:B:609:GLN:C	1:B:611:ALA:H	2.23	0.47
1:B:715:LEU:H	1:B:715:LEU:HD22	1.78	0.47
1:C:686:VAL:HG22	1:C:747:ARG:HD3	1.93	0.47
1:C:724:LYS:N	1:C:724:LYS:CD	2.72	0.47
1:D:476:PHE:HE2	1:D:503:ILE:HA	1.79	0.47
1:D:621:LYS:HG2	1:D:652:ASN:N	2.30	0.47
1:A:692:LEU:HD12	1:A:692:LEU:C	2.38	0.47
1:A:724:LYS:HB3	1:A:733:TYR:CD1	2.49	0.47
1:C:501:VAL:HA	1:C:511:ALA:HA	1.97	0.47
1:D:483:LEU:N	1:D:483:LEU:HD23	2.30	0.47
1:D:524:THR:OG1	1:D:527:ASP:HB2	2.14	0.47
1:B:609:GLN:O	1:B:611:ALA:N	2.47	0.47
1:B:621:LYS:HD3	1:B:621:LYS:HA	1.32	0.47
1:B:694:TRP:O	1:B:698:THR:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:TRP:HZ3	1:B:702:SER:O	1.98	0.47
1:C:693:MET:HE3	1:C:736:MET:HG2	1.96	0.47
1:D:537:MET:HG3	1:D:648:ALA:HB3	1.97	0.47
1:D:724:LYS:NZ	1:D:724:LYS:CB	2.73	0.47
1:A:741:HIS:HB2	1:A:747:ARG:HG2	1.97	0.47
1:A:759:ARG:HG2	1:A:760:ILE:N	2.30	0.47
1:B:647:LEU:HD23	1:B:647:LEU:O	2.14	0.47
1:B:687:TRP:HH2	1:B:721:ARG:NH2	2.13	0.47
1:C:519:LEU:HD12	1:C:528:LEU:CD2	2.45	0.47
1:D:670:MET:HE2	1:D:670:MET:HB3	1.71	0.47
1:A:657:TYR:CZ	1:A:660:THR:OG1	2.58	0.46
1:A:689:PHE:HE2	1:A:753:LEU:CD1	2.22	0.46
1:A:737:ARG:HD2	1:A:740:TRP:CE3	2.50	0.46
1:B:507:LYS:N	1:B:508:PRO:HD3	2.29	0.46
1:C:568:SER:HB3	1:C:636:GLU:N	2.29	0.46
1:C:729:THR:O	1:C:732:LEU:HD23	2.15	0.46
1:D:667:VAL:CG2	1:D:709:VAL:HG13	2.40	0.46
1:A:541:ILE:O	1:A:616:TYR:OH	2.29	0.46
1:D:568:SER:HB2	1:D:636:GLU:CB	2.44	0.46
1:D:606:CYS:SG	1:D:640:MET:HG2	2.56	0.46
1:D:749:THR:HG22	1:D:750:PHE:N	2.29	0.46
1:D:475:GLU:OE2	1:D:476:PHE:N	2.48	0.46
1:A:724:LYS:HB3	1:A:733:TYR:CD2	2.51	0.46
1:D:683:GLN:C	1:D:686:VAL:CG1	2.88	0.46
1:A:516:VAL:HB	1:A:518:MET:HE3	1.96	0.46
1:A:531:LEU:HD11	1:A:562:VAL:HG21	1.96	0.46
1:C:567:ALA:HB1	1:C:634:VAL:O	2.16	0.46
1:C:620:GLN:HB3	1:C:622:CYS:SG	2.56	0.46
2:C:1001:KX0:N04	2:C:1001:KX0:CL1	2.85	0.46
1:D:575:TYR:OH	1:D:579:ARG:NE	2.48	0.46
1:A:484:GLY:CA	1:A:497:MET:O	2.64	0.46
1:A:704:TYR:N	1:A:722:MET:CE	2.69	0.46
1:B:481:LEU:HD11	1:B:516:VAL:CG2	2.46	0.46
1:B:524:THR:HB	1:B:527:ASP:H	1.79	0.46
1:B:694:TRP:CG	1:B:722:MET:CE	2.99	0.46
1:B:518:MET:HE2	1:B:561:TYR:CD1	2.51	0.46
1:C:687:TRP:HZ3	1:C:691:VAL:HB	1.80	0.46
1:A:484:GLY:N	1:A:497:MET:O	2.48	0.46
1:A:725:PRO:HD2	1:A:728:CYS:HB2	1.96	0.46
1:D:495:VAL:HG12	1:D:517:LYS:CG	2.41	0.46
1:D:544:HIS:CD2	1:D:616:TYR:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:PRO:HG3	1:C:708:PRO:CB	2.46	0.46
1:A:623:ILE:O	1:A:623:ILE:HG13	2.16	0.46
1:C:524:THR:HB	1:C:527:ASP:H	1.81	0.46
1:C:635:THR:HB	1:C:639:VAL:O	2.16	0.46
1:C:683:GLN:O	1:C:686:VAL:HG22	2.16	0.46
1:B:536:GLU:OE1	1:B:536:GLU:HA	2.16	0.46
1:B:618:ALA:HB1	1:B:682:HIS:CD2	2.51	0.46
1:C:720:HIS:ND1	1:C:720:HIS:C	2.73	0.46
1:D:751:LYS:O	1:D:751:LYS:HD3	2.16	0.46
1:C:647:LEU:HD12	1:C:665:LEU:HD21	1.99	0.45
1:D:494:GLN:O	1:D:518:MET:N	2.32	0.45
1:D:672:PRO:CD	1:D:687:TRP:CH2	2.99	0.45
1:A:687:TRP:CD1	1:A:687:TRP:O	2.70	0.45
1:B:737:ARG:HA	1:B:737:ARG:HD2	1.74	0.45
1:B:531:LEU:C	1:B:531:LEU:CD1	2.85	0.45
1:B:551:LEU:HB2	1:B:563:ILE:HG22	1.97	0.45
1:D:528:LEU:C	1:D:528:LEU:CD2	2.90	0.45
1:A:608:TYR:CD2	1:A:761:LEU:HD23	2.52	0.45
1:A:689:PHE:CE2	1:A:753:LEU:HD12	2.51	0.45
1:B:571:ASN:HA	1:B:633:LEU:HA	1.98	0.45
1:C:679:VAL:HG23	1:C:679:VAL:O	2.16	0.45
1:D:531:LEU:HD11	1:D:560:LEU:HD12	1.98	0.45
1:B:651:ILE:CG2	1:B:655:ASP:HA	2.44	0.45
1:B:693:MET:HE1	1:B:735:MET:SD	2.57	0.45
1:C:475:GLU:CG	1:C:555:THR:OG1	2.63	0.45
1:C:687:TRP:O	1:C:687:TRP:CE3	2.70	0.45
1:B:538:MET:HB3	1:B:538:MET:HE2	1.62	0.45
1:B:694:TRP:CG	1:B:722:MET:HE1	2.51	0.45
1:D:749:THR:HG23	1:D:750:PHE:N	2.32	0.45
1:A:548:ILE:HB	1:A:642:ILE:O	2.16	0.45
1:B:694:TRP:CZ3	1:B:703:PRO:HA	2.52	0.45
1:C:664:ARG:CD	1:C:664:ARG:N	2.73	0.45
1:D:538:MET:HB2	1:D:550:LEU:HD23	1.99	0.45
1:B:474:TRP:CZ3	1:B:550:LEU:HD13	2.52	0.45
1:C:689:PHE:O	1:C:689:PHE:CD1	2.70	0.45
1:B:575:TYR:CD1	1:B:575:TYR:O	2.70	0.45
1:B:673:GLU:CD	1:B:744:PRO:HB3	2.42	0.45
1:C:600:PHE:CD1	1:C:600:PHE:O	2.70	0.45
1:D:470:GLU:HB2	1:D:475:GLU:CG	2.45	0.45
1:A:541:ILE:O	1:A:616:TYR:CZ	2.71	0.44
1:A:608:TYR:CD1	1:A:608:TYR:C	2.92	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:TYR:CD2	1:A:657:TYR:O	2.70	0.44
1:A:679:VAL:O	1:A:679:VAL:HG23	2.16	0.44
1:A:689:PHE:HD2	1:A:753:LEU:CD1	2.29	0.44
1:C:665:LEU:O	1:C:670:MET:HE3	2.16	0.44
1:D:475:GLU:HA	1:D:553:ALA:O	2.18	0.44
1:D:524:THR:OG1	1:D:527:ASP:CB	2.65	0.44
1:D:548:ILE:HD13	1:D:633:LEU:HD12	1.98	0.44
1:D:749:THR:HG23	1:D:750:PHE:H	1.81	0.44
1:A:708:PRO:HG2	1:A:711:GLU:HB3	2.00	0.44
1:B:614:MET:CG	1:B:627:LEU:HD21	2.47	0.44
1:B:621:LYS:HB3	1:B:652:ASN:HA	1.99	0.44
1:B:692:LEU:HD12	1:B:692:LEU:C	2.40	0.44
1:C:544:HIS:CG	1:C:616:TYR:CB	2.98	0.44
1:A:607:THR:HG22	1:A:757:LEU:HD11	1.86	0.44
1:B:650:ASP:OD1	1:B:652:ASN:N	2.43	0.44
1:D:542:GLY:N	1:D:616:TYR:CZ	2.86	0.44
1:B:671:ALA:HA	1:B:687:TRP:CD1	2.52	0.44
1:D:720:HIS:O	1:D:720:HIS:CG	2.70	0.44
1:A:638:ASN:OD1	1:A:638:ASN:N	2.48	0.44
1:A:647:LEU:CD1	1:A:665:LEU:HG	2.47	0.44
1:A:709:VAL:HG21	1:C:523:ALA:HB2	1.99	0.44
1:A:715:LEU:HD12	1:A:720:HIS:HB3	2.00	0.44
1:B:481:LEU:C	1:B:481:LEU:CD2	2.85	0.44
1:B:549:ASN:H	1:B:549:ASN:HD22	1.62	0.44
1:B:698:THR:HB	1:B:725:PRO:CB	2.47	0.44
1:C:474:TRP:CE3	1:C:474:TRP:HA	2.52	0.44
1:C:575:TYR:CD1	1:C:575:TYR:O	2.70	0.44
1:A:525:GLU:HB3	1:C:663:GLY:HA2	1.99	0.44
1:A:676:PHE:HB3	1:B:676:PHE:HB3	1.99	0.44
1:B:563:ILE:HG22	1:B:563:ILE:O	2.17	0.44
1:A:625:ARG:NH2	1:A:647:LEU:HD22	2.33	0.44
1:A:630:ARG:HH22	1:A:666:PRO:HG2	1.82	0.44
1:A:656:PTR:HD1	1:A:657:TYR:N	2.33	0.44
1:B:486:PRO:CB	1:B:496:VAL:HG22	2.47	0.44
1:C:548:ILE:HD12	1:C:641:LYS:CD	2.48	0.44
1:C:635:THR:OG1	1:C:639:VAL:O	2.34	0.44
1:A:520:LYS:O	1:A:521:ASP:C	2.61	0.44
1:A:550:LEU:HD12	1:A:551:LEU:H	1.83	0.44
1:A:657:TYR:O	1:A:657:TYR:CG	2.70	0.44
1:B:618:ALA:O	1:B:682:HIS:CE1	2.71	0.44
1:A:476:PHE:CE2	1:A:503:ILE:HD13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:687:TRP:CZ3	1:C:691:VAL:HB	2.53	0.43
1:D:720:HIS:ND1	1:D:720:HIS:C	2.72	0.43
1:B:504:ASP:CB	1:B:508:PRO:HD2	2.48	0.43
1:B:601:LYS:O	1:B:604:VAL:N	2.51	0.43
1:C:600:PHE:CD1	1:C:600:PHE:C	2.92	0.43
1:C:689:PHE:CD2	1:C:753:LEU:HD13	2.53	0.43
1:D:487:LEU:CD1	1:D:515:ALA:CB	2.96	0.43
1:D:575:TYR:O	1:D:575:TYR:CD1	2.71	0.43
1:A:477:PRO:HG2	1:A:480:LYS:CG	2.49	0.43
1:B:617:LEU:CD2	1:B:624:HIS:HB2	2.48	0.43
1:D:531:LEU:C	1:D:531:LEU:CD2	2.88	0.43
1:A:523:ALA:O	1:C:666:PRO:HA	2.19	0.43
1:B:624:HIS:C	1:B:624:HIS:ND1	2.72	0.43
1:C:623:ILE:HG22	1:C:682:HIS:HD2	1.83	0.43
1:A:693:MET:HE2	1:A:736:MET:CG	2.47	0.43
1:A:743:VAL:HA	1:A:744:PRO:HD2	1.86	0.43
1:B:727:ASN:HD22	1:B:727:ASN:H	1.64	0.43
1:C:481:LEU:HD11	1:C:498:ALA:HB1	1.99	0.43
1:C:542:GLY:C	1:C:543:LYS:CD	2.88	0.43
1:C:601:LYS:NZ	1:C:601:LYS:CB	2.81	0.43
1:C:686:VAL:HG21	1:C:747:ARG:CG	2.47	0.43
1:D:736:MET:HE2	1:D:740:TRP:CH2	2.53	0.43
1:A:546:ASN:N	1:A:546:ASN:ND2	2.60	0.43
1:A:664:ARG:N	1:A:664:ARG:CD	2.73	0.43
1:A:693:MET:HE3	1:A:693:MET:HB3	1.59	0.43
1:B:475:GLU:CD	1:B:556:GLN:H	2.27	0.43
1:C:519:LEU:HD12	1:C:528:LEU:HD21	1.99	0.43
1:C:627:LEU:HD12	1:C:627:LEU:HA	1.79	0.43
1:A:524:THR:O	1:A:527:ASP:HB2	2.18	0.43
1:B:567:ALA:HB1	1:B:634:VAL:O	2.19	0.43
1:A:496:VAL:HG22	1:A:518:MET:CE	2.49	0.43
1:A:572:LEU:HD22	1:A:640:MET:CE	2.49	0.43
1:A:656:PTR:HB2	1:B:743:VAL:HG21	1.98	0.43
1:C:568:SER:HB3	1:C:636:GLU:CB	2.49	0.43
1:C:600:PHE:HZ	1:C:729:THR:HG1	1.61	0.43
1:C:720:HIS:O	1:C:721:ARG:CG	2.67	0.43
1:A:683:GLN:HE22	1:A:749:THR:HA	1.83	0.43
1:D:724:LYS:HZ2	1:D:724:LYS:HB3	1.83	0.43
1:B:483:LEU:H	1:B:483:LEU:CD1	2.14	0.42
1:B:610:LEU:HD13	1:B:692:LEU:HD21	2.01	0.42
1:C:531:LEU:HD13	1:C:531:LEU:C	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:474:TRP:HE1	1:D:539:LYS:CG	2.22	0.42
1:A:572:LEU:HD12	1:A:572:LEU:C	2.43	0.42
1:A:548:ILE:CD1	1:A:633:LEU:HD12	2.50	0.42
1:C:691:VAL:HG13	1:C:692:LEU:N	2.33	0.42
1:C:694:TRP:CE3	1:C:722:MET:SD	3.12	0.42
1:D:575:TYR:CE1	1:D:579:ARG:CD	3.01	0.42
1:A:649:ARG:HH21	1:A:664:ARG:HH21	1.68	0.42
1:C:575:TYR:CD1	1:C:575:TYR:C	2.94	0.42
1:D:541:ILE:HG21	1:D:547:ILE:CD1	2.49	0.42
1:D:724:LYS:HB2	1:D:733:TYR:CD2	2.53	0.42
1:B:476:PHE:CE1	1:B:480:LYS:HB3	2.44	0.42
1:C:623:ILE:CG1	1:C:625:ARG:HG2	2.50	0.42
1:C:628:ALA:CB	1:C:669:TRP:NE1	2.82	0.42
1:A:495:VAL:CG2	1:A:517:LYS:HG3	2.49	0.42
1:A:503:ILE:HD12	1:A:503:ILE:C	2.43	0.42
1:A:756:ASP:O	1:A:760:ILE:HG13	2.19	0.42
1:B:483:LEU:N	1:B:483:LEU:CD1	2.73	0.42
1:B:708:PRO:HG2	1:B:711:GLU:CB	2.50	0.42
1:D:547:ILE:O	1:D:547:ILE:HG13	2.19	0.42
1:A:663:GLY:C	1:A:664:ARG:CD	2.85	0.42
1:C:694:TRP:HE1	1:C:725:PRO:HG3	1.70	0.42
1:D:694:TRP:HD1	1:D:736:MET:HE1	1.85	0.42
1:A:647:LEU:HD21	1:A:664:ARG:CG	2.48	0.42
1:B:535:MET:HE1	1:B:555:THR:HG22	2.01	0.42
1:D:514:VAL:HG23	1:D:514:VAL:O	2.20	0.42
1:D:651:ILE:HA	1:D:651:ILE:HD13	1.63	0.42
1:A:629:ALA:HB2	1:A:692:LEU:HD13	2.01	0.42
1:B:609:GLN:C	1:B:611:ALA:N	2.77	0.42
1:C:738:ASP:O	1:C:748:PRO:HD3	2.20	0.42
1:D:503:ILE:N	1:D:503:ILE:HD12	2.34	0.42
1:D:504:ASP:HB2	1:D:508:PRO:HG2	2.01	0.42
1:D:704:TYR:CE1	1:D:722:MET:CG	3.03	0.42
1:A:541:ILE:HD11	1:A:645:PHE:CE2	2.53	0.42
1:A:630:ARG:HG2	1:A:630:ARG:HH11	1.85	0.42
1:C:474:TRP:HE1	1:C:539:LYS:HG2	1.81	0.42
1:C:617:LEU:HD11	1:C:645:PHE:HE2	1.85	0.42
1:A:567:ALA:HB2	1:A:635:THR:HG22	2.02	0.41
1:B:710:GLU:OE1	1:D:560:LEU:N	2.48	0.41
1:C:572:LEU:HD23	1:C:572:LEU:C	2.45	0.41
1:D:724:LYS:NZ	1:D:724:LYS:HB3	2.33	0.41
1:B:549:ASN:O	1:B:564:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:LYS:HG3	1:B:635:THR:O	2.21	0.41
1:B:612:ARG:HA	1:B:754:VAL:HG22	2.01	0.41
1:B:715:LEU:CD2	1:B:715:LEU:N	2.81	0.41
1:C:474:TRP:CE3	1:C:552:GLY:HA2	2.54	0.41
1:C:651:ILE:HA	1:C:651:ILE:HD13	1.75	0.41
1:B:673:GLU:H	1:B:673:GLU:HG2	1.45	0.41
1:C:485:LYS:CB	1:C:486:PRO:CD	2.99	0.41
1:D:550:LEU:HD12	1:D:551:LEU:N	2.34	0.41
1:A:744:PRO:HG3	3:A:1002:CL:CL	2.50	0.41
1:B:487:LEU:CD2	1:B:497:MET:HB2	2.50	0.41
1:B:604:VAL:HG22	1:B:732:LEU:HD21	2.01	0.41
1:C:625:ARG:O	1:C:665:LEU:CD1	2.68	0.41
1:C:671:ALA:HB3	1:C:674:ALA:HB3	2.01	0.41
1:C:683:GLN:NE2	1:C:683:GLN:CA	2.71	0.41
1:C:687:TRP:O	1:C:687:TRP:HE3	2.02	0.41
1:A:540:MET:CE	1:A:650:ASP:OD2	2.69	0.41
1:A:704:TYR:CD1	1:A:704:TYR:N	2.88	0.41
1:A:727:ASN:OD1	1:A:727:ASN:N	2.54	0.41
1:B:545:LYS:HA	1:B:545:LYS:HD2	1.75	0.41
1:B:662:ASN:O	1:D:525:GLU:HG2	2.21	0.41
1:B:672:PRO:HD3	1:B:687:TRP:CD2	2.56	0.41
1:C:548:ILE:HG22	1:C:645:PHE:CE1	2.49	0.41
1:C:686:VAL:CG2	1:C:747:ARG:CG	2.98	0.41
1:A:545:LYS:HE3	1:A:639:VAL:CG1	2.50	0.41
1:A:640:MET:HE3	1:A:640:MET:HB3	1.83	0.41
1:C:474:TRP:CD1	1:C:539:LYS:HD3	2.56	0.41
1:C:575:TYR:CE1	1:C:579:ARG:NE	2.71	0.41
1:D:481:LEU:CD1	1:D:500:ALA:HB2	2.40	0.41
1:D:535:MET:HE3	1:D:539:LYS:HZ1	1.85	0.41
1:A:733:TYR:CZ	1:A:737:ARG:HD3	2.55	0.41
1:D:560:LEU:HD13	1:D:561:TYR:N	2.36	0.41
1:D:682:HIS:O	1:D:686:VAL:HG12	2.21	0.41
1:B:486:PRO:HB3	1:B:496:VAL:CG2	2.50	0.41
1:C:577:ARG:C	1:C:579:ARG:H	2.29	0.41
1:A:608:TYR:CD1	1:A:608:TYR:O	2.74	0.41
1:A:685:ASP:O	1:A:686:VAL:C	2.63	0.41
1:A:704:TYR:N	1:A:705:PRO:CD	2.84	0.41
1:A:739:CYS:O	1:A:747:ARG:HD3	2.20	0.41
1:B:518:MET:CE	1:B:561:TYR:CE1	3.04	0.41
1:B:614:MET:HB3	1:B:750:PHE:CD2	2.55	0.41
1:C:538:MET:HE1	1:C:564:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:541:ILE:HG21	1:C:547:ILE:CD1	2.51	0.41
1:C:550:LEU:HD12	1:C:550:LEU:HA	1.68	0.41
1:C:551:LEU:HD23	1:C:551:LEU:HA	1.77	0.41
1:C:570:GLY:O	1:C:634:VAL:HG12	2.20	0.41
1:C:581:PRO:CB	1:C:582:PRO:CD	2.96	0.41
1:C:617:LEU:HD23	1:C:622:CYS:HB2	2.03	0.41
1:D:497:MET:HE3	1:D:513:THR:HG21	2.02	0.41
1:D:710:GLU:H	1:D:710:GLU:CD	2.25	0.41
1:A:607:THR:HG21	1:A:757:LEU:HD11	2.03	0.41
1:A:712:LEU:HA	1:A:715:LEU:HD21	2.03	0.41
1:B:609:GLN:O	1:B:612:ARG:N	2.54	0.41
1:C:686:VAL:HG23	1:C:747:ARG:CD	2.41	0.41
1:C:759:ARG:HB2	1:C:759:ARG:NH2	2.36	0.41
1:B:575:TYR:CD1	1:B:575:TYR:C	2.97	0.40
1:B:693:MET:HE1	1:B:735:MET:CG	2.51	0.40
1:D:486:PRO:HA	1:D:496:VAL:HA	2.03	0.40
1:D:494:GLN:HE21	1:D:494:GLN:HB3	1.68	0.40
1:A:514:VAL:CG1	1:A:563:ILE:HB	2.50	0.40
1:A:716:LEU:HD23	1:A:716:LEU:HA	1.49	0.40
1:C:664:ARG:HD3	1:C:664:ARG:N	2.10	0.40
1:C:724:LYS:NZ	1:C:737:ARG:HG2	2.37	0.40
1:D:500:ALA:CA	1:D:503:ILE:HD11	2.50	0.40
1:A:620:GLN:OE1	1:A:620:GLN:HA	2.21	0.40
1:B:721:ARG:NH2	1:B:740:TRP:O	2.55	0.40
1:C:518:MET:HB3	1:C:518:MET:HE2	1.83	0.40
1:C:541:ILE:HG21	1:C:547:ILE:HD11	2.03	0.40
1:C:600:PHE:HE1	1:C:697:PHE:HE1	1.68	0.40
1:D:481:LEU:HD21	1:D:516:VAL:HG21	2.02	0.40
1:D:621:LYS:HG2	1:D:652:ASN:CA	2.52	0.40
1:D:661:THR:CA	1:D:678:ARG:CB	2.95	0.40
1:A:475:GLU:OE1	1:A:555:THR:HB	2.21	0.40
1:A:650:ASP:C	1:A:651:ILE:HD13	2.37	0.40
1:B:663:GLY:HA2	1:D:526:LYS:HB3	2.01	0.40
1:C:703:PRO:HB2	1:C:722:MET:HE1	2.01	0.40
1:A:548:ILE:HD13	1:A:633:LEU:HD12	2.03	0.40
1:A:569:LYS:HB2	1:A:634:VAL:HG13	2.03	0.40
1:B:694:TRP:CD2	1:B:722:MET:HE3	2.56	0.40
1:C:476:PHE:CZ	1:C:501:VAL:O	2.73	0.40
1:D:627:LEU:CD1	1:D:692:LEU:HD22	2.49	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	280/312 (90%)	273 (98%)	7 (2%)	0	100	100
1	B	278/312 (89%)	263 (95%)	13 (5%)	2 (1%)	18	50
1	C	267/312 (86%)	256 (96%)	11 (4%)	0	100	100
1	D	269/312 (86%)	264 (98%)	5 (2%)	0	100	100
All	All	1094/1248 (88%)	1056 (96%)	36 (3%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	507	LYS
1	B	469	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	229/272 (84%)	191 (83%)	38 (17%)	2	13
1	B	230/272 (85%)	178 (77%)	52 (23%)	1	6
1	C	214/272 (79%)	168 (78%)	46 (22%)	1	6
1	D	228/272 (84%)	171 (75%)	57 (25%)	0	4
All	All	901/1088 (83%)	708 (79%)	193 (21%)	1	6

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	479	ASP
1	A	495	VAL
1	A	503	ILE
1	A	519	LEU
1	A	524	THR
1	A	525	GLU
1	A	531	LEU
1	A	546	ASN
1	A	547	ILE
1	A	548	ILE
1	A	549	ASN
1	A	550	LEU
1	A	557	ASP
1	A	560	LEU
1	A	563	ILE
1	A	564	VAL
1	A	620	GLN
1	A	637	ASN
1	A	638	ASN
1	A	644	ASP
1	A	664	ARG
1	A	675	LEU
1	A	681	THR
1	A	683	GLN
1	A	686	VAL
1	A	693	MET
1	A	696	ILE
1	A	698	THR
1	A	699	LEU
1	A	715	LEU
1	A	717	LYS
1	A	727	ASN
1	A	728	CYS
1	A	732	LEU
1	A	741	HIS
1	A	752	GLN
1	A	757	LEU
1	A	759	ARG
1	B	476	PHE
1	B	481	LEU
1	B	482	THR
1	B	483	LEU
1	B	496	VAL

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Mol	Chain	Res	Type
1	B	512	VAL
1	B	514	VAL
1	B	524	THR
1	B	529	SER
1	B	536	GLU
1	B	547	ILE
1	B	549	ASN
1	B	550	LEU
1	B	556	GLN
1	B	560	LEU
1	B	564	VAL
1	B	568	SER
1	B	573	ARG
1	B	599	THR
1	B	601	LYS
1	B	607	THR
1	B	623	ILE
1	B	624	HIS
1	B	627	LEU
1	B	636	GLU
1	B	638	ASN
1	B	642	ILE
1	B	644	ASP
1	B	647	LEU
1	B	651	ILE
1	B	653	ASN
1	B	655	ASP
1	B	657	TYR
1	B	660	THR
1	B	665	LEU
1	B	673	GLU
1	B	679	VAL
1	B	681	THR
1	B	682	HIS
1	B	686	VAL
1	B	709	VAL
1	B	715	LEU
1	B	716	LEU
1	B	727	ASN
1	B	729	THR
1	B	732	LEU
1	B	734	MET

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Mol	Chain	Res	Type
1	B	741	HIS
1	B	749	THR
1	B	762	THR
1	B	763	LEU
1	B	764	THR
1	C	467	GLU
1	C	481	LEU
1	C	482	THR
1	C	495	VAL
1	C	497	MET
1	C	501	VAL
1	C	516	VAL
1	C	519	LEU
1	C	522	ASP
1	C	524	THR
1	C	529	SER
1	C	531	LEU
1	C	532	VAL
1	C	548	ILE
1	C	560	LEU
1	C	562	VAL
1	C	572	LEU
1	C	598	MET
1	C	601	LYS
1	C	606	CYS
1	C	617	LEU
1	C	620	GLN
1	C	623	ILE
1	C	630	ARG
1	C	632	VAL
1	C	633	LEU
1	C	637	ASN
1	C	647	LEU
1	C	651	ILE
1	C	667	VAL
1	C	675	LEU
1	C	681	THR
1	C	682	HIS
1	C	683	GLN
1	C	687	TRP
1	C	699	LEU
1	C	707	ILE

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Mol	Chain	Res	Type
1	C	724	LYS
1	C	728	CYS
1	C	732	LEU
1	C	734	MET
1	C	737	ARG
1	C	741	HIS
1	C	743	VAL
1	C	751	LYS
1	C	763	LEU
1	D	468	LEU
1	D	471	ASP
1	D	482	THR
1	D	501	VAL
1	D	503	ILE
1	D	512	VAL
1	D	525	GLU
1	D	528	LEU
1	D	531	LEU
1	D	548	ILE
1	D	550	LEU
1	D	555	THR
1	D	556	GLN
1	D	564	VAL
1	D	571	ASN
1	D	599	THR
1	D	601	LYS
1	D	607	THR
1	D	620	GLN
1	D	622	CYS
1	D	626	ASP
1	D	627	LEU
1	D	632	VAL
1	D	636	GLU
1	D	637	ASN
1	D	639	VAL
1	D	640	MET
1	D	644	ASP
1	D	650	ASP
1	D	651	ILE
1	D	657	TYR
1	D	664	ARG
1	D	670	MET

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Mol	Chain	Res	Type
1	D	673	GLU
1	D	675	LEU
1	D	679	VAL
1	D	681	THR
1	D	686	VAL
1	D	692	LEU
1	D	694	TRP
1	D	696	ILE
1	D	699	LEU
1	D	707	ILE
1	D	709	VAL
1	D	715	LEU
1	D	720	HIS
1	D	724	LYS
1	D	727	ASN
1	D	728	CYS
1	D	729	THR
1	D	738	ASP
1	D	741	HIS
1	D	745	SER
1	D	749	THR
1	D	752	GLN
1	D	755	GLU
1	D	760	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	683	GLN
1	A	746	GLN
1	B	544	HIS
1	B	549	ASN
1	B	556	GLN
1	B	727	ASN
1	C	683	GLN
1	C	741	HIS
1	D	494	GLN
1	D	549	ASN
1	D	556	GLN
1	D	662	ASN
1	D	746	GLN
1	D	752	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	PTR	A	656	1	15,16,17	0.71	0	17,22,24	0.98	0
1	PTR	B	656	1	15,16,17	0.72	0	17,22,24	1.17	1 (5%)

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
1	PTR	A	656	1	-	0/10/11/13	0/1/1/1
1	PTR	B	656	1	-	2/10/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	656	PTR	OH-CZ-CE1	2.05	125.35	119.22

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	656	PTR	N-CA-CB-CG
1	B	656	PTR	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	656	PTR	8	0
1	B	656	PTR	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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$
2	KX0	D	1001	-	32,32,32	4.75	11 (34%)	36,46,46	1.90	8 (22%)
2	KX0	A	1001	-	32,32,32	4.60	9 (28%)	36,46,46	1.76	8 (22%)
2	KX0	B	1001	-	32,32,32	4.40	8 (25%)	36,46,46	1.83	8 (22%)
2	KX0	C	1001	-	32,32,32	4.57	10 (31%)	36,46,46	1.63	9 (25%)

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
2	KX0	D	1001	-	-	6/8/16/16	0/4/5/5
2	KX0	A	1001	-	-	8/8/16/16	0/4/5/5
2	KX0	B	1001	-	-	6/8/16/16	0/4/5/5
2	KX0	C	1001	-	-	6/8/16/16	0/4/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	KX0	C05-N04	24.19	1.44	1.29
2	C	1001	KX0	C05-N04	23.41	1.43	1.29
2	A	1001	KX0	C05-N04	23.34	1.43	1.29
2	B	1001	KX0	C05-N04	22.03	1.43	1.29
2	A	1001	KX0	C16-N15	6.30	1.47	1.37
2	B	1001	KX0	C16-N15	6.15	1.47	1.37
2	C	1001	KX0	C16-N15	5.84	1.47	1.37
2	D	1001	KX0	C16-N15	5.78	1.46	1.37
2	A	1001	KX0	C14-N15	5.01	1.48	1.42
2	B	1001	KX0	C14-N15	4.68	1.48	1.42
2	C	1001	KX0	C14-N15	4.34	1.47	1.42
2	D	1001	KX0	C13-C05	4.26	1.55	1.49
2	D	1001	KX0	C14-N15	3.96	1.47	1.42
2	B	1001	KX0	C03-C16	-3.60	1.34	1.42
2	D	1001	KX0	C06-C05	3.49	1.55	1.49
2	C	1001	KX0	C13-C05	3.25	1.53	1.49
2	B	1001	KX0	C13-C05	3.22	1.53	1.49
2	A	1001	KX0	C13-C05	3.00	1.53	1.49
2	C	1001	KX0	C03-C16	-2.99	1.36	1.42
2	C	1001	KX0	C20-N23	2.95	1.44	1.37
2	A	1001	KX0	C16-N17	2.94	1.36	1.32
2	D	1001	KX0	C03-C16	-2.88	1.36	1.42
2	B	1001	KX0	C16-N17	2.85	1.36	1.32
2	A	1001	KX0	C20-N23	2.77	1.43	1.37
2	A	1001	KX0	C03-C16	-2.76	1.36	1.42
2	B	1001	KX0	C13-C14	-2.73	1.36	1.41
2	D	1001	KX0	C16-N17	2.68	1.36	1.32
2	D	1001	KX0	C13-C14	-2.47	1.37	1.41
2	C	1001	KX0	C16-N17	2.43	1.35	1.32
2	B	1001	KX0	C20-N23	2.41	1.43	1.37
2	D	1001	KX0	C03-N04	2.41	1.46	1.39
2	A	1001	KX0	C03-N04	2.24	1.46	1.39
2	A	1001	KX0	C13-C14	-2.23	1.37	1.41
2	D	1001	KX0	C20-N23	2.17	1.42	1.37
2	C	1001	KX0	C13-C14	-2.15	1.37	1.41
2	C	1001	KX0	C03-N04	2.09	1.45	1.39
2	D	1001	KX0	C02-N18	-2.05	1.31	1.34
2	C	1001	KX0	C06-C05	2.01	1.52	1.49

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	KX0	C01-C02-C03	-5.26	124.95	132.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	KX0	C16-N17-N18	5.07	107.20	103.32
2	D	1001	KX0	C16-N17-N18	4.85	107.04	103.32
2	B	1001	KX0	C16-N17-N18	4.75	106.96	103.32
2	D	1001	KX0	C13-C05-N04	-4.65	117.83	125.39
2	A	1001	KX0	C01-C02-C03	-4.63	125.80	132.11
2	C	1001	KX0	C16-N17-N18	4.09	106.45	103.32
2	C	1001	KX0	C01-C02-C03	-3.86	126.85	132.11
2	D	1001	KX0	C03-N04-C05	3.76	133.84	122.71
2	D	1001	KX0	C01-C02-C03	-3.70	127.07	132.11
2	B	1001	KX0	C01-C02-N18	3.21	126.88	121.81
2	B	1001	KX0	C03-N04-C05	3.21	132.20	122.71
2	D	1001	KX0	C14-C13-C05	2.98	125.06	121.85
2	D	1001	KX0	C28-N23-C24	-2.75	105.39	111.57
2	C	1001	KX0	C14-C13-C05	2.73	124.79	121.85
2	C	1001	KX0	C13-C05-N04	-2.67	121.06	125.39
2	A	1001	KX0	C01-C02-N18	2.63	125.96	121.81
2	B	1001	KX0	C19-C20-N23	-2.58	119.24	122.35
2	A	1001	KX0	C03-N04-C05	2.56	130.29	122.71
2	C	1001	KX0	C01-C02-N18	2.51	125.77	121.81
2	B	1001	KX0	C28-N23-C24	-2.43	106.09	111.57
2	A	1001	KX0	C28-N23-C24	-2.40	106.16	111.57
2	C	1001	KX0	C13-C14-N15	2.36	126.58	123.44
2	C	1001	KX0	C28-N23-C24	-2.30	106.40	111.57
2	C	1001	KX0	C22-N21-C20	2.26	121.11	117.41
2	A	1001	KX0	C14-C13-C05	2.22	124.24	121.85
2	C	1001	KX0	C03-N04-C05	2.16	129.09	122.71
2	D	1001	KX0	C08-C07-C06	2.14	123.67	119.80
2	B	1001	KX0	C13-C14-N15	2.13	126.28	123.44
2	D	1001	KX0	C27-O26-C25	2.11	116.72	109.88
2	A	1001	KX0	C22-N21-C20	2.11	120.86	117.41
2	B	1001	KX0	C07-C06-C11	2.09	120.23	117.79
2	A	1001	KX0	C13-C05-N04	-2.06	122.04	125.39

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	KX0	C19-C20-N23-C24
2	A	1001	KX0	N21-C20-N23-C24
2	A	1001	KX0	C13-C05-C06-C07
2	A	1001	KX0	C13-C05-C06-C11
2	A	1001	KX0	N04-C05-C06-C07

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Mol	Chain	Res	Type	Atoms
2	A	1001	KX0	N04-C05-C06-C11
2	B	1001	KX0	C19-C20-N23-C24
2	B	1001	KX0	N21-C20-N23-C24
2	B	1001	KX0	C13-C05-C06-C07
2	B	1001	KX0	C13-C05-C06-C11
2	B	1001	KX0	N04-C05-C06-C07
2	B	1001	KX0	N04-C05-C06-C11
2	C	1001	KX0	C13-C05-C06-C07
2	C	1001	KX0	C13-C05-C06-C11
2	C	1001	KX0	N04-C05-C06-C07
2	C	1001	KX0	N04-C05-C06-C11
2	D	1001	KX0	C19-C20-N23-C24
2	D	1001	KX0	N21-C20-N23-C24
2	D	1001	KX0	C13-C05-C06-C07
2	D	1001	KX0	C13-C05-C06-C11
2	D	1001	KX0	N04-C05-C06-C07
2	D	1001	KX0	N04-C05-C06-C11
2	C	1001	KX0	N21-C20-N23-C24
2	A	1001	KX0	C19-C20-N23-C28
2	C	1001	KX0	C19-C20-N23-C24
2	A	1001	KX0	N21-C20-N23-C28

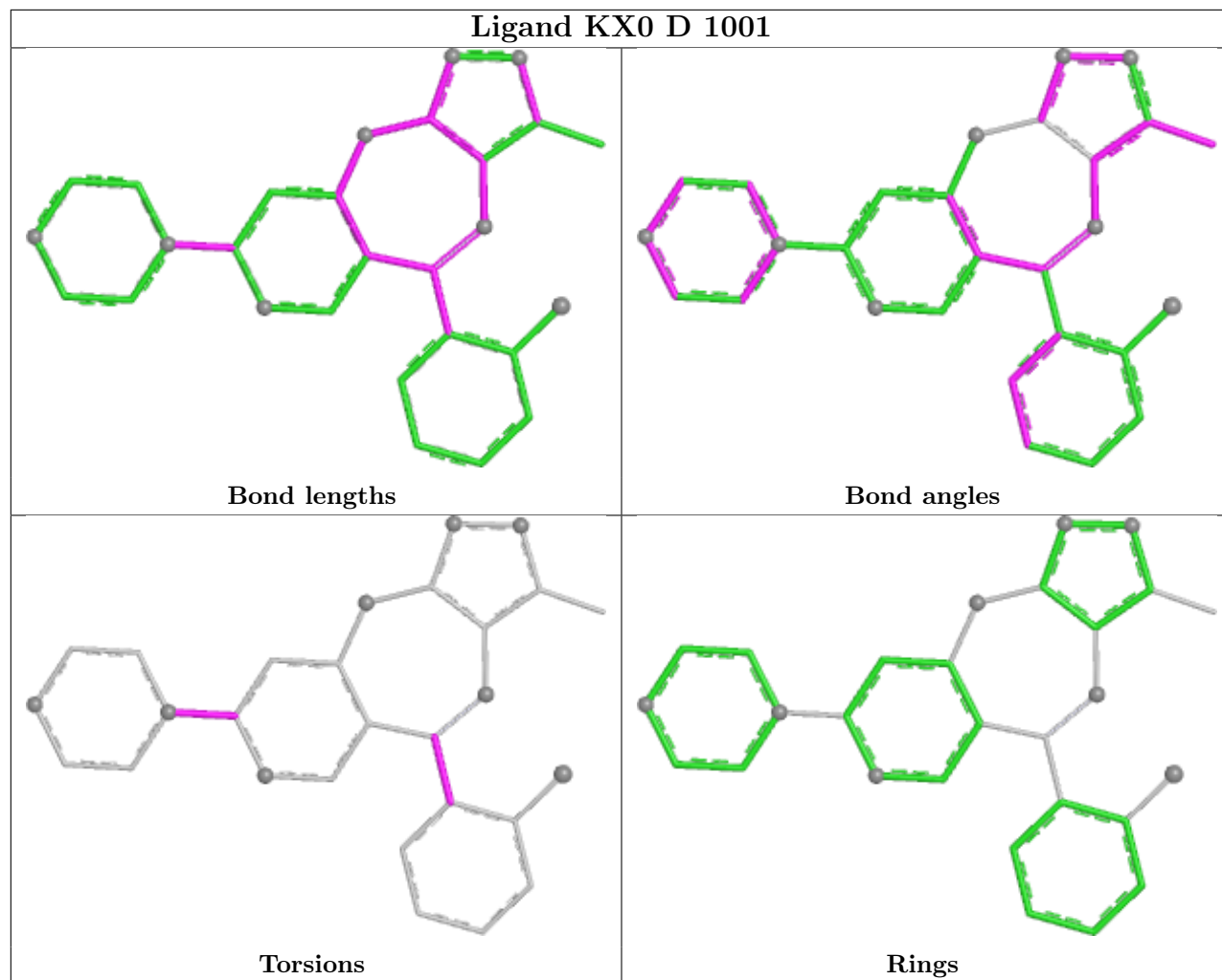
There are no ring outliers.

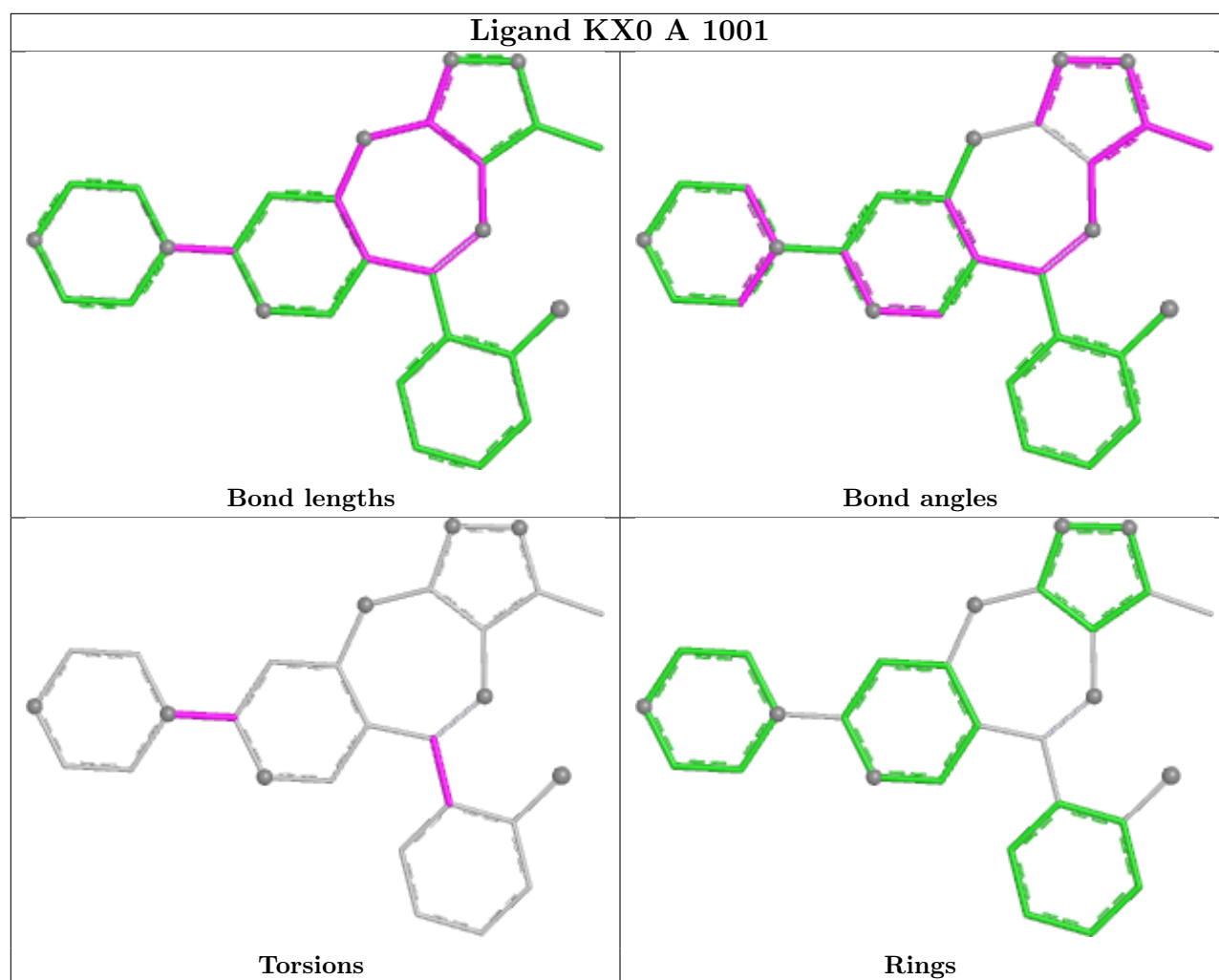
4 monomers are involved in 10 short contacts:

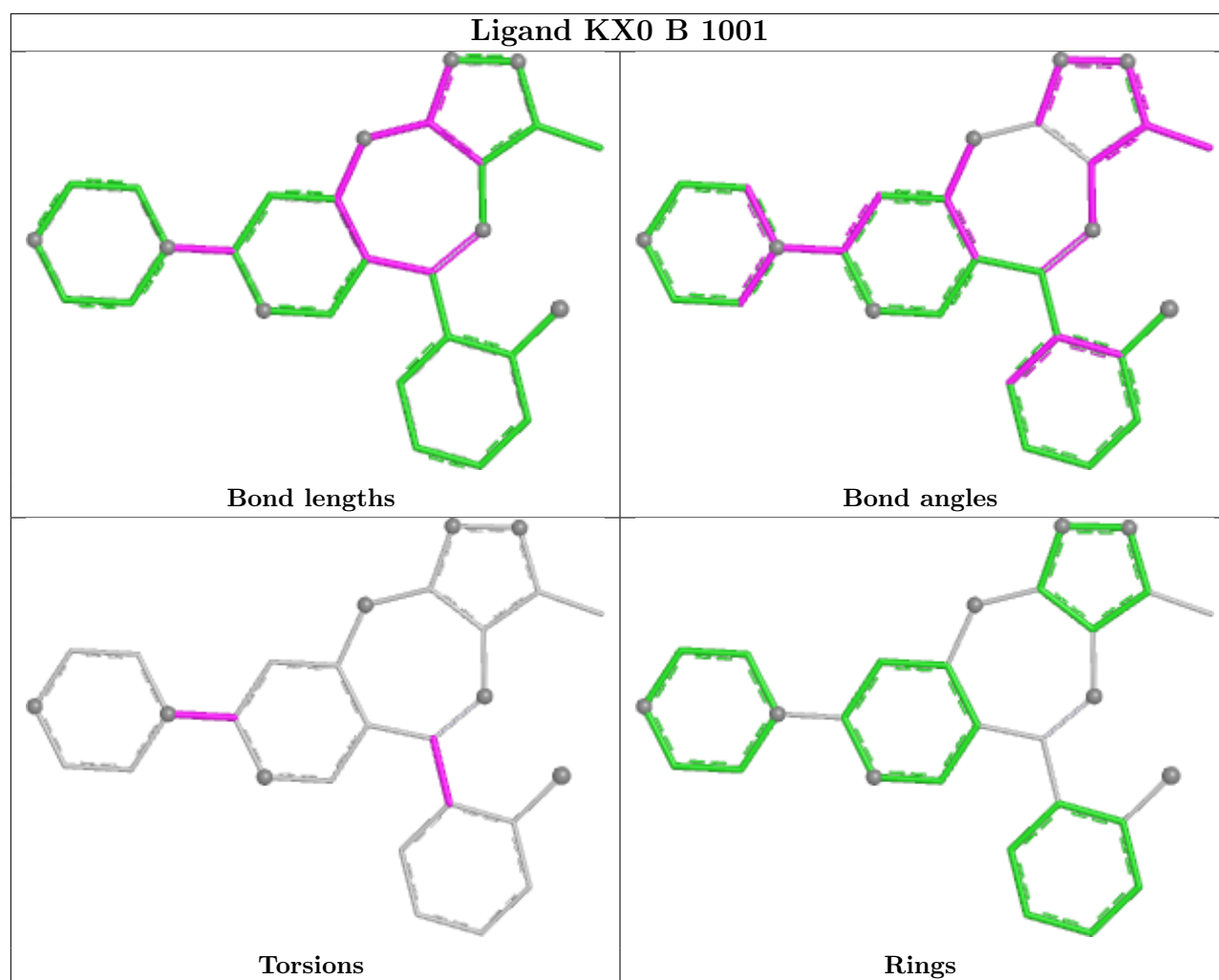
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1001	KX0	2	0
2	A	1001	KX0	4	0
2	B	1001	KX0	2	0
2	C	1001	KX0	2	0

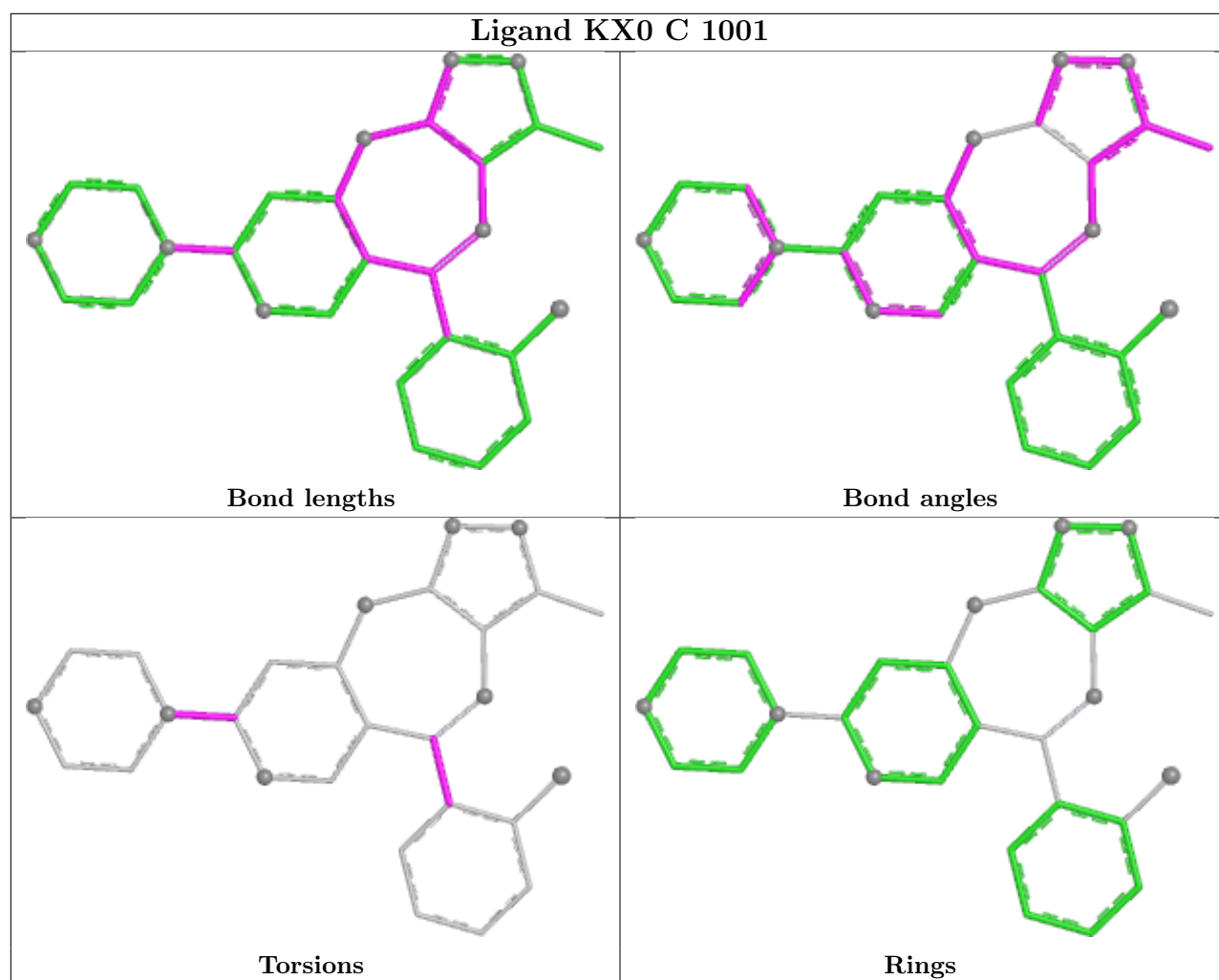
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	284/312 (91%)	0.15	2 (0%) 84 65	31, 54, 82, 102	0
1	B	282/312 (90%)	0.19	4 (1%) 73 50	37, 56, 92, 113	0
1	C	275/312 (88%)	0.21	3 (1%) 78 56	36, 66, 87, 138	0
1	D	277/312 (88%)	0.22	2 (0%) 84 65	42, 64, 89, 130	0
All	All	1118/1248 (89%)	0.19	11 (0%) 79 57	31, 61, 88, 138	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	683	GLN	2.7
1	B	742	ALA	2.4
1	B	657	TYR	2.4
1	C	566	TYR	2.3
1	A	655	ASP	2.3
1	B	522	ASP	2.3
1	B	471	ASP	2.1
1	D	661	THR	2.1
1	A	674	ALA	2.1
1	D	662	ASN	2.1
1	C	647	LEU	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PTR	A	656	16/17	0.85	0.14	65,70,84,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	PTR	B	656	16/17	0.90	0.12	45,58,74,82	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

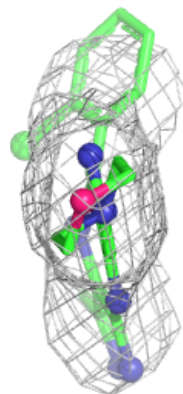
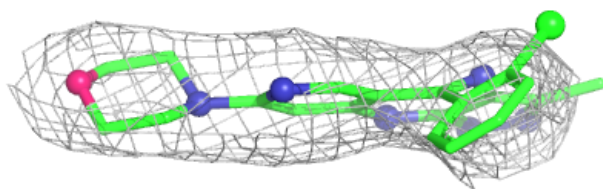
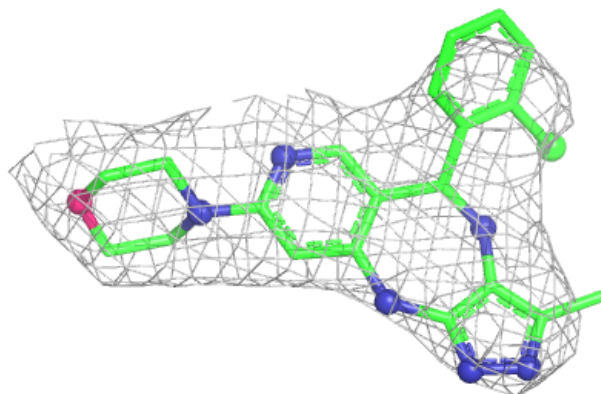
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	KX0	B	1001	28/28	0.87	0.14	41,59,77,104	0
2	KX0	C	1001	28/28	0.87	0.11	57,67,82,83	0
3	CL	A	1002	1/1	0.87	0.13	28,28,28,28	0
2	KX0	A	1001	28/28	0.88	0.12	39,59,69,76	0
2	KX0	D	1001	28/28	0.90	0.12	51,61,85,92	0

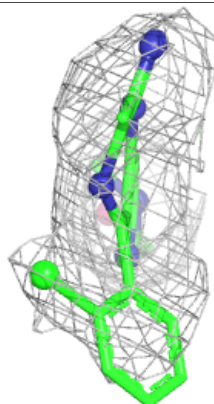
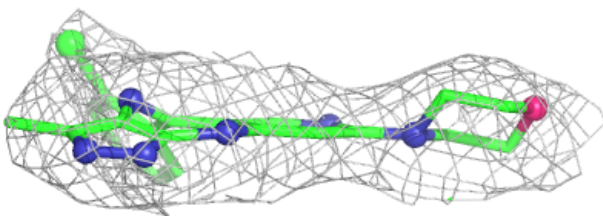
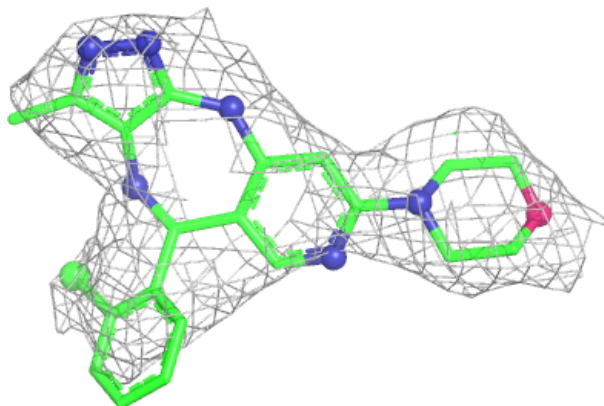
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KX0 B 1001:

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

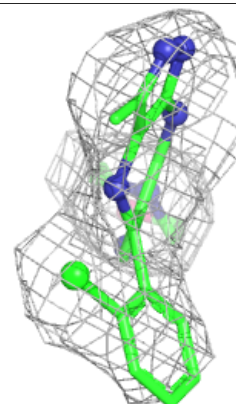
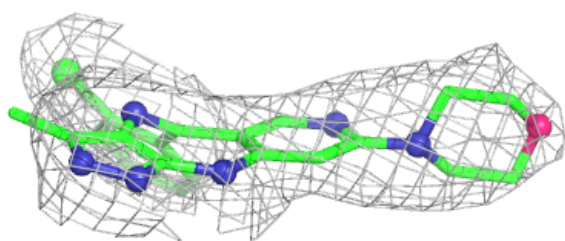
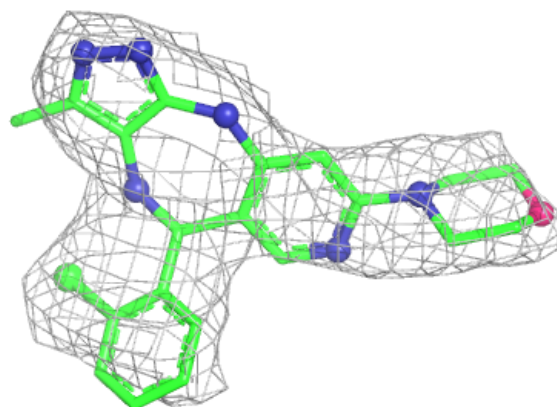
**Electron density around KX0 C 1001:**

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



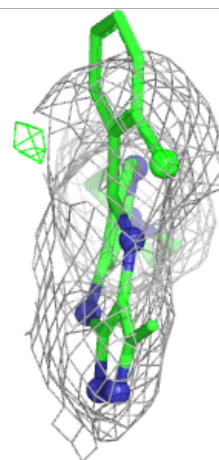
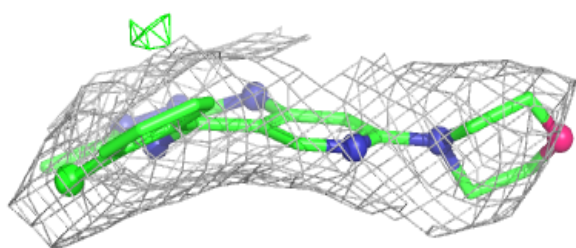
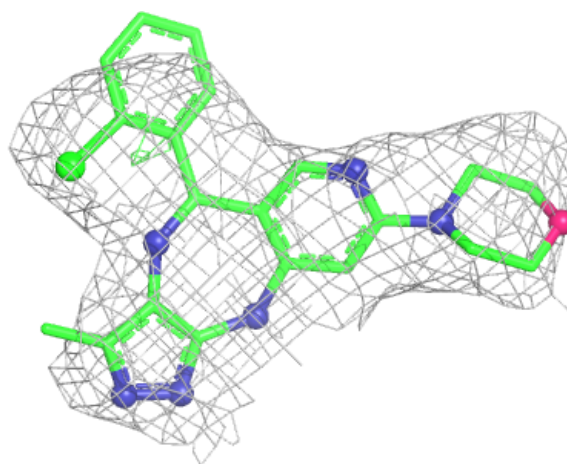
Electron density around KX0 A 1001:

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



Electron density around KX0 D 1001:

$2mF_o-DF_c$ (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.