



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:58 PM UTC

PDB ID : 6QXA / pdb_00006qxa
Title : Structure of membrane bound pyrophosphatase from *Thermotoga maritima* in complex with imidodiphosphate and N-[(2-amino-6-benzothiazolyl)methyl]-1H-indole-2-carboxamide (ATC)
Authors : Vidilaseris, K.; Goldman, A.
Deposited on : 2019-03-07
Resolution : 3.41 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

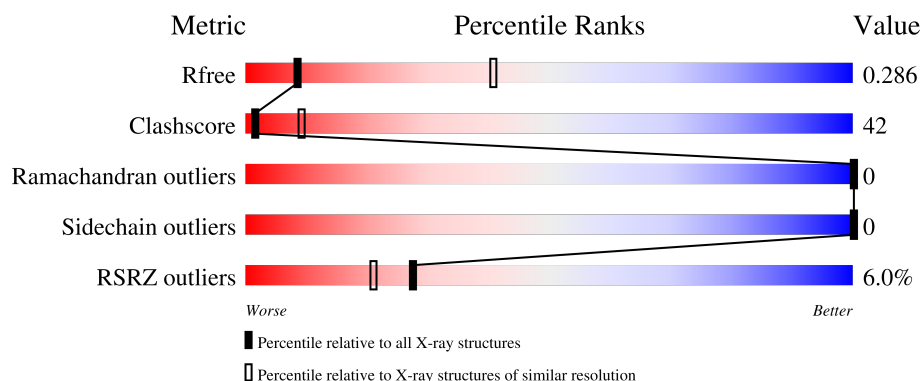
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	735	4% 43% 56%
1	B	735	8% 40% 57%
1	C	735	5% 43% 56%
1	D	735	6% 44% 54%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 21095 atoms, of which 53 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 K(+)-stimulated pyrophosphate-energized sodium pump.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	725	Total	C	N	O	S	0	0	0
			5260	3444	827	962	27			
1	B	715	Total	C	N	O	S	0	0	0
			5179	3397	810	946	26			
1	C	725	Total	C	N	O	S	0	0	0
			5267	3447	830	963	27			
1	D	719	Total	C	N	O	S	0	0	0
			5189	3407	804	951	27			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP Q9S5X0
A	-7	ARG	-	expression tag	UNP Q9S5X0
A	-6	GLY	-	expression tag	UNP Q9S5X0
A	-5	SER	-	expression tag	UNP Q9S5X0
A	-4	HIS	-	expression tag	UNP Q9S5X0
A	-3	HIS	-	expression tag	UNP Q9S5X0
A	-2	HIS	-	expression tag	UNP Q9S5X0
A	-1	HIS	-	expression tag	UNP Q9S5X0
A	0	HIS	-	expression tag	UNP Q9S5X0
A	1	HIS	-	expression tag	UNP Q9S5X0
A	353	LEU	VAL	conflict	UNP Q9S5X0
A	395	GLY	SER	conflict	UNP Q9S5X0
B	-8	MET	-	initiating methionine	UNP Q9S5X0
B	-7	ARG	-	expression tag	UNP Q9S5X0
B	-6	GLY	-	expression tag	UNP Q9S5X0
B	-5	SER	-	expression tag	UNP Q9S5X0
B	-4	HIS	-	expression tag	UNP Q9S5X0
B	-3	HIS	-	expression tag	UNP Q9S5X0
B	-2	HIS	-	expression tag	UNP Q9S5X0
B	-1	HIS	-	expression tag	UNP Q9S5X0
B	0	HIS	-	expression tag	UNP Q9S5X0

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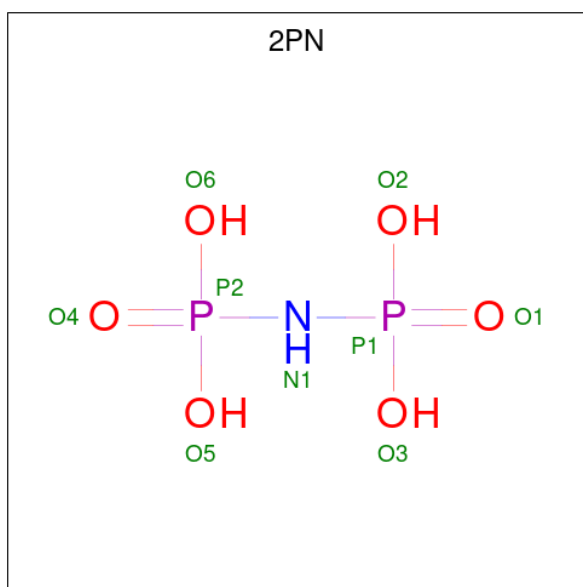
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	HIS	-	expression tag	UNP Q9S5X0
B	353	LEU	VAL	conflict	UNP Q9S5X0
B	395	GLY	SER	conflict	UNP Q9S5X0
C	-8	MET	-	initiating methionine	UNP Q9S5X0
C	-7	ARG	-	expression tag	UNP Q9S5X0
C	-6	GLY	-	expression tag	UNP Q9S5X0
C	-5	SER	-	expression tag	UNP Q9S5X0
C	-4	HIS	-	expression tag	UNP Q9S5X0
C	-3	HIS	-	expression tag	UNP Q9S5X0
C	-2	HIS	-	expression tag	UNP Q9S5X0
C	-1	HIS	-	expression tag	UNP Q9S5X0
C	0	HIS	-	expression tag	UNP Q9S5X0
C	1	HIS	-	expression tag	UNP Q9S5X0
C	353	LEU	VAL	conflict	UNP Q9S5X0
C	395	GLY	SER	conflict	UNP Q9S5X0
D	-8	MET	-	initiating methionine	UNP Q9S5X0
D	-7	ARG	-	expression tag	UNP Q9S5X0
D	-6	GLY	-	expression tag	UNP Q9S5X0
D	-5	SER	-	expression tag	UNP Q9S5X0
D	-4	HIS	-	expression tag	UNP Q9S5X0
D	-3	HIS	-	expression tag	UNP Q9S5X0
D	-2	HIS	-	expression tag	UNP Q9S5X0
D	-1	HIS	-	expression tag	UNP Q9S5X0
D	0	HIS	-	expression tag	UNP Q9S5X0
D	1	HIS	-	expression tag	UNP Q9S5X0
D	353	LEU	VAL	conflict	UNP Q9S5X0
D	395	GLY	SER	conflict	UNP Q9S5X0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total Mg 5 5	0	0
2	B	5	Total Mg 5 5	0	0
2	C	5	Total Mg 5 5	0	0
2	D	5	Total Mg 5 5	0	0

- Molecule 3 is IMIDODIPHOSPHORIC ACID (CCD ID: 2PN) (formula: H₅NO₆P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	N	O	P	0	0
			9	1	6	2		
3	B	1	Total	N	O	P	0	0
			9	1	6	2		
3	C	1	Total	N	O	P	0	0
			9	1	6	2		
3	D	1	Total	N	O	P	0	0
			9	1	6	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		
4	D	1	Total	Na	0	0
			1	1		

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

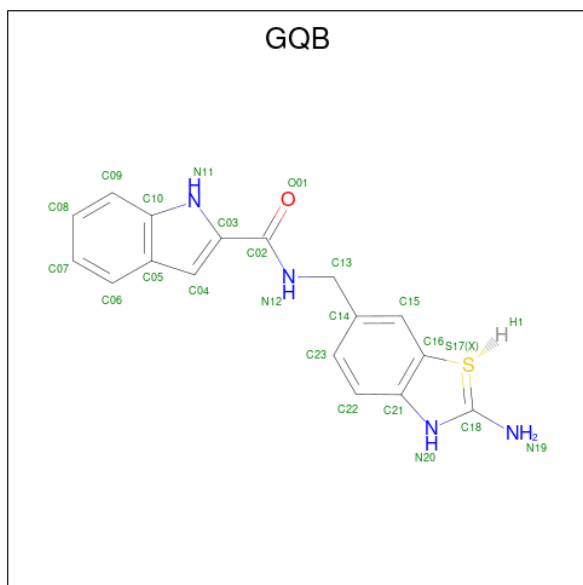
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		
5	B	1	Total	K	0	0
			1	1		

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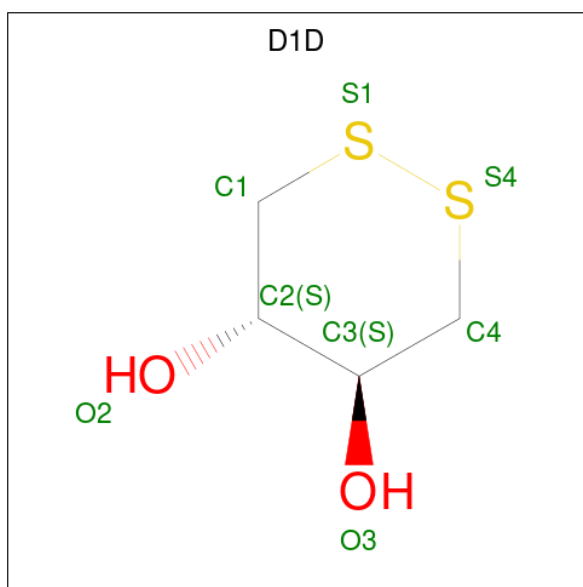
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total K 1 1	0	0

- Molecule 6 is {N}-[(2-azanyl-3 {H}-1,3-benzothiazol-6-yl)methyl]-1 {H}-indole-2-carboxamide (CCD ID: GQB) (formula: C₁₇H₁₆N₄OS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total 38	C 17	H 15	N 4	O 1	S 1	0	0
6	A	1	Total 38	C 17	H 15	N 4	O 1	S 1	0	0
6	C	1	Total 38	C 17	H 15	N 4	O 1	S 1	0	0

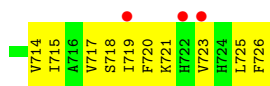
- Molecule 7 is (4S,5S)-1,2-DITHIANE-4,5-DIOL (CCD ID: D1D) (formula: C₄H₈O₂S₂).



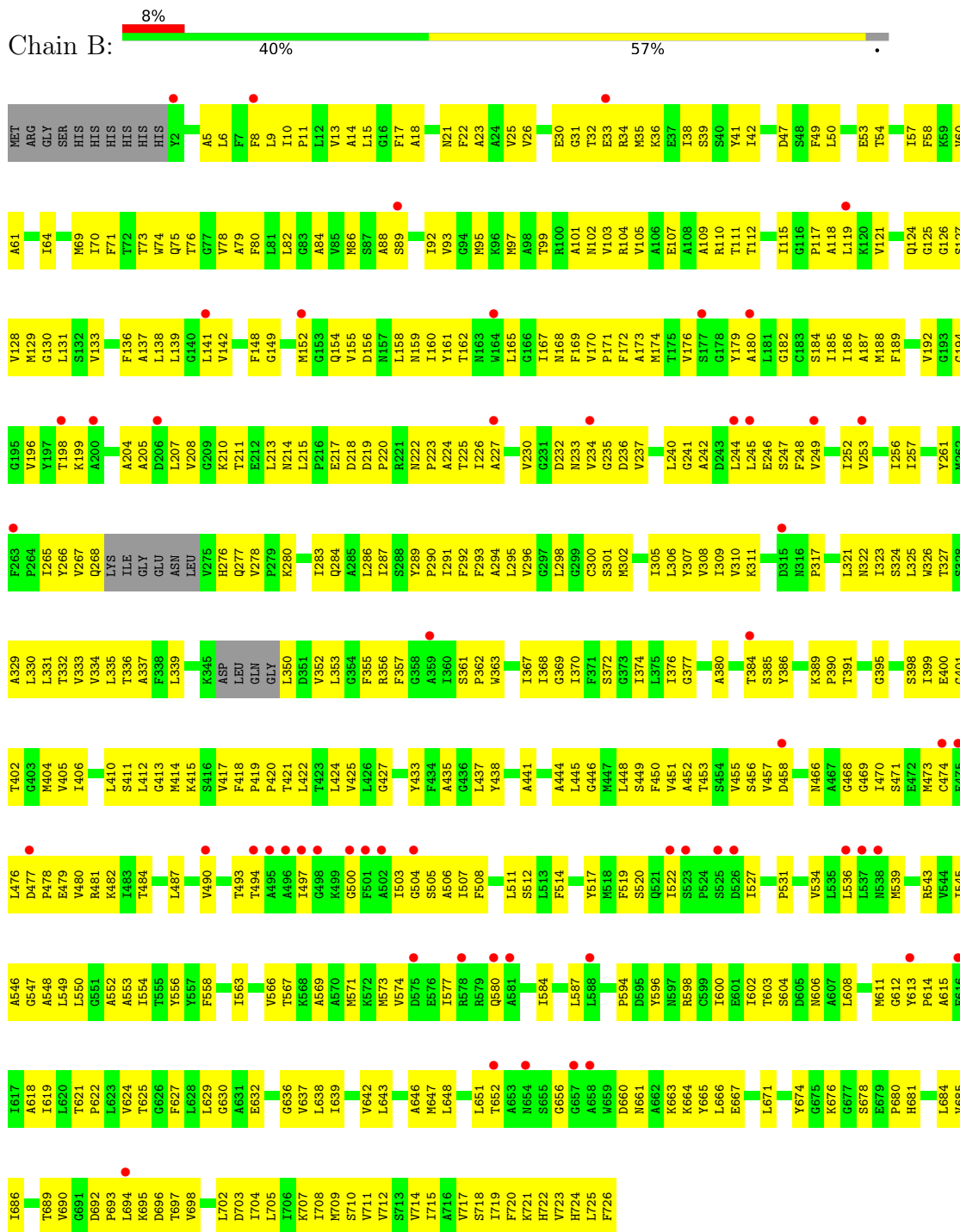
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	H	O	S	0	0
			16	4	8	2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	O	0	0
			1	1		
8	C	3	Total	O	0	0
			3	3		
8	D	4	Total	O	0	0
			4	4		

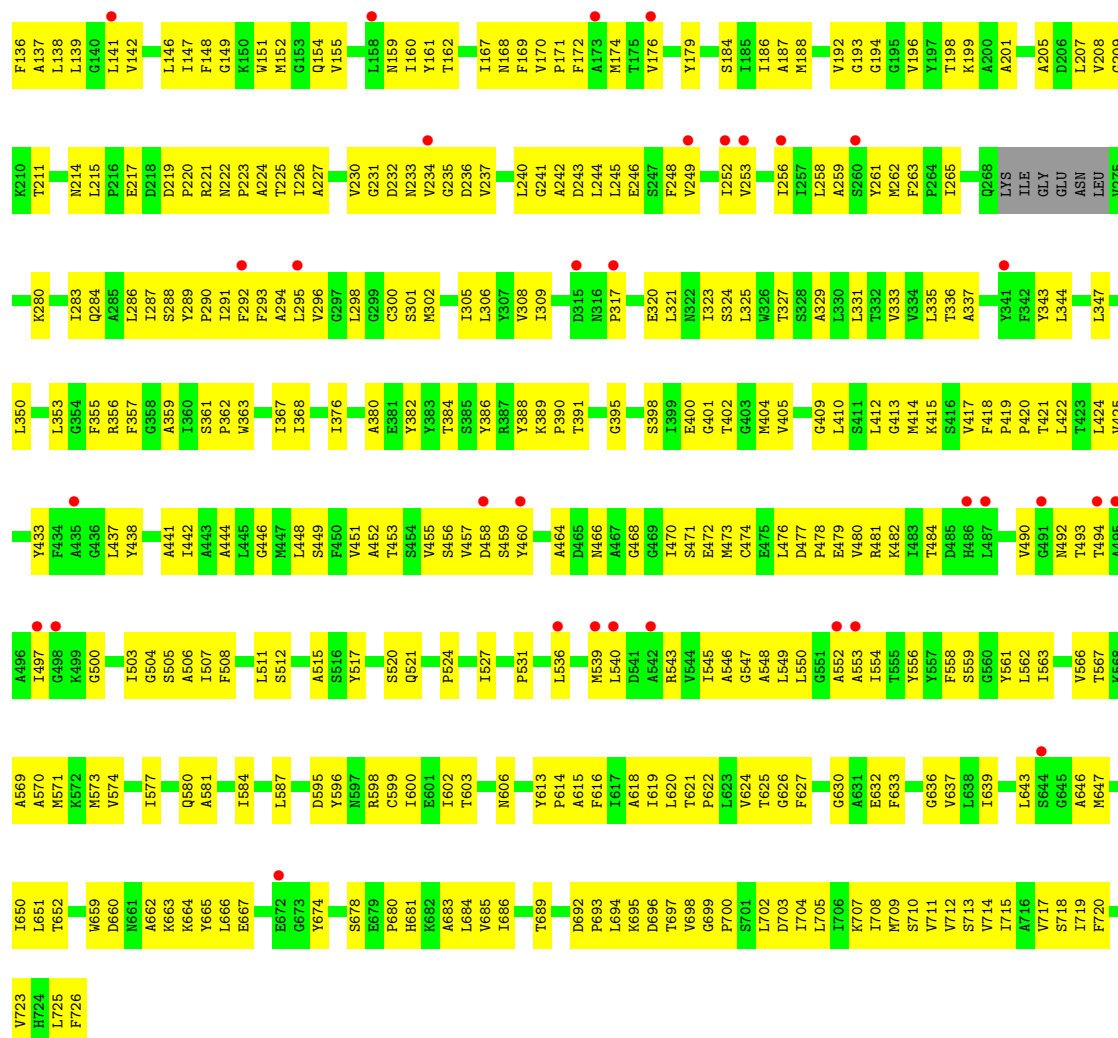


- Molecule 1: K(+)-stimulated pyrophosphate-energized sodium pump



- Molecule 1: K(+)-stimulated pyrophosphate-energized sodium pump





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.10Å 141.59Å 251.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.48 – 3.41 47.48 – 3.41	Depositor EDS
% Data completeness (in resolution range)	74.9 (47.48-3.41) 70.1 (47.48-3.41)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.228 , 0.284 0.231 , 0.286	Depositor DCC
R_{free} test set	2000 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å ²)	87.8	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	21095	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: D1D, MG, GQB, K, NA, 2PN

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	0.11	0/5373	0.26	0/7340
1	B	0.11	0/5289	0.26	0/7223
1	C	0.11	0/5379	0.26	0/7341
1	D	0.11	0/5302	0.25	0/7246
All	All	0.11	0/21343	0.26	0/29150

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5260	0	5236	452	0
1	B	5179	0	5167	472	0
1	C	5267	0	5267	479	0
1	D	5189	0	5149	445	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	9	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	9	0	1	0	0
3	C	9	0	0	0	0
3	D	9	0	1	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	46	30	0	2	0
6	C	23	15	0	0	0
7	C	8	8	8	1	0
8	A	1	0	0	0	0
8	C	3	0	0	1	0
8	D	4	0	0	0	0
All	All	21042	53	20830	1763	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 42.

All (1763) 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:308:VAL:HG21	1:D:324:SER:HB2	1.22	1.16
1:C:308:VAL:HG21	1:C:324:SER:HB2	1.24	1.09
1:A:14:ALA:HB2	1:A:298:LEU:HD21	1.37	1.06
1:B:308:VAL:HG21	1:B:324:SER:HB2	1.36	1.05
1:C:185:ILE:HG12	1:C:708:ILE:HD11	1.29	1.05
1:C:571:MET:HG3	1:D:404:MET:HE2	1.37	1.05
1:B:622:PRO:HG3	1:B:709:MET:HG3	1.38	1.05
1:C:76:THR:HG21	1:C:174:MET:HG3	1.40	1.04
1:D:259:ALA:HA	1:D:262:MET:HE2	1.40	1.03
1:C:39:SER:HB3	1:C:103:VAL:HG21	1.38	1.03
1:A:244:LEU:HD23	1:A:455:VAL:HG22	1.39	1.02
1:D:14:ALA:HB2	1:D:298:LEU:HD21	1.40	1.02
1:D:184:SER:HA	1:D:246:GLU:HG3	1.37	1.02
1:A:308:VAL:HG21	1:A:324:SER:HB2	1.42	1.00
1:C:43:ARG:HG2	1:C:99:THR:HB	1.43	1.00
1:A:571:MET:HG3	1:B:404:MET:HE2	1.40	0.99
1:C:14:ALA:HB2	1:C:298:LEU:HD21	1.42	0.99
1:B:39:SER:HB3	1:B:103:VAL:HG21	1.44	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:LEU:HD23	1:B:455:VAL:HG22	1.44	0.98
1:C:517:TYR:HB2	1:C:714:VAL:HG22	1.45	0.97
1:A:105:VAL:HG22	1:A:121:VAL:HG13	1.46	0.97
1:B:32:THR:H	1:B:35:MET:HE3	1.27	0.97
1:C:129:MET:HE2	1:C:241:GLY:HA3	1.48	0.96
1:C:244:LEU:HD23	1:C:455:VAL:HG22	1.47	0.96
1:C:622:PRO:HG3	1:C:709:MET:HG3	1.44	0.96
1:D:43:ARG:HG2	1:D:99:THR:HB	1.47	0.96
1:D:468:GLY:CA	1:D:484:THR:HG21	1.95	0.96
1:B:167:ILE:HD11	1:B:719:ILE:HD11	1.45	0.95
1:C:425:VAL:HG13	1:D:546:ALA:HB1	1.49	0.95
1:B:109:ALA:HB2	1:B:118:ALA:HB2	1.48	0.95
1:B:184:SER:HA	1:B:246:GLU:HG3	1.45	0.95
1:D:39:SER:HB3	1:D:103:VAL:HG21	1.45	0.95
1:A:39:SER:HB3	1:A:103:VAL:HG21	1.47	0.94
1:A:35:MET:HE2	1:A:476:LEU:HD21	1.50	0.94
1:B:517:TYR:HB2	1:B:714:VAL:HG22	1.50	0.93
1:D:25:VAL:HG11	1:D:97:MET:HE1	1.51	0.93
1:A:425:VAL:HG13	1:B:546:ALA:HB1	1.48	0.92
1:B:103:VAL:HG23	1:B:470:ILE:HD13	1.52	0.92
1:C:536:LEU:HD11	1:D:536:LEU:HD11	1.47	0.92
1:B:188:MET:HE3	1:B:614:PRO:HB2	1.52	0.92
1:D:468:GLY:HA3	1:D:484:THR:HG21	1.51	0.92
1:C:399:ILE:HD11	1:C:671:LEU:HD21	1.50	0.91
1:A:167:ILE:HD11	1:A:719:ILE:HD11	1.51	0.91
1:D:244:LEU:HD23	1:D:455:VAL:HG22	1.50	0.90
1:B:10:ILE:HD12	1:B:295:LEU:HB3	1.52	0.90
1:B:424:LEU:HD23	1:B:507:ILE:HD12	1.51	0.90
1:C:103:VAL:HG23	1:C:470:ILE:HD13	1.54	0.90
1:A:639:ILE:HD13	1:B:539:MET:HG2	1.51	0.90
1:B:110:ARG:HA	1:B:480:VAL:HG22	1.50	0.90
1:A:184:SER:HA	1:A:246:GLU:HG3	1.54	0.89
1:D:31:GLY:HA2	1:D:107:GLU:HG3	1.55	0.89
1:B:105:VAL:HG22	1:B:121:VAL:HG13	1.54	0.89
1:C:404:MET:HE2	1:D:571:MET:HG3	1.53	0.89
1:A:622:PRO:HG3	1:A:709:MET:HG3	1.55	0.88
1:C:25:VAL:HG11	1:C:97:MET:HE1	1.56	0.87
1:A:553:ALA:HB2	1:B:421:THR:HG21	1.56	0.87
1:B:14:ALA:HB2	1:B:298:LEU:HD21	1.54	0.87
1:B:317:PRO:HG2	1:B:490:VAL:HG21	1.55	0.87
1:A:399:ILE:HD11	1:A:671:LEU:HD21	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:546:ALA:HB1	1:D:425:VAL:HG13	1.55	0.87
1:C:138:LEU:HD13	1:C:295:LEU:HD23	1.57	0.87
1:B:32:THR:HG22	1:B:35:MET:HE3	1.56	0.86
1:D:437:LEU:HD13	1:D:515:ALA:HB2	1.55	0.86
1:A:317:PRO:HG2	1:A:490:VAL:HG21	1.57	0.86
1:D:138:LEU:HD13	1:D:295:LEU:HD23	1.56	0.86
1:C:530:PRO:HG2	1:C:533:LEU:HD13	1.57	0.86
1:B:444:ALA:HB2	1:B:508:PHE:HB3	1.57	0.86
1:B:162:THR:HG22	1:B:168:ASN:HD22	1.41	0.85
1:A:437:LEU:HD13	1:A:515:ALA:HB2	1.57	0.85
1:C:444:ALA:HB2	1:C:508:PHE:HB3	1.58	0.85
1:C:539:MET:HG2	1:D:539:MET:HG2	1.59	0.85
1:C:539:MET:HG3	1:D:539:MET:HE2	1.57	0.85
1:D:105:VAL:HG22	1:D:121:VAL:HG13	1.59	0.84
1:D:160:ILE:HD11	1:D:168:ASN:HB3	1.57	0.84
1:C:79:ALA:HB1	1:C:179:TYR:HB2	1.59	0.84
1:A:539:MET:HG2	1:B:639:ILE:HD13	1.57	0.84
1:B:587:LEU:HD21	1:B:594:PRO:HG3	1.59	0.84
1:A:192:VAL:HG11	1:A:614:PRO:HG3	1.58	0.84
1:D:336:THR:HG22	1:D:363:TRP:HD1	1.41	0.84
1:A:169:PHE:HB2	1:A:174:MET:HE3	1.60	0.84
1:B:31:GLY:HA2	1:B:107:GLU:HG3	1.60	0.84
1:C:105:VAL:HG22	1:C:121:VAL:HG13	1.60	0.83
1:A:404:MET:HE2	1:B:571:MET:HG3	1.60	0.83
1:A:306:LEU:HD12	1:A:309:ILE:HD11	1.59	0.83
1:A:138:LEU:HD13	1:A:295:LEU:HD23	1.60	0.83
1:D:517:TYR:HB2	1:D:714:VAL:HG22	1.59	0.83
1:A:639:ILE:CD1	1:B:539:MET:HG2	2.09	0.83
1:D:103:VAL:HG23	1:D:470:ILE:HD13	1.60	0.83
1:B:286:LEU:HB3	1:B:438:TYR:HE2	1.44	0.82
1:D:129:MET:HE2	1:D:241:GLY:HA3	1.60	0.82
1:B:584:ILE:HG23	1:B:587:LEU:HB2	1.62	0.82
1:C:344:LEU:HD22	1:C:347:LEU:HD11	1.61	0.82
1:B:137:ALA:HB2	1:B:245:LEU:HG	1.60	0.82
1:D:222:ASN:HB3	1:D:225:THR:HG23	1.61	0.82
1:B:399:ILE:HD11	1:B:671:LEU:HD21	1.62	0.82
1:A:188:MET:HE3	1:A:614:PRO:HB2	1.63	0.81
1:B:308:VAL:HG21	1:B:324:SER:CB	2.10	0.81
1:A:424:LEU:HD23	1:A:507:ILE:HD12	1.59	0.81
1:D:666:LEU:HD11	1:D:680:PRO:HB2	1.63	0.81
1:D:39:SER:HB3	1:D:103:VAL:CG2	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:MET:HE1	1:C:558:PHE:CZ	2.17	0.80
1:B:222:ASN:HB3	1:B:225:THR:HG23	1.63	0.80
1:C:199:LYS:HD2	1:C:696:ASP:HB2	1.64	0.80
1:D:492:ASN:ND2	1:D:660:ASP:OD2	2.15	0.80
1:B:580:GLN:O	1:B:584:ILE:HG22	1.80	0.79
1:C:418:PHE:HB3	1:C:419:PRO:HD3	1.63	0.79
1:D:308:VAL:HG21	1:D:324:SER:CB	2.07	0.79
1:C:262:MET:HE1	1:C:353:LEU:HB2	1.65	0.79
1:A:129:MET:HE2	1:A:241:GLY:HA3	1.64	0.79
1:B:32:THR:HG22	1:B:35:MET:CE	2.11	0.79
1:A:573:MET:HE3	1:A:599:CYS:HB3	1.64	0.79
1:C:39:SER:HB3	1:C:103:VAL:CG2	2.12	0.79
1:B:718:SER:HA	1:B:721:LYS:HD3	1.64	0.79
1:C:35:MET:CE	1:C:476:LEU:HD21	2.12	0.79
1:D:110:ARG:HA	1:D:480:VAL:HG22	1.63	0.78
1:A:418:PHE:HB3	1:A:419:PRO:HD3	1.64	0.78
1:C:184:SER:HA	1:C:246:GLU:HG3	1.64	0.78
1:A:325:LEU:HD23	1:A:453:THR:HG22	1.65	0.78
1:A:546:ALA:HB1	1:B:425:VAL:HG13	1.66	0.78
1:C:258:LEU:O	1:C:262:MET:HG3	1.84	0.78
1:C:537:LEU:HD23	1:C:639:ILE:HD11	1.64	0.78
1:C:553:ALA:HB2	1:D:421:THR:HG21	1.64	0.78
1:B:74:TRP:HH2	1:B:152:MET:HE1	1.48	0.78
1:C:76:THR:CG2	1:C:174:MET:HG3	2.14	0.78
1:C:444:ALA:HB2	1:C:508:PHE:CB	2.15	0.77
1:A:222:ASN:HB3	1:A:225:THR:HG23	1.65	0.77
1:B:39:SER:HB3	1:B:103:VAL:CG2	2.14	0.77
1:B:192:VAL:HG11	1:B:614:PRO:HG3	1.64	0.77
1:D:224:ALA:HB2	1:D:577:ILE:HD11	1.66	0.77
1:C:402:THR:HB	1:D:686:ILE:HD13	1.65	0.77
1:C:69:MET:HG2	1:C:74:TRP:HA	1.65	0.76
1:A:424:LEU:HD21	1:A:504:GLY:HA2	1.67	0.76
1:D:472:GLU:HG2	1:D:481:ARG:HD3	1.66	0.76
1:D:347:LEU:HB2	1:D:350:LEU:HD11	1.65	0.76
1:D:444:ALA:HB2	1:D:508:PHE:HB3	1.68	0.76
1:D:320:GLU:O	1:D:323:ILE:HG22	1.86	0.76
1:A:226:ILE:HD12	1:A:596:TYR:CD2	2.21	0.76
1:A:517:TYR:HB2	1:A:714:VAL:HG22	1.69	0.75
1:B:107:GLU:HG2	1:B:110:ARG:HH21	1.51	0.75
1:C:376:ILE:HD11	1:C:424:LEU:CD1	2.16	0.75
1:A:336:THR:HG22	1:A:363:TRP:HD1	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:PHE:HB3	1:B:419:PRO:HD3	1.69	0.75
1:C:74:TRP:O	1:C:78:VAL:HG23	1.86	0.75
1:C:448:LEU:HD13	1:C:505:SER:HB2	1.68	0.75
1:A:421:THR:HG21	1:B:553:ALA:HB2	1.68	0.75
1:D:398:SER:HA	1:D:405:VAL:HG22	1.68	0.74
1:A:39:SER:HB3	1:A:103:VAL:CG2	2.17	0.74
1:B:286:LEU:HB3	1:B:438:TYR:CE2	2.21	0.74
1:A:199:LYS:HD2	1:A:696:ASP:HB2	1.68	0.74
1:D:57:ILE:HD13	1:D:186:ILE:HD12	1.70	0.74
1:D:107:GLU:HG2	1:D:110:ARG:HH21	1.52	0.74
1:D:168:ASN:ND2	1:D:718:SER:OG	2.15	0.74
1:D:418:PHE:HB3	1:D:419:PRO:HD3	1.68	0.74
1:A:103:VAL:HG23	1:A:470:ILE:HD13	1.70	0.74
1:B:444:ALA:HB2	1:B:508:PHE:CB	2.17	0.74
1:A:539:MET:HG2	1:B:639:ILE:CD1	2.17	0.74
1:D:79:ALA:HB1	1:D:179:TYR:HB2	1.69	0.74
1:D:137:ALA:HB2	1:D:245:LEU:HG	1.69	0.74
1:A:244:LEU:CD2	1:A:455:VAL:HG22	2.16	0.73
1:D:74:TRP:HH2	1:D:152:MET:HE1	1.51	0.73
1:D:244:LEU:CD2	1:D:455:VAL:HG22	2.17	0.73
1:B:507:ILE:HD11	1:B:646:ALA:HB1	1.70	0.73
1:B:622:PRO:CG	1:B:709:MET:HG3	2.17	0.73
1:C:353:LEU:HD12	1:C:353:LEU:O	1.89	0.73
1:D:353:LEU:HD12	1:D:353:LEU:O	1.88	0.73
1:A:10:ILE:HD12	1:A:295:LEU:HB3	1.69	0.73
1:A:74:TRP:O	1:A:78:VAL:HG23	1.88	0.73
1:A:288:SER:HB2	1:A:343:TYR:OH	1.89	0.73
1:C:31:GLY:HA3	1:C:35:MET:SD	2.29	0.73
1:D:286:LEU:HD22	1:D:438:TYR:HE2	1.52	0.73
1:B:126:GLY:O	1:B:456:SER:HA	1.89	0.73
1:A:53:GLU:HG3	1:A:611:MET:HE1	1.70	0.72
1:A:471:SER:HA	1:A:476:LEU:HD13	1.69	0.72
1:B:138:LEU:HD13	1:B:295:LEU:HD23	1.71	0.72
1:C:424:LEU:HD23	1:C:507:ILE:HD12	1.70	0.72
1:D:35:MET:HE2	1:D:476:LEU:HD21	1.71	0.72
1:A:353:LEU:HD12	1:A:353:LEU:O	1.89	0.72
1:C:244:LEU:CD2	1:C:455:VAL:HG22	2.19	0.72
1:D:47:ASP:OD1	1:D:95:MET:HE1	1.90	0.72
1:D:243:ASP:CG	1:D:704:ILE:HD11	2.14	0.72
1:D:693:PRO:O	1:D:697:THR:OG1	2.06	0.72
1:D:622:PRO:HG3	1:D:709:MET:HG3	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:PRO:HG2	1:A:596:TYR:CE1	2.24	0.72
1:C:188:MET:HE1	1:C:558:PHE:HZ	1.54	0.72
1:A:137:ALA:HB2	1:A:245:LEU:HG	1.71	0.72
1:A:318:GLN:OE1	1:A:322:ASN:ND2	2.22	0.72
1:C:129:MET:HE2	1:C:241:GLY:CA	2.19	0.72
1:B:451:VAL:O	1:B:455:VAL:HG23	1.90	0.72
1:B:336:THR:HG22	1:B:363:TRP:HD1	1.55	0.72
1:A:82:LEU:O	1:A:86:MET:HG2	1.90	0.72
1:A:76:THR:OG1	1:A:174:MET:HG3	1.90	0.71
1:A:138:LEU:HD21	1:A:294:ALA:HB1	1.72	0.71
1:B:244:LEU:CD2	1:B:455:VAL:HG22	2.19	0.71
1:A:660:ASP:O	1:A:664:LYS:HG2	1.90	0.71
1:B:105:VAL:HA	1:B:121:VAL:HG11	1.72	0.71
1:B:693:PRO:O	1:B:697:THR:OG1	2.08	0.71
1:C:376:ILE:HD11	1:C:424:LEU:HD11	1.70	0.71
1:A:268:GLN:HG3	1:A:277:GLN:HE21	1.54	0.71
1:A:522:ILE:HD11	1:A:534:VAL:HG11	1.72	0.71
1:A:329:ALA:O	1:A:333:VAL:HG23	1.91	0.71
1:A:536:LEU:HD11	1:B:536:LEU:HD11	1.72	0.71
1:A:543:ARG:HH12	1:A:629:LEU:HD22	1.55	0.71
1:A:686:ILE:HD13	1:B:402:THR:HB	1.72	0.71
1:B:424:LEU:CD2	1:B:507:ILE:HD12	2.21	0.71
1:C:363:TRP:CE2	1:C:367:ILE:HD11	2.26	0.71
1:B:69:MET:HG2	1:B:74:TRP:HA	1.71	0.71
1:B:168:ASN:H	1:B:718:SER:CB	2.04	0.71
1:A:49:PHE:CD1	1:A:234:VAL:HG11	2.26	0.71
1:C:511:LEU:HD12	1:D:545:ILE:HD13	1.73	0.71
1:C:329:ALA:O	1:C:333:VAL:HG23	1.90	0.70
1:A:380:ALA:O	1:A:384:THR:HG22	1.91	0.70
1:C:336:THR:HG22	1:C:363:TRP:HD1	1.55	0.70
1:D:539:MET:HE2	1:D:639:ILE:HD13	1.74	0.70
1:A:74:TRP:HH2	1:A:152:MET:HE1	1.56	0.70
1:A:208:VAL:HG22	1:A:574:VAL:HG13	1.73	0.70
1:A:377:GLY:HA2	1:A:497:ILE:HG23	1.73	0.70
1:B:448:LEU:HD13	1:B:505:SER:HB2	1.74	0.70
1:C:25:VAL:CG1	1:C:97:MET:HE1	2.21	0.70
1:C:69:MET:HE2	1:C:74:TRP:HB2	1.71	0.70
1:D:194:GLY:HA3	1:D:235:GLY:HA2	1.73	0.70
1:D:437:LEU:HD13	1:D:515:ALA:CB	2.21	0.70
1:B:301:SER:CB	1:B:452:ALA:HB3	2.21	0.70
1:B:138:LEU:HD12	1:B:298:LEU:HD13	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ILE:HG22	1:A:298:LEU:HD22	1.74	0.70
1:D:8:PHE:CE2	1:D:146:LEU:HD21	2.26	0.70
1:D:31:GLY:HA3	1:D:35:MET:SD	2.31	0.70
1:D:103:VAL:CG2	1:D:470:ILE:HD13	2.21	0.70
1:D:336:THR:HG22	1:D:363:TRP:CD1	2.27	0.70
1:A:545:ILE:HG21	1:B:511:LEU:HD11	1.73	0.70
1:B:110:ARG:HA	1:B:480:VAL:CG2	2.22	0.70
1:B:627:PHE:CD1	1:B:720:PHE:HB3	2.27	0.69
1:D:105:VAL:HG22	1:D:121:VAL:CG1	2.22	0.69
1:C:47:ASP:OD1	1:C:95:MET:HE1	1.92	0.69
1:D:347:LEU:HB2	1:D:350:LEU:CD1	2.22	0.69
1:A:471:SER:CB	1:A:476:LEU:HD22	2.22	0.69
1:B:103:VAL:CG2	1:B:470:ILE:HD13	2.22	0.69
1:C:355:PHE:CD1	1:C:362:PRO:HD3	2.27	0.69
1:C:584:ILE:HG22	1:C:587:LEU:HB2	1.74	0.69
1:A:208:VAL:CG2	1:A:574:VAL:HG13	2.23	0.69
1:B:112:THR:HG21	1:B:117:PRO:HG2	1.73	0.69
1:A:224:ALA:HB2	1:A:577:ILE:HD11	1.74	0.69
1:C:421:THR:HG21	1:D:553:ALA:HB2	1.75	0.69
1:B:199:LYS:HD2	1:B:696:ASP:HB2	1.74	0.69
1:D:451:VAL:O	1:D:455:VAL:HG23	1.92	0.69
1:B:189:PHE:HE1	1:B:612:GLY:HA2	1.57	0.69
1:C:414:MET:HG2	1:C:651:LEU:HD11	1.75	0.69
1:D:76:THR:OG1	1:D:174:MET:HG3	1.93	0.69
1:D:82:LEU:O	1:D:86:MET:HG2	1.93	0.69
1:A:400:GLU:HG3	1:B:571:MET:HG2	1.74	0.69
1:A:451:VAL:O	1:A:455:VAL:HG23	1.93	0.69
1:B:353:LEU:HD12	1:B:353:LEU:O	1.92	0.69
1:B:522:ILE:HD11	1:B:534:VAL:HG11	1.73	0.69
1:D:35:MET:CE	1:D:476:LEU:HD21	2.23	0.69
1:C:86:MET:HE2	1:C:136:PHE:O	1.93	0.69
1:C:424:LEU:HD21	1:C:504:GLY:HA2	1.75	0.69
1:B:82:LEU:O	1:B:86:MET:HG2	1.93	0.68
1:B:129:MET:HE2	1:B:241:GLY:HA3	1.75	0.68
1:C:105:VAL:HA	1:C:121:VAL:HG11	1.75	0.68
1:C:222:ASN:HB3	1:C:225:THR:HG23	1.75	0.68
1:D:199:LYS:HD2	1:D:696:ASP:HB2	1.74	0.68
1:A:545:ILE:HD13	1:B:511:LEU:HD12	1.74	0.68
1:C:325:LEU:HD23	1:C:453:THR:HG22	1.75	0.68
1:D:188:MET:HE1	1:D:558:PHE:CZ	2.28	0.68
1:A:717:VAL:HA	1:A:720:PHE:CZ	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:LEU:HD12	1:C:298:LEU:HD13	1.74	0.68
1:C:167:ILE:HD11	1:C:719:ILE:HD11	1.75	0.68
1:D:133:VAL:HG13	1:D:245:LEU:HB2	1.75	0.68
1:B:49:PHE:CD1	1:B:234:VAL:HG11	2.28	0.68
1:B:199:LYS:HD3	1:B:692:ASP:HB3	1.73	0.68
1:C:14:ALA:CB	1:C:298:LEU:HD21	2.20	0.68
1:C:172:PHE:O	1:C:176:VAL:HG22	1.94	0.68
1:A:5:ALA:O	1:A:9:LEU:HD13	1.94	0.68
1:C:545:ILE:HD13	1:D:511:LEU:HD12	1.75	0.68
1:C:545:ILE:HG21	1:D:511:LEU:HD11	1.76	0.68
1:C:261:TYR:O	1:C:265:ILE:HD13	1.93	0.67
1:C:337:ALA:HB2	1:C:363:TRP:CE2	2.29	0.67
1:C:660:ASP:O	1:C:664:LYS:HG2	1.95	0.67
1:D:169:PHE:HB2	1:D:174:MET:HE3	1.76	0.67
1:A:109:ALA:HB2	1:A:118:ALA:HB2	1.76	0.67
1:B:10:ILE:HG22	1:B:298:LEU:HD22	1.76	0.67
1:B:138:LEU:HD21	1:B:294:ALA:HB1	1.76	0.67
1:A:437:LEU:HD13	1:A:515:ALA:CB	2.23	0.67
1:D:573:MET:HE3	1:D:599:CYS:HB3	1.77	0.67
1:A:53:GLU:CG	1:A:611:MET:HE1	2.24	0.67
1:B:596:TYR:O	1:B:600:ILE:HG12	1.95	0.67
1:D:448:LEU:HD13	1:D:505:SER:HB3	1.77	0.67
1:D:627:PHE:CD1	1:D:720:PHE:HB3	2.29	0.67
1:C:451:VAL:O	1:C:455:VAL:HG23	1.95	0.67
1:C:490:VAL:O	1:C:494:THR:HG23	1.94	0.67
1:D:168:ASN:HD22	1:D:718:SER:HG	1.39	0.67
1:A:35:MET:CE	1:A:476:LEU:HD21	2.23	0.66
1:A:58:PHE:O	1:A:62:ILE:HD13	1.96	0.66
1:A:571:MET:CG	1:B:404:MET:HE2	2.23	0.66
1:B:26:VAL:HA	1:B:104:ARG:CZ	2.25	0.66
1:B:79:ALA:HB1	1:B:179:TYR:HB2	1.77	0.66
1:C:124:GLN:O	1:C:128:VAL:HG23	1.95	0.66
1:C:598:ARG:O	1:C:602:ILE:HG12	1.95	0.66
1:A:149:GLY:CA	1:A:155:VAL:HG23	2.25	0.66
1:C:414:MET:HG2	1:C:651:LEU:CD1	2.26	0.66
1:A:84:ALA:HA	1:A:186:ILE:HG13	1.77	0.66
1:B:413:GLY:O	1:B:417:VAL:HG23	1.95	0.66
1:C:293:PHE:CE2	1:C:336:THR:HG21	2.31	0.66
1:B:199:LYS:HE2	1:B:199:LYS:HA	1.77	0.66
1:C:84:ALA:CB	1:C:186:ILE:HG13	2.26	0.66
1:C:318:GLN:OE1	1:C:322:ASN:ND2	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:545:ILE:HD13	1:D:511:LEU:CD1	2.25	0.66
1:A:299:GLY:HA2	1:A:302:MET:HE2	1.77	0.66
1:A:507:ILE:HD11	1:A:646:ALA:CB	2.25	0.66
1:B:162:THR:HG22	1:B:168:ASN:ND2	2.08	0.66
1:B:105:VAL:HG22	1:B:121:VAL:CG1	2.23	0.66
1:B:608:LEU:HA	1:B:611:MET:HE2	1.76	0.66
1:B:711:VAL:O	1:B:715:ILE:HG23	1.95	0.66
1:C:208:VAL:HG22	1:C:574:VAL:HG13	1.78	0.66
1:C:265:ILE:HG21	1:C:519:PHE:CE1	2.31	0.66
1:B:109:ALA:HB2	1:B:118:ALA:CB	2.26	0.66
1:C:571:MET:CG	1:D:404:MET:HE2	2.21	0.66
1:A:598:ARG:O	1:A:602:ILE:HG12	1.96	0.65
1:B:676:LYS:O	1:B:681:HIS:ND1	2.20	0.65
1:C:73:THR:OG1	1:C:76:THR:HG23	1.97	0.65
1:C:116:GLY:CA	1:C:313:PRO:HB2	2.26	0.65
1:C:686:ILE:HD13	1:D:402:THR:HB	1.79	0.65
1:D:5:ALA:O	1:D:9:LEU:HD13	1.95	0.65
1:D:25:VAL:CG1	1:D:97:MET:HE1	2.23	0.65
1:B:47:ASP:OD1	1:B:95:MET:HE1	1.95	0.65
1:C:292:PHE:O	1:C:296:VAL:HG23	1.96	0.65
1:D:619:ILE:HG12	1:D:708:ILE:HD11	1.78	0.65
1:C:548:ALA:HA	1:C:636:GLY:O	1.96	0.65
1:B:169:PHE:HB2	1:B:174:MET:HE3	1.76	0.65
1:C:126:GLY:O	1:C:456:SER:HA	1.96	0.65
1:C:185:ILE:CG1	1:C:708:ILE:HD11	2.16	0.65
1:A:492:ASN:ND2	1:A:660:ASP:OD2	2.29	0.65
1:A:35:MET:HE1	1:A:110:ARG:HD3	1.78	0.65
1:B:337:ALA:HB2	1:B:363:TRP:CZ2	2.31	0.65
1:C:318:GLN:O	1:C:322:ASN:ND2	2.27	0.65
1:C:587:LEU:HD21	1:C:594:PRO:HG3	1.78	0.65
1:D:14:ALA:CB	1:D:298:LEU:HD21	2.20	0.65
1:A:573:MET:SD	1:A:603:THR:HG23	2.37	0.65
1:B:156:ASP:O	1:B:280:LYS:HD3	1.97	0.65
1:D:471:SER:HA	1:D:476:LEU:HD13	1.80	0.65
1:A:652:THR:HB	1:A:694:LEU:O	1.97	0.64
1:C:643:LEU:HD12	1:D:643:LEU:HD12	1.79	0.64
1:A:293:PHE:CE2	1:A:336:THR:HG21	2.32	0.64
1:A:47:ASP:OD1	1:A:95:MET:HE1	1.96	0.64
1:C:247:SER:HA	1:C:707:LYS:HE3	1.79	0.64
1:A:530:PRO:HG2	1:A:533:LEU:HD13	1.79	0.64
1:B:329:ALA:O	1:B:333:VAL:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ASN:OD1	1:C:103:VAL:N	2.31	0.64
1:C:507:ILE:HG21	1:D:549:LEU:HD11	1.78	0.64
1:B:188:MET:HE1	1:B:558:PHE:CZ	2.33	0.64
1:D:199:LYS:HA	1:D:199:LYS:HE2	1.80	0.64
1:C:25:VAL:CB	1:C:97:MET:HE1	2.28	0.64
1:C:627:PHE:CD1	1:C:720:PHE:HB3	2.32	0.64
1:D:248:PHE:CZ	1:D:294:ALA:HB1	2.33	0.64
1:A:103:VAL:CG2	1:A:470:ILE:HD13	2.27	0.64
1:A:336:THR:HG22	1:A:363:TRP:CD1	2.32	0.64
1:A:666:LEU:HD23	1:A:666:LEU:O	1.98	0.64
1:B:507:ILE:HD11	1:B:646:ALA:CB	2.27	0.64
1:C:507:ILE:HD11	1:C:646:ALA:HB1	1.78	0.64
1:D:188:MET:HB2	1:D:704:ILE:CG2	2.27	0.64
1:B:703:ASP:OD1	1:B:704:ILE:N	2.31	0.64
1:B:172:PHE:O	1:B:176:VAL:HG22	1.97	0.64
1:B:712:VAL:O	1:B:715:ILE:HG13	1.98	0.64
1:C:424:LEU:CD2	1:C:507:ILE:HD12	2.27	0.64
1:C:543:ARG:HH12	1:C:629:LEU:HD22	1.61	0.63
1:D:329:ALA:O	1:D:333:VAL:HG23	1.97	0.63
1:A:444:ALA:HB2	1:A:508:PHE:HB3	1.81	0.63
1:C:169:PHE:HB2	1:C:174:MET:HE3	1.81	0.63
1:C:299:GLY:HA2	1:C:302:MET:HE2	1.79	0.63
1:C:703:ASP:OD1	1:C:704:ILE:N	2.30	0.63
1:D:413:GLY:O	1:D:417:VAL:HG23	1.99	0.63
1:B:268:GLN:HG3	1:B:277:GLN:HE21	1.63	0.63
1:C:192:VAL:HG11	1:C:614:PRO:HG3	1.79	0.63
1:D:265:ILE:HG22	1:D:531:PRO:HG3	1.80	0.63
1:B:421:THR:O	1:B:425:VAL:HG23	1.98	0.63
1:C:308:VAL:HG21	1:C:324:SER:CB	2.15	0.63
1:D:188:MET:HB2	1:D:704:ILE:HG21	1.81	0.63
1:A:507:ILE:HD11	1:A:646:ALA:HB1	1.80	0.63
1:B:102:ASN:OD1	1:B:103:VAL:N	2.32	0.63
1:A:105:VAL:HG22	1:A:121:VAL:CG1	2.26	0.63
1:B:208:VAL:HG11	1:B:577:ILE:CG2	2.28	0.63
1:C:84:ALA:HB1	1:C:186:ILE:HG13	1.80	0.63
1:D:138:LEU:HD21	1:D:294:ALA:HB1	1.81	0.63
1:D:258:LEU:O	1:D:262:MET:HG3	1.98	0.63
1:D:355:PHE:CD1	1:D:362:PRO:HD3	2.33	0.63
1:A:14:ALA:CB	1:A:298:LEU:HD21	2.22	0.63
1:C:11:PRO:O	1:C:15:LEU:HG	1.99	0.63
1:C:666:LEU:HD23	1:C:666:LEU:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:SER:HB3	1:A:715:ILE:HD11	1.80	0.63
1:C:138:LEU:HD12	1:C:298:LEU:CD1	2.29	0.63
1:C:286:LEU:HB3	1:C:438:TYR:CE2	2.34	0.63
1:C:301:SER:CB	1:C:452:ALA:HB3	2.29	0.63
1:C:112:THR:CB	1:C:117:PRO:HG2	2.29	0.62
1:D:68:LEU:HD13	1:D:76:THR:HG22	1.81	0.62
1:A:172:PHE:O	1:A:176:VAL:HG22	1.99	0.62
1:C:399:ILE:HD13	1:C:680:PRO:HB3	1.81	0.62
1:A:43:ARG:HG3	1:A:99:THR:HB	1.82	0.62
1:A:703:ASP:OD1	1:A:704:ILE:N	2.32	0.62
1:B:666:LEU:O	1:B:666:LEU:HD23	1.99	0.62
1:C:82:LEU:O	1:C:86:MET:HG2	1.99	0.62
1:C:380:ALA:O	1:C:384:THR:HG22	1.99	0.62
1:B:380:ALA:O	1:B:384:THR:HG22	2.00	0.62
1:D:172:PHE:O	1:D:176:VAL:HG22	2.00	0.62
1:D:414:MET:HG2	1:D:651:LEU:CD1	2.29	0.62
1:A:222:ASN:HB3	1:A:225:THR:CG2	2.30	0.62
1:D:301:SER:CB	1:D:452:ALA:HB3	2.29	0.62
1:A:95:MET:HE3	1:A:99:THR:HG21	1.81	0.62
1:A:424:LEU:CD2	1:A:507:ILE:HD12	2.30	0.62
1:A:105:VAL:HA	1:A:121:VAL:HG11	1.82	0.62
1:C:622:PRO:CG	1:C:709:MET:HG3	2.27	0.62
1:D:507:ILE:HD11	1:D:646:ALA:HB1	1.81	0.62
1:A:169:PHE:CB	1:A:174:MET:HE3	2.29	0.62
1:A:321:LEU:HD13	1:A:457:VAL:HG13	1.80	0.62
1:A:448:LEU:HD13	1:A:505:SER:HB2	1.82	0.61
1:D:380:ALA:O	1:D:384:THR:HG22	1.99	0.61
1:B:73:THR:HB	1:B:75:GLN:OE1	2.00	0.61
1:C:176:VAL:HB	1:C:253:VAL:HG13	1.82	0.61
1:C:514:PHE:CE1	1:C:638:LEU:HB3	2.35	0.61
1:B:168:ASN:H	1:B:718:SER:HB3	1.65	0.61
1:C:363:TRP:CZ2	1:C:367:ILE:HD11	2.35	0.61
1:A:11:PRO:HD3	1:A:295:LEU:HD22	1.82	0.61
1:A:247:SER:HA	1:A:707:LYS:HE3	1.80	0.61
1:C:35:MET:HE1	1:C:476:LEU:HD21	1.82	0.61
1:D:110:ARG:HA	1:D:480:VAL:CG2	2.29	0.61
1:B:138:LEU:HD12	1:B:298:LEU:CD1	2.31	0.61
1:A:545:ILE:HD13	1:B:511:LEU:CD1	2.30	0.61
1:B:105:VAL:HG22	1:B:121:VAL:HG22	1.82	0.61
1:B:300:CYS:SG	1:B:335:LEU:HD22	2.40	0.61
1:C:344:LEU:HD22	1:C:347:LEU:CD1	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:ILE:HG23	1:D:287:ILE:HG23	1.82	0.61
1:D:292:PHE:O	1:D:296:VAL:HG23	2.00	0.61
1:A:444:ALA:HB2	1:A:508:PHE:CB	2.31	0.61
1:A:573:MET:CE	1:A:599:CYS:HB3	2.31	0.61
1:C:267:VAL:HG11	1:C:274:LEU:HB3	1.81	0.61
1:D:129:MET:HE2	1:D:241:GLY:CA	2.31	0.61
1:A:25:VAL:HG21	1:A:97:MET:HE1	1.81	0.61
1:B:84:ALA:CB	1:B:186:ILE:HG13	2.31	0.61
1:B:112:THR:CB	1:B:117:PRO:HG2	2.31	0.61
1:B:309:ILE:HD12	1:B:310:VAL:HG23	1.83	0.61
1:A:507:ILE:HG21	1:B:549:LEU:HD11	1.83	0.61
1:B:124:GLN:O	1:B:128:VAL:HG23	2.01	0.61
1:B:176:VAL:HB	1:B:253:VAL:HG13	1.83	0.61
1:D:301:SER:HB3	1:D:452:ALA:HB3	1.83	0.61
1:A:42:ILE:HD12	1:A:43:ARG:N	2.16	0.61
1:A:710:SER:O	1:A:714:VAL:HG23	2.01	0.61
1:A:199:LYS:HA	1:A:199:LYS:HE2	1.83	0.60
1:B:336:THR:HG22	1:B:363:TRP:CD1	2.36	0.60
1:C:232:ASP:O	1:C:236:ASP:HB2	2.01	0.60
1:D:129:MET:HE1	1:D:237:VAL:O	2.01	0.60
1:C:530:PRO:CG	1:C:533:LEU:HD13	2.30	0.60
1:A:191:ARG:NH1	1:A:235:GLY:O	2.34	0.60
1:A:376:ILE:HD11	1:A:424:LEU:HD11	1.83	0.60
1:B:256:ILE:HG23	1:B:287:ILE:HG23	1.83	0.60
1:B:584:ILE:CG2	1:B:587:LEU:HB2	2.29	0.60
1:C:314:SER:HB2	1:C:320:GLU:OE2	2.02	0.60
1:D:127:SER:OG	1:D:305:ILE:HG21	2.01	0.60
1:D:548:ALA:HA	1:D:636:GLY:O	2.01	0.60
1:A:344:LEU:HD22	1:A:347:LEU:HD11	1.84	0.60
1:A:480:VAL:O	1:A:484:THR:HG23	2.00	0.60
1:B:292:PHE:O	1:B:296:VAL:HG23	2.01	0.60
1:B:321:LEU:HD13	1:B:457:VAL:HG13	1.82	0.60
1:C:400:GLU:HB2	1:C:404:MET:HG3	1.83	0.60
1:C:725:LEU:HD22	1:C:726:PHE:CZ	2.36	0.60
1:A:213:LEU:HB3	1:A:215:LEU:HD13	1.83	0.60
1:C:119:LEU:HD21	1:C:320:GLU:HG3	1.83	0.60
1:D:138:LEU:HD12	1:D:298:LEU:HD13	1.84	0.60
1:B:474:CYS:HB2	1:B:476:LEU:CD1	2.32	0.60
1:B:598:ARG:O	1:B:602:ILE:HG12	2.01	0.60
1:C:73:THR:O	1:C:76:THR:OG1	2.13	0.60
1:C:404:MET:HE2	1:D:571:MET:CG	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:TRP:CE2	1:D:367:ILE:HD11	2.37	0.60
1:D:703:ASP:OD1	1:D:704:ILE:N	2.34	0.60
1:A:306:LEU:CD1	1:A:309:ILE:HD11	2.31	0.60
1:A:347:LEU:HB2	1:A:350:LEU:CD1	2.32	0.60
1:D:117:PRO:O	1:D:121:VAL:HG12	2.02	0.60
1:B:240:LEU:HD12	1:B:244:LEU:HD13	1.83	0.60
1:C:69:MET:HG3	1:C:77:GLY:HA3	1.84	0.60
1:C:563:ILE:O	1:C:567:THR:HG23	2.01	0.60
1:D:141:LEU:HD21	1:D:252:ILE:HG21	1.84	0.60
1:C:129:MET:HE1	1:C:237:VAL:O	2.01	0.60
1:D:261:TYR:CE1	1:D:520:SER:HA	2.37	0.60
1:A:376:ILE:HD11	1:A:424:LEU:CD1	2.32	0.59
1:B:331:LEU:O	1:B:335:LEU:HD13	2.02	0.59
1:B:386:TYR:CD2	1:B:665:TYR:HB2	2.37	0.59
1:D:84:ALA:HA	1:D:186:ILE:HG13	1.82	0.59
1:D:444:ALA:HB2	1:D:508:PHE:CB	2.31	0.59
1:D:490:VAL:O	1:D:494:THR:HG23	2.02	0.59
1:D:543:ARG:HH22	1:D:726:PHE:C	2.10	0.59
1:D:596:TYR:O	1:D:600:ILE:HG12	2.02	0.59
1:B:223:PRO:HG2	1:B:577:ILE:HG12	1.84	0.59
1:D:226:ILE:HD11	1:D:473:MET:HE1	1.83	0.59
1:A:446:GLY:HA2	1:A:449:SER:HB3	1.83	0.59
1:B:298:LEU:HD23	1:B:302:MET:HE2	1.83	0.59
1:C:674:TYR:CD2	1:C:680:PRO:HG2	2.37	0.59
1:D:31:GLY:HA2	1:D:107:GLU:CG	2.31	0.59
1:D:69:MET:HG2	1:D:74:TRP:HA	1.84	0.59
1:D:217:GLU:OE2	1:D:663:LYS:NZ	2.35	0.59
1:D:563:ILE:O	1:D:567:THR:HG23	2.02	0.59
1:A:355:PHE:CD1	1:A:362:PRO:HD3	2.37	0.59
1:C:18:ALA:HB2	1:C:131:LEU:HB2	1.84	0.59
1:C:437:LEU:HD13	1:C:515:ALA:HB2	1.84	0.59
1:A:57:ILE:CD1	1:A:189:PHE:HB3	2.32	0.59
1:A:79:ALA:HB1	1:A:179:TYR:HB2	1.85	0.59
1:B:718:SER:O	1:B:721:LYS:HE3	2.03	0.59
1:C:10:ILE:HD12	1:C:295:LEU:HB3	1.84	0.59
1:D:187:ALA:HA	1:D:242:ALA:HB1	1.85	0.59
1:A:37:GLU:O	1:A:41:TYR:HD1	1.86	0.59
1:A:292:PHE:O	1:A:296:VAL:HG23	2.03	0.59
1:A:398:SER:HA	1:A:405:VAL:HG22	1.83	0.59
1:C:446:GLY:HA2	1:C:449:SER:HB3	1.83	0.59
1:D:73:THR:HB	1:D:75:GLN:OE1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ILE:HG13	1:A:508:PHE:HE1	1.67	0.59
1:C:103:VAL:CG2	1:C:470:ILE:HD13	2.30	0.59
1:D:507:ILE:HD11	1:D:646:ALA:CB	2.32	0.59
1:C:507:ILE:HD11	1:C:646:ALA:CB	2.33	0.59
1:D:112:THR:CB	1:D:117:PRO:HG2	2.33	0.59
1:D:199:LYS:HD3	1:D:692:ASP:HB3	1.84	0.59
1:A:725:LEU:HD23	1:A:725:LEU:O	2.02	0.59
1:B:301:SER:HB2	1:B:452:ALA:HB3	1.85	0.59
1:A:400:GLU:HB2	1:A:404:MET:HG3	1.85	0.58
1:B:160:ILE:O	1:B:160:ILE:HG23	2.02	0.58
1:D:148:PHE:O	1:D:154:GLN:HB2	2.03	0.58
1:A:124:GLN:O	1:A:128:VAL:HG23	2.03	0.58
1:A:268:GLN:CG	1:A:277:GLN:HE21	2.15	0.58
1:B:522:ILE:HD11	1:B:534:VAL:HG21	1.85	0.58
1:C:10:ILE:HG22	1:C:298:LEU:HD22	1.85	0.58
1:C:169:PHE:CB	1:C:174:MET:HE3	2.33	0.58
1:C:208:VAL:HG21	1:C:574:VAL:HA	1.85	0.58
1:D:474:CYS:HB2	1:D:476:LEU:CD1	2.33	0.58
1:A:127:SER:OG	1:A:305:ILE:HG21	2.03	0.58
1:A:293:PHE:CZ	1:A:336:THR:HG21	2.38	0.58
1:B:490:VAL:O	1:B:494:THR:HG23	2.03	0.58
1:C:120:LYS:HG3	1:C:313:PRO:HB3	1.85	0.58
1:C:511:LEU:HD11	1:D:545:ILE:HG21	1.85	0.58
1:A:548:ALA:HA	1:A:636:GLY:O	2.03	0.58
1:A:573:MET:HE3	1:A:599:CYS:CB	2.33	0.58
1:B:261:TYR:CE1	1:B:520:SER:HA	2.38	0.58
1:C:160:ILE:HG23	1:C:160:ILE:O	2.03	0.58
1:D:110:ARG:O	1:D:113:LYS:NZ	2.37	0.58
1:D:395:GLY:O	1:D:398:SER:OG	2.15	0.58
1:C:199:LYS:HE2	1:C:199:LYS:HA	1.84	0.58
1:C:218:ASP:HA	1:C:225:THR:HG22	1.85	0.58
1:C:717:VAL:HA	1:C:720:PHE:CE1	2.37	0.58
1:A:102:ASN:OD1	1:A:103:VAL:N	2.36	0.58
1:A:401:GLY:HA3	1:B:207:LEU:HD21	1.86	0.58
1:B:103:VAL:HG22	1:B:470:ILE:HG21	1.85	0.58
1:D:666:LEU:O	1:D:666:LEU:HD23	2.03	0.58
1:A:647:MET:HE2	1:A:647:MET:N	2.19	0.58
1:C:105:VAL:HG22	1:C:121:VAL:CG1	2.33	0.58
1:D:619:ILE:CG1	1:D:708:ILE:HD11	2.34	0.58
1:A:89:SER:O	1:A:93:VAL:HG23	2.04	0.58
1:B:84:ALA:HA	1:B:186:ILE:HG13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:LEU:CD1	1:D:545:ILE:HD13	2.33	0.58
1:C:517:TYR:OH	1:C:631:ALA:O	2.22	0.58
1:B:268:GLN:CG	1:B:277:GLN:HE21	2.16	0.58
1:B:326:TRP:O	1:B:330:LEU:HD13	2.04	0.58
1:B:356:ARG:HD2	1:B:433:TYR:O	2.04	0.58
1:C:73:THR:HB	1:C:75:GLN:OE1	2.04	0.58
1:D:188:MET:HE3	1:D:614:PRO:HB2	1.85	0.58
1:D:695:LYS:NZ	1:D:696:ASP:OD2	2.36	0.58
1:A:97:MET:HE2	1:A:128:VAL:HG21	1.86	0.57
1:A:413:GLY:O	1:A:417:VAL:HG23	2.03	0.57
1:B:26:VAL:HA	1:B:104:ARG:NH1	2.18	0.57
1:B:75:GLN:HA	1:B:78:VAL:CG2	2.33	0.57
1:B:548:ALA:HA	1:B:636:GLY:O	2.04	0.57
1:B:622:PRO:HG3	1:B:709:MET:CG	2.23	0.57
1:D:11:PRO:O	1:D:15:LEU:HG	2.03	0.57
1:D:97:MET:HE2	1:D:125:GLY:HA2	1.86	0.57
1:D:112:THR:OG1	1:D:117:PRO:HG2	2.04	0.57
1:A:31:GLY:HA3	1:A:35:MET:SD	2.44	0.57
1:A:84:ALA:CA	1:A:186:ILE:HG13	2.34	0.57
1:A:514:PHE:CE1	1:A:638:LEU:HB3	2.39	0.57
1:C:49:PHE:CD1	1:C:234:VAL:HG11	2.39	0.57
1:C:418:PHE:HE2	1:D:554:ILE:HG12	1.69	0.57
1:C:652:THR:HB	1:C:694:LEU:O	2.04	0.57
1:B:75:GLN:HA	1:B:78:VAL:HG22	1.86	0.57
1:C:7:PHE:O	1:C:10:ILE:HG13	2.04	0.57
1:C:57:ILE:CD1	1:C:189:PHE:HB3	2.35	0.57
1:C:474:CYS:HB2	1:C:476:LEU:CD1	2.33	0.57
1:D:219:ASP:O	1:D:225:THR:HG21	2.04	0.57
1:A:240:LEU:HD12	1:A:244:LEU:HD13	1.87	0.57
1:A:471:SER:HB2	1:A:476:LEU:HD22	1.85	0.57
1:B:129:MET:HE1	1:B:237:VAL:O	2.04	0.57
1:A:522:ILE:HD11	1:A:534:VAL:HG21	1.87	0.57
1:B:222:ASN:HB3	1:B:225:THR:CG2	2.33	0.57
1:B:337:ALA:HB2	1:B:363:TRP:CE2	2.39	0.57
1:C:413:GLY:O	1:C:417:VAL:HG23	2.03	0.57
1:D:471:SER:CB	1:D:476:LEU:HD22	2.35	0.57
1:D:558:PHE:CE1	1:D:562:LEU:HD11	2.39	0.57
1:B:265:ILE:HG21	1:B:519:PHE:CE1	2.39	0.57
1:C:116:GLY:O	1:C:120:LYS:HG3	2.03	0.57
1:C:199:LYS:HD3	1:C:692:ASP:HB3	1.86	0.57
1:D:414:MET:HG2	1:D:651:LEU:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:PHE:CB	1:B:174:MET:HE3	2.35	0.57
1:C:340:THR:CG2	1:C:362:PRO:HG2	2.34	0.57
1:C:725:LEU:O	1:C:725:LEU:HD23	2.04	0.57
1:D:49:PHE:CD1	1:D:234:VAL:HG11	2.40	0.57
1:D:263:PHE:CZ	1:D:280:LYS:HE2	2.39	0.57
1:A:138:LEU:HD21	1:A:294:ALA:CB	2.34	0.57
1:B:167:ILE:CD1	1:B:719:ILE:HD11	2.28	0.57
1:B:208:VAL:HG22	1:B:574:VAL:HG13	1.86	0.57
1:C:299:GLY:HA2	1:C:302:MET:CE	2.35	0.57
1:C:344:LEU:CD2	1:C:347:LEU:HD11	2.33	0.57
1:D:74:TRP:CH2	1:D:152:MET:HE1	2.38	0.57
1:D:700:PRO:O	1:D:704:ILE:HD12	2.05	0.57
1:A:148:PHE:O	1:A:154:GLN:HB2	2.05	0.57
1:A:331:LEU:O	1:A:335:LEU:HD13	2.05	0.57
1:A:490:VAL:O	1:A:494:THR:HG23	2.05	0.57
1:A:301:SER:CB	1:A:452:ALA:HB3	2.35	0.56
1:C:17:PHE:HB3	1:C:131:LEU:HD13	1.87	0.56
1:D:184:SER:CA	1:D:246:GLU:HG3	2.23	0.56
1:B:725:LEU:O	1:B:725:LEU:HD23	2.05	0.56
1:C:127:SER:OG	1:C:305:ILE:HG21	2.05	0.56
1:D:168:ASN:OD1	1:D:524:PRO:HD3	2.05	0.56
1:D:280:LYS:O	1:D:284:GLN:HG3	2.04	0.56
1:A:10:ILE:N	1:A:11:PRO:HD2	2.19	0.56
1:B:86:MET:HE2	1:B:136:PHE:O	2.05	0.56
1:C:293:PHE:CZ	1:C:336:THR:HG21	2.41	0.56
1:C:325:LEU:HD23	1:C:453:THR:CG2	2.34	0.56
1:C:402:THR:HG21	1:C:686:ILE:HG21	1.86	0.56
1:C:421:THR:O	1:C:425:VAL:HG23	2.05	0.56
1:D:704:ILE:O	1:D:708:ILE:HG22	2.05	0.56
1:B:112:THR:CG2	1:B:117:PRO:HG2	2.35	0.56
1:C:517:TYR:CB	1:C:714:VAL:HG22	2.28	0.56
1:D:39:SER:HA	1:D:42:ILE:HD11	1.86	0.56
1:D:573:MET:SD	1:D:603:THR:HG23	2.45	0.56
1:B:8:PHE:HD1	1:B:142:VAL:CG2	2.18	0.56
1:B:448:LEU:CD1	1:B:505:SER:HB2	2.35	0.56
1:C:398:SER:HB3	1:C:684:LEU:HD21	1.87	0.56
1:D:194:GLY:O	1:D:198:THR:HG22	2.05	0.56
1:D:209:GLY:O	1:D:214:ASN:N	2.39	0.56
1:D:400:GLU:HB2	1:D:404:MET:HG3	1.85	0.56
1:C:321:LEU:HD13	1:C:457:VAL:HG13	1.86	0.56
1:C:522:ILE:HD11	1:C:534:VAL:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:LEU:CD1	1:D:505:SER:HB3	2.35	0.56
1:A:248:PHE:O	1:A:252:ILE:HG13	2.05	0.56
1:B:60:VAL:O	1:B:64:ILE:HG12	2.06	0.56
1:B:101:ALA:O	1:B:105:VAL:HG23	2.06	0.56
1:B:280:LYS:O	1:B:284:GLN:HG3	2.06	0.56
1:C:596:TYR:O	1:C:600:ILE:HG12	2.05	0.56
1:D:126:GLY:O	1:D:456:SER:HA	2.06	0.56
1:A:299:GLY:HA2	1:A:302:MET:CE	2.35	0.56
1:B:385:SER:HA	1:B:661:ASN:HD22	1.71	0.56
1:C:89:SER:O	1:C:93:VAL:HG23	2.06	0.56
1:C:337:ALA:HB2	1:C:363:TRP:CZ2	2.41	0.56
1:C:422:LEU:O	1:C:422:LEU:HD23	2.06	0.56
1:D:102:ASN:OD1	1:D:103:VAL:N	2.37	0.56
1:D:219:ASP:OD1	1:D:220:PRO:HD2	2.06	0.56
1:A:120:LYS:HG3	1:A:313:PRO:HB3	1.88	0.56
1:A:185:ILE:HD13	1:A:619:ILE:HD11	1.88	0.56
1:A:656:GLY:HA3	1:A:695:LYS:HB2	1.88	0.56
1:B:277:GLN:HB3	1:B:352:VAL:HG11	1.87	0.56
1:C:116:GLY:HA3	1:C:313:PRO:HB2	1.86	0.56
1:D:112:THR:HG21	1:D:117:PRO:HG2	1.87	0.56
1:A:84:ALA:CB	1:A:186:ILE:HG13	2.36	0.56
1:B:53:GLU:HG3	1:B:611:MET:SD	2.46	0.56
1:B:199:LYS:CD	1:B:696:ASP:HB2	2.36	0.56
1:B:219:ASP:OD1	1:B:220:PRO:HD2	2.06	0.56
1:B:247:SER:HA	1:B:707:LYS:HE3	1.88	0.56
1:C:103:VAL:HG22	1:C:470:ILE:HG21	1.88	0.56
1:C:213:LEU:CB	1:C:215:LEU:HD13	2.36	0.56
1:A:57:ILE:HD11	1:A:611:MET:HE1	1.88	0.55
1:B:309:ILE:CD1	1:B:310:VAL:HG23	2.36	0.55
1:C:188:MET:HE3	1:C:614:PRO:HB2	1.87	0.55
1:D:468:GLY:N	1:D:484:THR:HG21	2.20	0.55
1:A:176:VAL:HB	1:A:253:VAL:HG13	1.88	0.55
1:B:155:VAL:HG22	1:B:172:PHE:CD2	2.41	0.55
1:C:25:VAL:CG2	1:C:124:GLN:HB3	2.36	0.55
1:C:208:VAL:HG23	1:C:574:VAL:HG22	1.88	0.55
1:A:252:ILE:HG12	1:A:445:LEU:HD13	1.87	0.55
1:A:347:LEU:HD12	1:A:350:LEU:HD11	1.88	0.55
1:A:422:LEU:HD23	1:A:422:LEU:O	2.06	0.55
1:A:578:ARG:O	1:A:582:ARG:HG2	2.07	0.55
1:C:80:PHE:HE2	1:C:185:ILE:HD12	1.70	0.55
1:C:97:MET:CE	1:C:125:GLY:HA2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:LEU:HD12	1:C:244:LEU:HD13	1.88	0.55
1:D:53:GLU:O	1:D:57:ILE:HG23	2.05	0.55
1:A:11:PRO:O	1:A:15:LEU:HG	2.06	0.55
1:A:414:MET:HG2	1:A:651:LEU:CD1	2.36	0.55
1:B:11:PRO:O	1:B:15:LEU:HG	2.07	0.55
1:B:380:ALA:HB3	1:B:497:ILE:HG12	1.87	0.55
1:C:398:SER:HB2	1:C:684:LEU:HG	1.89	0.55
1:D:300:CYS:SG	1:D:335:LEU:HD22	2.46	0.55
1:D:710:SER:O	1:D:714:VAL:HG23	2.06	0.55
1:B:301:SER:HB3	1:B:452:ALA:HB3	1.88	0.55
1:C:244:LEU:HD23	1:C:455:VAL:CG2	2.31	0.55
1:A:421:THR:O	1:A:425:VAL:HG23	2.06	0.55
1:B:296:VAL:HG21	1:B:339:LEU:HD22	1.89	0.55
1:A:474:CYS:HB2	1:A:476:LEU:CD1	2.37	0.55
1:A:621:THR:HB	1:A:622:PRO:HD3	1.88	0.55
1:A:718:SER:O	1:A:721:LYS:HE2	2.07	0.55
1:B:384:THR:CG2	1:B:493:THR:HG23	2.37	0.55
1:B:563:ILE:O	1:B:567:THR:HG23	2.07	0.55
1:C:120:LYS:CG	1:C:313:PRO:HB3	2.37	0.55
1:C:356:ARG:HG3	1:C:357:PHE:CD1	2.42	0.55
1:C:522:ILE:HD11	1:C:534:VAL:HG22	1.89	0.55
1:D:109:ALA:HB2	1:D:118:ALA:HB2	1.89	0.55
1:D:126:GLY:HA2	1:D:459:SER:OG	2.07	0.55
1:D:725:LEU:HD23	1:D:725:LEU:O	2.07	0.55
1:A:155:VAL:HG22	1:A:172:PHE:CD2	2.42	0.55
1:A:194:GLY:HA3	1:A:235:GLY:HA2	1.89	0.55
1:A:563:ILE:O	1:A:567:THR:HG23	2.07	0.55
1:B:479:GLU:O	1:B:482:LYS:HG2	2.07	0.55
1:C:386:TYR:HD2	1:C:665:TYR:HD2	1.53	0.55
1:C:521:GLN:NE2	1:C:631:ALA:HB1	2.23	0.55
1:D:31:GLY:CA	1:D:107:GLU:HG3	2.34	0.55
1:A:21:ASN:HB2	1:A:128:VAL:HG22	1.88	0.54
1:C:219:ASP:OD1	1:C:220:PRO:HD2	2.06	0.54
1:C:286:LEU:HB3	1:C:438:TYR:HE2	1.72	0.54
1:D:363:TRP:CZ2	1:D:367:ILE:HD11	2.42	0.54
1:D:421:THR:O	1:D:425:VAL:HG23	2.08	0.54
1:A:309:ILE:HD12	1:A:310:VAL:HG23	1.89	0.54
1:A:666:LEU:CD1	1:A:684:LEU:HD12	2.37	0.54
1:C:218:ASP:HA	1:C:225:THR:CG2	2.36	0.54
1:C:618:ALA:HB1	1:C:708:ILE:CG2	2.38	0.54
1:B:167:ILE:HG13	1:B:719:ILE:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ILE:O	1:B:295:LEU:HG	2.06	0.54
1:D:208:VAL:HG11	1:D:577:ILE:CG2	2.37	0.54
1:D:215:LEU:HD21	1:D:221:ARG:HB2	1.87	0.54
1:C:119:LEU:HD22	1:C:317:PRO:HA	1.88	0.54
1:C:336:THR:HG22	1:C:363:TRP:CD1	2.40	0.54
1:C:517:TYR:HB2	1:C:714:VAL:CG2	2.30	0.54
1:B:110:ARG:HD3	1:B:476:LEU:HD23	1.90	0.54
1:B:718:SER:HA	1:B:721:LYS:CD	2.35	0.54
1:C:137:ALA:HB2	1:C:245:LEU:HG	1.89	0.54
1:C:678:SER:HB2	1:C:680:PRO:HD2	1.89	0.54
1:D:39:SER:O	1:D:43:ARG:HG3	2.08	0.54
1:A:57:ILE:HG12	1:A:189:PHE:HB3	1.88	0.54
1:B:117:PRO:O	1:B:121:VAL:HG12	2.08	0.54
1:D:141:LEU:CD2	1:D:252:ILE:HG21	2.37	0.54
1:D:506:ALA:HB2	1:D:707:LYS:NZ	2.23	0.54
1:A:86:MET:HE2	1:A:136:PHE:O	2.07	0.54
1:A:219:ASP:OD1	1:A:220:PRO:HD2	2.06	0.54
1:B:95:MET:HE3	1:B:99:THR:HG21	1.90	0.54
1:B:503:ILE:HD11	1:B:646:ALA:HA	1.90	0.54
1:D:14:ALA:HA	1:D:302:MET:SD	2.47	0.54
1:B:704:ILE:O	1:B:708:ILE:HG22	2.07	0.54
1:C:97:MET:HE2	1:C:125:GLY:HA2	1.90	0.54
1:C:194:GLY:O	1:C:198:THR:HG22	2.08	0.54
1:C:340:THR:HG22	1:C:359:ALA:O	2.08	0.54
1:C:656:GLY:HA3	1:C:695:LYS:HB3	1.90	0.54
1:D:60:VAL:O	1:D:64:ILE:HG12	2.06	0.54
1:D:356:ARG:HD2	1:D:433:TYR:O	2.08	0.54
1:A:522:ILE:HD11	1:A:534:VAL:CG1	2.38	0.54
1:B:21:ASN:HB2	1:B:128:VAL:HG22	1.90	0.54
1:C:43:ARG:HG2	1:C:99:THR:CB	2.27	0.54
1:C:170:VAL:HB	1:C:173:ALA:HB3	1.88	0.54
1:A:377:GLY:CA	1:A:497:ILE:HG23	2.37	0.54
1:B:401:GLY:O	1:B:405:VAL:HG23	2.07	0.54
1:B:474:CYS:HB2	1:B:476:LEU:HD11	1.90	0.54
1:B:627:PHE:HE1	1:B:719:ILE:HG22	1.73	0.54
1:D:167:ILE:HD11	1:D:719:ILE:HD11	1.89	0.54
1:D:232:ASP:O	1:D:236:ASP:HB2	2.08	0.54
1:A:363:TRP:CE2	1:A:367:ILE:HD11	2.43	0.53
1:A:526:ASP:OD1	1:A:526:ASP:N	2.37	0.53
1:B:248:PHE:O	1:B:252:ILE:HG13	2.08	0.53
1:D:386:TYR:HD2	1:D:665:TYR:HD2	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:ILE:CG1	1:D:719:ILE:HD11	2.37	0.53
1:B:112:THR:HG21	1:B:117:PRO:CG	2.38	0.53
1:C:110:ARG:HA	1:C:480:VAL:HG22	1.90	0.53
1:C:115:ILE:HG13	1:C:483:ILE:HD12	1.90	0.53
1:D:222:ASN:HB3	1:D:225:THR:CG2	2.35	0.53
1:B:308:VAL:HG21	1:B:324:SER:CA	2.39	0.53
1:C:537:LEU:CD2	1:C:639:ILE:HD11	2.36	0.53
1:A:325:LEU:HD23	1:A:453:THR:CG2	2.36	0.53
1:A:448:LEU:O	1:A:451:VAL:HB	2.08	0.53
1:B:102:ASN:HB2	1:B:466:ASN:HB3	1.89	0.53
1:B:469:GLY:O	1:B:473:MET:HG3	2.08	0.53
1:B:615:ALA:O	1:B:619:ILE:HG13	2.09	0.53
1:C:409:GLY:HA3	1:C:659:TRP:CZ2	2.44	0.53
1:C:535:LEU:CA	1:D:540:LEU:HD22	2.38	0.53
1:D:86:MET:HE2	1:D:136:PHE:O	2.08	0.53
1:D:703:ASP:OD1	1:D:704:ILE:HD12	2.09	0.53
1:A:363:TRP:CH2	1:A:367:ILE:HD11	2.44	0.53
1:B:112:THR:OG1	1:B:117:PRO:HG2	2.08	0.53
1:B:130:GLY:HA2	1:B:455:VAL:HB	1.89	0.53
1:B:213:LEU:CB	1:B:215:LEU:HD13	2.39	0.53
1:C:188:MET:HB2	1:C:704:ILE:HG21	1.90	0.53
1:D:95:MET:HE3	1:D:99:THR:HG21	1.89	0.53
1:D:355:PHE:HB3	1:D:361:SER:HB2	1.90	0.53
1:A:545:ILE:HG21	1:B:511:LEU:CD1	2.38	0.53
1:B:188:MET:HB2	1:B:704:ILE:HG21	1.90	0.53
1:B:293:PHE:CE2	1:B:336:THR:HG21	2.44	0.53
1:C:10:ILE:N	1:C:11:PRO:HD2	2.23	0.53
1:B:110:ARG:HD3	1:B:476:LEU:CD2	2.38	0.53
1:B:194:GLY:O	1:B:198:THR:HG22	2.09	0.53
1:C:370:ILE:O	1:C:374:ILE:HG13	2.08	0.53
1:C:386:TYR:CD2	1:C:665:TYR:HB2	2.44	0.53
1:C:399:ILE:HD11	1:C:671:LEU:CD2	2.33	0.53
1:D:259:ALA:HA	1:D:262:MET:CE	2.27	0.53
1:D:547:GLY:O	1:D:637:VAL:HA	2.09	0.53
1:C:717:VAL:HA	1:C:720:PHE:CZ	2.43	0.53
1:B:80:PHE:CE2	1:B:182:GLY:HA2	2.44	0.53
1:C:398:SER:HA	1:C:405:VAL:HG22	1.90	0.53
1:C:584:ILE:CG2	1:C:587:LEU:HB2	2.38	0.53
1:D:10:ILE:N	1:D:11:PRO:HD2	2.24	0.53
1:B:218:ASP:HA	1:B:225:THR:CG2	2.38	0.52
1:B:248:PHE:CZ	1:B:294:ALA:HB1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ILE:O	1:C:160:ILE:CG2	2.57	0.52
1:D:141:LEU:HD21	1:D:252:ILE:CG2	2.39	0.52
1:D:493:THR:O	1:D:497:ILE:HG13	2.09	0.52
1:A:326:TRP:O	1:A:330:LEU:HD13	2.09	0.52
1:A:363:TRP:CZ2	1:A:367:ILE:HD11	2.44	0.52
1:B:119:LEU:HD22	1:B:317:PRO:HB3	1.91	0.52
1:B:725:LEU:HD22	1:B:726:PHE:CZ	2.44	0.52
1:D:149:GLY:HA2	1:D:155:VAL:HG23	1.92	0.52
1:D:422:LEU:HD23	1:D:422:LEU:O	2.08	0.52
1:A:53:GLU:HG2	1:A:57:ILE:HD11	1.91	0.52
1:B:422:LEU:O	1:B:422:LEU:HD23	2.09	0.52
1:C:84:ALA:HA	1:C:186:ILE:HG13	1.92	0.52
1:C:557:TYR:HD1	1:D:415:LYS:HA	1.73	0.52
1:C:562:LEU:HD13	1:C:697:THR:HG22	1.90	0.52
1:C:573:MET:SD	1:C:603:THR:HG23	2.49	0.52
1:D:170:VAL:HG13	1:D:171:PRO:HD2	1.92	0.52
1:D:674:TYR:HB3	1:D:678:SER:OG	2.10	0.52
1:A:53:GLU:HG2	1:A:57:ILE:CD1	2.39	0.52
1:B:84:ALA:HB1	1:B:186:ILE:HG13	1.90	0.52
1:B:619:ILE:HG12	1:B:708:ILE:HD11	1.91	0.52
1:C:213:LEU:HB2	1:C:215:LEU:HD13	1.91	0.52
1:D:199:LYS:CD	1:D:696:ASP:HB2	2.39	0.52
1:D:331:LEU:O	1:D:335:LEU:HD13	2.09	0.52
1:A:323:ILE:O	1:A:327:THR:HG23	2.10	0.52
1:A:584:ILE:HG22	1:A:587:LEU:HB2	1.91	0.52
1:A:705:LEU:HD23	1:A:705:LEU:C	2.34	0.52
1:C:400:GLU:HG3	1:D:571:MET:HG2	1.90	0.52
1:D:293:PHE:CE2	1:D:336:THR:HG21	2.44	0.52
1:D:398:SER:HA	1:D:405:VAL:CG2	2.39	0.52
1:A:291:ILE:O	1:A:295:LEU:HG	2.09	0.52
1:A:300:CYS:SG	1:A:335:LEU:HD22	2.50	0.52
1:A:573:MET:HE3	1:A:599:CYS:SG	2.50	0.52
1:B:363:TRP:CZ3	1:B:367:ILE:HD11	2.44	0.52
1:C:119:LEU:HD13	1:C:317:PRO:HB3	1.91	0.52
1:C:226:ILE:HD12	1:C:596:TYR:CD2	2.45	0.52
1:A:384:THR:HG21	1:A:493:THR:HA	1.92	0.52
1:B:410:LEU:O	1:B:414:MET:HG3	2.09	0.52
1:C:725:LEU:HD22	1:C:726:PHE:CE1	2.45	0.52
1:D:101:ALA:O	1:D:105:VAL:HG23	2.10	0.52
1:D:184:SER:HA	1:D:246:GLU:CG	2.26	0.52
1:D:479:GLU:O	1:D:482:LYS:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:MET:SD	1:B:603:THR:HG23	2.49	0.52
1:D:261:TYR:O	1:D:265:ILE:HD13	2.10	0.52
1:A:57:ILE:HG22	1:A:186:ILE:HD12	1.91	0.52
1:A:74:TRP:CH2	1:A:152:MET:HE1	2.40	0.52
1:A:187:ALA:HA	1:A:242:ALA:HB1	1.92	0.52
1:B:208:VAL:HG21	1:B:574:VAL:HA	1.92	0.52
1:B:395:GLY:O	1:B:398:SER:OG	2.22	0.52
1:B:652:THR:HB	1:B:694:LEU:O	2.10	0.52
1:D:622:PRO:HB3	1:D:713:SER:OG	2.09	0.52
1:A:322:ASN:HD22	1:A:322:ASN:N	2.08	0.52
1:B:127:SER:OG	1:B:305:ILE:HG21	2.10	0.52
1:B:133:VAL:HG13	1:B:245:LEU:HB2	1.92	0.52
1:C:208:VAL:HG11	1:C:577:ILE:CG2	2.39	0.52
1:D:291:ILE:O	1:D:295:LEU:HG	2.09	0.52
1:D:598:ARG:O	1:D:602:ILE:HG12	2.10	0.52
1:A:7:PHE:C	1:A:295:LEU:HD13	2.35	0.51
1:A:399:ILE:CD1	1:A:671:LEU:HD21	2.35	0.51
1:B:300:CYS:SG	1:B:332:THR:HA	2.50	0.51
1:C:573:MET:O	1:C:577:ILE:HG13	2.10	0.51
1:D:223:PRO:HB3	1:D:580:GLN:HE22	1.75	0.51
1:D:258:LEU:HD23	1:D:262:MET:HG3	1.92	0.51
1:D:323:ILE:O	1:D:327:THR:HG23	2.11	0.51
1:D:424:LEU:HD23	1:D:507:ILE:HD12	1.92	0.51
1:D:681:HIS:O	1:D:685:VAL:HG23	2.10	0.51
1:D:705:LEU:HD23	1:D:705:LEU:C	2.35	0.51
1:A:194:GLY:O	1:A:198:THR:HG22	2.10	0.51
1:A:390:PRO:HB2	1:A:412:LEU:HD11	1.91	0.51
1:B:42:ILE:HD12	1:B:226:ILE:HG23	1.90	0.51
1:B:266:TYR:CD1	1:B:531:PRO:HG2	2.45	0.51
1:B:629:LEU:HD23	1:B:726:PHE:HD2	1.75	0.51
1:C:69:MET:CE	1:C:74:TRP:HB2	2.40	0.51
1:C:545:ILE:HD13	1:D:511:LEU:HG	1.93	0.51
1:A:266:TYR:CE1	1:A:531:PRO:HG2	2.45	0.51
1:A:596:TYR:O	1:A:600:ILE:HG12	2.10	0.51
1:B:115:ILE:HG23	1:B:487:LEU:HD21	1.91	0.51
1:B:232:ASP:O	1:B:236:ASP:HB2	2.10	0.51
1:D:652:THR:HB	1:D:694:LEU:O	2.10	0.51
1:A:60:VAL:O	1:A:64:ILE:HG13	2.11	0.51
1:A:177:SER:CB	1:A:715:ILE:HD11	2.40	0.51
1:B:189:PHE:CE1	1:B:612:GLY:HA2	2.42	0.51
1:D:248:PHE:HZ	1:D:294:ALA:HB1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:VAL:CB	1:A:97:MET:HE1	2.41	0.51
1:A:129:MET:HE2	1:A:241:GLY:CA	2.37	0.51
1:B:41:TYR:CD2	1:B:226:ILE:HD13	2.45	0.51
1:B:660:ASP:O	1:B:664:LYS:HG3	2.11	0.51
1:C:102:ASN:HB2	1:C:466:ASN:HB3	1.92	0.51
1:C:248:PHE:O	1:C:252:ILE:HG13	2.11	0.51
1:C:288:SER:HB2	1:C:343:TYR:OH	2.11	0.51
1:C:291:ILE:O	1:C:295:LEU:HG	2.10	0.51
1:C:710:SER:O	1:C:714:VAL:HG23	2.11	0.51
1:A:188:MET:HE1	1:A:558:PHE:CZ	2.46	0.51
1:A:370:ILE:HG23	1:A:450:PHE:HE2	1.75	0.51
1:B:53:GLU:O	1:B:57:ILE:HG23	2.11	0.51
1:C:60:VAL:O	1:C:64:ILE:HG12	2.10	0.51
1:A:337:ALA:HB2	1:A:363:TRP:CZ2	2.45	0.51
1:A:404:MET:HE2	1:B:571:MET:CG	2.38	0.51
1:A:627:PHE:HE1	1:A:719:ILE:HG22	1.76	0.51
1:C:622:PRO:HG3	1:C:709:MET:CG	2.31	0.51
1:D:321:LEU:HD13	1:D:457:VAL:HG13	1.91	0.51
1:A:110:ARG:HA	1:A:480:VAL:HG22	1.92	0.51
1:B:78:VAL:HG21	1:B:148:PHE:CZ	2.45	0.51
1:C:95:MET:HE3	1:C:99:THR:HG21	1.93	0.51
1:C:301:SER:HB3	1:C:452:ALA:HB3	1.91	0.51
1:D:500:GLY:O	1:D:503:ILE:HG22	2.10	0.51
1:A:53:GLU:HG3	1:A:611:MET:CE	2.39	0.51
1:A:399:ILE:HD12	1:A:674:TYR:CE2	2.46	0.51
1:A:553:ALA:HB2	1:B:421:THR:CG2	2.36	0.51
1:B:107:GLU:O	1:B:111:THR:HG23	2.11	0.51
1:B:159:ASN:HB2	1:B:161:TYR:CE1	2.46	0.51
1:B:386:TYR:HD2	1:B:665:TYR:HD1	1.59	0.51
1:B:710:SER:O	1:B:714:VAL:HG23	2.11	0.51
1:C:133:VAL:HG13	1:C:245:LEU:HB2	1.93	0.51
1:C:227:ALA:HA	1:C:600:ILE:CD1	2.41	0.51
1:C:377:GLY:HA2	1:C:497:ILE:HG23	1.93	0.51
1:C:399:ILE:CD1	1:C:671:LEU:HD21	2.32	0.51
1:C:618:ALA:HB1	1:C:708:ILE:HG21	1.92	0.51
1:D:207:LEU:O	1:D:211:THR:HB	2.11	0.51
1:D:249:VAL:O	1:D:253:VAL:HG23	2.11	0.51
1:B:169:PHE:HB2	1:B:174:MET:CE	2.42	0.51
1:C:621:THR:HB	1:C:622:PRO:HD3	1.93	0.51
1:D:167:ILE:HG12	1:D:719:ILE:CG1	2.41	0.51
1:D:176:VAL:HB	1:D:253:VAL:HG13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:VAL:HG11	1:D:577:ILE:HG22	1.93	0.51
1:D:627:PHE:CE1	1:D:720:PHE:HB3	2.46	0.51
1:A:221:ARG:O	1:A:587:LEU:HD21	2.11	0.50
1:B:23:ALA:HA	1:B:26:VAL:HG12	1.93	0.50
1:B:38:ILE:HD12	1:B:474:CYS:SG	2.51	0.50
1:D:38:ILE:O	1:D:42:ILE:HG12	2.11	0.50
1:D:159:ASN:HB3	1:D:161:TYR:CE1	2.46	0.50
1:A:216:PRO:HG2	1:A:219:ASP:HB2	1.93	0.50
1:A:280:LYS:O	1:A:284:GLN:HG3	2.11	0.50
1:A:666:LEU:HD13	1:A:684:LEU:HD12	1.93	0.50
1:B:54:THR:O	1:B:57:ILE:HG13	2.10	0.50
1:B:648:LEU:O	1:B:652:THR:HG23	2.12	0.50
1:B:651:LEU:HD23	1:B:651:LEU:C	2.36	0.50
1:C:285:ALA:HB3	1:C:347:LEU:HD13	1.93	0.50
1:C:557:TYR:CD1	1:D:415:LYS:HA	2.46	0.50
1:C:718:SER:O	1:C:721:LYS:HE2	2.11	0.50
1:A:7:PHE:O	1:A:295:LEU:HD13	2.12	0.50
1:A:223:PRO:HA	1:A:596:TYR:CD1	2.46	0.50
1:B:119:LEU:HD13	1:B:317:PRO:HB3	1.92	0.50
1:B:322:ASN:HD22	1:B:322:ASN:C	2.18	0.50
1:C:647:MET:HE2	1:C:647:MET:N	2.27	0.50
1:D:89:SER:O	1:D:93:VAL:HG23	2.12	0.50
1:D:263:PHE:HB2	1:D:283:ILE:HG13	1.92	0.50
1:A:217:GLU:O	1:A:472:GLU:HG2	2.11	0.50
1:A:223:PRO:HG2	1:A:577:ILE:HG12	1.92	0.50
1:A:372:SER:HB2	1:A:447:MET:HE2	1.92	0.50
1:A:386:TYR:HD1	1:A:386:TYR:H	1.60	0.50
1:B:25:VAL:CB	1:B:97:MET:HE1	2.42	0.50
1:B:165:LEU:HB3	1:B:167:ILE:HD13	1.94	0.50
1:B:204:ALA:HB3	1:B:573:MET:HE2	1.92	0.50
1:B:233:ASN:OD1	1:B:466:ASN:ND2	2.44	0.50
1:C:545:ILE:HD13	1:D:511:LEU:CG	2.42	0.50
1:D:192:VAL:HG11	1:D:614:PRO:HG3	1.92	0.50
1:D:384:THR:CG2	1:D:493:THR:HG23	2.41	0.50
1:D:678:SER:HB2	1:D:680:PRO:HD2	1.94	0.50
1:A:308:VAL:HG21	1:A:324:SER:CB	2.28	0.50
1:A:402:THR:HG21	1:A:686:ILE:HG21	1.93	0.50
1:B:372:SER:O	1:B:376:ILE:HG13	2.11	0.50
1:B:390:PRO:HB2	1:B:412:LEU:HD11	1.92	0.50
1:C:437:LEU:HD13	1:C:515:ALA:CB	2.41	0.50
1:C:459:SER:O	1:C:462:PRO:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:HG13	1:A:245:LEU:HB2	1.92	0.50
1:A:477:ASP:OD1	1:A:478:PRO:HD2	2.12	0.50
1:B:187:ALA:HA	1:B:242:ALA:HB1	1.92	0.50
1:C:308:VAL:CG2	1:C:324:SER:HB2	2.17	0.50
1:C:340:THR:HG21	1:C:362:PRO:HG2	1.93	0.50
1:C:521:GLN:HG2	1:C:717:VAL:CG2	2.42	0.50
1:D:563:ILE:HD11	1:D:694:LEU:CD2	2.42	0.50
1:A:167:ILE:CD1	1:A:719:ILE:HD11	2.35	0.50
1:A:507:ILE:HD11	1:A:646:ALA:HB2	1.93	0.50
1:B:386:TYR:HA	1:B:391:THR:HB	1.94	0.50
1:B:621:THR:HB	1:B:622:PRO:HD3	1.92	0.50
1:D:30:GLU:O	1:D:107:GLU:HG3	2.11	0.50
1:D:84:ALA:CA	1:D:186:ILE:HG13	2.41	0.50
1:D:405:VAL:HG11	1:D:684:LEU:HD23	1.93	0.50
1:D:471:SER:HB2	1:D:476:LEU:HD22	1.94	0.50
1:A:402:THR:HB	1:B:686:ILE:HD13	1.92	0.50
1:A:471:SER:O	1:A:476:LEU:HD13	2.12	0.50
1:B:84:ALA:CA	1:B:186:ILE:HG13	2.41	0.50
1:B:88:ALA:O	1:B:92:ILE:HG13	2.12	0.50
1:B:168:ASN:OD1	1:B:721:LYS:HE2	2.11	0.50
1:C:115:ILE:HB	1:C:315:ASP:HA	1.92	0.50
1:A:84:ALA:HB1	1:A:186:ILE:HG13	1.94	0.50
1:A:622:PRO:CG	1:A:709:MET:HG3	2.35	0.50
1:B:61:ALA:HB2	1:B:186:ILE:HD11	1.94	0.50
1:B:129:MET:HE2	1:B:241:GLY:CA	2.41	0.50
1:B:267:VAL:HG12	1:B:276:HIS:HA	1.94	0.50
1:B:402:THR:HG21	1:B:686:ILE:HG21	1.93	0.50
1:B:517:TYR:CB	1:B:714:VAL:HG22	2.33	0.50
1:C:138:LEU:HD21	1:C:294:ALA:HB1	1.94	0.50
1:D:86:MET:HE3	1:D:136:PHE:HB3	1.94	0.50
1:D:88:ALA:O	1:D:92:ILE:HG13	2.12	0.49
1:D:615:ALA:O	1:D:619:ILE:HG13	2.12	0.49
1:A:356:ARG:HD2	1:A:433:TYR:O	2.12	0.49
1:A:547:GLY:O	1:A:637:VAL:HA	2.12	0.49
1:B:199:LYS:HD2	1:B:692:ASP:O	2.12	0.49
1:B:306:LEU:HD12	1:B:309:ILE:HD11	1.95	0.49
1:C:468:GLY:HA2	1:C:484:THR:HG21	1.94	0.49
1:C:627:PHE:CE1	1:C:720:PHE:HB3	2.48	0.49
1:D:160:ILE:CG2	1:D:527:ILE:HD12	2.42	0.49
1:D:460:TYR:HE2	1:D:490:VAL:HG12	1.76	0.49
1:A:263:PHE:HB3	1:A:264:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:SER:O	1:B:93:VAL:HG23	2.12	0.49
1:B:107:GLU:OE2	1:B:111:THR:HG21	2.13	0.49
1:C:84:ALA:CA	1:C:186:ILE:HG13	2.41	0.49
1:C:581:ALA:HB1	1:C:588:LEU:HD11	1.94	0.49
1:C:651:LEU:HD23	1:C:651:LEU:C	2.37	0.49
1:D:138:LEU:HD12	1:D:298:LEU:CD1	2.42	0.49
1:A:309:ILE:CD1	1:A:310:VAL:HG23	2.42	0.49
1:A:414:MET:HG2	1:A:651:LEU:HD12	1.94	0.49
1:B:105:VAL:CG2	1:B:121:VAL:HG22	2.42	0.49
1:B:218:ASP:HA	1:B:225:THR:HG22	1.95	0.49
1:B:363:TRP:CH2	1:B:367:ILE:HD11	2.47	0.49
1:B:419:PRO:N	1:B:420:PRO:HD2	2.28	0.49
1:A:192:VAL:HG11	1:A:614:PRO:CG	2.38	0.49
1:A:401:GLY:O	1:A:405:VAL:HG23	2.12	0.49
1:A:493:THR:O	1:A:497:ILE:HG13	2.12	0.49
1:A:651:LEU:C	1:A:651:LEU:HD23	2.37	0.49
1:D:613:TYR:N	1:D:614:PRO:HD2	2.27	0.49
1:D:621:THR:HB	1:D:622:PRO:HD3	1.94	0.49
1:A:82:LEU:HD23	1:A:144:VAL:HG23	1.94	0.49
1:A:363:TRP:CZ3	1:A:367:ILE:HD11	2.48	0.49
1:B:160:ILE:CG2	1:B:527:ILE:HD12	2.42	0.49
1:B:566:VAL:HG11	1:B:693:PRO:HB3	1.93	0.49
1:C:410:LEU:O	1:C:414:MET:HG3	2.12	0.49
1:D:155:VAL:O	1:D:155:VAL:HG12	2.13	0.49
1:D:240:LEU:HD21	1:D:458:ASP:CG	2.37	0.49
1:A:25:VAL:CG2	1:A:97:MET:HE1	2.42	0.49
1:A:347:LEU:HB2	1:A:350:LEU:HD11	1.94	0.49
1:B:377:GLY:HA2	1:B:497:ILE:HG23	1.95	0.49
1:B:514:PHE:CE1	1:B:638:LEU:HB3	2.46	0.49
1:D:409:GLY:HA3	1:D:659:TRP:CZ2	2.48	0.49
1:A:149:GLY:HA2	1:A:155:VAL:HG23	1.93	0.49
1:A:580:GLN:NE2	1:A:595:ASP:HB3	2.28	0.49
1:A:647:MET:HG3	1:B:552:ALA:HB1	1.94	0.49
1:B:226:ILE:O	1:B:230:VAL:HG23	2.13	0.49
1:B:437:LEU:H	1:B:437:LEU:HD22	1.78	0.49
1:C:109:ALA:HB2	1:C:118:ALA:HB2	1.95	0.49
1:C:535:LEU:HD22	1:D:540:LEU:HD23	1.95	0.49
1:D:97:MET:CE	1:D:125:GLY:HA2	2.42	0.49
1:D:561:TYR:HE2	1:D:614:PRO:HD3	1.78	0.49
1:A:553:ALA:CB	1:B:421:THR:HG21	2.36	0.49
1:A:667:GLU:HG2	1:A:681:HIS:NE2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:MET:CE	1:B:125:GLY:HA2	2.43	0.49
1:B:278:VAL:HG11	1:B:353:LEU:CD2	2.43	0.49
1:C:419:PRO:N	1:C:420:PRO:HD2	2.28	0.49
1:C:547:GLY:O	1:C:637:VAL:HA	2.12	0.49
1:D:7:PHE:O	1:D:10:ILE:HG13	2.12	0.49
1:D:288:SER:OG	1:D:343:TYR:OH	1.97	0.49
1:A:208:VAL:HG23	1:A:574:VAL:HG22	1.95	0.49
1:B:249:VAL:O	1:B:253:VAL:HG23	2.12	0.49
1:B:471:SER:O	1:B:476:LEU:HD13	2.12	0.49
1:B:522:ILE:HD11	1:B:534:VAL:CG1	2.42	0.49
1:B:678:SER:HB2	1:B:680:PRO:HD2	1.95	0.49
1:C:102:ASN:CB	1:C:466:ASN:HB3	2.43	0.49
1:C:115:ILE:HG21	1:C:317:PRO:HD3	1.95	0.49
1:A:474:CYS:HB2	1:A:476:LEU:HD11	1.95	0.48
1:B:102:ASN:CB	1:B:466:ASN:HB3	2.43	0.48
1:B:301:SER:OG	1:B:450:PHE:HA	2.12	0.48
1:C:112:THR:OG1	1:C:117:PRO:HG2	2.13	0.48
1:C:389:LYS:N	1:C:390:PRO:HD2	2.28	0.48
1:D:124:GLN:O	1:D:128:VAL:HG23	2.13	0.48
1:D:363:TRP:CD2	1:D:367:ILE:HD11	2.48	0.48
1:A:75:GLN:HB3	1:A:148:PHE:CD2	2.48	0.48
1:B:399:ILE:CD1	1:B:671:LEU:HD21	2.40	0.48
1:C:188:MET:HB2	1:C:704:ILE:CG2	2.44	0.48
1:C:373:GLY:HA3	1:C:447:MET:HG3	1.94	0.48
1:C:535:LEU:HB3	1:D:540:LEU:CD2	2.43	0.48
1:A:678:SER:HB2	1:A:680:PRO:HD2	1.95	0.48
1:C:119:LEU:HD13	1:C:317:PRO:CB	2.43	0.48
1:C:248:PHE:CZ	1:C:252:ILE:HD11	2.49	0.48
1:C:280:LYS:O	1:C:284:GLN:HG3	2.13	0.48
1:D:57:ILE:CD1	1:D:186:ILE:HD12	2.41	0.48
1:D:474:CYS:HB2	1:D:476:LEU:HD11	1.95	0.48
1:A:676:LYS:O	1:A:681:HIS:ND1	2.47	0.48
1:A:723:VAL:O	1:A:723:VAL:HG12	2.13	0.48
1:B:400:GLU:HB2	1:B:404:MET:HG3	1.94	0.48
1:B:705:LEU:HD23	1:B:705:LEU:C	2.38	0.48
1:C:248:PHE:HZ	1:C:294:ALA:HB1	1.78	0.48
1:C:493:THR:O	1:C:497:ILE:HG13	2.14	0.48
1:D:17:PHE:HB3	1:D:131:LEU:HD13	1.95	0.48
1:A:643:LEU:HD12	1:B:643:LEU:HD12	1.95	0.48
1:B:184:SER:HA	1:B:246:GLU:CG	2.31	0.48
1:B:569:ALA:HB2	1:B:606:ASN:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:698:VAL:HG12	1:C:702:LEU:HD11	1.96	0.48
1:D:169:PHE:CB	1:D:174:MET:HE3	2.41	0.48
1:A:169:PHE:HB2	1:A:174:MET:CE	2.38	0.48
1:A:184:SER:CA	1:A:246:GLU:HG3	2.35	0.48
1:A:355:PHE:HB3	1:A:361:SER:HB2	1.96	0.48
1:A:529:LYS:HD3	1:A:529:LYS:HA	1.50	0.48
1:A:549:LEU:HD11	1:B:507:ILE:HG21	1.96	0.48
1:A:698:VAL:O	1:A:702:LEU:HG	2.13	0.48
1:B:8:PHE:HD1	1:B:142:VAL:HG21	1.78	0.48
1:B:105:VAL:HG22	1:B:121:VAL:CG2	2.42	0.48
1:A:224:ALA:CB	1:A:577:ILE:HD11	2.43	0.48
1:B:188:MET:HB2	1:B:704:ILE:CG2	2.44	0.48
1:C:42:ILE:HD13	1:C:229:ASN:HB3	1.96	0.48
1:D:305:ILE:O	1:D:309:ILE:HG12	2.14	0.48
1:A:527:ILE:O	1:A:527:ILE:HG12	2.12	0.48
1:B:477:ASP:OD1	1:B:478:PRO:HD2	2.13	0.48
1:C:155:VAL:O	1:C:155:VAL:HG12	2.14	0.48
1:C:705:LEU:C	1:C:705:LEU:HD23	2.39	0.48
1:A:363:TRP:CD2	1:A:367:ILE:HD11	2.49	0.48
1:B:194:GLY:HA3	1:B:235:GLY:HA2	1.95	0.48
1:C:25:VAL:HG21	1:C:97:MET:HE1	1.96	0.48
1:C:222:ASN:HB3	1:C:225:THR:CG2	2.41	0.48
1:C:521:GLN:HG2	1:C:717:VAL:HG21	1.95	0.48
1:D:569:ALA:HB2	1:D:606:ASN:ND2	2.29	0.48
1:A:100:ARG:O	1:A:104:ARG:HG2	2.13	0.48
1:A:460:TYR:OH	1:A:487:LEU:HD22	2.13	0.48
1:D:441:ALA:HB2	1:D:512:SER:OG	2.13	0.48
1:A:471:SER:CA	1:A:476:LEU:HD13	2.42	0.47
1:A:648:LEU:O	1:A:652:THR:HG23	2.14	0.47
1:B:32:THR:OG1	1:B:33:GLU:N	2.44	0.47
1:B:325:LEU:HD23	1:B:453:THR:HG22	1.95	0.47
1:C:386:TYR:HA	1:C:391:THR:HB	1.95	0.47
1:D:662:ALA:C	1:D:684:LEU:HD13	2.39	0.47
1:A:226:ILE:HG13	1:A:473:MET:HE1	1.96	0.47
1:B:384:THR:HG21	1:B:493:THR:HA	1.95	0.47
1:B:584:ILE:HG23	1:B:584:ILE:O	2.14	0.47
1:A:337:ALA:HB2	1:A:363:TRP:CE2	2.49	0.47
1:A:613:TYR:N	1:A:614:PRO:HD2	2.28	0.47
1:B:22:PHE:O	1:B:26:VAL:HG12	2.14	0.47
1:B:404:MET:HA	1:B:404:MET:HE3	1.95	0.47
1:B:547:GLY:O	1:B:637:VAL:HA	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:LEU:O	1:C:185:ILE:HG13	2.15	0.47
1:C:418:PHE:HB3	1:C:419:PRO:CD	2.41	0.47
1:C:578:ARG:O	1:C:582:ARG:HG2	2.14	0.47
1:D:244:LEU:HD23	1:D:455:VAL:CG2	2.33	0.47
1:A:262:MET:SD	1:A:353:LEU:HD22	2.55	0.47
1:B:630:GLY:HA2	1:B:724:HIS:HB3	1.96	0.47
1:C:249:VAL:O	1:C:253:VAL:HG23	2.15	0.47
1:C:264:PRO:O	1:C:527:ILE:HD11	2.14	0.47
1:C:421:THR:CG2	1:D:553:ALA:HB2	2.43	0.47
1:C:647:MET:HE2	1:C:647:MET:HA	1.97	0.47
1:D:115:ILE:N	1:D:115:ILE:HD12	2.30	0.47
1:D:419:PRO:N	1:D:420:PRO:HD2	2.29	0.47
1:A:141:LEU:CD2	1:A:252:ILE:HG21	2.44	0.47
1:A:268:GLN:HG2	6:A:809:GQB:C10	2.44	0.47
1:B:613:TYR:N	1:B:614:PRO:HD2	2.29	0.47
1:D:105:VAL:HA	1:D:121:VAL:HG11	1.96	0.47
1:D:138:LEU:HD21	1:D:294:ALA:CB	2.44	0.47
1:D:581:ALA:HA	1:D:587:LEU:HD13	1.97	0.47
1:D:633:PHE:O	1:D:637:VAL:HG23	2.14	0.47
1:A:54:THR:HG22	1:A:58:PHE:HD2	1.80	0.47
1:A:155:VAL:O	1:A:155:VAL:HG12	2.14	0.47
1:B:11:PRO:HB2	1:B:139:LEU:HB2	1.96	0.47
1:C:326:TRP:O	1:C:330:LEU:HD13	2.15	0.47
1:D:147:ILE:O	1:D:151:TRP:HB3	2.15	0.47
1:A:192:VAL:O	1:A:196:VAL:HG23	2.15	0.47
1:A:226:ILE:O	1:A:230:VAL:HG23	2.14	0.47
1:A:356:ARG:HG3	1:A:357:PHE:CD1	2.50	0.47
1:B:10:ILE:N	1:B:11:PRO:HD2	2.30	0.47
1:B:225:THR:OG1	1:B:473:MET:HE2	2.13	0.47
1:B:227:ALA:HA	1:B:600:ILE:CD1	2.44	0.47
1:B:385:SER:HA	1:B:661:ASN:ND2	2.30	0.47
1:B:722:HIS:CD2	1:B:723:VAL:HG23	2.49	0.47
1:C:74:TRP:HH2	1:C:152:MET:HE1	1.79	0.47
1:C:112:THR:HG21	1:C:117:PRO:HG2	1.97	0.47
1:C:305:ILE:O	1:C:309:ILE:HG12	2.15	0.47
1:C:579:ARG:NH1	1:C:583:GLU:OE1	2.47	0.47
1:D:198:THR:HB	1:D:231:GLY:O	2.14	0.47
1:D:414:MET:HG2	1:D:651:LEU:HD11	1.96	0.47
1:D:616:PHE:O	1:D:620:LEU:HG	2.14	0.47
1:A:459:SER:O	1:A:462:PRO:HD2	2.15	0.47
1:A:550:LEU:O	1:A:554:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:THR:HG22	1:B:58:PHE:HD2	1.79	0.47
1:B:80:PHE:HE2	1:B:185:ILE:HD12	1.80	0.47
1:C:86:MET:HE3	1:C:136:PHE:HB3	1.96	0.47
1:D:248:PHE:O	1:D:252:ILE:HG13	2.15	0.47
1:D:410:LEU:O	1:D:414:MET:HG3	2.15	0.47
1:A:685:VAL:O	1:A:689:THR:HG23	2.15	0.47
1:B:97:MET:HE2	1:B:125:GLY:HA2	1.97	0.47
1:B:141:LEU:HD21	1:B:252:ILE:HG21	1.97	0.47
1:B:355:PHE:CD1	1:B:362:PRO:HD3	2.50	0.47
1:C:32:THR:OG1	1:C:33:GLU:N	2.47	0.47
1:C:43:ARG:CG	1:C:99:THR:HB	2.31	0.47
1:C:105:VAL:HG22	1:C:121:VAL:HG22	1.96	0.47
1:C:167:ILE:CD1	1:C:719:ILE:HD11	2.44	0.47
1:C:363:TRP:CD2	1:C:367:ILE:HD11	2.49	0.47
1:C:539:MET:CG	1:D:539:MET:HE2	2.39	0.47
1:D:25:VAL:CG2	1:D:124:GLN:HB3	2.45	0.47
1:D:214:ASN:C	1:D:215:LEU:HD12	2.39	0.47
1:D:240:LEU:HD12	1:D:244:LEU:HD13	1.96	0.47
1:B:18:ALA:HB2	1:B:131:LEU:HB2	1.97	0.47
1:B:398:SER:HA	1:B:405:VAL:HG22	1.97	0.47
1:C:204:ALA:HB3	1:C:573:MET:HE2	1.97	0.47
1:C:248:PHE:CZ	1:C:294:ALA:HB1	2.50	0.47
1:C:418:PHE:HA	1:D:553:ALA:HB1	1.97	0.47
1:C:553:ALA:HB2	1:D:421:THR:CG2	2.41	0.47
1:D:112:THR:CG2	1:D:117:PRO:HG2	2.45	0.47
1:D:504:GLY:O	1:D:508:PHE:HD1	1.98	0.47
1:D:692:ASP:HA	1:D:695:LYS:HE3	1.96	0.47
1:A:184:SER:O	1:A:708:ILE:HD11	2.15	0.46
1:B:323:ILE:O	1:B:327:THR:HG23	2.15	0.46
1:B:511:LEU:O	1:B:511:LEU:HD23	2.15	0.46
1:C:66:ILE:O	1:C:70:ILE:HG13	2.15	0.46
1:C:205:ALA:HB2	1:C:224:ALA:HB3	1.96	0.46
1:C:597:ASN:ND2	7:C:807:D1D:H1C1	2.31	0.46
1:D:167:ILE:HG12	1:D:719:ILE:HG13	1.96	0.46
1:D:233:ASN:OD1	1:D:466:ASN:ND2	2.48	0.46
1:A:80:PHE:HE2	1:A:185:ILE:HD12	1.81	0.46
1:B:17:PHE:HB3	1:B:131:LEU:HD13	1.96	0.46
1:B:493:THR:O	1:B:497:ILE:HG13	2.15	0.46
1:C:119:LEU:HD21	1:C:320:GLU:CG	2.45	0.46
1:C:226:ILE:O	1:C:230:VAL:HG23	2.15	0.46
1:C:296:VAL:HG11	1:C:335:LEU:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:LEU:HD22	1:D:317:PRO:HB3	1.97	0.46
1:B:70:ILE:HG22	1:B:71:PHE:CD1	2.51	0.46
1:B:155:VAL:O	1:B:155:VAL:HG12	2.14	0.46
1:B:208:VAL:HG11	1:B:577:ILE:HG22	1.96	0.46
1:C:616:PHE:O	1:C:620:LEU:HG	2.15	0.46
1:D:162:THR:HA	1:D:167:ILE:O	2.15	0.46
1:D:401:GLY:O	1:D:405:VAL:HG23	2.15	0.46
1:A:21:ASN:CB	1:A:128:VAL:HG22	2.45	0.46
1:C:119:LEU:CD2	1:C:317:PRO:HA	2.46	0.46
1:C:402:THR:CG2	1:C:686:ILE:HG21	2.46	0.46
1:C:477:ASP:OD1	1:C:478:PRO:HD2	2.14	0.46
1:A:25:VAL:HG21	1:A:97:MET:CE	2.45	0.46
1:B:180:ALA:HB2	1:B:253:VAL:HG21	1.98	0.46
1:B:424:LEU:HD21	1:B:504:GLY:HA2	1.98	0.46
1:C:571:MET:HG2	1:D:400:GLU:HG3	1.97	0.46
1:D:139:LEU:HA	1:D:142:VAL:HG12	1.97	0.46
1:D:215:LEU:CD2	1:D:221:ARG:HB2	2.46	0.46
1:D:626:GLY:HA2	1:D:630:GLY:O	2.15	0.46
1:A:170:VAL:HB	1:A:173:ALA:HB3	1.97	0.46
1:C:62:ILE:O	1:C:66:ILE:HG12	2.14	0.46
1:C:511:LEU:CD1	1:D:545:ILE:HG21	2.46	0.46
1:D:199:LYS:HE2	1:D:199:LYS:CA	2.44	0.46
1:D:363:TRP:CH2	1:D:367:ILE:HD11	2.51	0.46
1:A:109:ALA:HB2	1:A:118:ALA:CB	2.45	0.46
1:B:5:ALA:O	1:B:9:LEU:HD13	2.15	0.46
1:B:268:GLN:HG3	1:B:277:GLN:CG	2.45	0.46
1:C:205:ALA:HB2	1:C:224:ALA:CB	2.46	0.46
1:A:115:ILE:N	1:A:115:ILE:HD12	2.31	0.46
1:A:296:VAL:HG11	1:A:335:LEU:HB3	1.98	0.46
1:A:381:GLU:HG3	1:A:493:THR:HG21	1.97	0.46
1:A:571:MET:HG2	1:B:400:GLU:HG3	1.98	0.46
1:B:160:ILE:HG21	1:B:527:ILE:HD12	1.98	0.46
1:C:74:TRP:CH2	1:C:152:MET:HE1	2.51	0.46
1:C:208:VAL:CG2	1:C:574:VAL:HG13	2.44	0.46
1:D:32:THR:OG1	1:D:33:GLU:N	2.49	0.46
1:D:103:VAL:HG22	1:D:470:ILE:HG21	1.97	0.46
1:A:32:THR:HG23	1:A:35:MET:H	1.81	0.46
1:A:245:LEU:HD23	1:A:245:LEU:C	2.40	0.46
1:A:386:TYR:HD2	1:A:665:TYR:HD2	1.62	0.46
1:A:419:PRO:N	1:A:420:PRO:HD2	2.31	0.46
1:A:556:TYR:OH	1:B:556:TYR:OH	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:VAL:HG11	1:B:97:MET:HE1	1.97	0.46
1:C:549:LEU:HD11	1:D:507:ILE:HG21	1.98	0.46
1:D:723:VAL:O	1:D:723:VAL:HG12	2.16	0.46
1:A:418:PHE:HB3	1:A:419:PRO:CD	2.42	0.46
1:B:301:SER:O	1:B:305:ILE:HG13	2.15	0.46
1:B:550:LEU:O	1:B:554:ILE:HG13	2.16	0.46
1:C:154:GLN:HB3	1:C:171:PRO:HB2	1.98	0.46
1:C:395:GLY:O	1:C:398:SER:OG	2.16	0.46
1:D:521:GLN:HG2	1:D:717:VAL:CG2	2.46	0.46
1:D:698:VAL:O	1:D:702:LEU:HG	2.15	0.46
1:C:514:PHE:CZ	1:C:642:VAL:HG21	2.51	0.45
1:C:527:ILE:HG23	1:C:527:ILE:O	2.15	0.45
1:D:550:LEU:O	1:D:554:ILE:HG13	2.16	0.45
1:A:11:PRO:HD3	1:A:295:LEU:CD2	2.46	0.45
1:A:615:ALA:O	1:A:619:ILE:HG13	2.15	0.45
1:B:240:LEU:HD21	1:B:458:ASP:CG	2.41	0.45
1:C:25:VAL:HG21	1:C:97:MET:CE	2.47	0.45
1:A:301:SER:O	1:A:305:ILE:HG13	2.16	0.45
1:A:570:ALA:O	1:A:574:VAL:HG23	2.16	0.45
1:B:115:ILE:N	1:B:115:ILE:HD12	2.31	0.45
1:C:101:ALA:O	1:C:105:VAL:HG23	2.16	0.45
1:C:189:PHE:HD1	1:C:611:MET:HG2	1.81	0.45
1:C:363:TRP:O	1:C:367:ILE:HG13	2.15	0.45
1:C:647:MET:HE2	1:C:647:MET:CA	2.47	0.45
1:C:647:MET:HG3	1:D:552:ALA:HB1	1.98	0.45
1:D:194:GLY:HA3	1:D:235:GLY:CA	2.43	0.45
1:D:226:ILE:O	1:D:230:VAL:HG23	2.16	0.45
1:D:233:ASN:HA	1:D:237:VAL:CG2	2.46	0.45
1:D:361:SER:N	1:D:362:PRO:HD2	2.32	0.45
1:D:405:VAL:HG21	1:D:683:ALA:HB1	1.98	0.45
1:D:409:GLY:HA3	1:D:659:TRP:CE2	2.51	0.45
1:D:651:LEU:C	1:D:651:LEU:HD23	2.41	0.45
1:B:42:ILE:CD1	1:B:226:ILE:HG23	2.47	0.45
1:B:468:GLY:HA2	1:B:484:THR:HG21	1.99	0.45
1:B:707:LYS:O	1:B:711:VAL:HG23	2.16	0.45
1:C:278:VAL:HG21	1:C:353:LEU:HD23	1.98	0.45
1:C:448:LEU:O	1:C:451:VAL:HB	2.17	0.45
1:C:723:VAL:O	1:C:723:VAL:HG12	2.16	0.45
1:D:34:ARG:O	1:D:38:ILE:HG12	2.17	0.45
1:D:112:THR:HG21	1:D:117:PRO:CG	2.46	0.45
1:D:521:GLN:HG2	1:D:717:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:660:ASP:O	1:D:664:LYS:HG3	2.16	0.45
1:A:530:PRO:HB3	6:A:809:GQB:C08	2.47	0.45
1:B:717:VAL:HA	1:B:720:PHE:CZ	2.52	0.45
1:C:248:PHE:CE1	1:C:252:ILE:HD11	2.51	0.45
1:D:102:ASN:HB2	1:D:466:ASN:HB3	1.99	0.45
1:D:376:ILE:HD11	1:D:424:LEU:HD11	1.98	0.45
1:D:390:PRO:HB2	1:D:412:LEU:HD11	1.99	0.45
1:A:370:ILE:O	1:A:374:ILE:HG13	2.17	0.45
1:A:404:MET:HA	1:A:404:MET:HE3	1.98	0.45
1:A:500:GLY:O	1:A:503:ILE:HG22	2.16	0.45
1:B:6:LEU:O	1:B:6:LEU:HD23	2.17	0.45
1:B:252:ILE:HG23	1:B:290:PRO:HB2	1.99	0.45
1:B:543:ARG:HH22	1:B:726:PHE:C	2.25	0.45
1:D:84:ALA:CB	1:D:186:ILE:HG13	2.46	0.45
1:D:208:VAL:HG22	1:D:574:VAL:HG13	1.98	0.45
1:D:363:TRP:O	1:D:367:ILE:HG13	2.16	0.45
1:B:127:SER:HA	1:B:456:SER:HB2	1.98	0.45
1:B:167:ILE:HD11	1:B:719:ILE:CD1	2.31	0.45
1:C:202:ASP:HB2	8:C:902:HOH:O	2.15	0.45
1:C:223:PRO:CB	1:C:580:GLN:HE22	2.29	0.45
1:C:267:VAL:CG1	1:C:274:LEU:HB3	2.46	0.45
1:C:424:LEU:O	1:C:428:ILE:HG13	2.17	0.45
1:D:86:MET:HE3	1:D:136:PHE:CB	2.47	0.45
1:D:227:ALA:HA	1:D:600:ILE:CD1	2.46	0.45
1:D:301:SER:O	1:D:305:ILE:HG13	2.15	0.45
1:A:95:MET:HE3	1:A:99:THR:CG2	2.47	0.45
1:A:97:MET:CE	1:A:125:GLY:HA2	2.47	0.45
1:B:10:ILE:CG2	1:B:298:LEU:HD22	2.44	0.45
1:B:185:ILE:HG12	1:B:708:ILE:CD1	2.47	0.45
1:C:317:PRO:HG2	1:C:490:VAL:HG21	1.98	0.45
1:C:587:LEU:HD23	1:C:587:LEU:O	2.17	0.45
1:C:639:ILE:HD13	1:D:539:MET:HG3	1.99	0.45
1:D:224:ALA:CB	1:D:577:ILE:HD11	2.41	0.45
1:B:252:ILE:HG12	1:B:445:LEU:HD13	1.99	0.45
1:C:160:ILE:HG23	1:C:524:PRO:HB3	1.99	0.45
1:A:70:ILE:HG22	1:A:71:PHE:CD1	2.51	0.45
1:A:102:ASN:HB2	1:A:466:ASN:HB3	1.99	0.45
1:A:126:GLY:O	1:A:456:SER:HA	2.17	0.45
1:A:199:LYS:CD	1:A:696:ASP:HB2	2.41	0.45
1:A:301:SER:HB3	1:A:452:ALA:HB3	1.99	0.45
1:A:363:TRP:CE3	1:A:367:ILE:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:VAL:HG23	1:B:574:VAL:HG22	1.99	0.45
1:B:438:TYR:C	1:B:438:TYR:CD1	2.95	0.45
1:C:167:ILE:HG12	1:C:719:ILE:CG1	2.47	0.45
1:C:323:ILE:O	1:C:327:THR:HG23	2.17	0.45
1:C:444:ALA:HB2	1:C:508:PHE:HB2	1.94	0.45
1:D:149:GLY:CA	1:D:155:VAL:HG23	2.47	0.45
1:D:446:GLY:HA2	1:D:449:SER:HB3	1.97	0.45
1:D:685:VAL:O	1:D:689:THR:HG23	2.17	0.45
1:A:184:SER:OG	1:A:708:ILE:HG12	2.17	0.44
1:C:46:ALA:HB1	1:C:95:MET:SD	2.57	0.44
1:C:57:ILE:HG12	1:C:189:PHE:HB3	1.99	0.44
1:C:539:MET:CG	1:D:539:MET:HG2	2.40	0.44
1:A:17:PHE:HB3	1:A:131:LEU:HD13	1.99	0.44
1:A:32:THR:OG1	1:A:33:GLU:N	2.51	0.44
1:A:263:PHE:HB2	1:A:283:ILE:HG13	1.99	0.44
1:A:370:ILE:HG23	1:A:450:PHE:CE2	2.53	0.44
1:B:398:SER:HB2	1:B:684:LEU:HG	1.99	0.44
1:C:18:ALA:HB2	1:C:131:LEU:CB	2.47	0.44
1:C:355:PHE:CE1	1:C:362:PRO:HD3	2.52	0.44
1:C:448:LEU:CD1	1:C:505:SER:HB2	2.43	0.44
1:D:54:THR:O	1:D:57:ILE:HG13	2.17	0.44
1:A:223:PRO:HA	1:A:596:TYR:HD1	1.82	0.44
1:A:249:VAL:O	1:A:253:VAL:HG23	2.16	0.44
1:A:569:ALA:HB2	1:A:606:ASN:ND2	2.31	0.44
1:A:573:MET:O	1:A:577:ILE:HG13	2.15	0.44
1:B:103:VAL:HG23	1:B:470:ILE:CD1	2.35	0.44
1:B:278:VAL:HG11	1:B:353:LEU:HD21	1.99	0.44
1:C:80:PHE:CE2	1:C:182:GLY:HA2	2.52	0.44
1:C:149:GLY:O	1:C:155:VAL:HG23	2.16	0.44
1:C:216:PRO:HG2	1:C:219:ASP:HB2	1.97	0.44
1:C:227:ALA:HA	1:C:600:ILE:HD13	1.99	0.44
1:C:503:ILE:HD11	1:C:646:ALA:HA	1.98	0.44
1:C:535:LEU:HA	1:D:540:LEU:HD22	1.98	0.44
1:D:337:ALA:HB2	1:D:363:TRP:CZ2	2.52	0.44
1:D:464:ALA:O	1:D:484:THR:HG23	2.17	0.44
1:A:57:ILE:CG1	1:A:189:PHE:HB3	2.47	0.44
1:A:141:LEU:HD21	1:A:252:ILE:CG2	2.48	0.44
1:A:199:LYS:HE2	1:A:199:LYS:CA	2.47	0.44
1:A:259:ALA:HB2	1:A:438:TYR:HE2	1.82	0.44
1:A:262:MET:HE1	1:A:438:TYR:HB2	1.98	0.44
1:A:400:GLU:HG3	1:B:571:MET:CG	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:LEU:CD1	1:A:505:SER:HB2	2.46	0.44
1:B:367:ILE:O	1:B:368:ILE:C	2.61	0.44
1:B:619:ILE:CG1	1:B:708:ILE:HD11	2.48	0.44
1:C:6:LEU:HD23	1:C:6:LEU:O	2.18	0.44
1:C:265:ILE:HG22	1:C:531:PRO:HG3	1.99	0.44
1:D:53:GLU:OE2	1:D:193:GLY:HA3	2.17	0.44
1:D:344:LEU:HD22	1:D:347:LEU:HD11	1.99	0.44
1:A:410:LEU:O	1:A:414:MET:HG3	2.18	0.44
1:B:604:SER:O	1:B:608:LEU:HG	2.18	0.44
1:B:705:LEU:HA	1:B:708:ILE:HG22	1.99	0.44
1:C:53:GLU:OE2	1:C:193:GLY:HA3	2.17	0.44
1:C:57:ILE:HG22	1:C:186:ILE:HD12	2.00	0.44
1:C:96:LYS:O	1:C:100:ARG:HG3	2.18	0.44
1:D:188:MET:HE1	1:D:558:PHE:CE2	2.52	0.44
1:D:569:ALA:HB2	1:D:606:ASN:CB	2.47	0.44
1:D:647:MET:HE2	1:D:647:MET:HA	1.99	0.44
1:A:62:ILE:O	1:A:66:ILE:HG12	2.17	0.44
1:A:95:MET:O	1:A:99:THR:HG23	2.18	0.44
1:A:101:ALA:O	1:A:105:VAL:HG23	2.17	0.44
1:A:139:LEU:HA	1:A:142:VAL:HG12	1.99	0.44
1:B:141:LEU:HD21	1:B:252:ILE:CG2	2.47	0.44
1:B:188:MET:HE1	1:B:558:PHE:CE2	2.53	0.44
1:B:389:LYS:N	1:B:390:PRO:HD2	2.31	0.44
1:B:685:VAL:O	1:B:689:THR:HG23	2.17	0.44
1:C:115:ILE:HD12	1:C:115:ILE:N	2.32	0.44
1:C:221:ARG:O	1:C:587:LEU:HD21	2.17	0.44
1:C:367:ILE:O	1:C:368:ILE:C	2.61	0.44
1:C:613:TYR:N	1:C:614:PRO:HD2	2.32	0.44
1:D:196:VAL:HA	1:D:566:VAL:HG22	1.99	0.44
1:D:624:VAL:HG23	1:D:625:THR:N	2.33	0.44
1:A:23:ALA:HA	1:A:26:VAL:HG12	2.00	0.44
1:A:61:ALA:HB2	1:A:186:ILE:HD11	2.00	0.44
1:A:201:ALA:HB2	1:A:603:THR:HG21	2.00	0.44
1:A:227:ALA:HA	1:A:600:ILE:CD1	2.48	0.44
1:B:158:LEU:HD13	1:B:283:ILE:HG21	2.00	0.44
1:B:647:MET:N	1:B:647:MET:HE2	2.33	0.44
1:C:15:LEU:CD2	1:C:135:GLY:HA3	2.48	0.44
1:C:535:LEU:HB3	1:D:540:LEU:HD22	2.00	0.44
1:D:306:LEU:HA	1:D:309:ILE:HG12	2.00	0.44
1:D:367:ILE:O	1:D:368:ILE:C	2.60	0.44
1:A:208:VAL:HG21	1:A:574:VAL:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:HD12	1:A:258:LEU:HA	1.86	0.44
1:B:167:ILE:HD12	1:B:167:ILE:N	2.32	0.44
1:B:225:THR:CB	1:B:473:MET:HE2	2.47	0.44
1:B:723:VAL:O	1:B:723:VAL:HG12	2.18	0.44
1:C:199:LYS:HE2	1:C:199:LYS:CA	2.47	0.44
1:C:386:TYR:CB	1:C:665:TYR:HB2	2.46	0.44
1:D:230:VAL:O	1:D:234:VAL:HG23	2.17	0.44
1:D:558:PHE:CD2	1:D:705:LEU:HD12	2.53	0.44
1:A:219:ASP:O	1:A:225:THR:HG21	2.18	0.44
1:A:227:ALA:HA	1:A:600:ILE:HD13	2.00	0.44
1:A:232:ASP:O	1:A:237:VAL:HG23	2.18	0.44
1:B:76:THR:OG1	1:B:174:MET:HG3	2.17	0.44
1:B:268:GLN:HG3	1:B:277:GLN:HG2	1.99	0.44
1:B:437:LEU:HD22	1:B:437:LEU:N	2.33	0.44
1:C:88:ALA:O	1:C:92:ILE:HG13	2.18	0.44
1:C:545:ILE:HG21	1:D:511:LEU:CD1	2.44	0.44
1:D:424:LEU:HD21	1:D:504:GLY:HA2	2.00	0.44
1:A:189:PHE:HE1	1:A:612:GLY:HA2	1.83	0.43
1:A:262:MET:O	1:A:266:TYR:HD2	2.01	0.43
1:A:395:GLY:O	1:A:398:SER:OG	2.22	0.43
1:B:21:ASN:CB	1:B:128:VAL:HG22	2.47	0.43
1:B:214:ASN:C	1:B:215:LEU:HD12	2.43	0.43
1:C:15:LEU:HD21	1:C:135:GLY:HA3	1.99	0.43
1:C:615:ALA:O	1:C:619:ILE:HG13	2.18	0.43
1:C:647:MET:HB3	1:D:556:TYR:CE1	2.53	0.43
1:C:693:PRO:O	1:C:697:THR:HB	2.18	0.43
1:D:618:ALA:HB1	1:D:708:ILE:CG2	2.48	0.43
1:A:188:MET:HE1	1:A:558:PHE:CE1	2.53	0.43
1:A:298:LEU:HD23	1:A:298:LEU:C	2.43	0.43
1:A:344:LEU:O	1:A:359:ALA:HB2	2.18	0.43
1:A:367:ILE:O	1:A:368:ILE:C	2.61	0.43
1:A:511:LEU:HD12	1:B:545:ILE:HD13	2.00	0.43
1:B:23:ALA:HA	1:B:26:VAL:CG1	2.47	0.43
1:B:32:THR:HG22	1:B:35:MET:HE2	1.95	0.43
1:B:500:GLY:O	1:B:503:ILE:HG22	2.19	0.43
1:C:399:ILE:HD13	1:C:680:PRO:CB	2.48	0.43
1:D:25:VAL:CB	1:D:97:MET:HE1	2.47	0.43
1:D:35:MET:HE1	1:D:476:LEU:HD21	2.00	0.43
1:D:107:GLU:O	1:D:111:THR:HG23	2.18	0.43
1:D:298:LEU:HD23	1:D:298:LEU:C	2.42	0.43
1:A:266:TYR:CD1	1:A:531:PRO:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:GLN:HE22	1:A:595:ASP:HB3	1.82	0.43
1:A:624:VAL:HG23	1:A:625:THR:N	2.33	0.43
1:B:138:LEU:HD21	1:B:294:ALA:CB	2.46	0.43
1:B:170:VAL:HG13	1:B:171:PRO:HD2	2.00	0.43
1:C:481:ARG:HA	1:C:484:THR:OG1	2.18	0.43
1:C:558:PHE:CD2	1:C:705:LEU:HD12	2.54	0.43
1:D:188:MET:CB	1:D:704:ILE:HG21	2.46	0.43
1:D:359:ALA:O	1:D:362:PRO:HD2	2.18	0.43
1:A:120:LYS:HZ1	1:A:309:ILE:HA	1.84	0.43
1:A:666:LEU:HD23	1:A:666:LEU:C	2.43	0.43
1:B:34:ARG:O	1:B:38:ILE:HG13	2.18	0.43
1:B:666:LEU:HD23	1:B:666:LEU:C	2.43	0.43
1:C:80:PHE:CE2	1:C:185:ILE:HD12	2.51	0.43
1:C:500:GLY:O	1:C:503:ILE:HG22	2.17	0.43
1:C:624:VAL:HG23	1:C:625:THR:N	2.33	0.43
1:D:21:ASN:O	1:D:25:VAL:HG23	2.19	0.43
1:D:404:MET:HA	1:D:404:MET:HE3	2.01	0.43
1:D:717:VAL:HA	1:D:720:PHE:CZ	2.54	0.43
1:B:350:LEU:HB3	1:B:355:PHE:HD2	1.83	0.43
1:B:448:LEU:O	1:B:451:VAL:HB	2.18	0.43
1:C:263:PHE:HB3	1:C:264:PRO:HD3	2.00	0.43
1:C:421:THR:CB	1:D:553:ALA:HB2	2.48	0.43
1:C:663:LYS:O	1:C:667:GLU:HG3	2.19	0.43
1:D:198:THR:HB	1:D:231:GLY:C	2.43	0.43
1:D:325:LEU:HD23	1:D:453:THR:CG2	2.49	0.43
1:B:54:THR:HA	1:B:57:ILE:CG1	2.48	0.43
1:B:283:ILE:O	1:B:287:ILE:HG13	2.19	0.43
1:B:289:TYR:N	1:B:290:PRO:HD2	2.34	0.43
1:B:527:ILE:O	1:B:527:ILE:HG12	2.19	0.43
1:C:184:SER:HA	1:C:246:GLU:CG	2.43	0.43
1:C:306:LEU:HA	1:C:309:ILE:HG12	1.99	0.43
1:C:319:ARG:O	1:C:323:ILE:HG12	2.19	0.43
1:C:359:ALA:O	1:C:362:PRO:HD2	2.19	0.43
1:A:219:ASP:CG	1:A:220:PRO:HD2	2.42	0.43
1:B:25:VAL:CG2	1:B:124:GLN:HB3	2.49	0.43
1:B:330:LEU:O	1:B:334:VAL:HG23	2.19	0.43
1:B:514:PHE:CZ	1:B:642:VAL:HG21	2.54	0.43
1:C:396:LYS:O	1:C:399:ILE:HG12	2.19	0.43
1:C:632:GLU:CD	1:C:632:GLU:H	2.26	0.43
1:D:663:LYS:O	1:D:667:GLU:HG3	2.19	0.43
1:A:57:ILE:HG22	1:A:186:ILE:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ALA:O	1:A:92:ILE:HG13	2.18	0.43
1:A:296:VAL:CG1	1:A:335:LEU:HB3	2.49	0.43
1:A:522:ILE:HD11	1:A:534:VAL:CG2	2.48	0.43
1:B:26:VAL:HG23	1:B:104:ARG:NH2	2.33	0.43
1:B:245:LEU:HD23	1:B:245:LEU:C	2.44	0.43
1:B:446:GLY:HA2	1:B:449:SER:HB3	1.99	0.43
1:C:185:ILE:HD13	1:C:619:ILE:CD1	2.49	0.43
1:C:597:ASN:ND2	1:C:597:ASN:O	2.51	0.43
1:C:628:LEU:O	1:C:629:LEU:HD23	2.19	0.43
1:C:638:LEU:HD11	1:C:713:SER:OG	2.19	0.43
1:D:289:TYR:N	1:D:290:PRO:HD2	2.34	0.43
1:D:325:LEU:HD23	1:D:453:THR:HG22	2.01	0.43
1:A:627:PHE:CD1	1:A:720:PHE:HB3	2.53	0.43
1:B:15:LEU:HD21	1:B:136:PHE:N	2.34	0.43
1:B:185:ILE:HD13	1:B:619:ILE:HD11	2.00	0.43
1:B:213:LEU:HB3	1:B:215:LEU:HD13	2.00	0.43
1:B:265:ILE:CG1	1:B:522:ILE:HD12	2.48	0.43
1:B:457:VAL:HG12	1:B:494:THR:HB	2.01	0.43
1:C:54:THR:HG22	1:C:58:PHE:HD2	1.83	0.43
1:C:386:TYR:HB2	1:C:665:TYR:HB2	2.01	0.43
1:D:477:ASP:OD1	1:D:478:PRO:HD2	2.19	0.43
1:D:527:ILE:O	1:D:527:ILE:HG12	2.18	0.43
1:D:559:SER:HB3	1:D:698:VAL:HG11	1.99	0.43
1:A:22:PHE:O	1:A:26:VAL:HG12	2.19	0.43
1:A:80:PHE:CE2	1:A:182:GLY:HA2	2.53	0.43
1:A:154:GLN:CG	1:A:171:PRO:HB2	2.49	0.43
1:A:363:TRP:O	1:A:367:ILE:HG13	2.18	0.43
1:B:261:TYR:O	1:B:265:ILE:HD13	2.19	0.43
1:C:417:VAL:CG2	1:C:651:LEU:HB2	2.49	0.43
1:C:425:VAL:HG21	1:D:550:LEU:HB2	2.00	0.43
1:D:167:ILE:CD1	1:D:719:ILE:HD11	2.49	0.43
1:D:223:PRO:HG2	1:D:577:ILE:HG12	2.00	0.43
1:D:584:ILE:HG22	1:D:587:LEU:HB2	2.01	0.43
1:A:6:LEU:HD23	1:A:6:LEU:O	2.19	0.42
1:B:141:LEU:CD2	1:B:252:ILE:HG21	2.49	0.42
1:B:213:LEU:HB2	1:B:215:LEU:HD13	2.00	0.42
1:B:370:ILE:O	1:B:374:ILE:HG13	2.19	0.42
1:B:418:PHE:HB3	1:B:419:PRO:CD	2.45	0.42
1:B:527:ILE:O	1:B:527:ILE:HG23	2.18	0.42
1:C:25:VAL:HG11	1:C:97:MET:CE	2.36	0.42
1:A:72:THR:HA	1:A:163:ASN:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:HD12	1:A:298:LEU:HD13	2.01	0.42
1:A:381:GLU:O	1:A:385:SER:HB3	2.19	0.42
1:B:199:LYS:HE2	1:B:199:LYS:CA	2.48	0.42
1:B:386:TYR:H	1:B:386:TYR:HD1	1.66	0.42
1:C:11:PRO:HD3	1:C:295:LEU:HD22	2.00	0.42
1:C:22:PHE:HD1	1:C:97:MET:SD	2.42	0.42
1:C:149:GLY:CA	1:C:155:VAL:HG23	2.49	0.42
1:C:604:SER:O	1:C:608:LEU:HG	2.19	0.42
1:D:539:MET:CE	1:D:639:ILE:HG21	2.49	0.42
1:A:50:LEU:HD12	1:A:50:LEU:HA	1.91	0.42
1:A:214:ASN:C	1:A:215:LEU:HD12	2.44	0.42
1:A:365:SER:O	1:A:368:ILE:HB	2.19	0.42
1:A:587:LEU:O	1:A:587:LEU:HD23	2.19	0.42
1:A:643:LEU:O	1:A:647:MET:HG2	2.18	0.42
1:B:119:LEU:HD13	1:B:317:PRO:CB	2.49	0.42
1:C:325:LEU:CD2	1:C:453:THR:HG22	2.46	0.42
1:D:389:LYS:N	1:D:390:PRO:HD2	2.35	0.42
1:D:424:LEU:CD2	1:D:507:ILE:HD12	2.49	0.42
1:A:213:LEU:CB	1:A:215:LEU:HD13	2.48	0.42
1:A:379:TRP:CE2	1:A:419:PRO:HB3	2.55	0.42
1:B:26:VAL:HG23	1:B:104:ARG:HH22	1.84	0.42
1:C:79:ALA:O	1:C:179:TYR:HA	2.18	0.42
1:C:117:PRO:O	1:C:121:VAL:HG12	2.19	0.42
1:C:527:ILE:O	1:C:527:ILE:HG12	2.20	0.42
1:C:711:VAL:O	1:C:715:ILE:HG13	2.19	0.42
1:A:184:SER:HB2	1:A:708:ILE:HG13	2.01	0.42
1:A:320:GLU:OE1	1:A:320:GLU:HA	2.19	0.42
1:B:618:ALA:HB1	1:B:708:ILE:CG2	2.49	0.42
1:B:624:VAL:HG23	1:B:625:THR:N	2.35	0.42
1:C:386:TYR:HD2	1:C:665:TYR:CD2	2.36	0.42
1:C:630:GLY:H	1:C:724:HIS:CB	2.33	0.42
1:D:647:MET:HE2	1:D:647:MET:N	2.34	0.42
1:A:49:PHE:HD1	1:A:234:VAL:HG11	1.80	0.42
1:A:117:PRO:O	1:A:121:VAL:HG12	2.19	0.42
1:B:165:LEU:HG	1:B:167:ILE:HD11	2.00	0.42
1:B:386:TYR:CB	1:B:665:TYR:HB2	2.49	0.42
1:B:444:ALA:HB2	1:B:508:PHE:HB2	2.00	0.42
1:B:481:ARG:HA	1:B:484:THR:OG1	2.19	0.42
1:B:632:GLU:H	1:B:632:GLU:CD	2.28	0.42
1:C:219:ASP:CG	1:C:220:PRO:HD2	2.44	0.42
1:C:230:VAL:O	1:C:234:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:GLY:N	1:C:447:MET:HE2	2.34	0.42
1:C:666:LEU:HD13	1:C:684:LEU:HD12	2.01	0.42
1:D:25:VAL:HG11	1:D:97:MET:CE	2.36	0.42
1:D:160:ILE:HG21	1:D:527:ILE:HD12	2.01	0.42
1:D:194:GLY:C	1:D:235:GLY:HA3	2.44	0.42
1:D:263:PHE:CE1	1:D:280:LYS:HG2	2.54	0.42
1:D:570:ALA:O	1:D:574:VAL:HG23	2.20	0.42
1:D:712:VAL:O	1:D:715:ILE:HG12	2.19	0.42
1:A:163:ASN:OD1	1:A:167:ILE:HB	2.20	0.42
1:A:227:ALA:HB2	1:A:600:ILE:HD13	2.02	0.42
1:A:414:MET:HG2	1:A:651:LEU:HD11	2.00	0.42
1:A:543:ARG:HH11	1:A:629:LEU:HB3	1.84	0.42
1:B:543:ARG:HH22	1:B:726:PHE:CB	2.32	0.42
1:C:23:ALA:HA	1:C:26:VAL:HG12	2.00	0.42
1:C:361:SER:N	1:C:362:PRO:HD2	2.34	0.42
1:C:401:GLY:O	1:C:405:VAL:HG23	2.19	0.42
1:C:550:LEU:O	1:C:554:ILE:HG13	2.19	0.42
1:D:8:PHE:CD2	1:D:146:LEU:HD21	2.55	0.42
1:A:112:THR:HG21	1:A:117:PRO:HG2	2.01	0.42
1:A:232:ASP:O	1:A:236:ASP:HB2	2.20	0.42
1:A:248:PHE:CZ	1:A:294:ALA:HB1	2.54	0.42
1:A:361:SER:N	1:A:362:PRO:HD2	2.35	0.42
1:D:262:MET:SD	1:D:353:LEU:HD22	2.60	0.42
1:D:705:LEU:HA	1:D:708:ILE:HG22	2.01	0.42
1:D:707:LYS:O	1:D:711:VAL:HG23	2.20	0.42
1:A:86:MET:HE3	1:A:136:PHE:HB3	2.02	0.42
1:B:31:GLY:CA	1:B:107:GLU:HG3	2.41	0.42
1:B:361:SER:N	1:B:362:PRO:HD2	2.35	0.42
1:B:368:ILE:O	1:B:369:GLY:C	2.63	0.42
1:B:386:TYR:HB2	1:B:665:TYR:HB2	2.02	0.42
1:C:35:MET:HE2	1:C:476:LEU:HD21	1.96	0.42
1:C:141:LEU:CD2	1:C:252:ILE:HG21	2.50	0.42
1:C:555:THR:HG23	1:C:702:LEU:HD22	2.02	0.42
1:D:559:SER:HB3	1:D:698:VAL:CG1	2.49	0.42
1:A:253:VAL:O	1:A:257:ILE:HG13	2.20	0.42
1:A:258:LEU:O	1:A:262:MET:HG3	2.20	0.42
1:A:717:VAL:HG23	1:A:720:PHE:CE1	2.55	0.42
1:B:148:PHE:O	1:B:154:GLN:HB2	2.18	0.42
1:B:368:ILE:HG21	1:B:427:GLY:HA2	2.01	0.42
1:B:412:LEU:HD23	1:B:412:LEU:C	2.45	0.42
1:B:656:GLY:HA3	1:B:695:LYS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:GLU:HG3	1:C:611:MET:CE	2.50	0.42
1:C:666:LEU:CD1	1:C:684:LEU:HD12	2.50	0.42
1:C:684:LEU:HD23	1:C:684:LEU:HA	1.89	0.42
1:D:201:ALA:HB2	1:D:603:THR:HG21	2.02	0.42
1:A:725:LEU:HD22	1:A:726:PHE:CZ	2.55	0.41
1:B:219:ASP:CG	1:B:220:PRO:HD2	2.45	0.41
1:C:105:VAL:CG2	1:C:121:VAL:HG22	2.49	0.41
1:C:174:MET:SD	1:C:715:ILE:HG23	2.60	0.41
1:C:365:SER:O	1:C:368:ILE:HB	2.19	0.41
1:C:370:ILE:HG12	1:C:446:GLY:O	2.20	0.41
1:C:666:LEU:HD23	1:C:666:LEU:C	2.44	0.41
1:D:35:MET:HE2	1:D:476:LEU:HD11	2.01	0.41
1:D:130:GLY:HA2	1:D:455:VAL:HB	2.02	0.41
1:D:417:VAL:HA	1:D:650:ILE:HG21	2.02	0.41
1:D:666:LEU:HD23	1:D:666:LEU:C	2.44	0.41
1:A:53:GLU:HG2	1:A:611:MET:HE1	1.99	0.41
1:A:256:ILE:HG23	1:A:287:ILE:HG23	2.01	0.41
1:A:311:LYS:HG2	1:A:312:LYS:N	2.35	0.41
1:A:552:ALA:HB1	1:B:647:MET:HG3	2.02	0.41
1:B:74:TRP:CH2	1:B:152:MET:HE1	2.40	0.41
1:B:230:VAL:O	1:B:234:VAL:HG23	2.19	0.41
1:C:25:VAL:CG2	1:C:97:MET:HE1	2.50	0.41
1:C:90:ALA:HB1	1:C:133:VAL:HG22	2.01	0.41
1:C:282:THR:OG1	1:C:347:LEU:O	2.38	0.41
1:C:355:PHE:HB3	1:C:361:SER:HB2	2.02	0.41
1:C:643:LEU:CD1	1:D:643:LEU:HD12	2.48	0.41
1:D:219:ASP:CG	1:D:220:PRO:HD2	2.44	0.41
1:D:563:ILE:HD11	1:D:694:LEU:HD23	2.01	0.41
1:B:207:LEU:O	1:B:211:THR:HB	2.20	0.41
1:B:441:ALA:HB2	1:B:512:SER:OG	2.20	0.41
1:B:647:MET:HE2	1:B:647:MET:HA	2.02	0.41
1:C:107:GLU:O	1:C:111:THR:HG23	2.20	0.41
1:C:447:MET:HE1	1:C:508:PHE:HE2	1.85	0.41
1:C:630:GLY:H	1:C:724:HIS:HB3	1.83	0.41
1:D:573:MET:O	1:D:577:ILE:HG13	2.19	0.41
1:A:421:THR:CG2	1:B:553:ALA:HB2	2.45	0.41
1:B:9:LEU:O	1:B:13:VAL:HG23	2.20	0.41
1:B:54:THR:HG22	1:B:58:PHE:CD2	2.55	0.41
1:B:361:SER:HB3	1:B:435:ALA:HB2	2.01	0.41
1:C:686:ILE:O	1:C:690:VAL:HG23	2.20	0.41
1:D:188:MET:CA	1:D:704:ILE:HG21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:ALA:HB2	1:D:224:ALA:CB	2.50	0.41
1:A:199:LYS:HD2	1:A:692:ASP:O	2.21	0.41
1:A:293:PHE:CZ	1:A:366:ALA:HB1	2.56	0.41
1:B:50:LEU:HD22	1:B:95:MET:SD	2.60	0.41
1:A:399:ILE:HD12	1:A:674:TYR:CD2	2.56	0.41
1:B:244:LEU:HD23	1:B:455:VAL:CG2	2.31	0.41
1:B:419:PRO:CD	1:B:420:PRO:HD2	2.50	0.41
1:B:663:LYS:O	1:B:667:GLU:HG3	2.21	0.41
1:B:715:ILE:C	1:B:715:ILE:HD12	2.45	0.41
1:C:168:ASN:H	1:C:718:SER:HB3	1.85	0.41
1:D:527:ILE:O	1:D:527:ILE:HG23	2.19	0.41
1:D:580:GLN:OE1	1:D:595:ASP:HB3	2.20	0.41
1:D:632:GLU:H	1:D:632:GLU:CD	2.29	0.41
1:A:285:ALA:O	1:A:343:TYR:HE2	2.03	0.41
1:A:287:ILE:O	1:A:290:PRO:HD2	2.21	0.41
1:A:483:ILE:O	1:A:487:LEU:HG	2.21	0.41
1:A:557:TYR:CD1	1:B:415:LYS:HA	2.55	0.41
1:B:30:GLU:HG3	1:B:36:LYS:HE3	2.02	0.41
1:C:474:CYS:HB2	1:C:476:LEU:HD11	2.01	0.41
1:D:30:GLU:C	1:D:107:GLU:HG3	2.46	0.41
1:D:39:SER:HA	1:D:42:ILE:CD1	2.48	0.41
1:D:95:MET:O	1:D:99:THR:HG23	2.21	0.41
1:D:350:LEU:HD12	1:D:350:LEU:N	2.36	0.41
1:A:289:TYR:N	1:A:290:PRO:HD2	2.36	0.41
1:A:527:ILE:O	1:A:527:ILE:HG23	2.19	0.41
1:A:564:SER:HB2	1:B:411:SER:OG	2.21	0.41
1:B:298:LEU:HD23	1:B:298:LEU:C	2.46	0.41
1:C:187:ALA:HA	1:C:242:ALA:HB1	2.03	0.41
1:C:240:LEU:HD21	1:C:458:ASP:CG	2.46	0.41
1:D:205:ALA:HB2	1:D:224:ALA:HB3	2.01	0.41
1:D:245:LEU:HD23	1:D:245:LEU:C	2.46	0.41
1:D:386:TYR:HA	1:D:391:THR:HB	2.02	0.41
1:A:120:LYS:HE3	1:A:120:LYS:HB3	1.87	0.41
1:A:129:MET:HE1	1:A:237:VAL:O	2.20	0.41
1:A:306:LEU:O	1:A:309:ILE:HG13	2.20	0.41
1:A:406:ILE:HG21	1:B:690:VAL:HG11	2.02	0.41
1:A:641:THR:HG22	1:A:706:ILE:HG12	2.01	0.41
1:B:8:PHE:CD2	1:B:9:LEU:HD12	2.56	0.41
1:B:130:GLY:HA2	1:B:455:VAL:CG1	2.50	0.41
1:B:506:ALA:HB2	1:B:707:LYS:NZ	2.36	0.41
1:B:674:TYR:CD2	1:B:680:PRO:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:MET:HE2	1:C:203:MET:HB3	1.98	0.41
1:C:399:ILE:HD12	1:C:674:TYR:CE1	2.56	0.41
1:D:11:PRO:HD3	1:D:295:LEU:HD22	2.03	0.41
1:D:448:LEU:O	1:D:451:VAL:HB	2.20	0.41
1:D:587:LEU:O	1:D:587:LEU:HD23	2.21	0.41
1:D:647:MET:HE2	1:D:647:MET:CA	2.51	0.41
1:A:412:LEU:HD23	1:A:412:LEU:C	2.46	0.41
1:B:149:GLY:HA2	1:B:155:VAL:HG23	2.02	0.41
1:B:170:VAL:HB	1:B:173:ALA:HB3	2.03	0.41
1:B:205:ALA:HB2	1:B:224:ALA:HB3	2.03	0.41
1:B:208:VAL:CG2	1:B:574:VAL:HG13	2.50	0.41
1:B:627:PHE:HE1	1:B:719:ILE:CG2	2.32	0.41
1:B:698:VAL:O	1:B:702:LEU:HG	2.21	0.41
1:C:245:LEU:HD23	1:C:245:LEU:C	2.45	0.41
1:C:253:VAL:O	1:C:257:ILE:HG13	2.21	0.41
1:C:643:LEU:HD12	1:D:643:LEU:CD1	2.49	0.41
1:C:708:ILE:CG2	1:C:709:MET:N	2.84	0.41
1:D:337:ALA:HB2	1:D:363:TRP:CE2	2.56	0.41
1:D:376:ILE:HD11	1:D:424:LEU:CD1	2.50	0.41
1:A:356:ARG:HG3	1:A:357:PHE:CE1	2.56	0.40
1:A:368:ILE:O	1:A:369:GLY:C	2.64	0.40
1:A:471:SER:HA	1:A:476:LEU:CD1	2.47	0.40
1:A:690:VAL:HG11	1:B:406:ILE:HG21	2.03	0.40
1:B:167:ILE:HA	1:B:718:SER:HB2	2.03	0.40
1:C:5:ALA:O	1:C:9:LEU:HD13	2.20	0.40
1:C:162:THR:HA	1:C:167:ILE:O	2.21	0.40
1:C:208:VAL:HG11	1:C:577:ILE:HG22	2.02	0.40
1:A:112:THR:CB	1:A:117:PRO:HG2	2.51	0.40
1:A:663:LYS:O	1:A:667:GLU:HG3	2.20	0.40
1:B:31:GLY:HA2	1:B:107:GLU:CG	2.40	0.40
1:D:357:PHE:N	1:D:361:SER:OG	2.52	0.40
1:D:412:LEU:HD23	1:D:412:LEU:C	2.47	0.40
1:D:699:GLY:N	1:D:700:PRO:HD2	2.36	0.40
1:A:120:LYS:NZ	1:A:309:ILE:HA	2.36	0.40
1:A:185:ILE:HD13	1:A:619:ILE:CD1	2.49	0.40
1:A:369:GLY:O	1:A:370:ILE:C	2.64	0.40
1:A:717:VAL:HA	1:A:720:PHE:CE1	2.56	0.40
1:B:253:VAL:O	1:B:257:ILE:HG13	2.22	0.40
1:C:76:THR:HG22	1:C:174:MET:C	2.45	0.40
1:D:84:ALA:HB1	1:D:186:ILE:HG13	2.03	0.40
1:D:131:LEU:HD22	1:D:302:MET:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:LYS:HD2	1:D:692:ASP:O	2.22	0.40
1:D:539:MET:CE	1:D:639:ILE:HD13	2.47	0.40
1:A:53:GLU:O	1:A:57:ILE:HG13	2.21	0.40
1:A:82:LEU:HD23	1:A:144:VAL:CG2	2.51	0.40
1:A:142:VAL:O	1:A:146:LEU:HG	2.22	0.40
1:B:210:LYS:HE2	1:B:217:GLU:HB2	2.02	0.40
1:B:356:ARG:HG3	1:B:357:PHE:CD1	2.56	0.40
1:B:522:ILE:HD11	1:B:534:VAL:CG2	2.51	0.40
1:C:157:ASN:OD1	1:C:158:LEU:N	2.52	0.40
1:C:633:PHE:O	1:C:637:VAL:HG23	2.22	0.40
1:D:54:THR:HG22	1:D:58:PHE:HD2	1.86	0.40
1:D:382:TYR:HD1	1:D:388:TYR:CD2	2.39	0.40
1:D:442:ILE:HD13	1:D:442:ILE:HA	1.98	0.40
1:A:409:GLY:HA3	1:A:659:TRP:CZ2	2.57	0.40
1:B:95:MET:HE3	1:B:99:THR:CG2	2.51	0.40
1:B:192:VAL:O	1:B:196:VAL:HG23	2.21	0.40
1:B:307:TYR:CE1	1:B:311:LYS:HD3	2.57	0.40
1:B:402:THR:O	1:B:406:ILE:HG12	2.22	0.40
1:C:112:THR:CG2	1:C:117:PRO:HG2	2.52	0.40
1:C:125:GLY:HA3	1:C:463:ILE:CD1	2.52	0.40
1:C:246:GLU:OE2	1:C:707:LYS:HE2	2.22	0.40
1:C:584:ILE:HD13	1:C:584:ILE:HA	1.88	0.40
1:D:384:THR:HG21	1:D:493:THR:HA	2.04	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	723/735 (98%)	693 (96%)	30 (4%)	0	100	100
1	B	709/735 (96%)	679 (96%)	30 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	723/735 (98%)	690 (95%)	33 (5%)	0	100	100
1	D	715/735 (97%)	685 (96%)	30 (4%)	0	100	100
All	All	2870/2940 (98%)	2747 (96%)	123 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	526/575 (92%)	526 (100%)	0	100	100
1	B	519/575 (90%)	519 (100%)	0	100	100
1	C	529/575 (92%)	529 (100%)	0	100	100
1	D	518/575 (90%)	518 (100%)	0	100	100
All	All	2092/2300 (91%)	2092 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	A	268	GLN
1	A	277	GLN
1	A	318	GLN
1	A	322	ASN
1	A	466	ASN
1	A	606	ASN
1	B	229	ASN
1	B	284	GLN
1	C	154	GLN
1	C	214	ASN
1	C	268	GLN

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Mol	Chain	Res	Type
1	C	597	ASN
1	C	610	GLN
1	D	21	ASN
1	D	154	GLN
1	D	466	ASN
1	D	580	GLN
1	D	654	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 26 are monoatomic - leaving 8 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
6	GQB	A	809	-	22,26,26	2.72	9 (40%)	32,37,37	3.21	13 (40%)
7	D1D	C	807	-	8,8,8	2.34	4 (50%)	6,10,10	1.99	2 (33%)
3	2PN	B	806	5,2	8,8,8	2.68	6 (75%)	8,13,13	1.39	0
6	GQB	A	810	-	22,26,26	2.79	9 (40%)	32,37,37	2.98	14 (43%)
3	2PN	D	806	5,2	8,8,8	2.65	7 (87%)	8,13,13	1.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	2PN	A	806	5,2	8,8,8	2.66	6 (75%)	8,13,13	1.41	0
6	GQB	C	808	-	22,26,26	2.78	9 (40%)	32,37,37	3.16	13 (40%)
3	2PN	C	806	2	8,8,8	2.66	6 (75%)	8,13,13	1.39	0

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
6	GQB	A	809	-	-	5/9/25/25	0/4/4/4
7	D1D	C	807	-	-	-	0/1/1/1
3	2PN	B	806	5,2	-	2/2/6/6	-
6	GQB	A	810	-	-	1/9/25/25	0/4/4/4
3	2PN	D	806	5,2	-	2/2/6/6	-
3	2PN	A	806	5,2	-	1/2/6/6	-
6	GQB	C	808	-	-	5/9/25/25	0/4/4/4
3	2PN	C	806	2	-	0/2/6/6	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	810	GQB	C02-N12	7.36	1.46	1.33
6	C	808	GQB	C02-N12	7.22	1.45	1.33
6	A	809	GQB	C02-N12	7.01	1.45	1.33
6	C	808	GQB	C03-N11	4.32	1.44	1.38
6	A	809	GQB	C03-N11	4.27	1.44	1.38
6	A	810	GQB	C03-N11	4.19	1.44	1.38
6	A	809	GQB	C13-C14	4.16	1.60	1.51
6	C	808	GQB	C21-N20	4.06	1.46	1.38
6	A	809	GQB	C21-N20	4.01	1.46	1.38
6	A	810	GQB	C21-N20	3.97	1.46	1.38
7	C	807	D1D	C3-C2	3.87	1.58	1.52
6	C	808	GQB	C13-C14	3.87	1.60	1.51
6	A	810	GQB	C13-C14	3.76	1.59	1.51
3	B	806	2PN	P1-O1	3.57	1.51	1.46
3	C	806	2PN	P1-O1	3.56	1.51	1.46
6	A	810	GQB	C09-C10	3.56	1.45	1.39
3	A	806	2PN	P1-O1	3.54	1.51	1.46
3	D	806	2PN	P1-O1	3.50	1.51	1.46
3	D	806	2PN	P2-O4	3.50	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	806	2PN	P2-O4	3.49	1.51	1.46
3	C	806	2PN	P2-O4	3.49	1.51	1.46
3	B	806	2PN	P2-O4	3.48	1.51	1.46
6	A	809	GQB	C09-C10	3.48	1.45	1.39
6	C	808	GQB	C09-C10	3.47	1.45	1.39
7	C	807	D1D	C4-C3	3.33	1.58	1.52
6	A	809	GQB	C18-N19	3.17	1.38	1.32
6	C	808	GQB	C18-N19	3.16	1.38	1.32
6	A	810	GQB	C18-N19	3.16	1.38	1.32
6	A	810	GQB	C04-C03	3.14	1.42	1.37
6	A	810	GQB	C13-N12	3.14	1.52	1.46
6	C	808	GQB	C13-N12	3.06	1.52	1.46
7	C	807	D1D	O2-C2	-3.03	1.37	1.43
6	C	808	GQB	C04-C03	2.91	1.42	1.37
6	A	810	GQB	C03-C02	2.90	1.55	1.48
3	B	806	2PN	P1-N1	2.89	1.70	1.63
3	C	806	2PN	P1-N1	2.84	1.70	1.63
3	A	806	2PN	P1-N1	2.84	1.70	1.63
3	B	806	2PN	P2-N1	2.83	1.70	1.63
3	A	806	2PN	P2-N1	2.82	1.70	1.63
3	D	806	2PN	P2-N1	2.81	1.70	1.63
3	C	806	2PN	P2-N1	2.81	1.70	1.63
6	A	809	GQB	C13-N12	2.80	1.51	1.46
3	D	806	2PN	P1-N1	2.79	1.70	1.63
6	C	808	GQB	C03-C02	2.79	1.54	1.48
6	A	809	GQB	C04-C03	2.75	1.42	1.37
7	C	807	D1D	O3-C3	-2.63	1.37	1.43
6	A	809	GQB	C03-C02	2.53	1.54	1.48
3	B	806	2PN	P2-O6	-2.03	1.51	1.56
3	B	806	2PN	P2-O5	-2.03	1.51	1.56
3	C	806	2PN	P2-O6	-2.02	1.51	1.56
3	D	806	2PN	P1-O2	-2.02	1.51	1.56
3	D	806	2PN	P2-O5	-2.02	1.51	1.56
3	C	806	2PN	P2-O5	-2.01	1.51	1.56
3	A	806	2PN	P2-O6	-2.01	1.51	1.56
3	A	806	2PN	P2-O5	-2.01	1.51	1.56
3	D	806	2PN	P2-O6	-2.00	1.51	1.56

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	809	GQB	C03-C02-N12	11.10	132.07	116.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	808	GQB	C03-C02-N12	10.70	131.52	116.80
6	A	810	GQB	C03-C02-N12	8.10	127.94	116.80
6	C	808	GQB	N19-C18-N20	6.37	128.14	116.50
6	A	809	GQB	N19-C18-N20	6.36	128.12	116.50
6	A	810	GQB	N19-C18-N20	6.20	127.83	116.50
6	A	809	GQB	O01-C02-C03	-5.64	113.83	121.09
6	A	810	GQB	C13-N12-C02	5.34	129.70	122.07
6	C	808	GQB	O01-C02-C03	-5.24	114.34	121.09
6	A	809	GQB	O01-C02-N12	-5.13	114.09	123.35
6	C	808	GQB	O01-C02-N12	-5.10	114.14	123.35
6	A	809	GQB	C16-C21-N20	5.01	117.93	112.14
6	A	810	GQB	C16-C21-N20	4.72	117.60	112.14
6	C	808	GQB	C16-C21-N20	4.68	117.55	112.14
6	A	810	GQB	C04-C03-N11	-4.60	104.59	109.15
6	C	808	GQB	C04-C03-N11	-4.38	104.80	109.15
6	A	810	GQB	O01-C02-N12	-4.19	115.79	123.35
6	A	809	GQB	C04-C03-N11	-3.97	105.21	109.15
6	A	810	GQB	C14-C13-N12	3.86	121.21	113.07
6	A	810	GQB	O01-C02-C03	-3.74	116.27	121.09
6	A	809	GQB	C22-C21-C16	-3.37	116.31	120.51
7	C	807	D1D	O3-C3-C2	-3.35	102.84	110.20
6	C	808	GQB	C22-C21-C16	-3.21	116.52	120.51
6	A	810	GQB	C09-C10-C05	-3.11	119.31	122.13
6	A	810	GQB	C22-C21-C16	-3.10	116.66	120.51
6	C	808	GQB	C09-C10-C05	-2.84	119.56	122.13
6	A	810	GQB	C10-N11-C03	2.81	112.03	109.01
7	C	807	D1D	O2-C2-C1	-2.79	105.12	109.81
6	A	809	GQB	C13-C14-C15	2.75	126.50	120.63
6	A	809	GQB	C10-N11-C03	2.73	111.95	109.01
6	C	808	GQB	C10-N11-C03	2.59	111.79	109.01
6	A	810	GQB	C02-C03-N11	2.58	128.27	120.04
6	C	808	GQB	C02-C03-N11	2.55	128.20	120.04
6	A	810	GQB	C22-C21-N20	-2.51	125.74	130.83
6	A	809	GQB	C22-C21-N20	-2.51	125.76	130.83
6	C	808	GQB	C22-C21-N20	-2.42	125.93	130.83
6	A	809	GQB	C15-C16-C21	2.39	123.27	121.18
6	A	809	GQB	C09-C10-C05	-2.35	120.00	122.13
6	C	808	GQB	C13-N12-C02	2.35	125.42	122.07
6	C	808	GQB	C15-C16-C21	2.33	123.22	121.18
6	A	810	GQB	C15-C16-C21	2.27	123.17	121.18
6	A	809	GQB	C22-C23-C14	2.11	123.77	121.00

There are no chirality outliers.

All (16) torsion outliers are listed below:

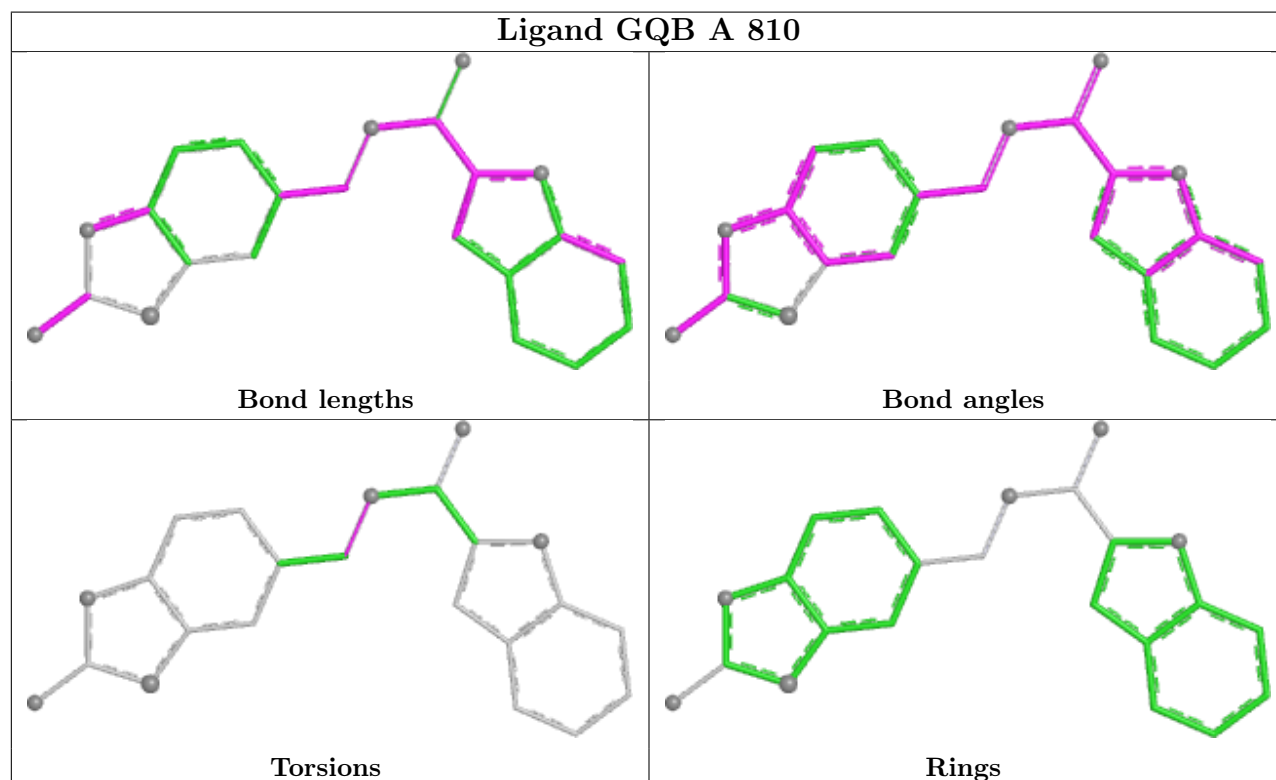
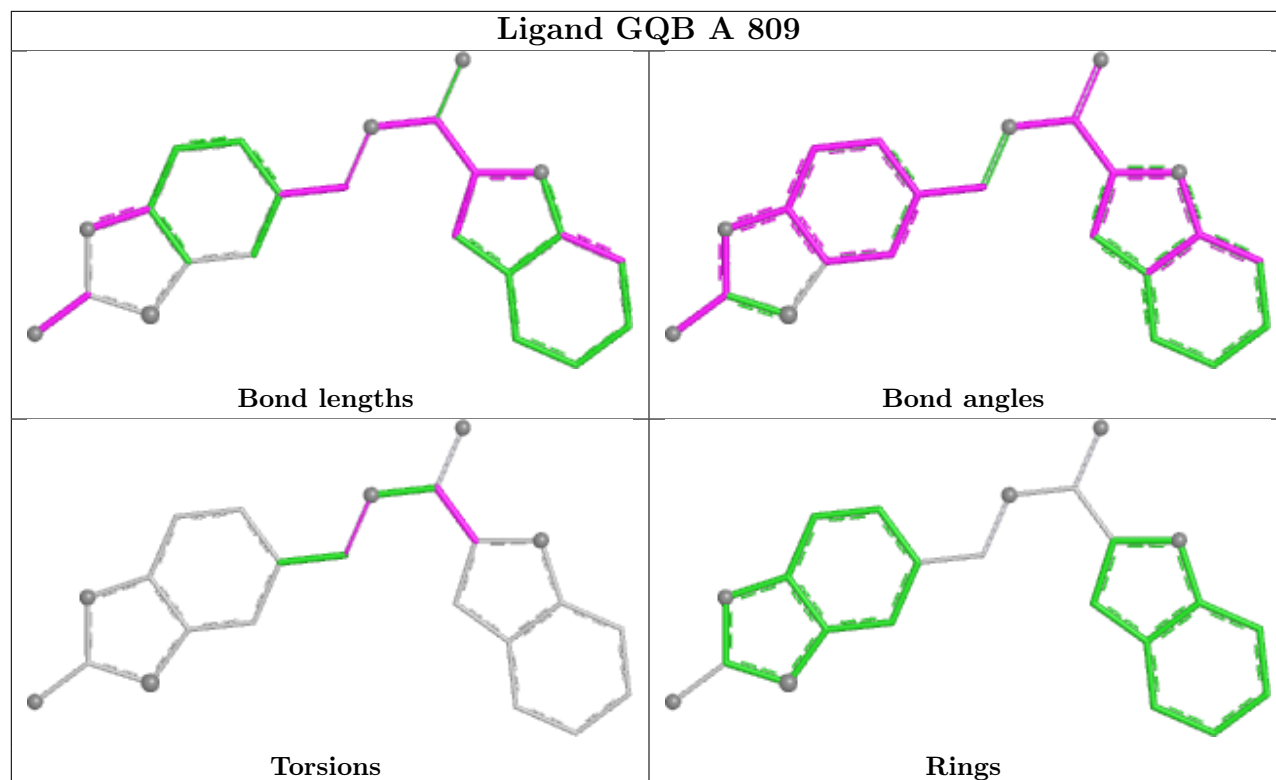
Mol	Chain	Res	Type	Atoms
3	B	806	2PN	P2-N1-P1-O1
3	B	806	2PN	P1-N1-P2-O4
3	D	806	2PN	P2-N1-P1-O1
3	D	806	2PN	P1-N1-P2-O4
6	A	809	GQB	N12-C02-C03-C04
6	A	809	GQB	N12-C02-C03-N11
6	A	809	GQB	O01-C02-C03-C04
6	A	809	GQB	O01-C02-C03-N11
6	A	809	GQB	C14-C13-N12-C02
6	A	810	GQB	C14-C13-N12-C02
6	C	808	GQB	N12-C02-C03-C04
6	C	808	GQB	N12-C02-C03-N11
6	C	808	GQB	O01-C02-C03-C04
6	C	808	GQB	O01-C02-C03-N11
6	C	808	GQB	C14-C13-N12-C02
3	A	806	2PN	P2-N1-P1-O1

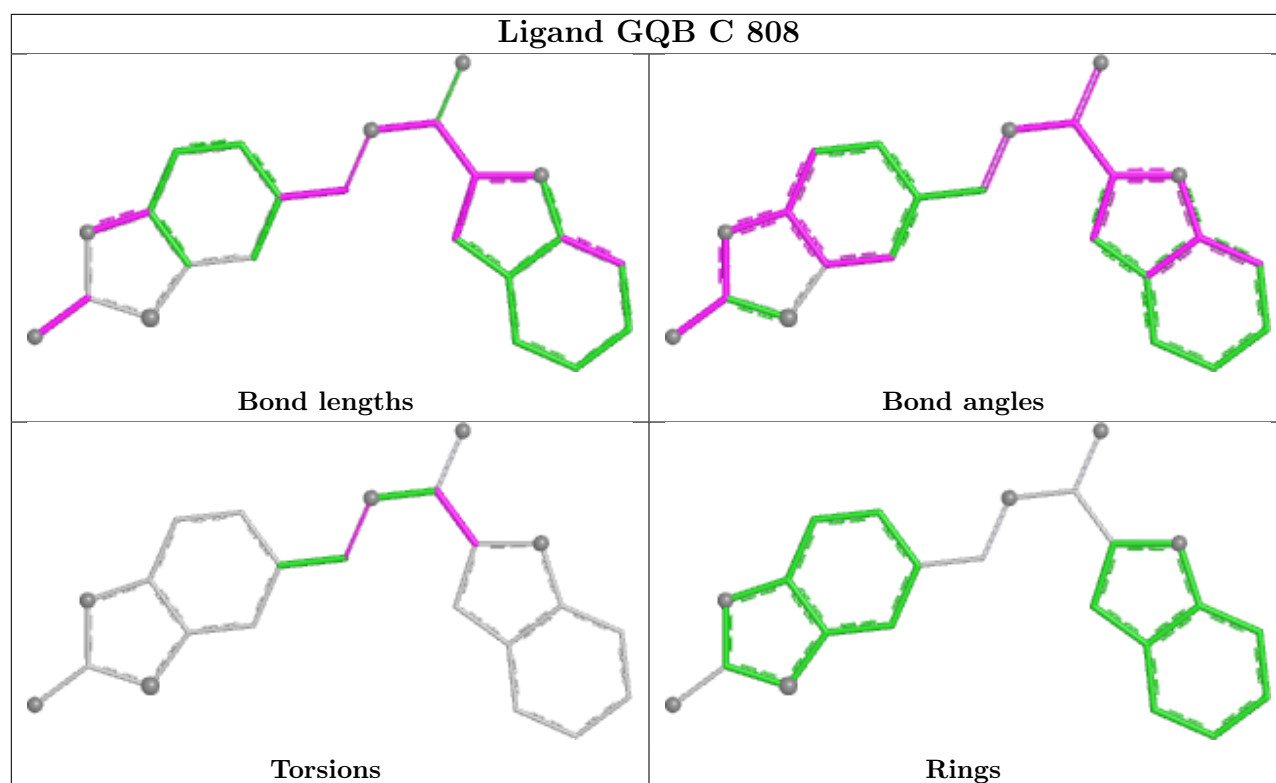
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	809	GQB	2	0
7	C	807	D1D	1	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	725/735 (98%)	0.32	31 (4%)	40	29	52, 79, 106, 148	0
1	B	715/735 (97%)	0.41	56 (7%)	19	16	56, 91, 127, 152	0
1	C	725/735 (98%)	0.38	40 (5%)	30	23	54, 81, 108, 135	0
1	D	719/735 (97%)	0.34	45 (6%)	26	20	53, 87, 111, 147	0
All	All	2884/2940 (98%)	0.36	172 (5%)	27	21	52, 85, 112, 152	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	272	GLU	5.9
1	C	701	SER	5.9
1	D	118	ALA	5.4
1	D	458	ASP	5.3
1	C	535	LEU	5.3
1	B	458	ASP	5.1
1	B	500	GLY	5.1
1	B	33	GLU	4.9
1	C	532	SER	4.8
1	D	498	GLY	4.7
1	D	119	LEU	4.6
1	B	490	VAL	4.5
1	C	605	ASP	4.2
1	C	254	SER	4.1
1	C	437	LEU	4.1
1	B	497	ILE	4.1
1	C	353	LEU	4.0
1	D	8	PHE	4.0
1	D	109	ALA	4.0
1	C	531	PRO	4.0
1	A	458	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	657	GLY	3.9
1	D	460	TYR	3.8
1	C	256	ILE	3.8
1	B	536	LEU	3.8
1	C	381	GLU	3.8
1	D	672	GLU	3.7
1	D	122	ALA	3.7
1	B	526	ASP	3.7
1	A	355	PHE	3.7
1	A	674	TYR	3.6
1	C	258	LEU	3.6
1	A	605	ASP	3.4
1	C	8	PHE	3.4
1	D	539	MET	3.4
1	A	723	VAL	3.4
1	B	245	LEU	3.4
1	C	4	ALA	3.4
1	D	491	GLY	3.3
1	B	575	ASP	3.3
1	B	89	SER	3.2
1	B	616	PHE	3.2
1	D	494	THR	3.2
1	D	497	ILE	3.2
1	B	588	LEU	3.1
1	A	590	GLY	3.1
1	D	317	PRO	3.1
1	A	668	ALA	3.1
1	C	325	LEU	3.1
1	B	249	VAL	3.1
1	A	259	ALA	3.1
1	B	141	LEU	3.1
1	B	658	ALA	3.0
1	B	253	VAL	3.0
1	C	494	THR	3.0
1	D	341	TYR	3.0
1	B	263	PHE	3.0
1	B	198	THR	3.0
1	B	578	ARG	2.9
1	B	502	ALA	2.9
1	D	173	ALA	2.9
1	B	234	VAL	2.9
1	C	262	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	353	LEU	2.9
1	A	613	TYR	2.9
1	D	7	PHE	2.9
1	A	207	LEU	2.9
1	C	318	GLN	2.8
1	B	180	ALA	2.8
1	C	536	LEU	2.8
1	D	253	VAL	2.8
1	B	522	ILE	2.8
1	B	475	GLU	2.8
1	C	282	THR	2.8
1	B	119	LEU	2.8
1	B	244	LEU	2.8
1	B	200	ALA	2.8
1	A	431	ALA	2.8
1	B	177	SER	2.8
1	A	351	ASP	2.7
1	B	496	ALA	2.7
1	C	278	VAL	2.7
1	C	659	TRP	2.7
1	D	234	VAL	2.7
1	D	540	LEU	2.7
1	B	152	MET	2.6
1	B	498	GLY	2.6
1	C	564	SER	2.6
1	C	490	VAL	2.6
1	D	542	ALA	2.6
1	C	514	PHE	2.6
1	A	475	GLU	2.6
1	B	164	TRP	2.6
1	B	474	CYS	2.6
1	A	676	LYS	2.6
1	B	494	THR	2.6
1	C	539	MET	2.5
1	A	722	HIS	2.5
1	D	260	SER	2.5
1	B	694	LEU	2.5
1	D	141	LEU	2.5
1	D	176	VAL	2.5
1	A	260	SER	2.5
1	B	525	SER	2.5
1	D	249	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	73	THR	2.5
1	C	49	PHE	2.5
1	D	117	PRO	2.5
1	D	295	LEU	2.5
1	D	536	LEU	2.5
1	B	580	GLN	2.5
1	D	487	LEU	2.5
1	C	388	TYR	2.5
1	B	581	ALA	2.4
1	C	670	ASN	2.4
1	D	553	ALA	2.4
1	A	666	LEU	2.4
1	C	165	LEU	2.4
1	C	424	LEU	2.4
1	B	654	ASN	2.4
1	A	435	ALA	2.4
1	D	12	LEU	2.4
1	D	53	GLU	2.4
1	B	227	ALA	2.3
1	A	539	MET	2.3
1	B	8	PHE	2.3
1	D	58	PHE	2.3
1	A	667	GLU	2.3
1	B	359	ALA	2.3
1	D	158	LEU	2.3
1	C	266	TYR	2.3
1	B	538	ASN	2.3
1	D	495	ALA	2.3
1	B	477	ASP	2.3
1	B	495	ALA	2.2
1	B	501	PHE	2.2
1	C	519	PHE	2.2
1	A	350	LEU	2.2
1	D	292	PHE	2.2
1	A	253	VAL	2.2
1	A	262	MET	2.2
1	A	476	LEU	2.2
1	B	537	LEU	2.2
1	C	323	ILE	2.2
1	C	715	ILE	2.2
1	D	256	ILE	2.2
1	C	351	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	315	ASP	2.2
1	B	652	THR	2.2
1	B	384	THR	2.1
1	C	533	LEU	2.1
1	D	552	ALA	2.1
1	C	349	GLY	2.1
1	B	2	TYR	2.1
1	C	286	LEU	2.1
1	A	719	ILE	2.1
1	B	613	TYR	2.1
1	A	669	GLY	2.1
1	C	491	GLY	2.1
1	A	608	LEU	2.1
1	D	435	ALA	2.1
1	D	644	SER	2.0
1	C	410	LEU	2.0
1	D	486	HIS	2.0
1	B	315	ASP	2.0
1	B	504	GLY	2.0
1	D	80	PHE	2.0
1	B	523	SER	2.0
1	D	252	ILE	2.0
1	A	386	TYR	2.0
1	B	206	ASP	2.0
1	D	42	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

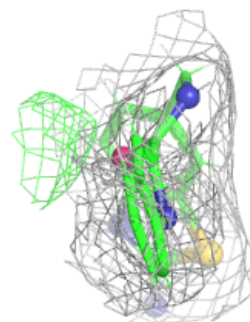
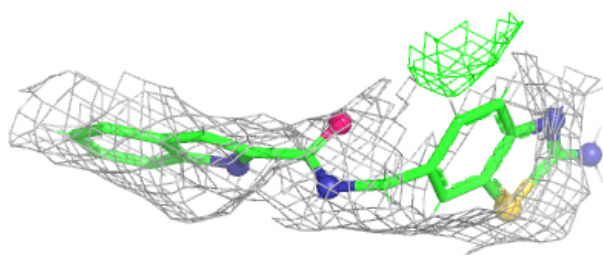
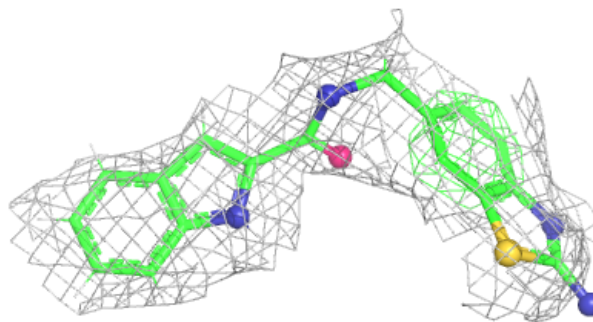
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GQB	C	808	23/23	0.54	0.15	112,138,182,185	0
6	GQB	A	810	23/23	0.75	0.13	92,110,132,136	0
2	MG	D	803	1/1	0.75	0.21	97,97,97,97	0
4	NA	D	807	1/1	0.77	0.15	74,74,74,74	0
5	K	A	808	1/1	0.78	0.15	110,110,110,110	0
5	K	D	808	1/1	0.80	0.11	92,92,92,92	0
6	GQB	A	809	23/23	0.80	0.10	68,104,127,139	0
7	D1D	C	807	8/8	0.81	0.13	90,116,135,135	0
5	K	B	808	1/1	0.82	0.17	106,106,106,106	0
2	MG	A	801	1/1	0.84	0.15	68,68,68,68	0
2	MG	B	804	1/1	0.85	0.22	85,85,85,85	0
2	MG	B	802	1/1	0.85	0.28	71,71,71,71	0
3	2PN	A	806	9/9	0.85	0.11	81,89,100,101	0
3	2PN	B	806	9/9	0.85	0.20	86,101,108,119	0
2	MG	A	804	1/1	0.86	0.16	79,79,79,79	0
2	MG	D	802	1/1	0.87	0.20	87,87,87,87	0
2	MG	D	804	1/1	0.87	0.21	81,81,81,81	0
3	2PN	D	806	9/9	0.88	0.14	90,93,98,102	0
2	MG	D	801	1/1	0.89	0.17	93,93,93,93	0
4	NA	A	807	1/1	0.89	0.09	70,70,70,70	0
2	MG	A	802	1/1	0.89	0.18	78,78,78,78	0
2	MG	A	805	1/1	0.89	0.09	71,71,71,71	0
3	2PN	C	806	9/9	0.89	0.14	77,80,92,94	0
2	MG	C	805	1/1	0.92	0.09	73,73,73,73	0
2	MG	C	802	1/1	0.93	0.17	72,72,72,72	0
2	MG	C	804	1/1	0.93	0.21	69,69,69,69	0
2	MG	A	803	1/1	0.94	0.17	64,64,64,64	0
2	MG	B	801	1/1	0.95	0.20	84,84,84,84	0
2	MG	D	805	1/1	0.95	0.08	95,95,95,95	0
2	MG	B	805	1/1	0.95	0.17	81,81,81,81	0
2	MG	C	801	1/1	0.96	0.14	65,65,65,65	0
2	MG	B	803	1/1	0.96	0.20	78,78,78,78	0
4	NA	B	807	1/1	0.98	0.05	68,68,68,68	0
2	MG	C	803	1/1	0.99	0.12	62,62,62,62	0

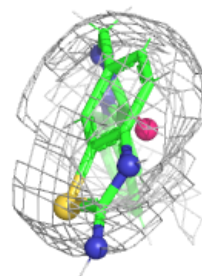
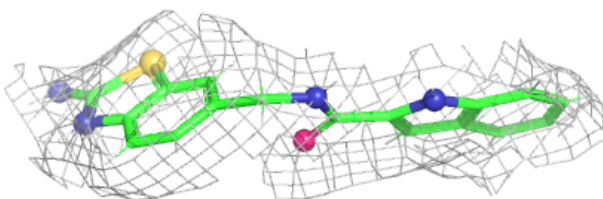
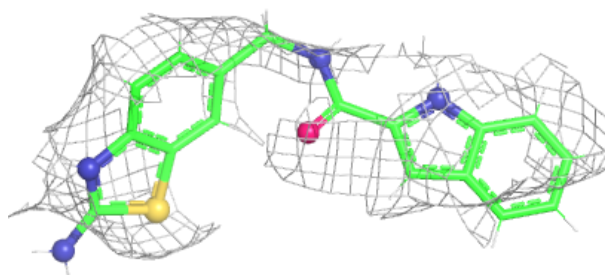
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GQB C 808:

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

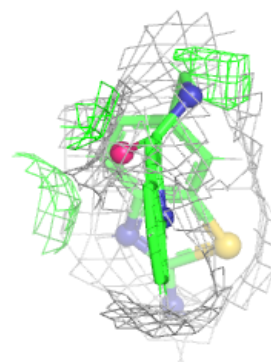
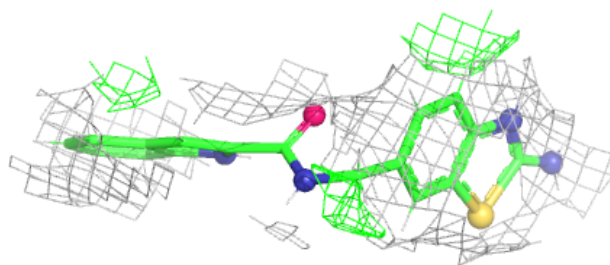
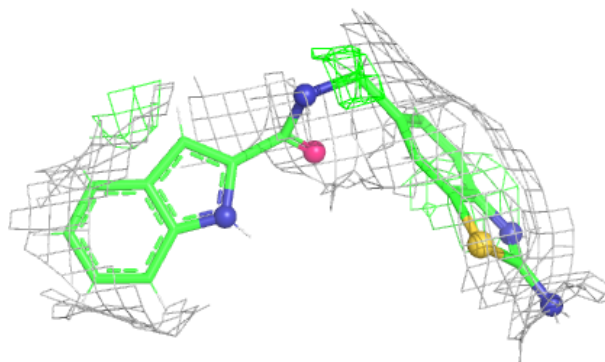
**Electron density around GQB A 810:**

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



Electron density around GQB A 809:

$2mF_o-DF_c$ (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.