



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:45 pm BST

PDB ID : 6B3W
Title : Structure of Hs/AcPRC2 in complex with 5,8-dichloro-7-(3,5-dimethyl-1,2-oxazol-4-yl)-2-[(4,6-dimethyl-2-oxo-1,2-dihydropyridin-3-yl)methyl]-3,4-dihydroisoquinolin-1(2H)-one
Authors : Gajiwala, K.S.; Brooun, A.; Liu, W.; Deng, Y.; Stewart, A.E.
Deposited on : 2017-09-25
Resolution : 3.05 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 : 2.11
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) : 2.11

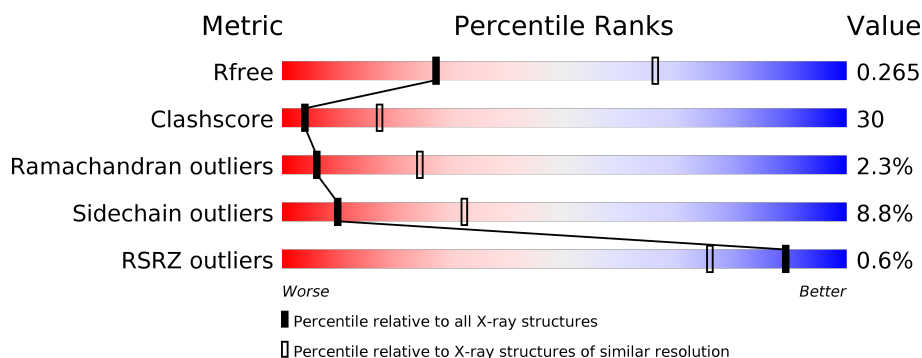
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	643	<div> <div></div> <div>36%31%5%28%</div> </div>
1	B	643	<div> <div>%</div> <div>37%29%6%28%</div> </div>
2	E	362	<div> <div></div> <div>48%46%..</div> </div>
2	F	362	<div> <div></div> <div>53%42%..</div> </div>
3	S	191	<div> <div>%</div> <div>30%32%5%33%</div> </div>
3	T	191	<div> <div></div> <div>22%38%6%.33%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15564 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 Enhancer of zeste 2 polycomb repressive complex 2 subunit, Enhancer of zeste 2 polycomb repressive complex 2 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3769	2365	678	688	38			
1	B	465	Total	C	N	O	S	0	0	0
			3777	2368	679	692	38			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	389	LEU	-	linker	UNP G1KPH4
A	390	GLY	-	linker	UNP G1KPH4
A	391	GLY	-	linker	UNP G1KPH4
A	392	GLY	-	linker	UNP G1KPH4
A	393	GLY	-	linker	UNP G1KPH4
A	394	SER	-	linker	UNP G1KPH4
A	395	GLY	-	linker	UNP G1KPH4
A	396	GLY	-	linker	UNP G1KPH4
A	397	GLY	-	linker	UNP G1KPH4
A	398	GLY	-	linker	UNP G1KPH4
A	399	SER	-	linker	UNP G1KPH4
A	400	GLY	-	linker	UNP G1KPH4
A	401	GLY	-	linker	UNP G1KPH4
A	402	GLY	-	linker	UNP G1KPH4
A	403	GLY	-	linker	UNP G1KPH4
A	404	SER	-	linker	UNP G1KPH4
A	405	ALA	-	linker	UNP G1KPH4
A	406	ALA	-	linker	UNP G1KPH4
A	407	ALA	-	linker	UNP G1KPH4
B	389	LEU	-	linker	UNP G1KPH4
B	390	GLY	-	linker	UNP G1KPH4
B	391	GLY	-	linker	UNP G1KPH4
B	392	GLY	-	linker	UNP G1KPH4
B	393	GLY	-	linker	UNP G1KPH4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	394	SER	-	linker	UNP G1KPH4
B	395	GLY	-	linker	UNP G1KPH4
B	396	GLY	-	linker	UNP G1KPH4
B	397	GLY	-	linker	UNP G1KPH4
B	398	GLY	-	linker	UNP G1KPH4
B	399	SER	-	linker	UNP G1KPH4
B	400	GLY	-	linker	UNP G1KPH4
B	401	GLY	-	linker	UNP G1KPH4
B	402	GLY	-	linker	UNP G1KPH4
B	403	GLY	-	linker	UNP G1KPH4
B	404	SER	-	linker	UNP G1KPH4
B	405	ALA	-	linker	UNP G1KPH4
B	406	ALA	-	linker	UNP G1KPH4
B	407	ALA	-	linker	UNP G1KPH4

- Molecule 2 is a protein called Polycomb protein EED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	358	Total	C	N	O	S	0	0	0
			2898	1834	509	534	21			
2	F	359	Total	C	N	O	S	0	0	0
			2906	1840	510	535	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	66	MET	-	expression tag	UNP O75530
F	66	MET	-	expression tag	UNP O75530

- Molecule 3 is a protein called Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	128	Total	C	N	O	S	0	0	0
			1070	675	185	198	12			
3	T	128	Total	C	N	O	S	0	0	0
			1070	675	185	198	12			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	535	MET	-	expression tag	UNP Q15022
S	536	ASP	-	expression tag	UNP Q15022

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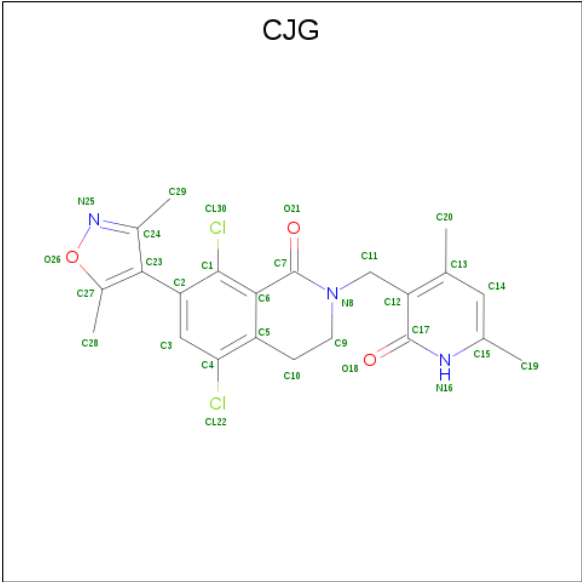
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Chain	Residue	Modelled	Actual	Comment	Reference
S	537	TYR	-	expression tag	UNP Q15022
S	538	LYS	-	expression tag	UNP Q15022
S	539	ASP	-	expression tag	UNP Q15022
S	540	ASP	-	expression tag	UNP Q15022
S	541	ASP	-	expression tag	UNP Q15022
S	542	ASP	-	expression tag	UNP Q15022
S	543	LYS	-	expression tag	UNP Q15022
S	544	GLY	-	expression tag	UNP Q15022
S	583	ASP	SER	conflict	UNP Q15022
T	535	MET	-	expression tag	UNP Q15022
T	536	ASP	-	expression tag	UNP Q15022
T	537	TYR	-	expression tag	UNP Q15022
T	538	LYS	-	expression tag	UNP Q15022
T	539	ASP	-	expression tag	UNP Q15022
T	540	ASP	-	expression tag	UNP Q15022
T	541	ASP	-	expression tag	UNP Q15022
T	542	ASP	-	expression tag	UNP Q15022
T	543	LYS	-	expression tag	UNP Q15022
T	544	GLY	-	expression tag	UNP Q15022
T	583	ASP	SER	conflict	UNP Q15022

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

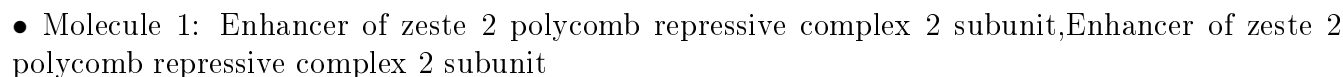
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	7	Total	Zn	0	0
			7	7		
4	A	7	Total	Zn	0	0
			7	7		

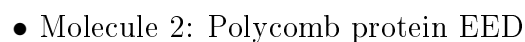
- Molecule 5 is 5,8-dichloro-7-(3,5-dimethyl-1,2-oxazol-4-yl)-2-[(4,6-dimethyl-2-oxo-1,2-dihydropyridin-3-yl)methyl]-3,4-dihydroisoquinolin-1(2H)-one (three-letter code: CJG) (formula: C₂₂H₂₁Cl₂N₃O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0	0
			30	22	2	3	3		
5	B	1	Total	C	Cl	N	O	0	0
			30	22	2	3	3		

- Molecule 1: Enhancer of zeste 2 polycomb repressive complex 2 subunit, Enhancer of zeste 2 polycomb repressive complex 2 subunit



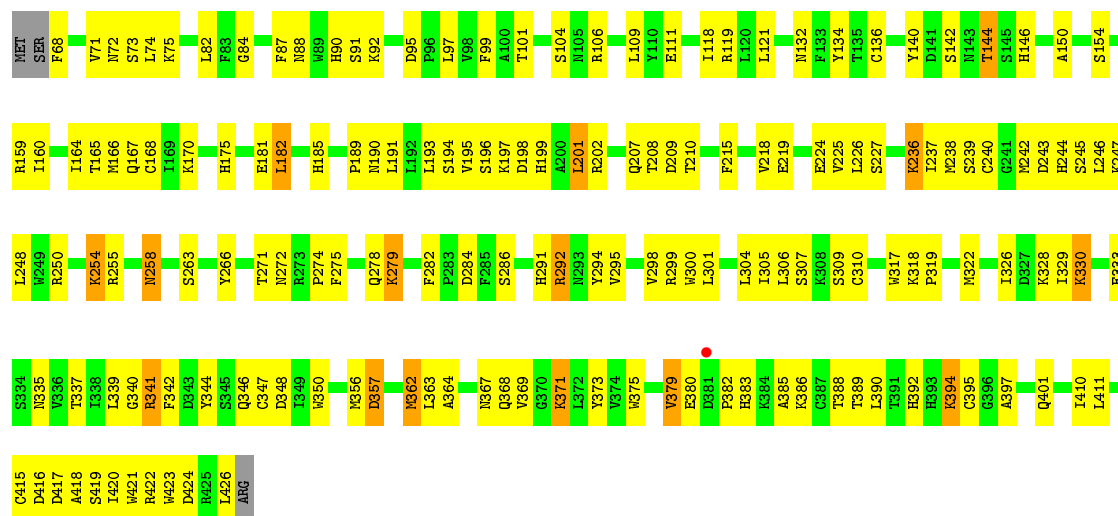


Response	Percentage
Yes	48%
No	46%

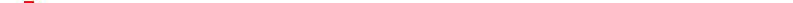


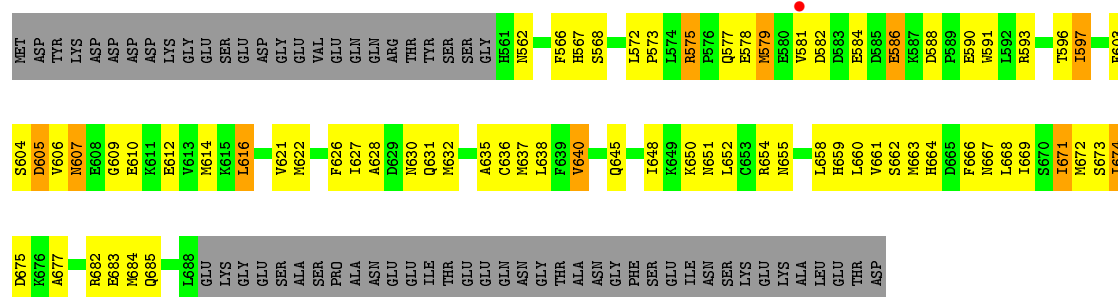
- Molecule 2: Polycomb protein EED

Chain F: 53% 42% 5%

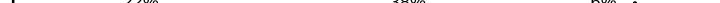


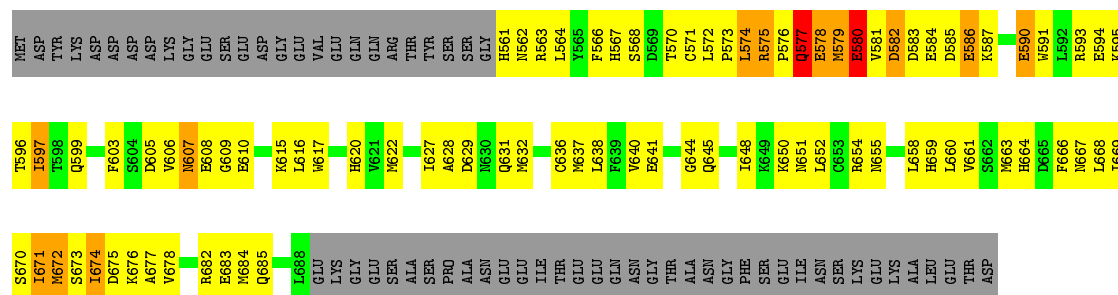
- Molecule 3: Polycomb protein SUZ12

Chain S: 



- Molecule 3: Polycomb protein SUZ12

Chain T:  22% 38% 6% 1% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.78Å 115.18Å 150.97Å 90.00° 102.58° 90.00°	Depositor
Resolution (Å)	147.34 – 3.05 147.34 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (147.34-3.05) 98.6 (147.34-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 3.01Å)	Xtriage
Refinement program	CNS 2005	Depositor
R, R_{free}	0.224 , 0.282 0.209 , 0.265	Depositor DCC
R_{free} test set	2404 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15564	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.91% 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: ZN, CJG

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	0.43	0/3850	0.55	0/5176
1	B	0.42	0/3856	0.55	0/5184
2	E	0.43	0/2972	0.59	0/4026
2	F	0.40	0/2980	0.58	0/4037
3	S	0.44	0/1091	0.56	0/1464
3	T	0.41	0/1091	0.56	0/1464
All	All	0.42	0/15840	0.56	0/21351

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
3	S	0	2
3	T	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	S	578	GLU	Peptide
3	S	582	ASP	Peptide
3	T	578	GLU	Peptide

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	3769	0	3657	229	0
1	B	3777	0	3672	228	0
2	E	2898	0	2812	193	0
2	F	2906	0	2823	171	0
3	S	1070	0	1052	88	0
3	T	1070	0	1052	109	0
4	A	7	0	0	0	0
4	B	7	0	0	0	0
5	A	30	0	0	0	0
5	B	30	0	0	0	0
All	All	15564	0	15068	921	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 30.

All (921) 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)
2:F:330:LYS:H	2:F:330:LYS:HD3	1.21	1.01
1:A:494:LYS:HB3	1:A:507:SER:HB3	1.44	0.99
1:A:357:ARG:HB3	1:A:357:ARG:HH11	1.27	0.99
3:T:628:ALA:H	3:T:631:GLN:HE21	1.08	0.98
2:F:367:ASN:HD22	2:F:371:LYS:HB2	1.26	0.98
2:E:367:ASN:HD22	2:E:371:LYS:HB2	1.27	0.97
1:A:567:ASN:HD22	1:A:569:ASP:H	1.05	0.95
2:E:330:LYS:HD3	2:E:330:LYS:H	1.30	0.95
2:F:193:LEU:HD22	2:F:237:ILE:HD13	1.48	0.94
2:E:165:THR:HG22	2:E:167:GLN:HG2	1.48	0.94
2:E:195:VAL:HG22	2:E:201:LEU:HD13	1.51	0.93
1:B:357:ARG:HB3	1:B:357:ARG:HH11	1.31	0.93
1:B:567:ASN:ND2	1:B:569:ASP:H	1.67	0.93
1:B:494:LYS:HB3	1:B:507:SER:HB3	1.49	0.92
1:A:96:ILE:HG12	1:A:97:PRO:HD2	1.50	0.92
1:A:567:ASN:ND2	1:A:569:ASP:H	1.67	0.91
2:E:224:GLU:HB3	2:E:242:MET:HG3	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLN:HE22	1:A:31:ARG:HD3	1.33	0.91
3:T:628:ALA:H	3:T:631:GLN:NE2	1.67	0.90
1:A:293:THR:HG22	1:A:445:GLN:HE21	1.37	0.90
2:E:425:ARG:HH21	2:E:425:ARG:HG2	1.36	0.90
1:B:293:THR:HG22	1:B:445:GLN:HE21	1.37	0.88
1:B:567:ASN:HD22	1:B:569:ASP:H	1.22	0.88
3:T:627:ILE:H	3:T:631:GLN:HE22	1.19	0.88
1:B:96:ILE:HG12	1:B:97:PRO:HD2	1.54	0.87
2:F:224:GLU:HB3	2:F:242:MET:HG3	1.56	0.87
2:F:175:HIS:HE1	2:F:194:SER:OG	1.57	0.86
1:B:460:LYS:HD3	1:B:460:LYS:H	1.42	0.85
2:E:425:ARG:HH21	2:E:425:ARG:CG	1.88	0.85
2:E:197:LYS:HA	2:E:224:GLU:HG3	1.58	0.85
2:F:197:LYS:HA	2:F:224:GLU:HG3	1.58	0.84
2:F:165:THR:HG22	2:F:167:GLN:HG2	1.59	0.84
2:E:68:PHE:HB2	2:E:390:LEU:HD11	1.60	0.83
1:A:460:LYS:H	1:A:460:LYS:HD3	1.44	0.83
1:A:580:LYS:NZ	3:T:581:VAL:HG13	1.94	0.83
2:E:254:LYS:HE2	2:E:254:LYS:H	1.44	0.83
1:B:567:ASN:C	1:B:567:ASN:HD22	1.82	0.83
1:B:580:LYS:NZ	3:S:581:VAL:HG13	1.94	0.82
3:T:627:ILE:H	3:T:631:GLN:NE2	1.78	0.82
1:A:293:THR:HG22	1:A:445:GLN:NE2	1.95	0.82
1:A:424:ARG:NH1	2:E:170:LYS:HA	1.95	0.81
2:E:340:GLY:HA3	2:E:382:PRO:HG3	1.61	0.81
2:F:330:LYS:HD3	2:F:330:LYS:N	1.96	0.81
3:S:628:ALA:H	3:S:631:GLN:HE21	1.27	0.81
3:S:628:ALA:H	3:S:631:GLN:NE2	1.78	0.81
2:E:159:ARG:HH11	2:E:159:ARG:HG2	1.46	0.81
3:T:606:VAL:CG1	3:T:610:GLU:HG3	2.10	0.81
3:T:655:ASN:HA	3:T:658:LEU:HD13	1.63	0.81
2:E:341:ARG:O	2:E:382:PRO:HB2	1.80	0.80
1:A:510:HIS:NE2	3:T:580:GLU:HA	1.97	0.80
3:S:671:ILE:O	3:S:674:ILE:HG22	1.81	0.79
1:A:119:ASN:ND2	1:A:542:ILE:HD11	1.98	0.79
1:A:355:ILE:O	1:A:359:ILE:HG13	1.83	0.78
1:B:94:GLN:HE22	2:E:119:ARG:HA	1.47	0.78
3:S:567:HIS:HA	3:S:581:VAL:HG23	1.65	0.78
3:T:593:ARG:O	3:T:596:THR:HG22	1.83	0.78
1:B:418:GLN:HA	1:B:418:GLN:HE21	1.48	0.78
2:E:175:HIS:HE1	2:E:194:SER:OG	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:409:SER:HA	2:E:425:ARG:HD2	1.66	0.78
1:A:123:GLU:HG2	1:A:124:ASP:N	1.98	0.78
3:T:628:ALA:N	3:T:631:GLN:HE21	1.82	0.77
1:A:39:LYS:HD3	2:F:380:GLU:CB	2.15	0.77
2:F:326:ILE:HA	2:F:329:ILE:HD12	1.66	0.77
2:E:394:LYS:HB3	2:E:421:TRP:HH2	1.49	0.76
1:A:39:LYS:HD3	2:F:380:GLU:HB3	1.66	0.76
1:A:85:VAL:HG11	2:F:74:LEU:HD23	1.68	0.76
3:S:627:ILE:H	3:S:631:GLN:HE22	1.34	0.76
1:A:119:ASN:HD22	1:A:542:ILE:HD11	1.50	0.76
1:A:224:THR:O	1:A:228:LEU:HG	1.86	0.75
2:F:340:GLY:HA3	2:F:382:PRO:HG3	1.69	0.75
1:A:171:PHE:O	1:A:175:VAL:HG23	1.87	0.75
1:B:460:LYS:HD3	1:B:460:LYS:N	2.01	0.75
2:F:319:PRO:HG2	2:F:329:ILE:HD13	1.65	0.75
1:B:460:LYS:H	1:B:460:LYS:CD	1.99	0.75
3:S:627:ILE:H	3:S:631:GLN:NE2	1.84	0.75
1:A:39:LYS:HD3	2:F:380:GLU:HG3	1.68	0.75
1:A:67:PRO:HG3	2:F:95:ASP:OD2	1.87	0.74
2:F:254:LYS:HE2	2:F:254:LYS:H	1.53	0.74
1:B:122:VAL:HG22	1:B:543:ILE:HG22	1.68	0.74
1:A:94:GLN:HE22	2:F:119:ARG:HA	1.51	0.74
2:E:367:ASN:ND2	2:E:371:LYS:HB2	2.00	0.74
1:A:555:TYR:HE2	1:A:563:LEU:HD11	1.53	0.73
1:B:253:ASP:OD1	3:S:654:ARG:HB2	1.88	0.73
2:F:190:ASN:ND2	2:F:207:GLN:HB2	2.02	0.73
2:E:330:LYS:HE2	2:E:333:GLU:OE1	1.89	0.73
2:E:425:ARG:NH2	2:E:425:ARG:HG2	2.03	0.72
1:B:249:THR:N	1:B:250:PRO:HD3	2.04	0.72
2:F:201:LEU:HB2	2:F:215:PHE:HB2	1.71	0.72
2:F:367:ASN:ND2	2:F:371:LYS:HB2	2.03	0.72
3:S:648:ILE:HD13	3:S:685:GLN:HA	1.71	0.71
3:T:578:GLU:HG3	3:T:580:GLU:CD	2.10	0.71
3:S:581:VAL:O	3:S:581:VAL:HG22	1.90	0.71
2:E:397:ALA:HB2	2:E:417:ASP:OD2	1.90	0.71
1:B:273:PHE:HB2	1:B:280:TYR:CE1	2.26	0.71
1:B:464:ASN:H	1:B:464:ASN:ND2	1.89	0.71
2:F:301:LEU:HD13	2:F:356:MET:HE1	1.72	0.71
2:E:379:VAL:HG21	2:E:385:ALA:HA	1.73	0.70
1:B:355:ILE:O	1:B:359:ILE:HG13	1.91	0.70
3:T:606:VAL:HG13	3:T:610:GLU:HG3	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:606:VAL:CG1	3:S:610:GLU:HG3	2.22	0.70
1:A:460:LYS:HD3	1:A:460:LYS:N	2.06	0.70
1:B:123:GLU:HG2	1:B:124:ASP:N	2.07	0.70
2:E:330:LYS:HD3	2:E:330:LYS:N	2.04	0.69
2:E:97:LEU:HD12	2:E:410:ILE:HD12	1.74	0.69
1:A:249:THR:N	1:A:250:PRO:HD3	2.06	0.69
1:B:168:ASP:HB3	1:B:235:LEU:HD11	1.74	0.69
1:B:494:LYS:HD3	1:B:507:SER:HA	1.74	0.69
2:E:392:HIS:CE1	2:E:394:LYS:HB2	2.27	0.69
2:F:72:ASN:OD1	2:F:73:SER:N	2.26	0.68
1:B:171:PHE:O	1:B:175:VAL:HG23	1.93	0.68
1:A:460:LYS:CD	1:A:460:LYS:H	2.05	0.68
1:B:102:ASN:HD22	1:B:102:ASN:N	1.90	0.68
2:F:371:LYS:HD3	2:F:389:THR:CG2	2.24	0.68
1:B:524:PHE:CE1	1:B:618:GLU:HB2	2.29	0.68
1:B:85:VAL:HG11	2:E:74:LEU:HD23	1.76	0.68
2:E:326:ILE:HA	2:E:329:ILE:HD12	1.75	0.68
3:S:593:ARG:O	3:S:596:THR:HG22	1.93	0.68
1:B:368:TYR:O	1:B:371:ARG:HB3	1.94	0.68
1:B:177:ALA:HA	1:B:180:GLN:NE2	2.09	0.67
1:A:122:VAL:HG22	1:A:543:ILE:HG22	1.76	0.67
1:A:365:ARG:O	1:A:368:TYR:N	2.27	0.67
1:B:24:MET:O	1:B:28:GLN:HB2	1.94	0.67
1:B:365:ARG:O	1:B:368:TYR:N	2.27	0.67
2:F:250:ARG:HG3	2:F:284:ASP:CG	2.14	0.67
2:F:193:LEU:HD11	2:F:201:LEU:HD12	1.75	0.67
2:F:330:LYS:H	2:F:330:LYS:CD	1.98	0.67
2:F:394:LYS:HB3	2:F:421:TRP:HH2	1.60	0.67
1:A:574:ALA:O	1:A:582:ARG:NH1	2.27	0.67
1:A:528:PRO:O	1:A:529:VAL:HG23	1.95	0.67
1:B:464:ASN:HD22	1:B:464:ASN:H	1.41	0.67
2:F:68:PHE:HB2	2:F:390:LEU:HD11	1.77	0.67
1:B:251:ASN:HA	3:S:607:ASN:ND2	2.10	0.67
3:T:606:VAL:HG12	3:T:610:GLU:HG3	1.76	0.67
1:A:425:GLN:NE2	1:A:426:PRO:HD2	2.10	0.66
3:T:567:HIS:HA	3:T:581:VAL:HG23	1.77	0.66
1:B:445:GLN:OE1	1:B:445:GLN:HA	1.94	0.66
1:A:39:LYS:HD3	2:F:380:GLU:CG	2.25	0.66
1:A:425:GLN:HE21	1:A:425:GLN:HA	1.60	0.66
1:A:590:PRO:HB3	1:A:621:PHE:HA	1.78	0.66
2:F:218:VAL:HG11	3:T:591:TRP:CE3	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:671:ILE:O	3:T:674:ILE:HG22	1.96	0.66
1:A:20:LYS:O	1:A:24:MET:HB2	1.95	0.66
2:E:68:PHE:HA	2:E:424:ASP:O	1.95	0.66
3:S:674:ILE:O	3:S:674:ILE:HG12	1.96	0.66
3:T:654:ARG:O	3:T:658:LEU:HD12	1.95	0.66
1:B:96:ILE:CG1	1:B:97:PRO:HD2	2.25	0.66
1:B:450:CYS:HB3	1:B:453:ARG:HG3	1.78	0.66
2:F:371:LYS:HD3	2:F:389:THR:HG21	1.78	0.66
1:A:280:TYR:OH	3:T:659:HIS:HD2	1.79	0.66
2:F:144:THR:HG22	2:F:146:HIS:CD2	2.31	0.66
2:F:279:LYS:HD3	2:F:279:LYS:N	2.11	0.66
2:E:415:CYS:HB2	2:E:419:SER:OG	1.95	0.65
2:E:250:ARG:HG3	2:E:284:ASP:CG	2.17	0.65
3:S:579:MET:HG3	3:S:579:MET:O	1.97	0.65
3:S:606:VAL:HG12	3:S:610:GLU:HG3	1.78	0.65
2:F:195:VAL:HG22	2:F:201:LEU:HD13	1.78	0.65
1:A:96:ILE:CG1	1:A:97:PRO:HD2	2.25	0.65
1:B:538:TYR:HH	1:B:564:PHE:HE2	1.43	0.65
3:S:654:ARG:O	3:S:658:LEU:HD12	1.97	0.65
3:T:674:ILE:O	3:T:674:ILE:HG12	1.96	0.65
1:A:358:LEU:HD21	3:T:675:ASP:HB3	1.77	0.64
2:E:357:ASP:OD1	2:E:362:MET:HB2	1.97	0.64
2:F:190:ASN:HD22	2:F:207:GLN:HB2	1.62	0.64
2:E:104:SER:O	2:E:132:ASN:HA	1.96	0.64
1:A:67:PRO:HG3	2:F:95:ASP:CG	2.18	0.64
1:B:345:ILE:HG22	1:B:355:ILE:HD13	1.79	0.64
2:E:425:ARG:HH21	2:E:425:ARG:CB	2.10	0.64
1:B:611:ARG:HD2	1:B:612:ALA:O	1.97	0.64
2:E:254:LYS:CE	2:E:254:LYS:H	2.10	0.64
1:B:65:ILE:HD12	1:B:65:ILE:N	2.13	0.64
1:B:101:LEU:HD22	2:E:168:CYS:HB2	1.79	0.64
1:B:178:LEU:HD13	1:B:211:ILE:HG23	1.80	0.63
2:E:181:GLU:HG3	2:E:182:LEU:H	1.61	0.63
2:F:294:TYR:OH	2:F:310:CYS:HB3	1.97	0.63
1:B:458:ARG:HA	1:B:484:THR:HG21	1.81	0.63
1:A:333:TRP:CH2	1:A:362:LYS:HG3	2.33	0.63
2:F:330:LYS:HE2	2:F:333:GLU:OE1	1.98	0.63
1:B:119:ASN:HB3	1:B:542:ILE:HD11	1.78	0.63
1:B:490:HIS:C	1:B:492:ASP:H	2.02	0.63
2:E:184:PHE:CZ	2:E:192:LEU:HD13	2.33	0.63
2:E:341:ARG:HG3	2:E:341:ARG:HH11	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:588:ASP:OD1	3:S:593:ARG:HD3	1.98	0.63
1:A:57:ASN:O	1:A:61:LYS:HG3	1.98	0.63
2:F:254:LYS:CE	2:F:254:LYS:H	2.11	0.63
2:F:68:PHE:HA	2:F:424:ASP:O	1.99	0.63
1:B:259:SER:OG	1:B:342:ARG:NH2	2.32	0.63
1:B:119:ASN:ND2	1:B:542:ILE:HD11	2.14	0.63
2:F:195:VAL:HG13	2:F:225:VAL:HB	1.80	0.63
2:E:367:ASN:HB2	2:E:371:LYS:O	1.99	0.62
1:B:580:LYS:HZ3	3:S:581:VAL:HG13	1.64	0.62
2:F:274:PRO:HD3	3:T:578:GLU:OE2	1.99	0.62
2:F:319:PRO:HG2	2:F:329:ILE:CD1	2.29	0.62
3:S:628:ALA:N	3:S:631:GLN:HE21	1.96	0.62
2:F:181:GLU:HG3	2:F:182:LEU:H	1.64	0.62
1:B:522:GLY:HA2	1:B:585:ASN:HD21	1.63	0.62
2:E:159:ARG:HG2	2:E:159:ARG:NH1	2.14	0.62
1:A:251:ASN:HA	3:T:607:ASN:ND2	2.14	0.62
1:A:86:THR:HG22	1:A:87:SER:N	2.15	0.62
1:A:262:ARG:HB2	1:A:343:VAL:HA	1.82	0.62
1:B:251:ASN:OD1	1:B:252:ILE:N	2.32	0.62
1:A:523:ILE:HG23	1:A:619:LEU:HD12	1.82	0.62
1:B:177:ALA:HA	1:B:180:GLN:HE22	1.64	0.62
2:F:227:SER:HB3	2:F:240:CYS:SG	2.39	0.62
3:S:655:ASN:HA	3:S:658:LEU:HD13	1.81	0.62
1:A:177:ALA:HA	1:A:180:GLN:NE2	2.15	0.62
1:B:293:THR:HG22	1:B:445:GLN:NE2	2.11	0.62
2:E:154:SER:HA	2:E:178:ALA:HB1	1.82	0.62
3:T:658:LEU:HD12	3:T:658:LEU:H	1.64	0.62
1:A:102:ASN:HD22	1:A:102:ASN:N	1.98	0.61
1:A:368:TYR:O	1:A:371:ARG:HB3	2.00	0.61
1:B:418:GLN:CA	1:B:418:GLN:HE21	2.13	0.61
1:B:86:THR:HG22	1:B:87:SER:N	2.14	0.61
2:F:198:ASP:O	2:F:199:HIS:HB2	2.00	0.61
2:F:238:MET:HE2	2:F:248:LEU:CD1	2.30	0.61
1:B:459:CYS:SG	1:B:468:CYS:HB2	2.40	0.61
1:A:555:TYR:CE2	1:A:563:LEU:HD11	2.34	0.61
2:E:306:LEU:HD12	2:E:356:MET:CE	2.31	0.61
1:B:122:VAL:CG2	1:B:543:ILE:HG22	2.30	0.61
2:E:319:PRO:HG2	2:E:329:ILE:HD13	1.82	0.61
1:A:102:ASN:HD22	1:A:102:ASN:H	1.46	0.61
1:A:524:PHE:CE1	1:A:618:GLU:HB2	2.36	0.61
1:B:480:ASP:O	1:B:481:LEU:HD23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:THR:HG21	2:E:359:TRP:CE3	2.35	0.61
1:A:450:CYS:HB3	1:A:453:ARG:HG3	1.81	0.61
1:A:567:ASN:C	1:A:567:ASN:HD22	2.03	0.61
2:E:346:GLN:O	2:E:368:GLN:HG2	2.01	0.61
2:F:236:LYS:HD2	2:F:300:TRP:CH2	2.36	0.61
2:E:198:ASP:O	2:E:199:HIS:HB2	2.01	0.60
3:T:658:LEU:HA	3:T:661:VAL:HG12	1.83	0.60
1:A:365:ARG:O	1:A:367:VAL:N	2.34	0.60
1:B:67:PRO:HG3	2:E:95:ASP:OD2	2.01	0.60
1:B:531:LYS:HG2	1:B:532:ASN:ND2	2.16	0.60
2:E:330:LYS:CD	2:E:330:LYS:H	2.07	0.60
3:T:636:CYS:O	3:T:640:VAL:HG12	2.02	0.60
1:A:445:GLN:OE1	1:A:445:GLN:HA	2.02	0.60
1:B:224:THR:O	1:B:228:LEU:HG	2.01	0.60
3:S:659:HIS:CE1	3:S:663:MET:HE1	2.36	0.60
3:T:581:VAL:HG22	3:T:581:VAL:O	2.02	0.60
1:B:234:GLU:C	1:B:236:THR:H	2.05	0.60
2:E:193:LEU:HD11	2:E:201:LEU:HD12	1.84	0.60
2:F:263:SER:HA	2:F:275:PHE:CE1	2.37	0.60
1:A:352:PHE:HA	1:A:355:ILE:HB	1.83	0.60
1:B:580:LYS:HE2	3:S:584:GLU:HG3	1.82	0.60
1:A:357:ARG:HH11	1:A:357:ARG:CB	2.08	0.59
2:E:394:LYS:HB3	2:E:421:TRP:CH2	2.36	0.59
2:E:201:LEU:HB2	2:E:215:PHE:HB2	1.84	0.59
1:B:550:ARG:NH1	1:B:550:ARG:HB2	2.17	0.59
2:E:156:GLY:HA2	2:E:179:ILE:HG13	1.85	0.59
1:A:333:TRP:HB3	1:A:337:GLU:OE1	2.02	0.59
2:F:304:LEU:HD13	2:F:339:LEU:HD12	1.84	0.59
2:F:379:VAL:HG21	2:F:385:ALA:HA	1.84	0.59
1:B:253:ASP:OD2	3:S:652:LEU:HA	2.02	0.59
1:A:86:THR:HG22	1:A:87:SER:H	1.68	0.59
3:S:671:ILE:HA	3:S:674:ILE:HG22	1.85	0.59
2:E:240:CYS:HB2	2:E:295:VAL:HB	1.85	0.59
1:A:464:ASN:ND2	1:A:464:ASN:H	2.01	0.59
1:B:528:PRO:O	1:B:529:VAL:HG23	2.02	0.59
2:E:319:PRO:O	2:E:329:ILE:HD11	2.02	0.59
1:A:251:ASN:OD1	1:A:252:ILE:N	2.35	0.59
1:B:272:LEU:HD11	3:S:603:PHE:CZ	2.38	0.58
1:A:480:ASP:O	1:A:481:LEU:HD23	2.04	0.58
1:A:550:ARG:NH1	1:A:550:ARG:HB2	2.18	0.58
3:T:563:ARG:HG2	3:T:564:LEU:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ARG:HG3	2:E:92:LYS:HD3	1.84	0.58
1:B:102:ASN:HD22	1:B:102:ASN:H	1.48	0.58
1:B:22:GLU:O	1:B:26:LEU:HD23	2.02	0.58
1:A:253:ASP:OD1	3:T:654:ARG:HB2	2.02	0.58
1:A:352:PHE:HZ	1:A:371:ARG:HH11	1.50	0.58
1:A:38:VAL:HG22	2:F:339:LEU:HD22	1.85	0.58
2:F:239:SER:O	2:F:246:LEU:HA	2.03	0.58
1:A:39:LYS:CD	2:F:380:GLU:HB3	2.34	0.58
1:B:458:ARG:HA	1:B:484:THR:CG2	2.34	0.58
2:E:74:LEU:HD13	2:E:118:ILE:HD12	1.86	0.58
1:A:494:LYS:HD3	1:A:507:SER:HA	1.85	0.58
1:B:168:ASP:HB3	1:B:235:LEU:CD1	2.34	0.57
1:B:418:GLN:HA	1:B:418:GLN:NE2	2.19	0.57
2:E:294:TYR:OH	2:E:310:CYS:HB3	2.04	0.57
2:E:409:SER:HA	2:E:425:ARG:HG3	1.86	0.57
1:A:450:CYS:HB3	1:A:453:ARG:CG	2.34	0.57
2:E:263:SER:HA	2:E:275:PHE:CE1	2.39	0.57
2:F:346:GLN:O	2:F:368:GLN:HG2	2.04	0.57
3:S:567:HIS:HA	3:S:581:VAL:CG2	2.33	0.57
3:T:664:HIS:CE1	3:T:671:ILE:HG12	2.40	0.57
1:A:230:GLU:HG2	1:A:233:LYS:HD2	1.86	0.57
2:E:341:ARG:NH1	2:E:341:ARG:HG3	2.20	0.57
2:F:175:HIS:CE1	2:F:194:SER:OG	2.49	0.57
2:F:238:MET:HA	2:F:247:LYS:O	2.05	0.57
1:B:555:TYR:HE2	1:B:563:LEU:HD11	1.68	0.57
2:E:154:SER:HA	2:E:178:ALA:CB	2.34	0.57
3:S:660:LEU:O	3:S:669:ILE:HD11	2.04	0.57
1:A:618:GLU:HG2	1:A:620:PHE:CE2	2.40	0.57
1:B:46:ARG:NH2	2:E:360:GLN:O	2.34	0.57
1:A:89:LEU:HD22	2:F:72:ASN:HA	1.86	0.57
1:B:365:ARG:O	1:B:367:VAL:N	2.38	0.57
2:E:409:SER:HA	2:E:425:ARG:CD	2.34	0.57
2:F:363:LEU:HD23	2:F:364:ALA:N	2.20	0.57
2:F:272:ASN:HB3	3:T:577:GLN:HB3	1.86	0.57
1:A:418:GLN:CA	1:A:418:GLN:HE21	2.17	0.57
2:E:193:LEU:HD22	2:E:237:ILE:HD13	1.86	0.57
2:F:111:GLU:HB2	2:F:121:LEU:HD11	1.87	0.57
2:F:226:LEU:HD22	2:F:350:TRP:HZ3	1.70	0.57
1:A:490:HIS:C	1:A:492:ASP:H	2.08	0.56
1:B:459:CYS:O	1:B:484:THR:OG1	2.21	0.56
2:E:417:ASP:O	2:E:418:ALA:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:GLN:NE2	1:B:50:GLN:HE22	2.01	0.56
2:F:341:ARG:HH11	2:F:341:ARG:HG3	1.69	0.56
1:A:87:SER:HA	2:F:73:SER:O	2.05	0.56
1:B:224:THR:HG22	1:B:227:GLU:OE2	2.04	0.56
2:F:254:LYS:O	2:F:258:ASN:HB2	2.06	0.56
3:T:577:GLN:N	3:T:577:GLN:OE1	2.37	0.56
1:A:580:LYS:HZ1	3:T:581:VAL:HG13	1.67	0.56
2:E:291:HIS:HE1	2:E:307:SER:OG	1.87	0.56
2:E:306:LEU:HD12	2:E:356:MET:HE2	1.88	0.56
2:F:193:LEU:HD22	2:F:237:ILE:CD1	2.27	0.56
1:A:515:PRO:HD3	3:T:566:PHE:CE2	2.40	0.56
1:A:513:LEU:HD22	3:T:568:SER:HA	1.87	0.56
3:T:567:HIS:HA	3:T:581:VAL:CG2	2.36	0.56
1:A:425:GLN:NE2	1:A:425:GLN:HA	2.20	0.56
1:B:464:ASN:ND2	1:B:464:ASN:N	2.52	0.56
1:A:494:LYS:CB	1:A:507:SER:HB3	2.29	0.56
2:E:390:LEU:HD22	2:E:390:LEU:N	2.21	0.56
3:S:636:CYS:O	3:S:640:VAL:HG12	2.06	0.56
1:A:253:ASP:OD2	3:T:652:LEU:HA	2.06	0.56
3:T:595:LYS:O	3:T:599:GLN:HG3	2.06	0.56
3:T:628:ALA:N	3:T:631:GLN:NE2	2.46	0.56
1:B:340:MET:HG3	1:B:344:LEU:HD12	1.88	0.55
2:F:218:VAL:HG11	3:T:591:TRP:CZ3	2.42	0.55
3:T:607:ASN:HB2	3:T:609:GLY:H	1.70	0.55
3:T:658:LEU:HA	3:T:661:VAL:CG1	2.36	0.55
1:B:341:PHE:O	1:B:345:ILE:HG23	2.07	0.55
2:E:229:ASP:OD2	2:E:299:ARG:HA	2.06	0.55
2:F:255:ARG:HD2	2:F:278:GLN:OE1	2.06	0.55
2:F:410:ILE:HG22	2:F:411:LEU:N	2.21	0.55
3:S:682:ARG:HH11	3:S:682:ARG:HG2	1.71	0.55
1:A:348:TYR:O	1:A:349:TYR:HB2	2.04	0.55
1:B:345:ILE:HG22	1:B:355:ILE:CD1	2.36	0.55
2:E:144:THR:HG22	2:E:146:HIS:CG	2.42	0.55
1:A:178:LEU:HD12	1:A:215:ILE:HD11	1.88	0.55
1:B:121:MET:CE	1:B:542:ILE:HB	2.37	0.55
1:A:418:GLN:HE21	1:A:418:GLN:HA	1.71	0.55
1:B:618:GLU:HG2	1:B:620:PHE:CE2	2.42	0.55
3:S:607:ASN:C	3:S:609:GLY:N	2.60	0.55
1:B:94:GLN:NE2	2:E:118:ILE:O	2.40	0.55
2:E:138:TRP:CE2	2:E:149:LEU:HD13	2.42	0.55
2:E:208:THR:HG23	2:E:210:THR:OG1	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:390:LEU:HD22	2:E:390:LEU:H	1.71	0.55
3:T:583:ASP:O	3:T:584:GLU:HG3	2.06	0.55
1:B:352:PHE:HB3	1:B:367:VAL:HB	1.88	0.55
2:E:190:ASN:ND2	2:E:207:GLN:HB2	2.21	0.54
2:E:71:VAL:O	2:E:72:ASN:HB2	2.06	0.54
3:T:576:PRO:C	3:T:578:GLU:H	2.11	0.54
1:A:270:HIS:HB3	1:A:294:TYR:CE2	2.42	0.54
1:B:110:MET:HE3	1:B:113:TRP:HE1	1.72	0.54
2:F:104:SER:O	2:F:132:ASN:HA	2.06	0.54
1:B:116:LEU:HD22	1:B:577:LYS:HB2	1.90	0.54
1:B:590:PRO:HB3	1:B:621:PHE:HA	1.88	0.54
2:F:254:LYS:CD	2:F:254:LYS:H	2.21	0.54
1:B:258:LYS:O	1:B:335:GLY:HA3	2.07	0.54
1:B:625:TYR:C	1:B:627:GLN:H	2.08	0.54
2:E:294:TYR:CZ	2:E:350:TRP:HB3	2.43	0.54
2:F:341:ARG:O	2:F:382:PRO:HB2	2.07	0.54
2:E:164:ILE:HG22	2:E:164:ILE:O	2.08	0.54
3:T:574:LEU:HD11	3:T:578:GLU:CD	2.27	0.54
1:B:357:ARG:CB	1:B:357:ARG:HH11	2.14	0.54
1:B:494:LYS:HB3	1:B:507:SER:CB	2.32	0.54
2:F:197:LYS:O	2:F:197:LYS:HG2	2.07	0.54
1:A:424:ARG:HH11	2:E:170:LYS:HA	1.70	0.54
2:E:238:MET:HA	2:E:247:LYS:O	2.08	0.54
2:E:319:PRO:HB2	2:E:329:ILE:HD13	1.89	0.54
2:E:304:LEU:HD13	2:E:339:LEU:HD12	1.89	0.54
2:F:82:LEU:HD13	2:F:101:THR:HG23	1.90	0.54
3:T:648:ILE:HD13	3:T:685:GLN:HA	1.90	0.54
1:B:54:GLU:OE2	1:B:58:GLN:OE1	2.26	0.54
2:E:363:LEU:HD23	2:E:364:ALA:N	2.22	0.54
2:F:159:ARG:HH11	2:F:159:ARG:HG2	1.71	0.54
1:B:524:PHE:HE1	1:B:618:GLU:HB2	1.73	0.54
1:A:273:PHE:HB2	1:A:280:TYR:CE1	2.43	0.54
2:F:208:THR:HG23	2:F:210:THR:OG1	2.08	0.54
1:A:580:LYS:HZ2	3:T:581:VAL:HG13	1.71	0.54
2:E:218:VAL:HG11	3:S:591:TRP:CE3	2.42	0.53
2:F:82:LEU:HD13	2:F:101:THR:CG2	2.38	0.53
1:A:12:PRO:O	1:A:16:ARG:HG3	2.08	0.53
1:A:295:LYS:HB2	1:A:295:LYS:NZ	2.23	0.53
2:E:82:LEU:HD13	2:E:101:THR:HG23	1.89	0.53
2:F:238:MET:HE2	2:F:248:LEU:HD12	1.91	0.53
2:F:306:LEU:HD12	2:F:356:MET:CE	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:HIS:CE1	3:T:581:VAL:H	2.26	0.53
1:B:574:ALA:O	1:B:582:ARG:NH1	2.41	0.53
2:E:197:LYS:HG3	2:E:224:GLU:CD	2.29	0.53
2:E:239:SER:O	2:E:246:LEU:HA	2.08	0.53
3:S:575:ARG:NE	3:S:577:GLN:HE22	2.07	0.53
1:A:291:PRO:HG3	2:E:146:HIS:HE1	1.72	0.53
1:A:45:ASN:O	1:A:48:LYS:HB2	2.08	0.53
1:B:117:GLN:CD	1:B:508:LYS:HZ3	2.12	0.53
1:B:180:GLN:HG2	1:B:181:LEU:HD12	1.90	0.53
2:F:164:ILE:O	2:F:164:ILE:HG22	2.06	0.53
2:F:390:LEU:HB3	2:F:423:TRP:CH2	2.43	0.53
3:S:666:PHE:O	3:S:667:ASN:HB2	2.09	0.53
1:B:494:LYS:CB	1:B:507:SER:HB3	2.33	0.53
2:F:291:HIS:HE1	2:F:307:SER:OG	1.92	0.53
1:A:39:LYS:CD	2:F:380:GLU:HG3	2.38	0.53
1:B:567:ASN:ND2	1:B:567:ASN:C	2.53	0.53
1:B:567:ASN:HD22	1:B:568:ASN:N	2.06	0.53
3:T:637:MET:O	3:T:641:GLU:HG3	2.09	0.53
1:B:361:THR:O	1:B:362:LYS:HG3	2.09	0.53
2:E:219:GLU:HA	2:E:219:GLU:OE1	2.08	0.53
3:S:632:MET:HG3	3:S:668:LEU:HB3	1.90	0.53
1:B:425:GLN:HA	1:B:425:GLN:HE21	1.73	0.53
2:F:415:CYS:HB2	2:F:419:SER:OG	2.08	0.53
1:A:524:PHE:HE1	1:A:618:GLU:HB2	1.74	0.52
1:B:30:LYS:O	1:B:31:ARG:C	2.48	0.52
1:A:45:ASN:ND2	2:F:304:LEU:HG	2.24	0.52
1:B:567:ASN:ND2	1:B:570:PHE:H	2.06	0.52
2:E:236:LYS:HD2	2:E:248:LEU:HD11	1.91	0.52
2:E:279:LYS:HD3	2:E:279:LYS:N	2.24	0.52
2:F:382:PRO:HG2	2:F:383:HIS:CD2	2.45	0.52
1:A:224:THR:HG22	1:A:227:GLU:OE2	2.10	0.52
1:A:39:LYS:NZ	2:F:380:GLU:HG3	2.24	0.52
3:S:593:ARG:O	3:S:597:ILE:HG23	2.09	0.52
3:T:682:ARG:C	3:T:684:MET:H	2.11	0.52
1:A:613:ILE:HG23	1:A:617:GLU:OE1	2.09	0.52
1:B:270:HIS:HB3	1:B:294:TYR:CE2	2.45	0.52
2:E:266:TYR:CD1	2:E:275:PHE:HB2	2.44	0.52
2:F:181:GLU:HG3	2:F:182:LEU:N	2.24	0.52
1:A:581:ILE:HG13	1:A:581:ILE:O	2.08	0.52
2:F:367:ASN:HB2	2:F:371:LYS:O	2.10	0.52
1:B:12:PRO:O	1:B:16:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:181:GLU:HG3	2:E:182:LEU:N	2.24	0.52
3:T:590:GLU:H	3:T:590:GLU:CD	2.13	0.52
1:A:263:GLU:O	1:A:263:GLU:HG3	2.09	0.52
2:E:226:LEU:HD11	2:E:242:MET:HG2	1.92	0.52
1:A:274:CYS:SG	1:A:276:ARG:HB2	2.50	0.52
1:A:590:PRO:CB	1:A:621:PHE:HA	2.40	0.52
3:T:644:GLY:O	3:T:648:ILE:HG13	2.10	0.52
1:B:86:THR:HG22	1:B:87:SER:H	1.73	0.51
2:E:222:ARG:HH12	2:E:288:ARG:NH1	2.07	0.51
3:S:658:LEU:HA	3:S:661:VAL:HG12	1.92	0.51
3:T:593:ARG:HG2	3:T:622:MET:HE2	1.91	0.51
1:A:68:VAL:HG11	2:F:109:LEU:HD23	1.92	0.51
1:B:178:LEU:HB3	1:B:211:ILE:HD13	1.91	0.51
2:E:395:CYS:HA	2:E:421:TRP:CZ2	2.45	0.51
1:B:117:GLN:NE2	1:B:508:LYS:NZ	2.58	0.51
1:B:586:HIS:CG	1:B:587:SER:N	2.78	0.51
1:B:515:PRO:HD3	3:S:566:PHE:CE2	2.45	0.51
2:F:97:LEU:HD12	2:F:410:ILE:HD12	1.91	0.51
1:A:363:THR:C	1:A:365:ARG:N	2.62	0.51
2:F:243:ASP:O	2:F:244:HIS:HB2	2.11	0.51
2:F:318:LYS:HG2	2:F:337:THR:HB	1.93	0.51
1:A:180:GLN:HG2	1:A:181:LEU:HD12	1.92	0.51
1:B:425:GLN:NE2	1:B:426:PRO:HD2	2.26	0.51
3:S:659:HIS:CE1	3:S:663:MET:CE	2.93	0.51
1:A:512:LEU:O	1:A:523:ILE:HD12	2.10	0.51
1:B:57:ASN:ND2	2:E:406:ARG:HH21	2.09	0.51
2:E:271:THR:O	3:S:575:ARG:NH2	2.43	0.51
1:B:67:PRO:HG3	2:E:95:ASP:CG	2.31	0.51
3:T:578:GLU:HB3	3:T:579:MET:O	2.11	0.51
2:E:73:SER:HA	2:E:420:ILE:O	2.11	0.51
2:F:197:LYS:HG3	2:F:224:GLU:CD	2.31	0.51
3:T:597:ILE:HB	3:T:615:LYS:HD3	1.92	0.51
1:B:352:PHE:HA	1:B:355:ILE:HB	1.93	0.50
2:F:71:VAL:O	2:F:72:ASN:HB2	2.11	0.50
3:T:682:ARG:C	3:T:684:MET:N	2.64	0.50
1:A:28:GLN:NE2	1:A:31:ARG:HD3	2.15	0.50
1:A:340:MET:HG3	1:A:344:LEU:HD12	1.92	0.50
1:A:418:GLN:NE2	1:A:418:GLN:HA	2.27	0.50
2:E:254:LYS:CD	2:E:254:LYS:H	2.24	0.50
2:F:198:ASP:O	2:F:199:HIS:CB	2.59	0.50
2:F:73:SER:HA	2:F:420:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:TYR:OH	3:S:674:ILE:HG23	2.12	0.50
1:B:51:GLU:O	1:B:55:ILE:HG13	2.11	0.50
2:E:196:SER:OG	2:E:197:LYS:N	2.45	0.50
1:B:120:PHE:O	1:B:541:GLU:HA	2.11	0.50
2:E:195:VAL:CG2	2:E:201:LEU:HD13	2.34	0.50
2:F:254:LYS:HE2	2:F:254:LYS:N	2.25	0.50
1:A:23:TYR:CE2	1:A:27:ARG:HD3	2.47	0.50
1:A:88:ASP:O	1:A:89:LEU:HD12	2.12	0.50
3:S:606:VAL:HG13	3:S:610:GLU:HG3	1.90	0.50
1:B:464:ASN:HA	1:B:471:TYR:CD1	2.46	0.50
1:B:87:SER:HA	2:E:73:SER:O	2.11	0.50
1:A:39:LYS:NZ	1:A:43:ASN:HD21	2.10	0.50
1:A:496:VAL:HG12	1:A:497:SER:N	2.26	0.50
2:E:243:ASP:O	2:E:244:HIS:HB2	2.11	0.50
2:F:238:MET:HE3	2:F:305:ILE:HD11	1.94	0.50
2:F:319:PRO:CG	2:F:329:ILE:HD13	2.39	0.50
2:E:198:ASP:O	2:E:199:HIS:CB	2.59	0.50
2:F:341:ARG:NH1	2:F:341:ARG:HG3	2.26	0.50
3:S:682:ARG:C	3:S:684:MET:N	2.64	0.50
1:A:86:THR:CG2	1:A:87:SER:H	2.24	0.50
1:B:541:GLU:OE1	1:B:551:ARG:NH2	2.45	0.50
2:F:386:LYS:NZ	2:F:388:THR:HG22	2.27	0.50
3:S:659:HIS:HE1	3:S:663:MET:HE1	1.74	0.50
1:A:177:ALA:HA	1:A:180:GLN:HE22	1.77	0.49
1:A:547:GLU:HG3	1:A:551:ARG:HD2	1.92	0.49
1:A:83:CYS:HB2	2:F:106:ARG:NH2	2.27	0.49
1:B:277:CYS:HB2	1:B:279:LYS:HE3	1.94	0.49
1:B:550:ARG:HB2	1:B:550:ARG:CZ	2.42	0.49
2:F:226:LEU:HD11	2:F:242:MET:HG2	1.94	0.49
1:B:209:ASP:OD1	1:B:229:LYS:HD3	2.12	0.49
2:E:109:LEU:N	2:E:109:LEU:HD12	2.27	0.49
1:B:71:MET:HB2	2:E:122:GLN:HG2	1.94	0.49
2:E:390:LEU:HB3	2:E:423:TRP:CH2	2.47	0.49
3:T:574:LEU:HD11	3:T:578:GLU:OE2	2.12	0.49
3:T:660:LEU:HB3	3:T:674:ILE:HG13	1.94	0.49
1:A:224:THR:OG1	1:A:225:ALA:N	2.45	0.49
1:B:30:LYS:HE2	1:B:170:ILE:HG12	1.94	0.49
1:B:86:THR:CG2	1:B:87:SER:H	2.23	0.49
1:B:263:GLU:O	1:B:263:GLU:HG3	2.12	0.49
3:T:671:ILE:HA	3:T:674:ILE:HG22	1.93	0.49
1:B:422:HIS:O	1:B:422:HIS:ND1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:MET:HE3	1:B:542:ILE:HB	1.94	0.49
2:E:346:GLN:O	2:E:367:ASN:OD1	2.31	0.49
1:A:494:LYS:HB3	1:A:507:SER:CB	2.30	0.49
3:S:636:CYS:SG	3:S:663:MET:HE3	2.52	0.49
1:A:480:ASP:OD1	3:T:629:ASP:HB2	2.12	0.49
1:A:30:LYS:HE3	1:A:33:ARG:HH12	1.78	0.49
1:B:119:ASN:CB	1:B:542:ILE:HD11	2.43	0.49
2:F:87:PHE:CD2	2:F:99:PHE:HB3	2.48	0.49
3:S:671:ILE:CA	3:S:674:ILE:HG22	2.43	0.49
1:B:476:GLU:OE1	1:B:504:GLN:HG2	2.12	0.49
1:B:119:ASN:HD22	1:B:542:ILE:HD11	1.78	0.49
3:T:675:ASP:C	3:T:677:ALA:N	2.66	0.49
1:A:178:LEU:HD13	1:A:211:ILE:HG23	1.93	0.49
1:A:182:ASP:OD2	1:A:208:SER:HB2	2.13	0.49
3:S:593:ARG:HG2	3:S:622:MET:CE	2.42	0.48
3:S:593:ARG:HG2	3:S:622:MET:HE2	1.93	0.48
3:T:585:ASP:O	3:T:587:LYS:N	2.46	0.48
1:B:512:LEU:HD23	3:S:581:VAL:HG12	1.95	0.48
2:F:193:LEU:CD2	2:F:237:ILE:HD13	2.32	0.48
1:A:116:LEU:HD22	1:A:577:LYS:HB2	1.95	0.48
1:A:464:ASN:HA	1:A:471:TYR:CD1	2.48	0.48
1:B:441:GLU:CD	1:B:475:ARG:HH22	2.17	0.48
1:B:87:SER:C	1:B:89:LEU:H	2.17	0.48
2:F:357:ASP:OD1	2:F:362:MET:HB2	2.13	0.48
1:A:522:GLY:HA2	1:A:585:ASN:HD21	1.79	0.48
1:A:579:ASN:O	1:A:582:ARG:HG2	2.13	0.48
1:B:259:SER:OG	1:B:342:ARG:CZ	2.62	0.48
2:E:195:VAL:HG22	2:E:201:LEU:CD1	2.32	0.48
2:E:357:ASP:OD1	2:E:357:ASP:N	2.47	0.48
2:F:309:SER:OG	2:F:310:CYS:N	2.46	0.48
1:A:116:LEU:CD1	3:T:591:TRP:HZ2	2.26	0.48
1:A:63:ARG:NH2	2:F:90:HIS:HD2	2.12	0.48
3:T:593:ARG:HG2	3:T:622:MET:CE	2.44	0.48
3:T:673:SER:C	3:T:675:ASP:H	2.17	0.48
1:A:534:PHE:HA	1:A:608:PHE:CD1	2.49	0.48
1:B:461:ALA:O	1:B:462:GLN:HB2	2.14	0.48
2:E:158:ILE:O	2:E:171:HIS:HA	2.14	0.48
2:E:72:ASN:OD1	2:E:73:SER:N	2.40	0.48
2:F:417:ASP:O	2:F:418:ALA:HB3	2.13	0.48
3:T:675:ASP:HA	3:T:678:VAL:HG23	1.96	0.48
1:A:333:TRP:CE3	1:A:337:GLU:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:ALA:O	1:A:462:GLN:HB2	2.14	0.48
1:A:567:ASN:ND2	1:A:570:PHE:H	2.11	0.48
1:B:180:GLN:HB3	1:B:180:GLN:HE21	1.47	0.48
1:B:572:VAL:HG11	1:B:605:ILE:HD12	1.95	0.48
3:S:607:ASN:C	3:S:609:GLY:H	2.15	0.48
1:A:26:LEU:O	1:A:27:ARG:C	2.53	0.48
2:E:68:PHE:CB	2:E:390:LEU:HD11	2.39	0.48
2:F:266:TYR:CD1	2:F:275:PHE:HB2	2.48	0.48
3:S:575:ARG:HE	3:S:577:GLN:HE22	1.61	0.48
3:S:660:LEU:HB3	3:S:674:ILE:HG13	1.95	0.48
1:A:272:LEU:HD11	3:T:603:PHE:CZ	2.49	0.48
3:T:654:ARG:O	3:T:658:LEU:CD1	2.61	0.48
1:A:361:THR:O	1:A:362:LYS:HE2	2.13	0.47
1:A:458:ARG:HA	1:A:484:THR:CG2	2.43	0.47
1:B:230:GLU:HG2	1:B:233:LYS:HD2	1.95	0.47
1:B:592:CYS:HB2	1:B:620:PHE:O	2.14	0.47
2:E:390:LEU:HB3	2:E:423:TRP:CZ3	2.48	0.47
3:S:658:LEU:H	3:S:658:LEU:HD12	1.77	0.47
3:T:595:LYS:HE3	3:T:599:GLN:OE1	2.15	0.47
1:A:459:CYS:O	1:A:484:THR:OG1	2.28	0.47
1:A:541:GLU:OE1	1:A:551:ARG:NH2	2.43	0.47
1:B:490:HIS:C	1:B:492:ASP:N	2.68	0.47
2:E:195:VAL:HG13	2:E:225:VAL:HB	1.95	0.47
2:F:319:PRO:O	2:F:329:ILE:HD11	2.14	0.47
1:A:224:THR:HG23	1:A:227:GLU:H	1.78	0.47
1:A:265:SER:O	3:T:658:LEU:HD23	2.15	0.47
1:A:41:MET:CE	2:F:322:MET:SD	3.03	0.47
1:A:592:CYS:SG	1:A:619:LEU:HD22	2.54	0.47
1:B:348:TYR:O	1:B:349:TYR:HB2	2.15	0.47
2:E:254:LYS:O	2:E:258:ASN:HB2	2.15	0.47
2:E:346:GLN:HB3	2:E:368:GLN:HE21	1.79	0.47
2:E:371:LYS:HD3	2:E:389:THR:CG2	2.43	0.47
2:E:409:SER:HA	2:E:425:ARG:CG	2.44	0.47
2:E:76:GLU:OE2	2:E:110:TYR:OH	2.21	0.47
2:F:294:TYR:CZ	2:F:350:TRP:HB3	2.49	0.47
3:S:682:ARG:NH1	3:S:682:ARG:HG2	2.30	0.47
1:A:351:ASN:OD1	1:A:353:CYS:HB2	2.15	0.47
1:B:102:ASN:N	1:B:102:ASN:ND2	2.61	0.47
2:E:238:MET:HE3	2:E:305:ILE:HD11	1.96	0.47
1:B:496:VAL:HG12	1:B:497:SER:N	2.30	0.47
2:E:309:SER:OG	2:E:310:CYS:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:617:TRP:CZ2	3:T:663:MET:HE1	2.50	0.47
1:A:259:SER:OG	1:A:342:ARG:NH2	2.48	0.47
1:B:280:TYR:OH	3:S:659:HIS:HD2	1.97	0.47
2:F:410:ILE:CG2	2:F:411:LEU:N	2.77	0.47
1:B:564:PHE:HD1	1:B:626:SER:HB3	1.80	0.47
2:F:292:ARG:HB2	2:F:292:ARG:HE	1.48	0.47
3:S:654:ARG:O	3:S:658:LEU:CD1	2.63	0.47
3:T:574:LEU:HD11	3:T:578:GLU:CG	2.45	0.47
1:A:28:GLN:NE2	1:A:31:ARG:HB3	2.30	0.47
1:A:577:LYS:HE2	3:T:591:TRP:CH2	2.50	0.47
2:F:159:ARG:NH1	2:F:159:ARG:HG2	2.30	0.47
2:F:159:ARG:C	2:F:160:ILE:HD13	2.35	0.47
2:F:271:THR:O	3:T:575:ARG:NH2	2.47	0.47
3:S:575:ARG:NE	3:S:577:GLN:NE2	2.63	0.47
1:B:522:GLY:CA	1:B:585:ASN:HD21	2.28	0.46
2:E:351:TYR:CE1	2:E:353:ARG:NH2	2.82	0.46
2:E:369:VAL:O	2:E:371:LYS:N	2.48	0.46
3:S:673:SER:C	3:S:675:ASP:H	2.18	0.46
1:B:110:MET:CE	1:B:113:TRP:HE1	2.28	0.46
3:T:658:LEU:CA	3:T:661:VAL:HG12	2.44	0.46
1:A:122:VAL:CG2	1:A:543:ILE:HG22	2.44	0.46
1:A:333:TRP:CE2	1:A:370:PHE:CD2	3.04	0.46
1:A:550:ARG:CZ	1:A:550:ARG:HB2	2.44	0.46
1:A:70:ILE:CD1	1:A:96:ILE:HD11	2.45	0.46
3:S:658:LEU:HA	3:S:661:VAL:CG1	2.45	0.46
1:B:42:PHE:O	1:B:45:ASN:HB3	2.15	0.46
2:F:306:LEU:HD12	2:F:356:MET:HE2	1.98	0.46
1:B:268:SER:O	1:B:272:LEU:HB3	2.15	0.46
1:B:538:TYR:OH	1:B:564:PHE:HE2	1.97	0.46
2:E:140:TYR:CE1	2:E:189:PRO:HG3	2.50	0.46
3:T:563:ARG:HG2	3:T:564:LEU:N	2.29	0.46
1:A:18:ARG:O	1:A:19:VAL:C	2.54	0.46
1:A:36:ASP:O	1:A:37:GLU:C	2.54	0.46
2:E:243:ASP:OD1	2:E:245:SER:HB3	2.15	0.46
2:E:390:LEU:H	2:E:390:LEU:CD2	2.28	0.46
2:E:74:LEU:N	2:E:74:LEU:HD12	2.30	0.46
2:F:369:VAL:O	2:F:369:VAL:HG23	2.15	0.46
2:F:394:LYS:HB3	2:F:421:TRP:CH2	2.46	0.46
1:B:234:GLU:C	1:B:236:THR:N	2.68	0.46
1:B:625:TYR:C	1:B:627:GLN:N	2.69	0.46
2:F:392:HIS:CE1	2:F:394:LYS:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ALA:O	1:B:335:GLY:HA3	2.16	0.46
1:B:295:LYS:NZ	1:B:295:LYS:HB2	2.30	0.46
1:B:464:ASN:HD22	1:B:464:ASN:N	2.02	0.46
2:E:375:TRP:CD1	2:E:387:CYS:HB2	2.51	0.46
1:A:9:GLU:N	1:A:210:LYS:HZ2	2.14	0.46
1:A:567:ASN:C	1:A:567:ASN:ND2	2.69	0.46
1:B:579:ASN:OD1	1:B:579:ASN:N	2.48	0.46
2:F:136:CYS:HA	2:F:150:ALA:O	2.16	0.46
2:F:333:GLU:OE2	2:F:335:ASN:HB2	2.16	0.46
2:F:397:ALA:HB2	2:F:417:ASP:OD2	2.15	0.46
3:T:566:PHE:CD1	3:T:573:PRO:HA	2.51	0.46
1:A:180:GLN:HG2	1:A:181:LEU:N	2.30	0.45
1:A:460:LYS:CD	1:A:460:LYS:N	2.75	0.45
1:B:226:GLU:HA	1:B:229:LYS:HE3	1.97	0.45
2:E:141:ASP:C	2:E:141:ASP:OD1	2.55	0.45
3:T:660:LEU:HD22	3:T:674:ILE:HA	1.97	0.45
1:A:41:MET:O	1:A:45:ASN:HB2	2.17	0.45
1:B:86:THR:O	1:B:87:SER:HB2	2.15	0.45
3:T:578:GLU:O	3:T:579:MET:HG2	2.16	0.45
2:F:298:VAL:O	2:F:299:ARG:HD3	2.15	0.45
2:F:330:LYS:N	2:F:330:LYS:CD	2.64	0.45
3:S:566:PHE:CE1	3:S:573:PRO:HB3	2.52	0.45
3:S:660:LEU:HD22	3:S:674:ILE:HA	1.97	0.45
1:A:586:HIS:CG	1:A:587:SER:N	2.84	0.45
1:B:255:PRO:HG2	1:B:256:ASN:OD1	2.17	0.45
1:B:262:ARG:HA	1:B:343:VAL:HG22	1.97	0.45
1:B:117:GLN:NE2	1:B:508:LYS:HZ2	2.15	0.45
2:E:319:PRO:HG2	2:E:326:ILE:HD12	1.98	0.45
1:A:546:ASP:O	1:A:549:ASP:HB2	2.17	0.45
1:B:224:THR:HG23	1:B:227:GLU:H	1.82	0.45
1:B:249:THR:HG23	1:B:249:THR:O	2.16	0.45
1:B:262:ARG:HG3	1:B:263:GLU:N	2.31	0.45
2:E:201:LEU:CD2	2:E:225:VAL:HG11	2.46	0.45
2:F:144:THR:HG22	2:F:146:HIS:CG	2.52	0.45
2:F:167:GLN:OE1	2:F:167:GLN:HA	2.15	0.45
3:S:682:ARG:C	3:S:684:MET:H	2.20	0.45
1:A:16:ARG:HD2	1:A:217:SER:CB	2.47	0.45
1:A:258:LYS:O	1:A:335:GLY:HA3	2.16	0.45
1:B:30:LYS:HE2	1:B:170:ILE:CG1	2.47	0.45
1:B:47:GLN:NE2	1:B:50:GLN:NE2	2.65	0.45
1:B:541:GLU:O	1:B:572:VAL:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:240:CYS:HA	2:E:245:SER:O	2.17	0.45
2:F:84:GLY:HA2	2:F:401:GLN:OE1	2.15	0.45
3:T:566:PHE:CE1	3:T:573:PRO:HB3	2.51	0.45
1:A:180:GLN:HB3	1:A:180:GLN:HE21	1.51	0.45
1:A:357:ARG:NH1	1:A:357:ARG:HB3	2.11	0.45
1:B:522:GLY:HA2	1:B:585:ASN:ND2	2.29	0.45
1:B:584:ALA:O	1:B:623:TYR:OH	2.29	0.45
2:E:400:ARG:HA	2:E:400:ARG:HD3	1.77	0.45
2:F:342:PHE:HD1	2:F:375:TRP:CD1	2.35	0.45
3:S:612:GLU:OE1	3:S:612:GLU:HA	2.16	0.45
3:S:621:VAL:HA	3:S:626:PHE:CE2	2.52	0.45
1:A:114:SER:HA	1:A:115:PRO:HD3	1.77	0.45
1:A:34:ARG:HA	1:A:37:GLU:HB2	1.99	0.45
1:B:213:GLU:HG3	1:B:214:ALA:N	2.32	0.45
1:B:345:ILE:O	1:B:349:TYR:HA	2.17	0.45
2:E:147:PRO:O	2:E:148:LEU:HD23	2.16	0.45
2:E:392:HIS:HE1	2:E:394:LYS:HB2	1.76	0.45
3:T:606:VAL:HG13	3:T:610:GLU:CG	2.45	0.45
3:T:672:MET:O	3:T:676:LYS:HB2	2.16	0.45
3:T:682:ARG:HH11	3:T:682:ARG:HG2	1.82	0.45
1:A:572:VAL:HG11	1:A:605:ILE:HD12	1.98	0.45
1:B:547:GLU:HG3	1:B:551:ARG:HD2	1.99	0.45
1:B:588:VAL:HG12	1:B:624:ARG:NH2	2.31	0.45
2:E:111:GLU:HB2	2:E:121:LEU:HD11	1.98	0.45
2:E:182:LEU:O	2:E:183:LYS:HG2	2.16	0.45
2:E:243:ASP:O	2:E:244:HIS:CB	2.65	0.45
2:E:313:ALA:HA	2:E:344:TYR:CE2	2.52	0.45
2:F:219:GLU:HA	2:F:219:GLU:OE1	2.16	0.45
2:F:243:ASP:OD1	2:F:245:SER:HB3	2.17	0.45
2:F:197:LYS:HG3	2:F:224:GLU:OE1	2.16	0.45
2:F:246:LEU:HD22	2:F:317:TRP:HZ2	1.82	0.45
3:S:671:ILE:C	3:S:674:ILE:HG22	2.37	0.45
3:T:659:HIS:CE1	3:T:663:MET:HE1	2.51	0.45
1:A:446:CYS:O	1:A:453:ARG:NH2	2.50	0.44
1:A:625:TYR:C	1:A:627:GLN:H	2.21	0.44
3:T:651:ASN:O	3:T:651:ASN:CG	2.54	0.44
1:A:41:MET:HE1	2:F:322:MET:SD	2.57	0.44
2:E:218:VAL:HG11	3:S:591:TRP:CZ3	2.51	0.44
3:T:660:LEU:O	3:T:669:ILE:HD11	2.16	0.44
1:A:345:ILE:HG22	1:A:355:ILE:CD1	2.47	0.44
1:A:567:ASN:HD22	1:A:569:ASP:N	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:ARG:HH12	1:B:617:GLU:CD	2.21	0.44
2:E:109:LEU:N	2:E:109:LEU:CD1	2.80	0.44
3:S:575:ARG:HE	3:S:577:GLN:NE2	2.16	0.44
3:S:621:VAL:HA	3:S:626:PHE:HE2	1.81	0.44
3:T:617:TRP:O	3:T:620:HIS:HB3	2.18	0.44
1:B:168:ASP:OD2	1:B:235:LEU:HD11	2.16	0.44
2:E:124:TYR:CD2	2:E:124:TYR:N	2.86	0.44
2:E:285:PHE:CZ	2:E:319:PRO:HB3	2.52	0.44
2:E:97:LEU:HD12	2:E:410:ILE:CD1	2.44	0.44
3:T:607:ASN:C	3:T:609:GLY:N	2.71	0.44
1:A:256:ASN:N	1:A:256:ASN:OD1	2.50	0.44
1:B:180:GLN:HG2	1:B:181:LEU:N	2.32	0.44
1:A:580:LYS:HD3	3:T:568:SER:OG	2.18	0.44
1:A:249:THR:N	1:A:250:PRO:CD	2.79	0.44
2:E:319:PRO:CG	2:E:329:ILE:HD13	2.48	0.44
2:E:363:LEU:C	2:E:363:LEU:HD23	2.38	0.44
1:A:70:ILE:HD12	2:F:121:LEU:O	2.17	0.44
2:F:196:SER:OG	2:F:197:LYS:N	2.51	0.44
2:F:294:TYR:O	2:F:294:TYR:CD1	2.71	0.44
3:T:584:GLU:C	3:T:586:GLU:H	2.20	0.44
3:T:670:SER:OG	3:T:672:MET:HG3	2.18	0.44
1:A:101:LEU:HD22	2:F:168:CYS:HB2	2.00	0.44
1:A:209:ASP:OD1	1:A:229:LYS:HD3	2.18	0.44
1:A:490:HIS:C	1:A:492:ASP:N	2.70	0.44
1:A:71:MET:SD	2:F:166:MET:SD	3.16	0.44
1:B:355:ILE:HG22	1:B:355:ILE:O	2.16	0.43
2:F:170:LYS:NZ	2:F:209:ASP:OD1	2.51	0.43
3:S:632:MET:O	3:S:635:ALA:HB3	2.18	0.43
1:A:252:ILE:HA	1:A:257:ALA:HB2	2.00	0.43
1:A:333:TRP:CE2	1:A:370:PHE:HD2	2.35	0.43
1:B:531:LYS:HG2	1:B:532:ASN:HD22	1.82	0.43
2:E:74:LEU:CD1	2:E:118:ILE:HD12	2.48	0.43
3:T:579:MET:N	3:T:579:MET:CE	2.81	0.43
1:A:290:THR:HB	1:A:421:ASP:OD1	2.18	0.43
2:F:109:LEU:HD12	2:F:109:LEU:N	2.33	0.43
2:F:159:ARG:HG2	2:F:168:CYS:SG	2.59	0.43
3:T:632:MET:HG3	3:T:668:LEU:HB3	2.00	0.43
1:B:66:GLN:HA	1:B:67:PRO:HD3	1.87	0.43
2:E:159:ARG:NH1	2:E:168:CYS:SG	2.92	0.43
2:E:301:LEU:HD13	2:E:356:MET:HE1	1.99	0.43
1:A:120:PHE:O	1:A:541:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ASP:O	1:A:185:ASP:HB2	2.17	0.43
1:A:290:THR:OG1	1:A:293:THR:HG23	2.19	0.43
1:A:345:ILE:O	1:A:349:TYR:HA	2.18	0.43
1:A:51:GLU:O	1:A:55:ILE:HG13	2.19	0.43
1:B:258:LYS:C	1:B:335:GLY:HA3	2.39	0.43
1:B:445:GLN:OE1	1:B:445:GLN:CA	2.65	0.43
1:B:46:ARG:HH22	2:E:360:GLN:C	2.16	0.43
3:S:604:SER:O	3:S:605:ASP:HB2	2.18	0.43
3:S:648:ILE:HD13	3:S:685:GLN:CA	2.47	0.43
1:A:13:ILE:O	1:A:17:LYS:CG	2.66	0.43
1:B:262:ARG:HB2	1:B:343:VAL:HA	2.00	0.43
2:E:319:PRO:CB	2:E:329:ILE:HD13	2.49	0.43
2:E:88:ASN:OD1	2:E:88:ASN:C	2.57	0.43
1:A:361:THR:O	1:A:362:LYS:CD	2.67	0.43
1:A:89:LEU:HD13	2:F:73:SER:HB3	2.00	0.43
1:B:224:THR:OG1	1:B:225:ALA:N	2.52	0.43
1:B:450:CYS:HB3	1:B:453:ARG:CG	2.47	0.43
2:E:144:THR:HG22	2:E:146:HIS:CD2	2.54	0.43
2:E:82:LEU:HD13	2:E:101:THR:CG2	2.49	0.43
3:S:607:ASN:CB	3:S:610:GLU:HG2	2.49	0.43
1:A:464:ASN:HD22	1:A:464:ASN:H	1.65	0.43
1:A:531:LYS:HG2	1:A:532:ASN:ND2	2.34	0.43
1:A:580:LYS:HD3	3:T:568:SER:CB	2.49	0.43
2:E:98:VAL:HG13	2:E:110:TYR:O	2.19	0.43
2:E:205:ASN:C	2:E:205:ASN:OD1	2.57	0.43
2:E:298:VAL:HG13	2:E:298:VAL:O	2.18	0.43
3:S:650:LYS:O	3:S:651:ASN:HB3	2.19	0.43
1:A:255:PRO:HG2	1:A:256:ASN:OD1	2.19	0.43
1:B:14:CYS:O	1:B:17:LYS:HB3	2.19	0.43
2:E:155:ARG:O	2:E:157:ILE:HG13	2.19	0.43
2:E:167:GLN:OE1	2:E:167:GLN:HA	2.18	0.43
2:F:294:TYR:CD1	2:F:294:TYR:C	2.92	0.43
3:S:607:ASN:HB2	3:S:610:GLU:H	1.83	0.43
1:B:580:LYS:NZ	3:S:581:VAL:CG1	2.75	0.42
1:B:84:SER:HB3	1:B:95:VAL:HG22	2.01	0.42
1:A:458:ARG:HA	1:A:484:THR:HG21	2.01	0.42
1:B:34:ARG:HH12	2:E:322:MET:CE	2.32	0.42
1:A:213:GLU:HG3	1:A:214:ALA:N	2.33	0.42
1:A:219:PHE:O	1:A:221:ASP:N	2.53	0.42
1:A:358:LEU:HD21	3:T:675:ASP:CB	2.48	0.42
1:A:541:GLU:O	1:A:572:VAL:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:LYS:HD3	1:B:478:ASP:OD2	2.18	0.42
1:B:579:ASN:O	1:B:582:ARG:HG2	2.19	0.42
2:F:364:ALA:HA	2:F:373:TYR:O	2.19	0.42
3:S:628:ALA:N	3:S:631:GLN:NE2	2.55	0.42
3:S:658:LEU:CA	3:S:661:VAL:HG12	2.49	0.42
3:T:579:MET:O	3:T:580:GLU:C	2.58	0.42
1:A:210:LYS:O	1:A:213:GLU:HG2	2.20	0.42
1:A:459:CYS:SG	1:A:468:CYS:HB2	2.59	0.42
3:S:568:SER:H	3:S:581:VAL:CG2	2.33	0.42
1:B:512:LEU:O	1:B:523:ILE:HD12	2.19	0.42
2:F:238:MET:HE2	2:F:248:LEU:HD13	2.00	0.42
3:S:661:VAL:HG13	3:S:662:SER:N	2.34	0.42
3:S:675:ASP:C	3:S:677:ALA:N	2.72	0.42
1:A:296:ARG:CZ	3:T:664:HIS:CE1	3.03	0.42
1:A:359:ILE:O	1:A:359:ILE:HG22	2.20	0.42
1:B:177:ALA:O	1:B:178:LEU:C	2.57	0.42
1:A:421:ASP:O	2:E:167:GLN:NE2	2.53	0.42
2:F:226:LEU:HD12	2:F:295:VAL:O	2.19	0.42
2:F:294:TYR:CE1	2:F:350:TRP:HB2	2.53	0.42
2:F:390:LEU:HB3	2:F:423:TRP:CZ3	2.54	0.42
3:S:586:GLU:HB3	3:S:588:ASP:O	2.19	0.42
1:A:102:ASN:ND2	1:A:102:ASN:N	2.64	0.42
1:A:338:ALA:O	1:A:341:PHE:HB3	2.19	0.42
1:B:249:THR:N	1:B:250:PRO:CD	2.80	0.42
1:B:272:LEU:HD23	3:S:614:MET:CE	2.49	0.42
2:E:208:THR:HG21	2:E:263:SER:O	2.20	0.42
2:F:356:MET:HA	2:F:362:MET:O	2.20	0.42
3:T:577:GLN:CD	3:T:577:GLN:H	2.23	0.42
1:A:284:LEU:HD23	1:A:284:LEU:O	2.20	0.42
1:A:526:LYS:HG2	1:A:526:LYS:O	2.18	0.42
1:B:250:PRO:O	1:B:251:ASN:HB3	2.20	0.42
1:B:363:THR:C	1:B:365:ARG:N	2.73	0.42
2:E:352:MET:HB3	2:E:352:MET:HE3	1.89	0.42
2:F:243:ASP:O	2:F:244:HIS:CB	2.67	0.42
1:A:65:ILE:HG13	2:F:90:HIS:HB3	2.01	0.42
3:T:666:PHE:O	3:T:667:ASN:HB2	2.20	0.42
1:B:180:GLN:O	1:B:184:ARG:HG3	2.19	0.42
1:B:250:PRO:O	1:B:251:ASN:CB	2.67	0.42
1:B:352:PHE:CD1	1:B:367:VAL:HG12	2.55	0.42
1:B:530:GLN:O	1:B:531:LYS:C	2.58	0.42
1:B:98:LEU:HD13	2:E:125:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:367:ASN:O	2:E:398:ALA:HA	2.20	0.42
2:E:417:ASP:O	2:E:418:ALA:CB	2.68	0.42
3:T:650:LYS:HB2	3:T:652:LEU:HD12	2.02	0.42
1:A:611:ARG:HD2	1:A:612:ALA:O	2.20	0.42
1:B:541:GLU:HG3	1:B:577:LYS:HG3	2.01	0.42
1:B:590:PRO:CB	1:B:621:PHE:HA	2.49	0.42
2:E:201:LEU:HD21	2:E:225:VAL:HG11	2.01	0.42
2:E:227:SER:HB3	2:E:240:CYS:SG	2.60	0.42
2:F:357:ASP:OD1	2:F:357:ASP:N	2.51	0.42
2:F:395:CYS:HA	2:F:421:TRP:CZ2	2.55	0.42
3:S:674:ILE:O	3:S:674:ILE:CG1	2.66	0.42
1:B:479:PRO:HB3	1:B:491:TRP:HH2	1.85	0.41
2:E:369:VAL:O	2:E:369:VAL:HG23	2.20	0.41
2:F:185:HIS:HB2	2:F:191:LEU:HB2	2.02	0.41
2:F:193:LEU:HD11	2:F:201:LEU:HB3	2.02	0.41
2:F:344:TYR:HE1	2:F:347:CYS:HB3	1.85	0.41
1:A:186:GLU:OE2	1:A:186:GLU:N	2.53	0.41
1:A:16:ARG:HB3	1:A:218:MET:CE	2.50	0.41
1:B:296:ARG:CZ	3:S:664:HIS:CE1	3.02	0.41
2:E:159:ARG:HG2	2:E:168:CYS:SG	2.60	0.41
2:F:134:TYR:OH	2:F:154:SER:HB3	2.20	0.41
1:A:295:LYS:HZ1	1:A:295:LYS:HB2	1.85	0.41
1:B:436:ALA:O	1:B:437:GLN:CB	2.68	0.41
1:B:441:GLU:OE2	1:B:475:ARG:NH1	2.51	0.41
1:B:513:LEU:HD22	3:S:568:SER:HA	2.01	0.41
2:E:136:CYS:HB3	2:E:151:VAL:HG12	2.02	0.41
2:E:169:ILE:O	2:E:170:LYS:HG3	2.20	0.41
3:T:659:HIS:CE1	3:T:663:MET:CE	3.03	0.41
3:T:673:SER:O	3:T:675:ASP:N	2.53	0.41
1:A:119:ASN:HB3	1:A:542:ILE:HD11	2.01	0.41
1:B:107:VAL:HG13	2:E:173:VAL:HG11	2.02	0.41
2:E:397:ALA:HB3	2:E:415:CYS:HB3	2.02	0.41
2:F:118:ILE:HD11	2:F:422:ARG:HB2	2.02	0.41
3:T:570:THR:O	3:T:571:CYS:HB2	2.20	0.41
1:A:94:GLN:NE2	2:F:118:ILE:O	2.53	0.41
2:F:346:GLN:O	2:F:367:ASN:OD1	2.38	0.41
3:S:616:LEU:HA	3:S:616:LEU:HD12	1.76	0.41
3:T:607:ASN:CB	3:T:609:GLY:H	2.32	0.41
1:A:177:ALA:O	1:A:178:LEU:C	2.59	0.41
1:B:83:CYS:HB2	2:E:106:ARG:NH2	2.36	0.41
1:B:53:THR:CG2	2:E:359:TRP:CE3	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:88:ASN:C	2:F:88:ASN:OD1	2.59	0.41
1:A:280:TYR:OH	3:T:659:HIS:CD2	2.68	0.41
2:E:184:PHE:CE2	2:E:192:LEU:HD13	2.55	0.41
2:E:319:PRO:HG2	2:E:329:ILE:CD1	2.49	0.41
2:E:395:CYS:CA	2:E:421:TRP:CZ2	3.03	0.41
2:E:78:HIS:O	2:E:79:ASN:HB2	2.20	0.41
3:T:607:ASN:C	3:T:609:GLY:H	2.24	0.41
1:A:462:GLN:O	1:A:463:CYS:HB2	2.21	0.41
1:B:494:LYS:HD3	1:B:507:SER:CA	2.47	0.41
2:E:294:TYR:CE1	2:E:350:TRP:HB2	2.55	0.41
1:A:479:PRO:HB3	1:A:491:TRP:HH2	1.86	0.41
2:E:205:ASN:CG	2:E:208:THR:HG22	2.41	0.41
2:E:226:LEU:HD22	2:E:350:TRP:HZ3	1.84	0.41
2:F:140:TYR:CZ	2:F:189:PRO:HG3	2.56	0.41
3:T:584:GLU:C	3:T:586:GLU:N	2.74	0.41
2:F:282:PHE:CE2	3:T:594:GLU:HB3	2.56	0.41
1:A:431:CYS:O	1:A:435:ILE:HG13	2.21	0.41
1:A:595:LYS:HE2	1:A:608:PHE:CE2	2.57	0.41
1:B:449:GLU:O	1:B:450:CYS:C	2.59	0.41
1:B:541:GLU:CG	1:B:577:LYS:HG3	2.51	0.41
1:B:523:ILE:HG22	1:B:584:ALA:HA	2.02	0.41
2:E:242:MET:HB3	2:E:242:MET:HE2	1.80	0.41
1:A:464:ASN:ND2	1:A:464:ASN:N	2.63	0.40
2:E:150:ALA:HA	2:E:159:ARG:O	2.21	0.40
2:E:136:CYS:HA	2:E:150:ALA:O	2.20	0.40
1:B:178:LEU:HD12	1:B:215:ILE:HD11	2.02	0.40
1:B:26:LEU:O	1:B:27:ARG:C	2.59	0.40
1:B:178:LEU:CD1	1:B:211:ILE:HG23	2.50	0.40
1:B:273:PHE:CD1	1:B:273:PHE:C	2.94	0.40
1:B:68:VAL:HG11	2:E:109:LEU:HD23	2.04	0.40
2:F:74:LEU:HD13	2:F:118:ILE:HD12	2.02	0.40
2:F:92:LYS:HB2	2:F:95:ASP:OD2	2.21	0.40
3:S:637:MET:O	3:S:640:VAL:HG13	2.21	0.40
3:T:564:LEU:HA	3:T:564:LEU:HD12	1.69	0.40
1:B:121:MET:HE1	1:B:542:ILE:HB	2.03	0.40
2:E:185:HIS:HA	2:E:186:PRO:HD3	1.80	0.40
2:E:319:PRO:HG2	2:E:326:ILE:CD1	2.51	0.40
1:A:85:VAL:CG1	2:F:74:LEU:HD23	2.45	0.40
1:B:280:TYR:CG	3:S:614:MET:HG2	2.56	0.40
3:T:650:LYS:O	3:T:651:ASN:HB3	2.20	0.40
1:A:345:ILE:HG22	1:A:355:ILE:HD13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:THR:O	1:A:365:ARG:N	2.54	0.40
1:B:581:ILE:HG13	1:B:581:ILE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	449/643 (70%)	386 (86%)	53 (12%)	10 (2%)	6	25
1	B	451/643 (70%)	383 (85%)	57 (13%)	11 (2%)	6	23
2	E	356/362 (98%)	322 (90%)	30 (8%)	4 (1%)	14	42
2	F	357/362 (99%)	329 (92%)	26 (7%)	2 (1%)	25	55
3	S	126/191 (66%)	102 (81%)	18 (14%)	6 (5%)	2	11
3	T	126/191 (66%)	101 (80%)	16 (13%)	9 (7%)	1	5
All	All	1865/2392 (78%)	1623 (87%)	200 (11%)	42 (2%)	6	24

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	SER
1	B	87	SER
1	B	250	PRO
3	S	579	MET
3	S	605	ASP
3	T	586	GLU
3	T	605	ASP
1	A	250	PRO
1	A	257	ALA
1	A	261	GLN

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Mol	Chain	Res	Type
1	A	366	GLN
1	B	366	GLN
2	E	379	VAL
2	F	379	VAL
3	S	683	GLU
3	T	577	GLN
3	T	579	MET
3	T	580	GLU
3	T	683	GLU
1	A	349	TYR
1	A	462	GLN
1	B	235	LEU
1	B	261	GLN
1	B	349	TYR
1	B	462	GLN
1	B	491	TRP
2	E	144	THR
2	E	370	GLY
2	E	416	ASP
3	T	562	ASN
3	T	582	ASP
1	A	258	LYS
1	A	491	TRP
1	B	251	ASN
2	F	144	THR
3	S	562	ASN
3	S	630	ASN
1	B	258	LYS
1	B	257	ALA
3	T	674	ILE
1	A	528	PRO
3	S	674	ILE

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	418/560 (75%)	383 (92%)	35 (8%)	11	34
1	B	420/560 (75%)	376 (90%)	44 (10%)	7	23
2	E	321/325 (99%)	299 (93%)	22 (7%)	15	42
2	F	322/325 (99%)	300 (93%)	22 (7%)	16	42
3	S	122/175 (70%)	110 (90%)	12 (10%)	8	26
3	T	122/175 (70%)	106 (87%)	16 (13%)	4	15
All	All	1725/2120 (81%)	1574 (91%)	151 (9%)	10	32

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	MET
1	A	36	ASP
1	A	39	LYS
1	A	42	PHE
1	A	90	ASP
1	A	98	LEU
1	A	102	ASN
1	A	112	SER
1	A	116	LEU
1	A	117	GLN
1	A	121	MET
1	A	123	GLU
1	A	168	ASP
1	A	180	GLN
1	A	186	GLU
1	A	261	GLN
1	A	262	ARG
1	A	275	ARG
1	A	277	CYS
1	A	295	LYS
1	A	296	ARG
1	A	357	ARG
1	A	418	GLN
1	A	458	ARG
1	A	460	LYS
1	A	464	ASN
1	A	484	THR
1	A	502	SER
1	A	510	HIS
1	A	513	LEU

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Mol	Chain	Res	Type
1	A	560	CYS
1	A	567	ASN
1	A	576	ARG
1	A	577	LYS
1	A	597	MET
1	B	9	GLU
1	B	13	ILE
1	B	27	ARG
1	B	28	GLN
1	B	30	LYS
1	B	31	ARG
1	B	40	SER
1	B	57	ASN
1	B	62	GLN
1	B	90	ASP
1	B	98	LEU
1	B	99	LYS
1	B	102	ASN
1	B	112	SER
1	B	116	LEU
1	B	117	GLN
1	B	121	MET
1	B	123	GLU
1	B	168	ASP
1	B	180	GLN
1	B	186	GLU
1	B	210	LYS
1	B	262	ARG
1	B	275	ARG
1	B	277	CYS
1	B	284	LEU
1	B	294	TYR
1	B	295	LYS
1	B	296	ARG
1	B	357	ARG
1	B	418	GLN
1	B	442	LYS
1	B	458	ARG
1	B	460	LYS
1	B	464	ASN
1	B	468	CYS
1	B	484	THR

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Mol	Chain	Res	Type
1	B	502	SER
1	B	513	LEU
1	B	529	VAL
1	B	549	ASP
1	B	560	CYS
1	B	567	ASN
1	B	577	LYS
2	E	75	LYS
2	E	112	CYS
2	E	159	ARG
2	E	177	ASN
2	E	182	LEU
2	E	201	LEU
2	E	202	ARG
2	E	254	LYS
2	E	255	ARG
2	E	258	ASN
2	E	328	LYS
2	E	330	LYS
2	E	341	ARG
2	E	348	ASP
2	E	357	ASP
2	E	362	MET
2	E	371	LYS
2	E	381	ASP
2	E	388	THR
2	E	394	LYS
2	E	416	ASP
2	E	425	ARG
2	F	75	LYS
2	F	91	SER
2	F	142	SER
2	F	182	LEU
2	F	201	LEU
2	F	202	ARG
2	F	236	LYS
2	F	254	LYS
2	F	258	ASN
2	F	279	LYS
2	F	286	SER
2	F	292	ARG
2	F	328	LYS

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Mol	Chain	Res	Type
2	F	330	LYS
2	F	341	ARG
2	F	348	ASP
2	F	357	ASP
2	F	362	MET
2	F	371	LYS
2	F	394	LYS
2	F	416	ASP
2	F	426	LEU
3	S	572	LEU
3	S	575	ARG
3	S	586	GLU
3	S	590	GLU
3	S	597	ILE
3	S	607	ASN
3	S	616	LEU
3	S	638	LEU
3	S	640	VAL
3	S	645	GLN
3	S	671	ILE
3	S	672	MET
3	T	561	HIS
3	T	572	LEU
3	T	574	LEU
3	T	575	ARG
3	T	577	GLN
3	T	580	GLU
3	T	582	ASP
3	T	590	GLU
3	T	597	ILE
3	T	607	ASN
3	T	608	GLU
3	T	616	LEU
3	T	638	LEU
3	T	645	GLN
3	T	671	ILE
3	T	672	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN

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Mol	Chain	Res	Type
1	A	43	ASN
1	A	94	GLN
1	A	102	ASN
1	A	117	GLN
1	A	119	ASN
1	A	180	GLN
1	A	264	GLN
1	A	418	GLN
1	A	445	GLN
1	A	464	ASN
1	A	467	GLN
1	A	504	GLN
1	A	532	ASN
1	A	545	GLN
1	A	567	ASN
1	A	585	ASN
1	A	603	HIS
1	B	43	ASN
1	B	47	GLN
1	B	50	GLN
1	B	57	ASN
1	B	58	GLN
1	B	62	GLN
1	B	66	GLN
1	B	94	GLN
1	B	117	GLN
1	B	180	GLN
1	B	264	GLN
1	B	418	GLN
1	B	425	GLN
1	B	429	ASN
1	B	445	GLN
1	B	464	ASN
1	B	467	GLN
1	B	504	GLN
1	B	532	ASN
1	B	545	GLN
1	B	567	ASN
1	B	585	ASN
2	E	146	HIS
2	E	175	HIS
2	E	199	HIS

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Mol	Chain	Res	Type
2	E	244	HIS
2	E	291	HIS
2	E	367	ASN
2	E	368	GLN
2	E	383	HIS
2	F	90	HIS
2	F	146	HIS
2	F	175	HIS
2	F	199	HIS
2	F	244	HIS
2	F	291	HIS
2	F	335	ASN
2	F	367	ASN
2	F	383	HIS
3	S	562	ASN
3	S	567	HIS
3	S	631	GLN
3	S	645	GLN
3	S	659	HIS
3	S	664	HIS
3	S	667	ASN
3	T	562	ASN
3	T	631	GLN
3	T	642	ASN
3	T	645	GLN
3	T	659	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CJG	A	708	-	28,33,33	2.51	11 (39%)	29,50,50	1.99	6 (20%)
5	CJG	B	708	-	28,33,33	2.31	12 (42%)	29,50,50	2.02	6 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CJG	A	708	-	-	1/8/21/21	0/4/4/4
5	CJG	B	708	-	-	2/8/21/21	0/4/4/4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	708	CJG	C17-C12	5.92	1.54	1.41
5	A	708	CJG	C14-C13	5.86	1.48	1.39
5	A	708	CJG	C2-C1	5.15	1.45	1.39
5	B	708	CJG	C17-C12	5.15	1.52	1.41
5	B	708	CJG	C14-C13	5.13	1.47	1.39
5	B	708	CJG	C2-C1	4.80	1.44	1.39
5	B	708	CJG	C17-N16	3.85	1.39	1.33
5	A	708	CJG	C17-N16	3.64	1.39	1.33
5	A	708	CJG	C11-C12	3.02	1.53	1.51
5	A	708	CJG	C6-C7	2.96	1.54	1.47
5	A	708	CJG	C2-C23	-2.88	1.46	1.50
5	B	708	CJG	C3-C4	2.80	1.43	1.38
5	B	708	CJG	C11-C12	2.58	1.53	1.51
5	A	708	CJG	C6-C5	2.51	1.45	1.40
5	B	708	CJG	C6-C1	2.50	1.45	1.39
5	B	708	CJG	C6-C5	2.45	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	708	CJG	C6-C7	2.44	1.53	1.47
5	A	708	CJG	C6-C1	2.39	1.45	1.39
5	B	708	CJG	C15-N16	2.35	1.39	1.34
5	A	708	CJG	C4-C5	2.32	1.43	1.39
5	A	708	CJG	C15-N16	2.24	1.39	1.34
5	B	708	CJG	C14-C15	-2.08	1.34	1.38
5	B	708	CJG	C3-C2	2.02	1.43	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	708	CJG	C17-N16-C15	5.70	124.90	116.89
5	A	708	CJG	C17-N16-C15	5.64	124.81	116.89
5	B	708	CJG	C11-C12-C13	5.01	127.31	119.75
5	A	708	CJG	C11-C12-C13	4.75	126.92	119.75
5	A	708	CJG	C20-C13-C12	3.90	126.78	122.01
5	B	708	CJG	C20-C13-C14	-3.86	112.36	119.49
5	B	708	CJG	C20-C13-C12	3.79	126.65	122.01
5	A	708	CJG	C20-C13-C14	-3.66	112.72	119.49
5	B	708	CJG	C9-C10-C5	-2.45	107.60	111.63
5	A	708	CJG	O21-C7-C6	-2.22	120.11	124.25
5	A	708	CJG	C9-C10-C5	-2.18	108.05	111.63
5	B	708	CJG	O21-C7-C6	-2.08	120.36	124.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

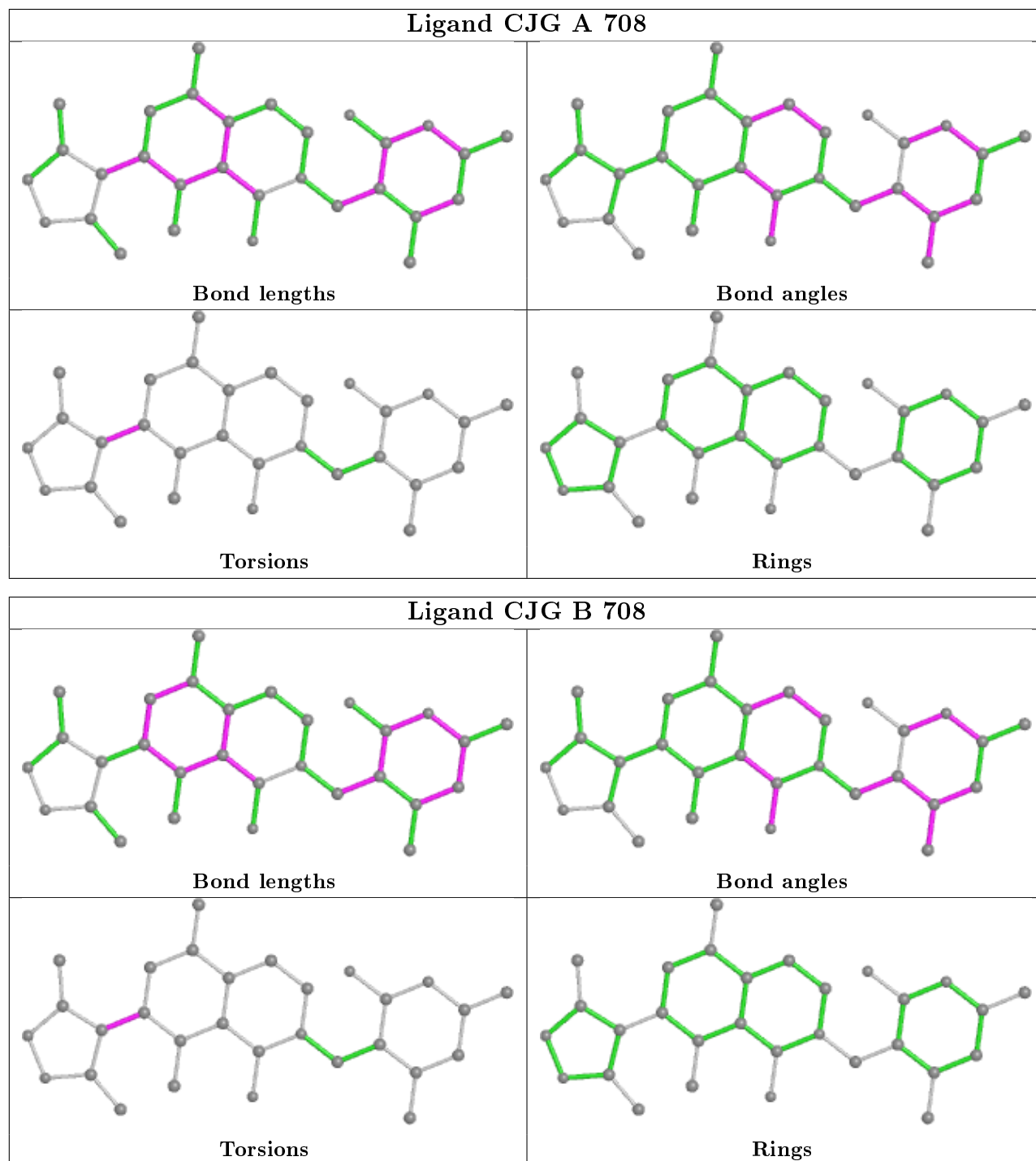
Mol	Chain	Res	Type	Atoms
5	B	708	CJG	C3-C2-C23-C24
5	A	708	CJG	C3-C2-C23-C24
5	B	708	CJG	C3-C2-C23-C27

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	463/643 (72%)	0.00	3 (0%) 89 76	31, 69, 105, 118	0
1	B	465/643 (72%)	-0.01	5 (1%) 80 60	34, 68, 106, 117	0
2	E	358/362 (98%)	-0.06	1 (0%) 94 85	34, 57, 80, 116	0
2	F	359/362 (99%)	-0.08	1 (0%) 94 85	35, 57, 80, 116	0
3	S	128/191 (67%)	-0.05	1 (0%) 86 70	43, 70, 109, 114	0
3	T	128/191 (67%)	0.01	0 100 100	41, 70, 109, 120	0
All	All	1901/2392 (79%)	-0.03	11 (0%) 89 76	31, 63, 103, 120	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166	ILE	3.8
1	A	291	PRO	3.0
1	B	494	LYS	3.0
2	E	385	ALA	2.7
2	F	381	ASP	2.6
3	S	581	VAL	2.5
1	B	367	VAL	2.4
1	A	263	GLU	2.2
1	A	367	VAL	2.2
1	B	293	THR	2.2
1	B	287	PHE	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

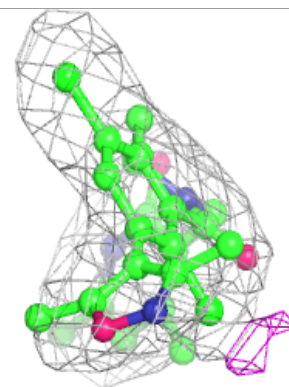
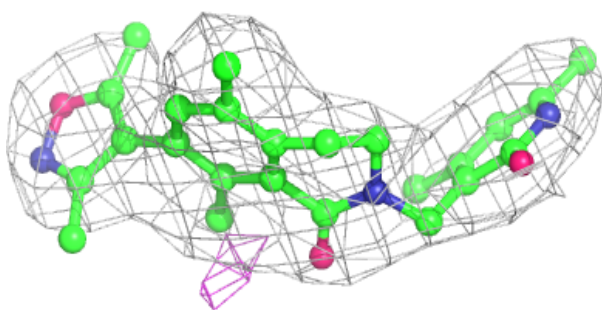
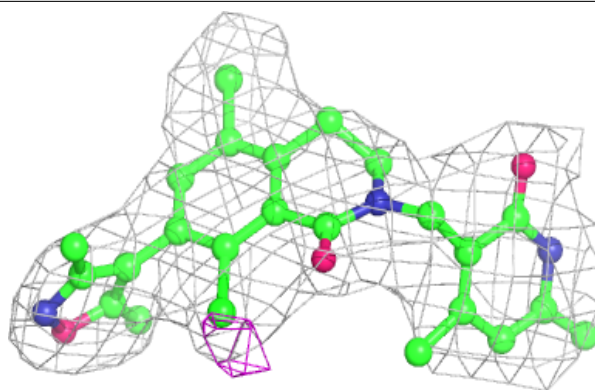
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CJG	B	708	30/30	0.97	0.22	47,52,55,57	0
4	ZN	A	701	1/1	0.97	0.19	44,44,44,44	1
4	ZN	B	706	1/1	0.97	0.22	58,58,58,58	1
5	CJG	A	708	30/30	0.97	0.25	43,49,57,60	0
4	ZN	B	701	1/1	0.97	0.24	58,58,58,58	1
4	ZN	B	702	1/1	0.98	0.17	44,44,44,44	1
4	ZN	B	704	1/1	0.99	0.18	32,32,32,32	1
4	ZN	B	703	1/1	0.99	0.22	42,42,42,42	1
4	ZN	A	702	1/1	0.99	0.19	37,37,37,37	1
4	ZN	A	705	1/1	0.99	0.22	35,35,35,35	1
4	ZN	A	704	1/1	0.99	0.21	49,49,49,49	1
4	ZN	A	707	1/1	0.99	0.19	27,27,27,27	1
4	ZN	B	707	1/1	0.99	0.21	32,32,32,32	1
4	ZN	A	703	1/1	0.99	0.24	47,47,47,47	1
4	ZN	A	706	1/1	1.00	0.22	27,27,27,27	1
4	ZN	B	705	1/1	1.00	0.23	48,48,48,48	1

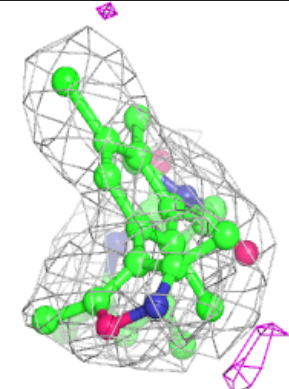
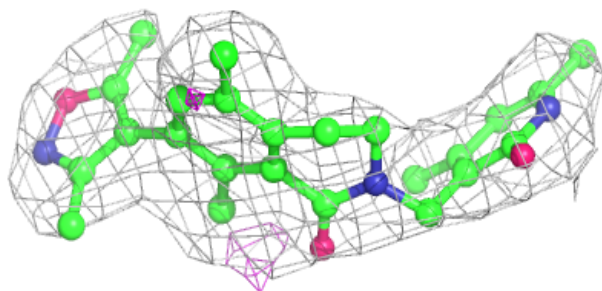
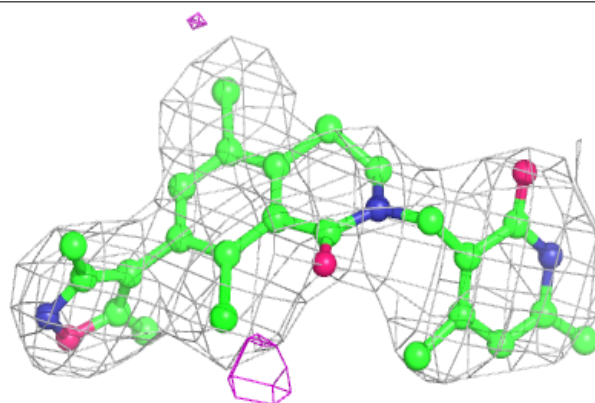
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CJG B 708:

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

**Electron density around CJG A 708:**

$2mF_o-DF_c$ (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.