



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 10:22 pm BST

PDB ID : 1XKH
Title : Pyoverdine outer membrane receptor FpvA from *Pseudomonas aeruginosa* PAO1 bound to pyoverdine
Authors : Cobessi, D.; Celia, H.; Folschweiller, N.; Schalk, I.J.; Abdallah, M.A.; Pattus, F.
Deposited on : 2004-09-29
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

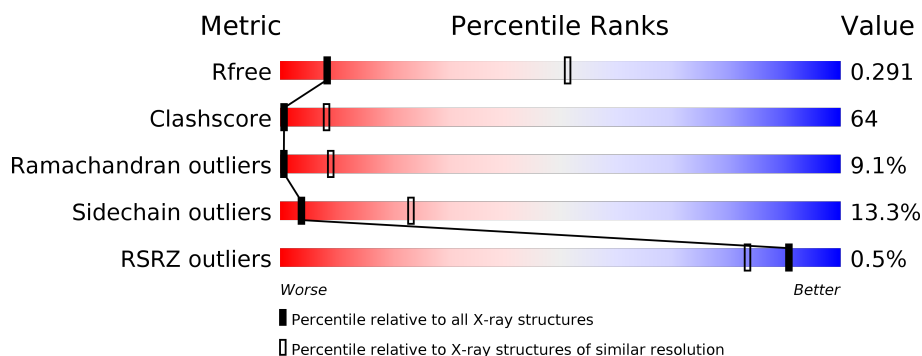
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	687	<div> <div>24%</div> <div>61%</div> <div>14%</div> <div>.</div> </div>
1	B	687	<div> <div>24%</div> <div>59%</div> <div>15%</div> <div>.</div> </div>
1	C	687	<div> <div>%</div> <div>25%</div> <div>59%</div> <div>15%</div> <div>.</div> </div>
2	I	8	<div> <div>13%</div> <div>63%</div> <div>25%</div> </div>
2	J	8	<div> <div>25%</div> <div>50%</div> <div>25%</div> </div>
2	K	8	<div> <div>25%</div> <div>50%</div> <div>25%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FHO	K	5	-	-	-	X
3	SO4	B	2002	-	-	X	-
4	PVE	I	1	X	-	-	-
4	PVE	J	1	X	-	-	-
4	PVE	K	1	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16719 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ferripyoverdine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	687	Total	C	N	O	Se	0	0	0
			5474	3449	933	1080	12			
1	B	687	Total	C	N	O	Se	0	0	0
			5474	3449	933	1080	12			
1	C	687	Total	C	N	O	Se	0	0	0
			5474	3449	933	1080	12			

- Molecule 2 is a protein called Pyoverdin C-E.

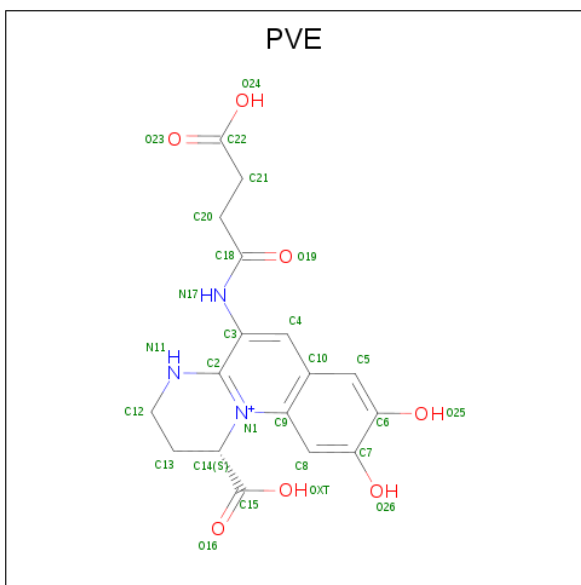
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	8	Total	C	N	O	0	0	0
			68	38	14	16			
2	J	8	Total	C	N	O	0	0	0
			68	38	14	16			
2	K	8	Total	C	N	O	0	0	0
			68	38	14	16			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is (1S)-1-CARBOXY-5-[(3-CARBOXYPROPANOYL)AMINO]-8,9-DIHYDROXY-1,2,3,4-TETRAHYDROPYRIMIDO[1,2-A]QUINOLIN-11-IUM (three-letter code: PVE) (formula: C₁₇H₁₈N₃O₇).

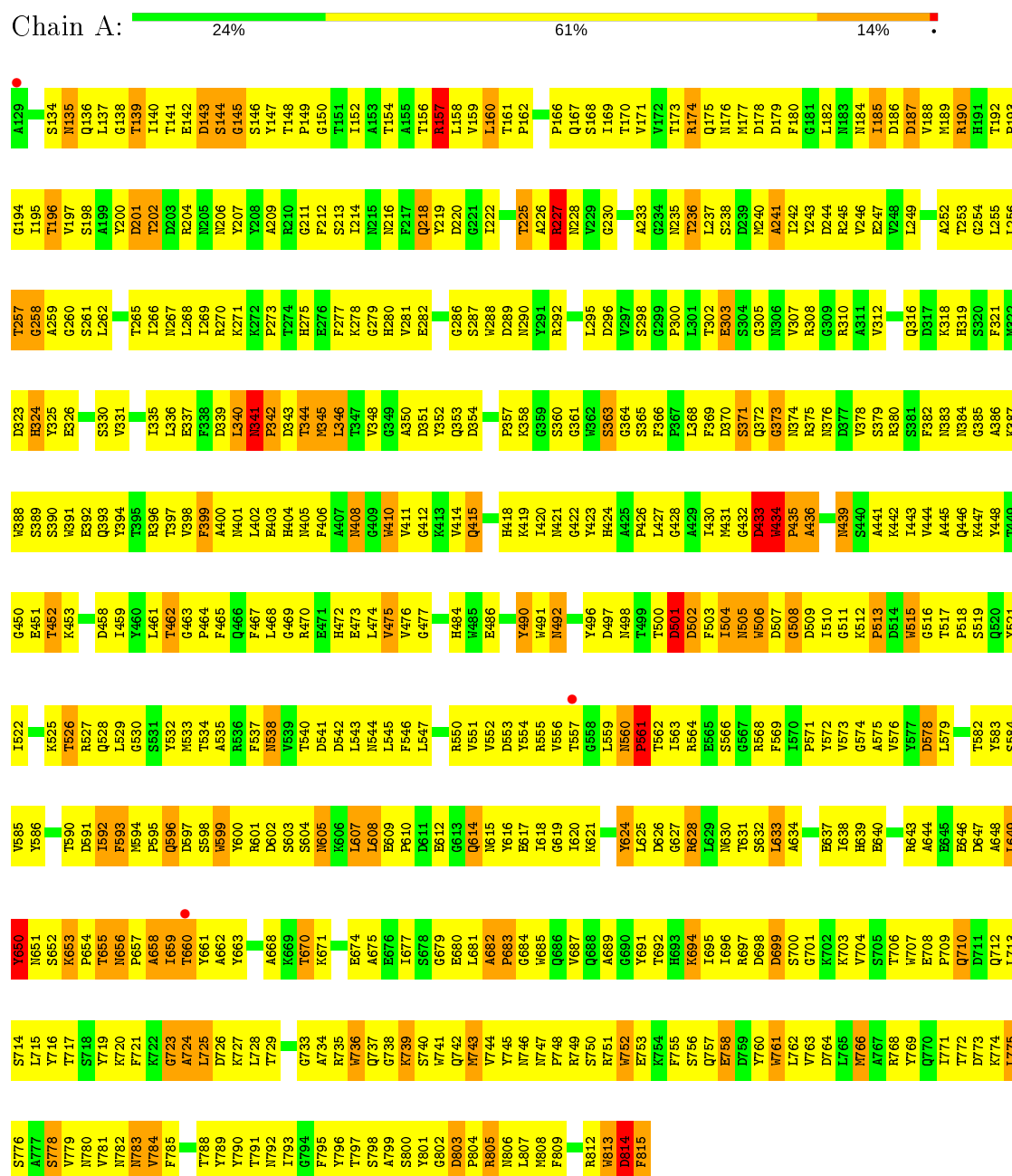


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	I	1	Total 26	C 17	N 3	O 6	0	0
4	J	1	Total 26	C 17	N 3	O 6	0	0
4	K	1	Total 26	C 17	N 3	O 6	0	0

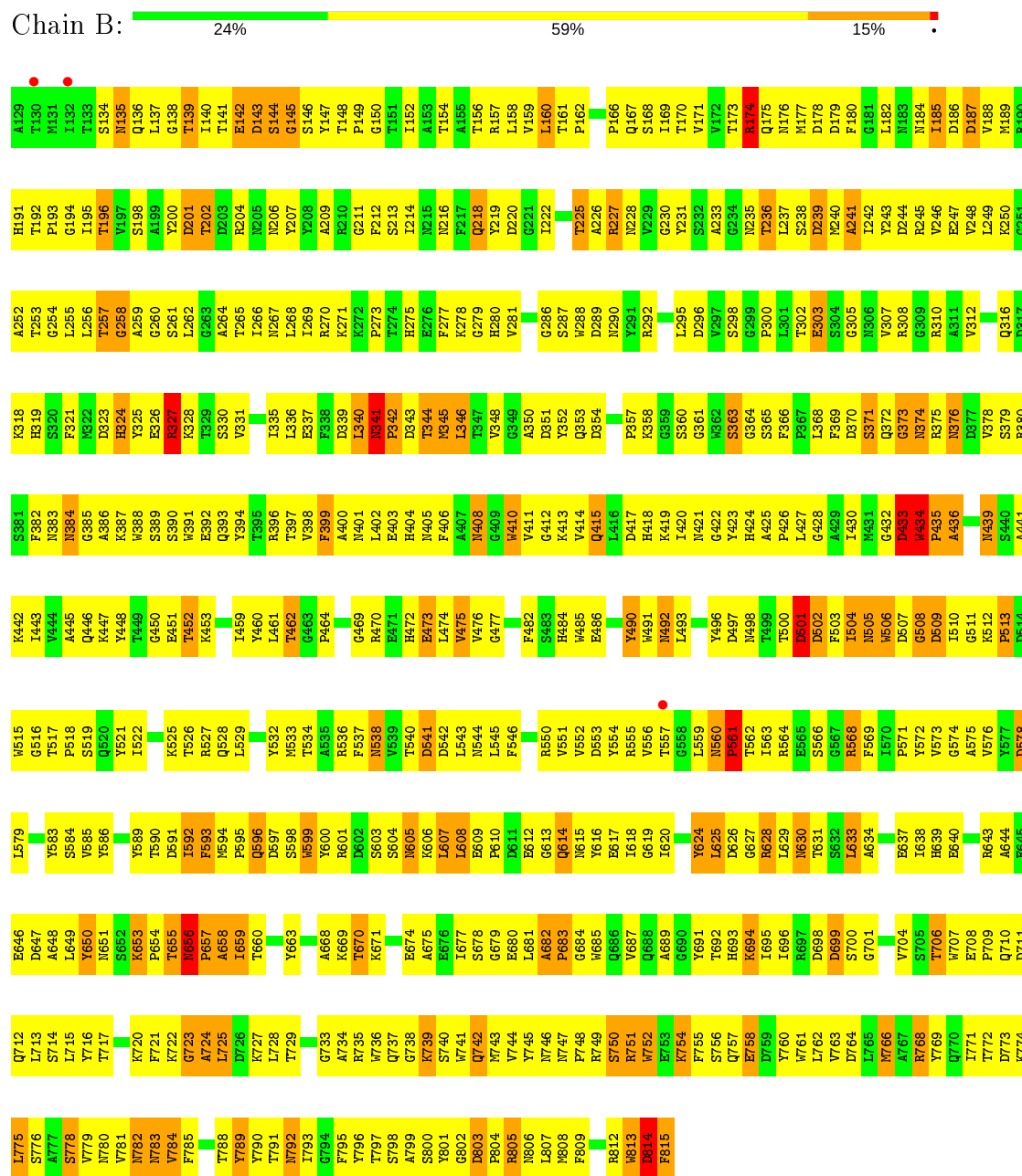
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

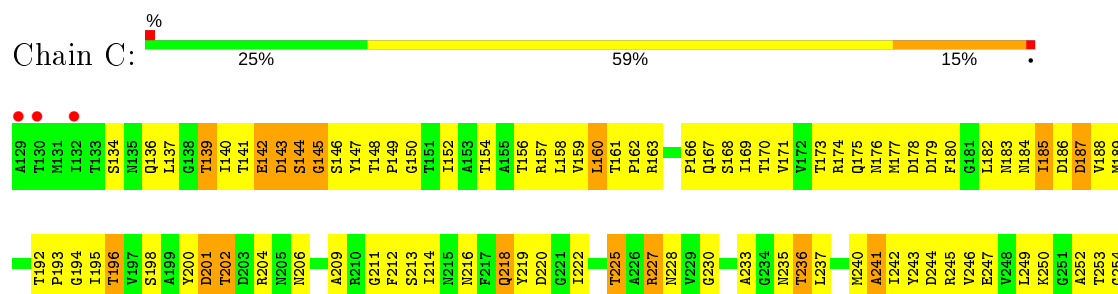
- Molecule 1: Ferripyoverdine receptor

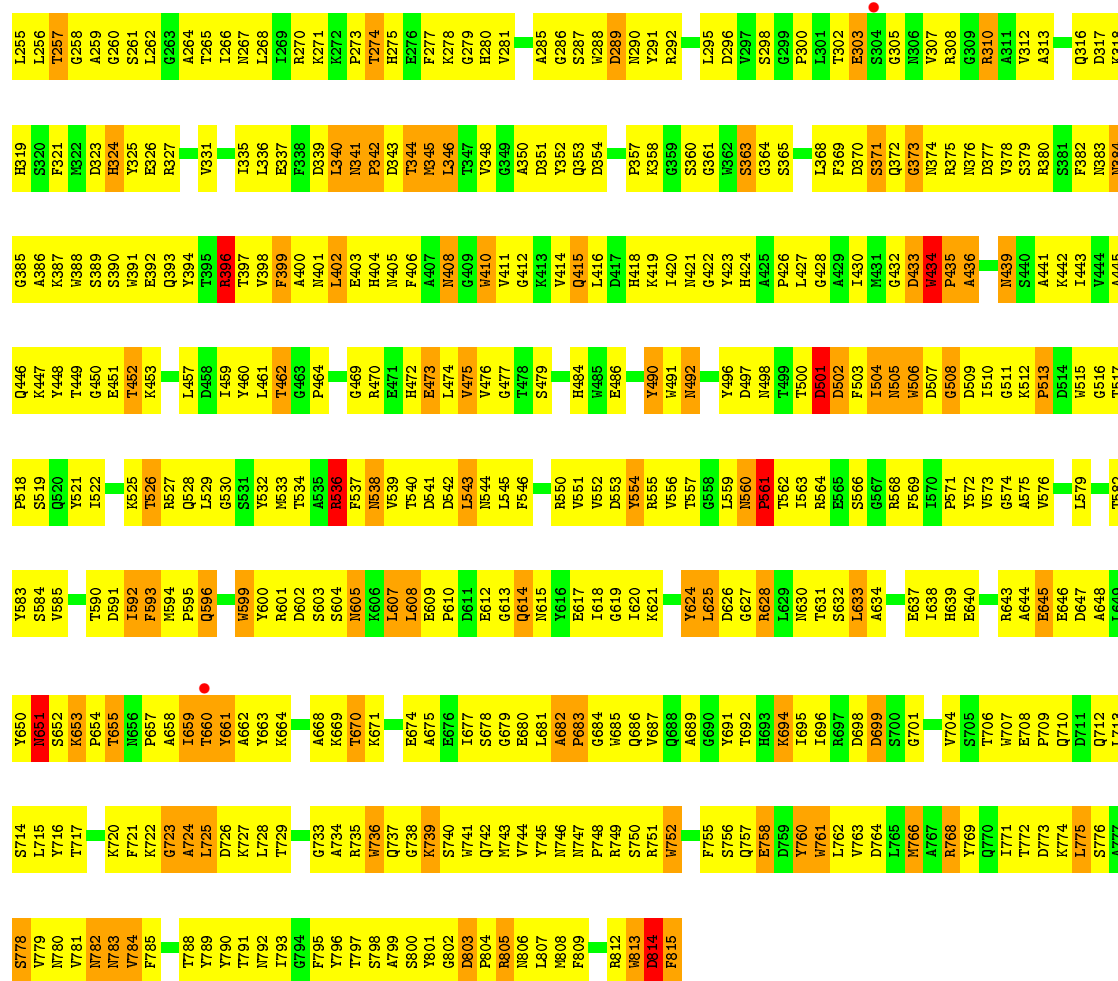


● Molecule 1: Ferripyoverdine receptor

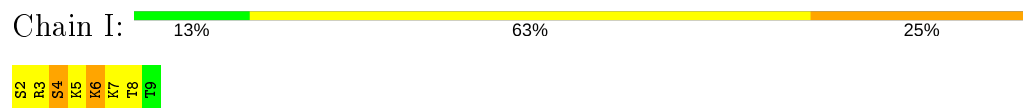


● Molecule 1: Ferripyoverdine receptor





• Molecule 2: Pyoverdin C-E



• Molecule 2: Pyoverdin C-E



• Molecule 2: Pyoverdin C-E



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.45Å 231.34Å 121.69Å 90.00° 104.57° 90.00°	Depositor
Resolution (Å)	20.00 – 3.60 19.99 – 3.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.60) 99.1 (19.99-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.62Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.259 , 0.288 0.260 , 0.291	Depositor DCC
R_{free} test set	2105 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	74.5	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	16719	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DSN, FHO, PVE, SO4

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	0.49	0/5606	0.72	3/7599 (0.0%)
1	B	0.50	0/5606	0.72	3/7599 (0.0%)
1	C	0.50	0/5606	0.74	3/7599 (0.0%)
2	I	0.67	0/31	1.07	0/36
2	J	0.76	0/31	1.03	0/36
2	K	0.71	0/31	0.95	0/36
All	All	0.50	0/16911	0.73	9/22905 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
1	C	0	4
2	I	0	5
2	J	0	5
2	K	0	4
All	All	0	25

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	434	TRP	N-CA-C	5.91	126.96	111.00
1	A	434	TRP	N-CA-C	5.79	126.63	111.00
1	C	434	TRP	N-CA-C	5.78	126.61	111.00
1	C	346	LEU	N-CA-C	-5.61	95.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	LEU	N-CA-C	-5.58	95.95	111.00
1	A	346	LEU	N-CA-C	-5.38	96.47	111.00
1	B	813	TRP	N-CA-C	5.38	125.52	111.00
1	A	813	TRP	N-CA-C	5.34	125.42	111.00
1	C	813	TRP	N-CA-C	5.33	125.40	111.00

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	ARG	Sidechain
1	A	190	ARG	Sidechain
1	A	227	ARG	Sidechain
1	B	174	ARG	Sidechain
1	B	227	ARG	Sidechain
1	B	327	ARG	Sidechain
1	B	751	ARG	Sidechain
1	C	310	ARG	Sidechain
1	C	396	ARG	Sidechain
1	C	536	ARG	Sidechain
1	C	768	ARG	Sidechain
2	I	2	DSN	Peptide
2	I	3	ARG	Sidechain,Peptide
2	I	4	DSN	Peptide
2	I	5	FHO	Peptide
2	J	2	DSN	Peptide
2	J	3	ARG	Sidechain,Peptide
2	J	4	DSN	Peptide
2	J	5	FHO	Peptide
2	K	3	ARG	Sidechain,Peptide
2	K	4	DSN	Peptide
2	K	5	FHO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5474	0	5154	673	0
1	B	5474	0	5154	708	0
1	C	5474	0	5154	691	0
2	I	68	0	65	3	0
2	J	68	0	65	2	0
2	K	68	0	65	2	0
3	A	5	0	0	0	0
3	B	5	0	0	2	0
3	C	5	0	0	0	0
4	I	26	0	13	1	0
4	J	26	0	13	3	0
4	K	26	0	13	1	0
All	All	16719	0	15696	2076	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 64.

All (2076) 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:B:768:ARG:HG3	1:B:778:SER:CB	1.61	1.31
1:A:189:MSE:CE	1:A:195:ILE:HD13	1.68	1.23
1:B:768:ARG:CG	1:B:778:SER:HB3	1.70	1.21
1:C:352:TYR:CD1	1:C:396:ARG:HG2	1.78	1.19
1:A:227:ARG:HD3	1:A:594:MSE:HE1	1.28	1.11
1:A:474:LEU:HD12	1:A:475:VAL:H	1.08	1.10
1:B:681:LEU:HD22	1:B:687:VAL:HG11	1.32	1.09
1:C:352:TYR:HD1	1:C:396:ARG:HG2	1.04	1.09
1:C:352:TYR:HD1	1:C:396:ARG:CG	1.66	1.09
1:A:189:MSE:HE1	1:A:195:ILE:HD13	1.09	1.08
1:B:227:ARG:HD3	1:B:594:MSE:HE1	1.30	1.08
1:C:554:TYR:CD2	1:C:595:PRO:HG3	1.89	1.08
1:B:371:SER:HB2	1:B:436:ALA:HA	1.34	1.05
1:C:370:ASP:HA	1:C:435:PRO:HD2	1.40	1.04
1:A:371:SER:HB2	1:A:436:ALA:HA	1.36	1.03
1:C:474:LEU:HD11	1:C:533:MSE:HG3	1.39	1.03
1:B:474:LEU:HD11	1:B:533:MSE:HG3	1.42	1.02
1:B:659:ILE:HG12	1:B:660:THR:H	1.21	1.02
1:A:681:LEU:HD22	1:A:687:VAL:HG11	1.38	1.01
1:C:227:ARG:HD3	1:C:594:MSE:HE1	1.06	1.01
1:C:371:SER:HB2	1:C:436:ALA:HA	1.39	1.01
1:A:370:ASP:HA	1:A:435:PRO:HD2	1.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:TYR:HA	1:A:173:THR:HG21	1.42	1.00
1:B:370:ASP:HA	1:B:435:PRO:HD2	1.39	1.00
1:C:768:ARG:HB2	1:C:778:SER:HB3	1.44	0.98
1:B:280:HIS:HB2	1:B:813:TRP:HB3	1.42	0.97
1:B:134:SER:HA	1:B:139:THR:HA	1.46	0.97
1:B:474:LEU:HD12	1:B:475:VAL:H	1.30	0.97
1:C:280:HIS:HB2	1:C:813:TRP:HB3	1.47	0.97
1:A:474:LEU:HD11	1:A:533:MSE:HG3	1.45	0.97
1:B:653:LYS:HD3	1:B:653:LYS:H	1.27	0.96
1:C:536:ARG:HG3	1:C:536:ARG:O	1.62	0.96
1:B:246:VAL:HG23	1:B:268:LEU:HD23	1.45	0.96
1:B:147:TYR:HA	1:B:173:THR:HG21	1.46	0.96
1:C:134:SER:HA	1:C:139:THR:HA	1.48	0.96
1:C:339:ASP:O	1:C:340:LEU:HG	1.66	0.96
1:A:189:MSE:HE1	1:A:195:ILE:CD1	1.95	0.96
1:C:147:TYR:HA	1:C:173:THR:HG21	1.46	0.96
1:C:227:ARG:CD	1:C:594:MSE:HE1	1.95	0.96
1:B:434:TRP:HB3	1:B:441:ALA:HB1	1.48	0.95
1:C:776:SER:HB2	1:C:812:ARG:HB2	1.48	0.95
1:A:182:LEU:HD22	1:A:187:ASP:O	1.66	0.95
1:A:776:SER:HB2	1:A:812:ARG:HB2	1.48	0.95
1:C:474:LEU:HD12	1:C:475:VAL:H	1.32	0.95
1:A:339:ASP:O	1:A:340:LEU:HG	1.66	0.95
1:A:782:ASN:HB2	1:A:806:ASN:HB2	1.47	0.95
1:B:659:ILE:HG12	1:B:660:THR:N	1.82	0.95
1:B:776:SER:HB2	1:B:812:ARG:HB2	1.47	0.94
1:A:280:HIS:HB2	1:A:813:TRP:HB3	1.47	0.94
1:C:771:ILE:HG13	1:C:772:THR:HG23	1.49	0.94
1:A:154:THR:HB	1:A:247:GLU:OE2	1.68	0.93
1:A:246:VAL:HG23	1:A:268:LEU:HD23	1.49	0.93
1:A:542:ASP:HA	1:A:578:ASP:OD2	1.68	0.93
1:A:695:ILE:HD11	1:A:710:GLN:NE2	1.82	0.93
1:B:518:PRO:HG2	1:B:521:TYR:OH	1.67	0.93
1:C:286:GLY:HA3	1:C:808:MSE:HG3	1.50	0.93
1:B:339:ASP:O	1:B:340:LEU:HG	1.66	0.93
1:B:771:ILE:HG13	1:B:772:THR:HG23	1.50	0.93
1:C:286:GLY:CA	1:C:808:MSE:HG3	1.99	0.93
1:A:771:ILE:HG13	1:A:772:THR:HG23	1.49	0.93
1:B:154:THR:HB	1:B:247:GLU:OE2	1.68	0.92
1:A:462:THR:HB	1:A:475:VAL:HG23	1.51	0.92
1:A:134:SER:HA	1:A:139:THR:HA	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:GLN:HB3	1:A:267:ASN:OD1	1.69	0.92
1:A:467:PHE:CE2	1:A:468:LEU:HD23	2.04	0.92
1:B:136:GLN:HG3	1:B:413:LYS:NZ	1.85	0.91
1:C:154:THR:HB	1:C:247:GLU:OE2	1.68	0.91
1:A:434:TRP:HB3	1:A:441:ALA:HB1	1.49	0.91
1:A:252:ALA:HB3	1:A:590:THR:HB	1.52	0.91
1:B:518:PRO:HG2	1:B:521:TYR:CZ	2.06	0.91
1:C:341:ASN:HB3	1:C:342:PRO:CD	2.01	0.91
1:A:394:TYR:CZ	1:A:422:GLY:HA3	2.06	0.91
1:C:645:GLU:HG2	1:C:664:LYS:NZ	1.86	0.91
1:B:568:ARG:HD3	1:B:569:PHE:H	1.34	0.91
1:C:462:THR:HB	1:C:475:VAL:HG23	1.52	0.91
1:A:474:LEU:HD12	1:A:475:VAL:N	1.86	0.91
1:C:394:TYR:CZ	1:C:422:GLY:HA3	2.05	0.91
1:C:252:ALA:HB3	1:C:590:THR:HB	1.53	0.91
1:A:637:GLU:HG3	1:A:671:LYS:HB3	1.53	0.90
1:B:599:TRP:HE3	1:B:599:TRP:N	1.69	0.90
1:C:434:TRP:HB3	1:C:441:ALA:HB1	1.50	0.90
1:B:568:ARG:HD3	1:B:569:PHE:N	1.87	0.90
1:B:812:ARG:HG3	1:B:813:TRP:H	1.36	0.90
1:A:812:ARG:HG3	1:A:813:TRP:H	1.34	0.90
1:B:754:LYS:H	1:B:754:LYS:HD2	1.35	0.90
1:C:812:ARG:HG3	1:C:813:TRP:H	1.35	0.90
1:C:188:VAL:HG11	1:C:246:VAL:HG11	1.52	0.90
1:B:252:ALA:HB3	1:B:590:THR:HB	1.53	0.89
1:C:258:GLY:HA3	1:C:528:GLN:OE1	1.71	0.89
1:A:599:TRP:HE3	1:A:599:TRP:N	1.70	0.89
1:B:768:ARG:HG3	1:B:778:SER:HB3	0.90	0.89
1:C:782:ASN:HB2	1:C:806:ASN:HB2	1.55	0.88
1:B:462:THR:HB	1:B:475:VAL:HG23	1.55	0.88
1:C:236:THR:HG23	1:C:237:LEU:CD2	2.04	0.88
1:C:637:GLU:HG3	1:C:671:LYS:HB3	1.56	0.88
1:B:637:GLU:HG3	1:B:671:LYS:HB3	1.56	0.87
1:A:599:TRP:H	1:A:599:TRP:HE3	1.19	0.87
1:B:258:GLY:HA3	1:B:528:GLN:OE1	1.75	0.87
1:C:243:TYR:CD2	1:C:268:LEU:HB3	2.09	0.87
1:C:271:LYS:HD2	1:C:310:ARG:CZ	2.04	0.87
1:B:782:ASN:HB2	1:B:806:ASN:HB2	1.57	0.86
1:B:653:LYS:N	1:B:653:LYS:HD3	1.86	0.86
1:B:188:VAL:HG11	1:B:246:VAL:HG11	1.57	0.86
1:A:258:GLY:HA3	1:A:528:GLN:OE1	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:ARG:HE	1:C:569:PHE:H	1.23	0.85
1:C:189:MSE:HE2	1:C:266:ILE:HD11	1.59	0.85
1:B:341:ASN:HB3	1:B:342:PRO:CD	2.07	0.85
1:B:394:TYR:CZ	1:B:422:GLY:HA3	2.12	0.85
1:A:324:HIS:HE1	1:A:383:ASN:HB3	1.42	0.84
1:A:526:THR:HG23	1:A:556:VAL:HG23	1.60	0.84
1:A:360:SER:HB3	1:A:390:SER:HA	1.58	0.84
1:A:776:SER:H	1:A:812:ARG:HB3	1.43	0.84
1:B:136:GLN:HG3	1:B:413:LYS:HZ2	1.39	0.84
1:B:599:TRP:HE3	1:B:599:TRP:H	1.19	0.84
1:B:357:PRO:O	1:B:390:SER:HB2	1.78	0.84
1:B:762:LEU:HD21	1:B:789:TYR:HE2	1.43	0.84
1:A:188:VAL:HG11	1:A:246:VAL:HG11	1.60	0.84
1:C:227:ARG:HD3	1:C:594:MSE:CE	2.01	0.84
1:C:324:HIS:HE1	1:C:383:ASN:HB3	1.43	0.84
1:C:776:SER:H	1:C:812:ARG:HB3	1.43	0.84
1:A:198:SER:HB3	1:A:206:ASN:ND2	1.93	0.84
1:B:236:THR:HG23	1:B:237:LEU:CD2	2.08	0.83
1:B:655:THR:HG23	1:B:659:ILE:HD12	1.58	0.83
1:B:779:VAL:HG21	1:B:809:PHE:CE1	2.11	0.83
1:C:764:ASP:HB3	1:C:782:ASN:O	1.78	0.83
1:B:747:ASN:HB3	1:B:748:PRO:HD3	1.61	0.83
1:C:416:LEU:CD2	1:C:457:LEU:CD1	2.56	0.83
1:B:776:SER:H	1:B:812:ARG:HB3	1.43	0.83
1:C:271:LYS:CD	1:C:310:ARG:NH2	2.41	0.83
1:C:526:THR:HG23	1:C:556:VAL:HG23	1.60	0.83
1:C:352:TYR:CD1	1:C:396:ARG:CG	2.51	0.83
1:A:568:ARG:HE	1:A:569:PHE:H	1.21	0.82
1:B:352:TYR:HD1	1:B:396:ARG:HB3	1.44	0.82
1:C:560:ASN:ND2	1:C:561:PRO:HD2	1.95	0.82
1:A:364:GLY:HA3	1:A:798:SER:HB2	1.62	0.82
1:C:659:ILE:HG23	1:C:660:THR:H	1.45	0.82
1:B:364:GLY:HA3	1:B:798:SER:HB2	1.62	0.82
1:A:681:LEU:HD22	1:A:687:VAL:CG1	2.08	0.82
1:C:360:SER:HB3	1:C:390:SER:HA	1.60	0.82
1:A:352:TYR:HD1	1:A:396:ARG:HB3	1.45	0.82
1:C:357:PRO:O	1:C:390:SER:HB2	1.80	0.82
1:B:360:SER:HB3	1:B:390:SER:HA	1.61	0.81
1:A:747:ASN:HB3	1:A:748:PRO:HD3	1.59	0.81
1:A:583:TYR:HB3	1:A:620:ILE:HD11	1.61	0.81
1:B:526:THR:HG22	1:B:556:VAL:HG23	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ASN:HB3	1:B:342:PRO:HD2	1.62	0.81
1:B:189:MSE:HE2	1:B:266:ILE:HD11	1.59	0.81
1:A:560:ASN:ND2	1:A:561:PRO:HD2	1.96	0.81
1:B:560:ASN:ND2	1:B:561:PRO:HD2	1.96	0.81
1:A:357:PRO:O	1:A:390:SER:HB2	1.80	0.81
1:C:646:GLU:HB2	1:C:661:TYR:OH	1.81	0.80
1:C:236:THR:HG23	1:C:237:LEU:HD22	1.64	0.80
1:C:599:TRP:N	1:C:599:TRP:HE3	1.78	0.80
1:B:789:TYR:CE1	1:B:802:GLY:HA3	2.16	0.80
1:B:583:TYR:HB3	1:B:620:ILE:HD11	1.64	0.80
1:C:583:TYR:HB3	1:C:620:ILE:HD11	1.64	0.80
1:A:344:THR:HG21	1:A:405:ASN:HD21	1.47	0.80
1:C:341:ASN:HB3	1:C:342:PRO:HD2	1.62	0.79
1:A:292:ARG:HD2	1:A:316:GLN:CD	2.03	0.79
1:B:599:TRP:N	1:B:599:TRP:CE3	2.48	0.79
1:B:779:VAL:CG2	1:B:809:PHE:CD1	2.65	0.79
1:C:601:ARG:HG3	1:C:601:ARG:HH11	1.48	0.79
1:A:764:ASP:HB3	1:A:782:ASN:O	1.83	0.79
1:B:443:ILE:HD13	1:B:510:ILE:HD12	1.64	0.79
1:C:364:GLY:HA3	1:C:798:SER:HB2	1.64	0.79
1:B:324:HIS:HE1	1:B:383:ASN:HB3	1.48	0.79
1:B:643:ARG:HH12	1:B:704:VAL:HG21	1.47	0.79
1:A:560:ASN:HD22	1:A:561:PRO:HD2	1.48	0.78
1:B:763:VAL:HG11	1:B:785:PHE:CE2	2.18	0.78
1:B:601:ARG:HH11	1:B:601:ARG:HG3	1.48	0.78
1:C:661:TYR:HD1	1:C:662:ALA:H	1.31	0.78
1:A:768:ARG:HG3	1:A:778:SER:HB3	1.64	0.78
1:C:402:LEU:HD12	1:C:414:VAL:CG1	2.14	0.78
1:C:271:LYS:HD2	1:C:310:ARG:NH2	1.98	0.78
1:C:560:ASN:HD22	1:C:561:PRO:HD2	1.46	0.78
1:C:189:MSE:CE	1:C:266:ILE:HD11	2.12	0.78
1:A:198:SER:HB3	1:A:206:ASN:HD21	1.47	0.77
1:C:275:HIS:O	1:C:300:PRO:HG3	1.84	0.77
1:C:584:SER:O	1:C:620:ILE:HG13	1.84	0.77
1:A:599:TRP:CE3	1:A:599:TRP:N	2.49	0.77
1:B:560:ASN:HD22	1:B:561:PRO:HD2	1.48	0.77
1:B:643:ARG:NH1	1:B:704:VAL:HG21	1.99	0.77
1:A:344:THR:HG21	1:A:405:ASN:ND2	2.00	0.77
1:C:645:GLU:HG2	1:C:664:LYS:HZ2	1.47	0.77
1:A:341:ASN:HB3	1:A:342:PRO:CD	2.14	0.76
1:B:184:ASN:OD1	1:B:186:ASP:HB2	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:681:LEU:HD22	1:B:687:VAL:CG1	2.11	0.76
1:A:601:ARG:HH11	1:A:601:ARG:HG3	1.51	0.76
1:B:391:TRP:HD1	1:B:391:TRP:O	1.68	0.76
1:A:387:LYS:HD2	1:A:509:ASP:HB3	1.67	0.76
1:A:474:LEU:CD1	1:A:475:VAL:H	1.93	0.76
1:A:763:VAL:HG13	1:A:784:VAL:HB	1.67	0.76
1:C:369:PHE:O	1:C:433:ASP:HA	1.85	0.76
1:C:763:VAL:HG13	1:C:784:VAL:HB	1.66	0.76
1:A:275:HIS:O	1:A:300:PRO:HG3	1.85	0.76
1:A:443:ILE:HD13	1:A:510:ILE:HD12	1.67	0.76
1:B:253:THR:HG21	1:B:265:THR:OG1	1.84	0.76
1:A:341:ASN:HB3	1:A:342:PRO:HD2	1.67	0.76
1:A:584:SER:O	1:A:620:ILE:HG13	1.86	0.76
1:C:252:ALA:HB3	1:C:590:THR:CB	2.16	0.76
1:B:779:VAL:HG21	1:B:809:PHE:CD1	2.21	0.76
1:B:584:SER:O	1:B:620:ILE:HG13	1.86	0.75
1:B:252:ALA:HB3	1:B:590:THR:CB	2.15	0.75
1:C:331:VAL:HB	1:C:353:GLN:HG3	1.68	0.75
1:C:600:TYR:OH	2:K:2:DSN:HB3	1.86	0.75
1:A:189:MSE:HE3	1:A:195:ILE:HD13	1.67	0.75
1:A:625:LEU:HD13	1:A:628:ARG:HH12	1.50	0.75
1:A:655:THR:HG23	1:A:656:ASN:H	1.50	0.75
1:A:252:ALA:HB3	1:A:590:THR:CB	2.15	0.75
1:B:280:HIS:HB2	1:B:813:TRP:CB	2.16	0.75
1:A:762:LEU:HD21	1:A:789:TYR:HE2	1.52	0.75
1:B:625:LEU:O	1:B:627:GLY:N	2.18	0.75
1:A:253:THR:HG21	1:A:265:THR:OG1	1.85	0.75
1:A:643:ARG:HH12	1:A:704:VAL:HG21	1.51	0.75
1:C:599:TRP:N	1:C:599:TRP:CE3	2.53	0.75
1:B:445:ALA:O	1:B:446:GLN:HG3	1.87	0.75
1:C:253:THR:HG21	1:C:265:THR:OG1	1.87	0.75
1:C:559:LEU:HG	1:C:559:LEU:O	1.87	0.74
1:A:391:TRP:CE3	1:A:427:LEU:HD11	2.23	0.74
1:A:434:TRP:CE3	1:A:434:TRP:HA	2.22	0.74
1:B:331:VAL:HB	1:B:353:GLN:HG3	1.68	0.74
1:B:391:TRP:CD1	1:B:391:TRP:O	2.40	0.74
1:B:189:MSE:HE2	1:B:266:ILE:CD1	2.17	0.74
1:B:275:HIS:O	1:B:300:PRO:HG3	1.87	0.74
1:C:189:MSE:CE	1:C:266:ILE:CD1	2.65	0.74
1:C:643:ARG:HH12	1:C:704:VAL:HG21	1.52	0.74
1:C:443:ILE:HD13	1:C:510:ILE:HD12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:MSE:CE	1:A:195:ILE:CD1	2.60	0.74
1:B:754:LYS:HD3	1:B:754:LYS:O	1.88	0.73
1:C:292:ARG:HD2	1:C:316:GLN:CD	2.09	0.73
1:C:768:ARG:CB	1:C:778:SER:HB3	2.19	0.73
1:A:185:ILE:CD1	1:A:189:MSE:HG2	2.18	0.73
1:A:434:TRP:HB3	1:A:441:ALA:CB	2.18	0.73
1:B:292:ARG:HD2	1:B:316:GLN:CD	2.09	0.73
1:A:369:PHE:O	1:A:433:ASP:HA	1.88	0.73
1:A:397:THR:HB	1:A:419:LYS:HG3	1.68	0.73
1:C:762:LEU:HD21	1:C:789:TYR:HE2	1.51	0.73
1:A:380:ARG:HA	1:A:801:TYR:CD2	2.23	0.73
1:A:625:LEU:O	1:A:627:GLY:N	2.20	0.73
4:J:1:PVE:H11	4:J:1:PVE:H212	1.53	0.73
1:A:227:ARG:HD3	1:A:594:MSE:CE	2.13	0.73
1:A:537:PHE:HE2	1:A:547:LEU:HD12	1.53	0.73
1:B:629:LEU:HD12	1:B:630:ASN:H	1.54	0.73
1:C:340:LEU:HB2	1:C:343:ASP:HB2	1.70	0.73
1:B:189:MSE:CE	1:B:266:ILE:HD11	2.19	0.73
1:C:434:TRP:HB3	1:C:441:ALA:CB	2.18	0.73
1:A:496:TYR:CD1	1:A:513:PRO:HB3	2.24	0.73
1:A:633:LEU:HD23	1:A:633:LEU:O	1.89	0.72
1:B:380:ARG:HA	1:B:801:TYR:CD2	2.24	0.72
1:C:445:ALA:O	1:C:446:GLN:HG3	1.88	0.72
1:A:340:LEU:HB2	1:A:343:ASP:HB2	1.69	0.72
1:C:365:SER:C	1:C:384:ASN:HD22	1.92	0.72
1:B:559:LEU:O	1:B:559:LEU:HD23	1.89	0.72
1:A:194:GLY:HA2	1:A:712:GLN:OE1	1.89	0.72
1:A:763:VAL:HG11	1:A:785:PHE:CE2	2.24	0.72
1:B:434:TRP:HB3	1:B:441:ALA:CB	2.19	0.72
1:A:695:ILE:HD11	1:A:710:GLN:HE21	1.55	0.72
1:C:380:ARG:HA	1:C:801:TYR:CD2	2.25	0.72
1:C:747:ASN:HB3	1:C:748:PRO:HD3	1.70	0.72
1:A:240:MSE:O	1:A:242:ILE:N	2.23	0.72
1:B:369:PHE:O	1:B:433:ASP:HA	1.90	0.72
1:B:474:LEU:HD11	1:B:533:MSE:CG	2.20	0.72
1:B:768:ARG:CB	1:B:778:SER:HB3	2.20	0.72
1:C:335:ILE:C	1:C:336:LEU:HD12	2.11	0.72
1:B:340:LEU:HB2	1:B:343:ASP:HB2	1.70	0.71
1:C:352:TYR:CE1	1:C:396:ARG:HD2	2.25	0.71
1:C:271:LYS:HD3	1:C:310:ARG:NH2	2.04	0.71
1:B:376:ASN:HD21	1:B:435:PRO:HG2	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:TYR:CD1	1:C:513:PRO:HB3	2.24	0.71
1:A:192:THR:HB	1:A:195:ILE:HD12	1.73	0.71
1:B:763:VAL:HG13	1:B:784:VAL:HB	1.72	0.71
1:C:184:ASN:OD1	1:C:186:ASP:HB2	1.90	0.71
1:C:643:ARG:NH1	1:C:704:VAL:HG21	2.05	0.71
1:A:643:ARG:NH1	1:A:704:VAL:HG21	2.04	0.71
1:C:552:VAL:HG22	1:C:553:ASP:N	2.05	0.71
1:B:189:MSE:CE	1:B:266:ILE:CD1	2.68	0.71
1:C:397:THR:HB	1:C:419:LYS:HG3	1.73	0.71
1:C:625:LEU:O	1:C:627:GLY:N	2.22	0.71
1:A:402:LEU:O	1:A:402:LEU:HD12	1.91	0.71
1:B:218:GLN:HB3	1:B:267:ASN:OD1	1.91	0.71
1:B:240:MSE:O	1:B:242:ILE:N	2.24	0.71
1:B:273:PRO:HG3	1:B:337:GLU:HG3	1.73	0.71
1:B:659:ILE:CG1	1:B:660:THR:H	2.00	0.71
1:C:554:TYR:CD2	1:C:595:PRO:CG	2.71	0.71
1:A:168:SER:HB2	1:A:617:GLU:OE2	1.91	0.71
1:B:764:ASP:HB3	1:B:782:ASN:O	1.91	0.71
1:B:169:ILE:HD13	1:B:249:LEU:HA	1.71	0.70
1:B:192:THR:HB	1:B:195:ILE:HD12	1.73	0.70
1:B:397:THR:HB	1:B:419:LYS:HG3	1.72	0.70
1:C:240:MSE:O	1:C:242:ILE:N	2.23	0.70
1:A:467:PHE:CE2	1:A:468:LEU:CD2	2.74	0.70
1:B:135:ASN:HD22	1:B:135:ASN:N	1.88	0.70
1:B:227:ARG:CD	1:B:594:MSE:HE1	2.16	0.70
1:A:652:SER:O	1:A:654:PRO:HD3	1.91	0.70
1:B:496:TYR:CD1	1:B:513:PRO:HB3	2.27	0.70
1:B:233:ALA:HB2	1:B:423:TYR:HB3	1.73	0.70
1:A:233:ALA:HB2	1:A:423:TYR:HB3	1.74	0.70
1:B:194:GLY:HA2	1:B:712:GLN:OE1	1.92	0.70
1:B:335:ILE:C	1:B:336:LEU:HD12	2.12	0.70
1:C:233:ALA:HB2	1:C:423:TYR:HB3	1.74	0.70
1:C:386:ALA:HB3	1:C:389:SER:HB2	1.74	0.70
1:C:601:ARG:HG3	1:C:601:ARG:NH1	2.06	0.70
1:C:683:PRO:HG2	1:C:684:GLY:H	1.57	0.70
1:C:242:ILE:O	1:C:271:LYS:HG3	1.92	0.70
1:B:386:ALA:HB3	1:B:389:SER:HB2	1.73	0.70
1:A:559:LEU:HD23	1:A:559:LEU:O	1.92	0.70
1:C:189:MSE:HE2	1:C:266:ILE:CD1	2.22	0.70
1:A:335:ILE:C	1:A:336:LEU:HD12	2.13	0.70
1:B:144:SER:O	1:B:146:SER:N	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:754:LYS:N	1:B:754:LYS:HD2	2.03	0.69
1:A:768:ARG:CB	1:A:778:SER:HB3	2.23	0.69
1:B:552:VAL:HG22	1:B:553:ASP:N	2.07	0.69
1:C:763:VAL:HG11	1:C:785:PHE:CE2	2.27	0.69
1:B:140:ILE:HG22	1:B:141:THR:N	2.07	0.69
1:C:169:ILE:HD13	1:C:249:LEU:HA	1.73	0.69
1:A:376:ASN:HD21	1:A:435:PRO:HG2	1.57	0.69
1:B:720:LYS:HG3	1:B:729:THR:OG1	1.92	0.69
1:C:506:TRP:CZ2	1:C:508:GLY:HA2	2.28	0.69
1:C:246:VAL:HG23	1:C:268:LEU:HD23	1.74	0.69
1:B:352:TYR:CD1	1:B:396:ARG:HB3	2.27	0.69
1:B:605:ASN:OD1	1:B:658:ALA:HB2	1.93	0.69
1:C:720:LYS:HG3	1:C:729:THR:OG1	1.92	0.69
1:A:470:ARG:HH11	1:A:470:ARG:HG2	1.57	0.69
1:A:331:VAL:HB	1:A:353:GLN:HG3	1.73	0.69
1:A:552:VAL:HG22	1:A:553:ASP:N	2.07	0.69
1:B:447:LYS:HE2	3:B:2002:SO4:O4	1.93	0.69
1:B:492:ASN:HB2	1:B:519:SER:OG	1.92	0.69
1:A:169:ILE:HD13	1:A:249:LEU:HA	1.74	0.68
1:C:538:ASN:CB	1:C:544:ASN:ND2	2.56	0.68
1:C:140:ILE:HG22	1:C:141:THR:N	2.08	0.68
1:C:470:ARG:HH11	1:C:470:ARG:HG2	1.59	0.68
1:A:439:ASN:OD1	1:A:502:ASP:HB2	1.93	0.68
1:A:659:ILE:HG12	1:A:660:THR:H	1.58	0.68
1:B:762:LEU:HD21	1:B:789:TYR:CE2	2.28	0.68
1:C:169:ILE:CD1	1:C:249:LEU:HA	2.23	0.68
1:C:340:LEU:O	1:C:341:ASN:HB2	1.93	0.68
1:A:140:ILE:HG22	1:A:141:THR:N	2.09	0.68
1:A:506:TRP:CZ2	1:A:508:GLY:HA2	2.29	0.68
1:A:647:ASP:H	1:A:663:TYR:HA	1.59	0.68
1:B:654:PRO:O	1:B:656:ASN:N	2.24	0.68
1:C:271:LYS:CD	1:C:310:ARG:CZ	2.72	0.68
1:C:402:LEU:HD12	1:C:414:VAL:HG13	1.74	0.68
1:B:601:ARG:HG3	1:B:601:ARG:NH1	2.07	0.68
1:A:601:ARG:NH1	1:A:601:ARG:HG3	2.08	0.68
1:C:192:THR:HB	1:C:195:ILE:HD12	1.75	0.68
1:C:218:GLN:HB3	1:C:267:ASN:OD1	1.92	0.68
1:C:652:SER:O	1:C:654:PRO:HD3	1.94	0.68
1:A:646:GLU:HA	1:A:663:TYR:CD2	2.27	0.68
1:B:625:LEU:HD13	1:B:628:ARG:HH12	1.58	0.68
1:B:174:ARG:HD2	1:B:177:MSE:HE3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ILE:HD11	1:C:249:LEU:CD1	2.24	0.68
1:A:238:SER:HA	1:A:353:GLN:HE22	1.57	0.67
1:A:720:LYS:HG3	1:A:729:THR:OG1	1.94	0.67
1:B:158:LEU:HD21	1:B:473:GLU:HG3	1.76	0.67
1:A:625:LEU:C	1:A:627:GLY:H	1.98	0.67
1:B:776:SER:CB	1:B:812:ARG:HB2	2.23	0.67
1:B:403:GLU:HB3	1:B:413:LYS:HG3	1.76	0.67
1:B:779:VAL:HG23	1:B:809:PHE:CD1	2.30	0.67
1:C:746:ASN:HD21	1:C:749:ARG:CG	2.07	0.67
1:A:352:TYR:CD1	1:A:396:ARG:HB3	2.28	0.67
1:A:412:GLY:HA3	1:A:461:LEU:HD23	1.76	0.67
1:B:625:LEU:C	1:B:627:GLY:H	1.98	0.67
1:A:271:LYS:NZ	1:A:310:ARG:NH2	2.42	0.67
1:B:402:LEU:O	1:B:402:LEU:HD12	1.95	0.67
1:A:169:ILE:HD11	1:A:249:LEU:CD1	2.24	0.67
1:B:168:SER:HB2	1:B:617:GLU:OE2	1.94	0.67
1:A:189:MSE:HE3	1:A:195:ILE:HG21	1.77	0.67
1:A:657:PRO:C	1:A:659:ILE:H	1.95	0.67
1:C:638:ILE:N	1:C:670:THR:O	2.21	0.67
1:A:492:ASN:HB2	1:A:519:SER:OG	1.95	0.67
1:A:445:ALA:O	1:A:446:GLN:HG3	1.94	0.67
1:A:746:ASN:HD22	1:A:749:ARG:HB2	1.59	0.67
1:B:280:HIS:CE1	1:B:812:ARG:HH21	2.12	0.67
1:B:345:MSE:O	1:B:402:LEU:HA	1.94	0.67
1:B:421:ASN:O	1:B:452:THR:HG22	1.95	0.66
1:B:517:THR:HB	1:B:518:PRO:HD2	1.77	0.66
1:C:645:GLU:HG2	1:C:664:LYS:HZ3	1.59	0.66
1:B:506:TRP:CZ2	1:B:508:GLY:HA2	2.30	0.66
1:A:683:PRO:HG2	1:A:684:GLY:H	1.60	0.66
1:A:194:GLY:CA	1:A:712:GLN:OE1	2.44	0.66
1:B:169:ILE:CD1	1:B:249:LEU:HA	2.25	0.66
1:B:412:GLY:HA3	1:B:461:LEU:HD23	1.77	0.66
1:B:647:ASP:H	1:B:663:TYR:HA	1.60	0.66
1:C:144:SER:O	1:C:146:SER:N	2.26	0.66
1:A:342:PRO:C	1:A:344:THR:H	1.99	0.66
1:C:625:LEU:C	1:C:627:GLY:H	1.99	0.66
1:C:647:ASP:H	1:C:663:TYR:HA	1.58	0.66
1:A:638:ILE:N	1:A:670:THR:O	2.21	0.66
1:C:345:MSE:O	1:C:402:LEU:HA	1.95	0.66
1:C:412:GLY:HA3	1:C:461:LEU:HD23	1.77	0.66
1:A:266:ILE:HG22	1:A:267:ASN:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:ARG:CG	1:A:778:SER:HB3	2.25	0.66
1:A:776:SER:CB	1:A:812:ARG:HB2	2.25	0.66
1:B:791:THR:HG22	1:B:800:SER:O	1.95	0.66
1:C:280:HIS:HB2	1:C:813:TRP:CB	2.25	0.66
1:C:554:TYR:CG	1:C:595:PRO:HG3	2.30	0.66
1:A:682:ALA:CB	1:A:683:PRO:CD	2.73	0.66
1:B:194:GLY:CA	1:B:712:GLN:OE1	2.44	0.66
1:B:774:LYS:HD3	1:B:814:ASP:OD2	1.96	0.66
1:A:227:ARG:CD	1:A:594:MSE:HE1	2.17	0.66
1:B:422:GLY:HA2	1:B:451:GLU:HA	1.78	0.66
1:C:319:HIS:CG	1:C:326:GLU:HG2	2.31	0.66
1:C:416:LEU:HD23	1:C:457:LEU:HD12	1.78	0.66
1:C:605:ASN:OD1	1:C:658:ALA:HB2	1.96	0.66
1:C:695:ILE:HD11	1:C:710:GLN:HE21	1.60	0.65
1:B:474:LEU:CD1	1:B:475:VAL:H	2.06	0.65
1:B:683:PRO:HG2	1:B:684:GLY:H	1.61	0.65
1:B:695:ILE:HD11	1:B:710:GLN:HE21	1.61	0.65
1:B:376:ASN:ND2	1:B:435:PRO:HG2	2.12	0.65
1:A:422:GLY:HA2	1:A:451:GLU:HA	1.77	0.65
1:B:185:ILE:O	1:B:185:ILE:HD13	1.96	0.65
1:B:474:LEU:HD12	1:B:475:VAL:N	2.08	0.65
1:C:474:LEU:CD1	1:C:475:VAL:H	2.08	0.65
1:C:682:ALA:CB	1:C:683:PRO:CD	2.74	0.65
1:A:697:ARG:NH2	1:A:703:LYS:HZ2	1.95	0.65
1:A:719:TYR:CE2	1:A:721:PHE:HD1	2.13	0.65
1:C:134:SER:HB3	1:C:139:THR:HB	1.79	0.65
1:C:434:TRP:HA	1:C:434:TRP:CE3	2.32	0.65
1:C:625:LEU:HD13	1:C:628:ARG:HH12	1.61	0.65
1:C:813:TRP:O	1:C:814:ASP:HB2	1.97	0.65
1:A:184:ASN:OD1	1:A:186:ASP:HB2	1.96	0.65
1:A:746:ASN:ND2	1:A:749:ARG:HB2	2.12	0.65
1:B:434:TRP:CE3	1:B:434:TRP:HA	2.32	0.65
1:B:387:LYS:HG3	1:B:509:ASP:HA	1.78	0.65
1:C:185:ILE:CD1	1:C:189:MSE:HG2	2.27	0.65
1:A:190:ARG:NH1	1:A:197:VAL:HG11	2.11	0.64
1:A:387:LYS:HG3	1:A:509:ASP:HA	1.78	0.64
1:B:629:LEU:HD12	1:B:630:ASN:N	2.13	0.64
1:C:185:ILE:HD13	1:C:185:ILE:O	1.97	0.64
1:C:209:ALA:HB2	1:C:214:ILE:HD11	1.78	0.64
1:B:682:ALA:CB	1:B:683:PRO:CD	2.75	0.64
1:C:387:LYS:HD2	1:C:509:ASP:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:LEU:HD12	1:C:402:LEU:O	1.97	0.64
1:A:209:ALA:HB2	1:A:214:ILE:HD11	1.78	0.64
1:B:136:GLN:CG	1:B:413:LYS:NZ	2.60	0.64
1:C:474:LEU:HD12	1:C:475:VAL:N	2.10	0.64
1:C:776:SER:CB	1:C:812:ARG:HB2	2.26	0.64
1:C:439:ASN:OD1	1:C:502:ASP:HB2	1.97	0.64
1:A:657:PRO:O	1:A:659:ILE:HG22	1.97	0.64
1:A:391:TRP:CZ3	1:A:427:LEU:HD11	2.33	0.64
1:B:233:ALA:HA	1:B:393:GLN:OE1	1.98	0.64
1:C:736:TRP:HA	1:C:760:TYR:O	1.98	0.64
1:A:319:HIS:CG	1:A:326:GLU:HG2	2.33	0.64
1:B:342:PRO:C	1:B:344:THR:H	2.00	0.64
1:B:746:ASN:HD22	1:B:749:ARG:HB2	1.62	0.64
1:C:492:ASN:HB2	1:C:519:SER:OG	1.96	0.64
1:A:350:ALA:HB2	1:A:398:VAL:HG22	1.80	0.64
1:B:177:MSE:HA	1:B:182:LEU:HD12	1.80	0.64
1:B:185:ILE:CD1	1:B:189:MSE:HG2	2.28	0.64
1:B:741:TRP:HA	1:B:755:PHE:O	1.97	0.64
1:C:169:ILE:HD11	1:C:249:LEU:HD12	1.80	0.64
1:A:147:TYR:HA	1:A:173:THR:CG2	2.25	0.63
1:A:421:ASN:O	1:A:452:THR:HG22	1.98	0.63
1:A:467:PHE:HD2	1:A:468:LEU:HG	1.62	0.63
1:B:169:ILE:HD11	1:B:249:LEU:CD1	2.28	0.63
1:A:370:ASP:O	1:A:372:GLN:N	2.31	0.63
1:C:416:LEU:HD22	1:C:457:LEU:CD1	2.28	0.63
1:C:538:ASN:HB2	1:C:544:ASN:ND2	2.13	0.63
1:A:376:ASN:ND2	1:A:435:PRO:HG2	2.13	0.63
1:B:136:GLN:HG2	1:B:137:LEU:H	1.64	0.63
1:B:134:SER:CA	1:B:139:THR:HA	2.25	0.63
1:A:345:MSE:O	1:A:402:LEU:HA	1.99	0.63
1:B:134:SER:HB3	1:B:139:THR:HB	1.79	0.63
1:A:434:TRP:HE3	1:A:434:TRP:HA	1.63	0.63
1:B:236:THR:HG23	1:B:237:LEU:HD22	1.79	0.63
1:C:422:GLY:HA2	1:C:451:GLU:HA	1.79	0.63
1:C:568:ARG:HE	1:C:569:PHE:N	1.95	0.63
1:A:287:SER:O	1:A:290:ASN:HB2	1.99	0.63
1:A:364:GLY:HA3	1:A:798:SER:CB	2.28	0.63
1:B:246:VAL:CG2	1:B:268:LEU:HD23	2.26	0.63
1:B:364:GLY:HA3	1:B:798:SER:CB	2.28	0.63
1:C:342:PRO:C	1:C:344:THR:H	2.00	0.63
1:C:370:ASP:O	1:C:372:GLN:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:677:ILE:HG12	1:C:678:SER:N	2.13	0.63
1:C:783:ASN:HB3	1:C:805:ARG:HA	1.81	0.63
1:A:774:LYS:HD3	1:A:814:ASP:OD2	1.98	0.62
1:B:768:ARG:HG3	1:B:778:SER:OG	1.97	0.62
1:A:169:ILE:CD1	1:A:249:LEU:HA	2.29	0.62
1:A:655:THR:HG23	1:A:656:ASN:N	2.14	0.62
1:B:236:THR:HG23	1:B:237:LEU:HD23	1.78	0.62
1:B:166:PRO:HG3	1:B:546:PHE:CD2	2.34	0.62
1:C:134:SER:CA	1:C:139:THR:HA	2.26	0.62
1:C:387:LYS:HG3	1:C:509:ASP:HA	1.81	0.62
1:C:791:THR:HG22	1:C:800:SER:O	1.99	0.62
1:A:240:MSE:HE2	1:A:240:MSE:HA	1.81	0.62
1:B:350:ALA:HB2	1:B:398:VAL:HG22	1.79	0.62
1:C:593:PHE:HB3	1:C:612:GLU:HG3	1.79	0.62
1:B:638:ILE:N	1:B:670:THR:O	2.21	0.62
1:C:364:GLY:HA3	1:C:798:SER:CB	2.30	0.62
1:A:625:LEU:HD13	1:A:628:ARG:NH1	2.13	0.62
1:A:646:GLU:HA	1:A:663:TYR:HD2	1.64	0.62
1:B:813:TRP:O	1:B:814:ASP:HB2	1.99	0.62
1:C:216:ASN:HD21	1:C:261:SER:H	1.45	0.62
1:C:402:LEU:CD1	1:C:414:VAL:CG1	2.78	0.62
1:A:169:ILE:HD11	1:A:249:LEU:HD12	1.81	0.62
1:C:421:ASN:O	1:C:452:THR:HG22	1.99	0.62
1:C:546:PHE:O	1:C:573:VAL:HA	1.99	0.62
1:C:661:TYR:CD1	1:C:662:ALA:N	2.67	0.62
1:C:774:LYS:HD3	1:C:814:ASP:OD2	2.00	0.62
1:B:589:TYR:HE1	1:B:614:GLN:HB3	1.64	0.62
1:A:136:GLN:HG2	1:A:137:LEU:H	1.63	0.62
1:A:136:GLN:HG2	1:A:137:LEU:N	2.15	0.62
1:A:174:ARG:HD2	1:A:177:MSE:HE3	1.82	0.62
1:A:538:ASN:H	1:A:538:ASN:HD22	1.48	0.62
1:B:209:ALA:HB2	1:B:214:ILE:HD11	1.82	0.62
1:B:554:TYR:CG	1:B:595:PRO:HG3	2.35	0.62
1:A:682:ALA:HB1	1:A:683:PRO:CD	2.30	0.62
1:A:791:THR:HG22	1:A:800:SER:O	1.99	0.62
1:A:273:PRO:HG3	1:A:337:GLU:HG3	1.82	0.61
1:A:596:GLN:HG2	1:A:600:TYR:HD2	1.65	0.61
1:B:475:VAL:O	1:B:475:VAL:HG22	2.00	0.61
1:C:554:TYR:CE2	1:C:595:PRO:HG3	2.35	0.61
1:C:682:ALA:HB1	1:C:683:PRO:CD	2.30	0.61
1:C:698:ASP:O	1:C:701:GLY:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:782:ASN:HB3	1:C:806:ASN:HD22	1.65	0.61
1:B:167:GLN:NE2	1:B:572:TYR:CE1	2.69	0.61
1:B:650:TYR:CE1	1:B:654:PRO:HD2	2.35	0.61
1:C:380:ARG:HH11	1:C:380:ARG:HG3	1.65	0.61
1:A:656:ASN:O	1:A:659:ILE:HB	2.00	0.61
1:A:783:ASN:HB3	1:A:805:ARG:HA	1.82	0.61
1:B:538:ASN:HB3	1:B:544:ASN:OD1	2.00	0.61
1:B:546:PHE:O	1:B:573:VAL:HA	2.00	0.61
1:A:281:VAL:O	1:A:281:VAL:HG13	1.99	0.61
1:A:568:ARG:HE	1:A:569:PHE:N	1.95	0.61
1:A:781:VAL:HB	1:A:807:LEU:CD1	2.31	0.61
1:B:287:SER:O	1:B:290:ASN:HB2	2.01	0.61
1:B:391:TRP:CE3	1:B:427:LEU:HD11	2.35	0.61
1:B:655:THR:HA	1:B:659:ILE:HD12	1.82	0.61
1:C:273:PRO:HG3	1:C:337:GLU:HG3	1.81	0.61
1:C:416:LEU:HD22	1:C:457:LEU:HD13	1.81	0.61
1:A:216:ASN:HD21	1:A:261:SER:H	1.47	0.61
1:A:262:LEU:CD1	1:A:640:GLU:HG3	2.31	0.61
1:B:538:ASN:H	1:B:538:ASN:HD22	1.48	0.61
1:C:166:PRO:HG3	1:C:546:PHE:CD2	2.35	0.61
1:A:736:TRP:HA	1:A:760:TYR:O	2.00	0.61
1:B:340:LEU:O	1:B:341:ASN:HB2	1.99	0.61
1:B:600:TYR:O	1:B:607:LEU:HA	1.99	0.61
1:B:698:ASP:O	1:B:701:GLY:N	2.33	0.61
1:A:593:PHE:HB3	1:A:612:GLU:HG3	1.82	0.61
1:B:593:PHE:HB3	1:B:612:GLU:HG3	1.83	0.61
1:C:240:MSE:HE2	1:C:240:MSE:HA	1.83	0.61
1:C:262:LEU:CD1	1:C:640:GLU:HG3	2.30	0.61
1:C:596:GLN:HG2	1:C:600:TYR:HD2	1.65	0.61
1:C:183:ASN:HD21	1:C:808:MSE:HE1	1.65	0.61
1:A:340:LEU:CB	1:A:343:ASP:HB2	2.30	0.61
1:A:434:TRP:CB	1:A:441:ALA:HB1	2.29	0.61
1:A:166:PRO:HG3	1:A:546:PHE:CD2	2.35	0.61
1:A:600:TYR:O	1:A:607:LEU:HA	2.00	0.61
1:C:771:ILE:HG13	1:C:772:THR:CG2	2.28	0.61
1:A:144:SER:O	1:A:146:SER:N	2.29	0.61
1:A:467:PHE:CD2	1:A:468:LEU:HD23	2.35	0.61
1:B:246:VAL:O	1:B:246:VAL:HG13	2.01	0.61
1:C:552:VAL:CG1	1:C:593:PHE:HZ	2.13	0.61
1:B:380:ARG:HH11	1:B:380:ARG:HG3	1.66	0.60
1:B:262:LEU:CD1	1:B:640:GLU:HG3	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:LYS:HD3	1:B:694:LYS:O	2.01	0.60
1:C:782:ASN:CB	1:C:806:ASN:HD22	2.14	0.60
1:C:348:VAL:HG12	1:C:400:ALA:HA	1.83	0.60
1:B:319:HIS:CG	1:B:326:GLU:HG2	2.37	0.60
1:B:736:TRP:HA	1:B:760:TYR:O	2.00	0.60
1:B:746:ASN:ND2	1:B:749:ARG:HB2	2.17	0.60
1:B:771:ILE:HG13	1:B:772:THR:CG2	2.29	0.60
1:A:280:HIS:HB2	1:A:813:TRP:CB	2.26	0.60
1:A:280:HIS:O	1:A:295:LEU:HD12	2.00	0.60
1:A:386:ALA:HB3	1:A:389:SER:HB2	1.81	0.60
1:B:281:VAL:O	1:B:281:VAL:HG13	1.98	0.60
1:C:506:TRP:CH2	1:C:508:GLY:HA2	2.36	0.60
1:A:540:THR:CG2	1:A:542:ASP:OD2	2.49	0.60
1:A:134:SER:CA	1:A:139:THR:HA	2.28	0.60
1:A:659:ILE:HG12	1:A:660:THR:N	2.17	0.60
1:C:271:LYS:HB3	1:C:310:ARG:NH1	2.17	0.60
1:C:158:LEU:HD21	1:C:473:GLU:HG3	1.84	0.60
1:A:344:THR:CG2	1:A:405:ASN:ND2	2.64	0.60
1:C:746:ASN:ND2	1:C:749:ARG:CG	2.65	0.60
1:B:655:THR:HG23	1:B:659:ILE:CD1	2.28	0.60
1:B:677:ILE:HG12	1:B:678:SER:N	2.15	0.60
1:C:776:SER:H	1:C:812:ARG:CB	2.15	0.60
1:A:506:TRP:CH2	1:A:508:GLY:HA2	2.36	0.60
1:A:682:ALA:HB1	1:A:683:PRO:HD3	1.84	0.60
1:A:134:SER:HB3	1:A:139:THR:HB	1.84	0.60
1:B:260:GLY:O	1:B:594:MSE:HB2	2.01	0.60
1:B:391:TRP:CD1	1:B:393:GLN:HG3	2.36	0.60
1:B:783:ASN:HB3	1:B:805:ARG:HA	1.82	0.60
1:C:536:ARG:CG	1:C:536:ARG:O	2.42	0.60
1:A:596:GLN:HG2	1:A:600:TYR:CD2	2.37	0.59
1:C:741:TRP:HA	1:C:755:PHE:O	2.02	0.59
1:A:554:TYR:CG	1:A:595:PRO:HG3	2.36	0.59
1:B:391:TRP:HD1	1:B:393:GLN:HG3	1.67	0.59
1:C:340:LEU:CB	1:C:343:ASP:HB2	2.32	0.59
1:C:596:GLN:HG2	1:C:600:TYR:CD2	2.37	0.59
1:C:600:TYR:O	1:C:607:LEU:HA	2.01	0.59
1:A:380:ARG:HH11	1:A:380:ARG:HG3	1.67	0.59
1:B:340:LEU:CB	1:B:343:ASP:HB2	2.32	0.59
1:A:698:ASP:O	1:A:701:GLY:N	2.35	0.59
1:A:697:ARG:NH2	1:A:703:LYS:NZ	2.50	0.59
1:B:350:ALA:CB	1:B:398:VAL:HG22	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:SER:H	1:B:812:ARG:CB	2.15	0.59
1:B:782:ASN:HB3	1:B:806:ASN:HD22	1.67	0.59
1:C:216:ASN:HA	1:C:227:ARG:HH21	1.66	0.59
1:C:681:LEU:HD22	1:C:687:VAL:HG11	1.84	0.59
1:C:689:ALA:HB2	1:C:715:LEU:HD12	1.83	0.59
1:B:136:GLN:HG2	1:B:137:LEU:N	2.16	0.59
1:C:200:TYR:HD1	1:C:795:PHE:CZ	2.21	0.59
1:C:177:MSE:HA	1:C:182:LEU:HD12	1.83	0.59
4:J:1:PVE:H212	4:J:1:PVE:N11	2.16	0.59
1:A:185:ILE:O	1:A:185:ILE:HD13	2.03	0.59
1:A:260:GLY:O	1:A:594:MSE:HB2	2.03	0.59
1:A:813:TRP:O	1:A:814:ASP:HB2	2.01	0.59
1:B:434:TRP:CB	1:B:441:ALA:HB1	2.30	0.59
1:B:543:LEU:HA	1:B:576:VAL:O	2.02	0.59
1:C:529:LEU:HB2	1:C:553:ASP:OD2	2.03	0.59
1:B:447:LYS:HD2	1:B:515:TRP:CD1	2.38	0.59
1:B:596:GLN:HG2	1:B:600:TYR:HD2	1.68	0.59
1:B:682:ALA:HB1	1:B:683:PRO:CD	2.32	0.59
1:C:346:LEU:HA	1:C:402:LEU:HB3	1.83	0.59
1:C:655:THR:OG1	1:C:659:ILE:HD12	2.01	0.59
1:A:745:TYR:HB2	1:A:752:TRP:HE1	1.67	0.59
1:B:706:THR:OG1	1:B:741:TRP:CD1	2.53	0.59
1:C:287:SER:O	1:C:290:ASN:HB2	2.03	0.59
1:C:682:ALA:HB1	1:C:683:PRO:HD3	1.85	0.59
1:A:246:VAL:O	1:A:246:VAL:HG13	2.03	0.58
1:A:344:THR:HG1	1:A:404:HIS:HA	1.66	0.58
1:B:240:MSE:HE2	1:B:240:MSE:HA	1.85	0.58
1:B:324:HIS:CE1	1:B:383:ASN:HB3	2.35	0.58
1:C:243:TYR:CE2	1:C:268:LEU:HB3	2.37	0.58
1:A:546:PHE:O	1:A:573:VAL:HA	2.03	0.58
1:A:768:ARG:HB2	1:A:778:SER:HB3	1.85	0.58
1:C:236:THR:HG23	1:C:237:LEU:HD23	1.80	0.58
1:C:474:LEU:CD1	1:C:533:MSE:HG3	2.25	0.58
1:C:745:TYR:HB2	1:C:752:TRP:HE1	1.68	0.58
1:A:324:HIS:CE1	1:A:383:ASN:HB3	2.31	0.58
1:A:771:ILE:HG13	1:A:772:THR:CG2	2.29	0.58
1:C:350:ALA:HB2	1:C:398:VAL:HG22	1.84	0.58
1:C:365:SER:C	1:C:384:ASN:ND2	2.56	0.58
1:C:511:GLY:O	1:C:513:PRO:HD3	2.03	0.58
1:A:776:SER:H	1:A:812:ARG:CB	2.15	0.58
1:A:538:ASN:N	1:A:538:ASN:HD22	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:MSE:HE1	1:C:266:ILE:CD1	2.32	0.58
1:C:394:TYR:CE1	1:C:422:GLY:HA3	2.38	0.58
1:C:691:TYR:HA	1:C:712:GLN:O	2.04	0.58
1:B:370:ASP:O	1:B:372:GLN:N	2.36	0.58
1:C:432:GLY:O	1:C:433:ASP:C	2.42	0.58
1:B:185:ILE:HG23	1:B:186:ASP:N	2.19	0.58
1:C:228:ASN:HA	2:K:3:ARG:HH11	1.66	0.58
1:A:619:GLY:HA3	1:A:634:ALA:HB2	1.86	0.58
1:A:657:PRO:C	1:A:659:ILE:N	2.57	0.58
1:C:185:ILE:HG23	1:C:186:ASP:N	2.18	0.58
1:C:416:LEU:CD2	1:C:457:LEU:HD12	2.32	0.58
1:C:447:LYS:HD2	1:C:515:TRP:CD1	2.39	0.58
1:C:358:LYS:HA	1:C:390:SER:HB3	1.86	0.58
1:B:432:GLY:O	1:B:433:ASP:C	2.42	0.57
1:B:691:TYR:HA	1:B:712:GLN:O	2.03	0.57
1:C:218:GLN:OE1	1:C:265:THR:HG21	2.04	0.57
1:A:357:PRO:HD2	1:A:392:GLU:HA	1.85	0.57
1:B:655:THR:HG22	1:B:655:THR:O	2.03	0.57
1:C:552:VAL:HG11	1:C:593:PHE:CZ	2.39	0.57
1:C:683:PRO:HG2	1:C:684:GLY:N	2.18	0.57
1:A:370:ASP:O	1:A:371:SER:C	2.43	0.57
1:A:350:ALA:CB	1:A:398:VAL:HG22	2.35	0.57
1:B:169:ILE:HD11	1:B:249:LEU:HD12	1.86	0.57
1:B:446:GLN:HG2	1:B:491:TRP:HB3	1.86	0.57
1:B:754:LYS:HD3	1:B:754:LYS:C	2.24	0.57
1:A:741:TRP:HA	1:A:755:PHE:O	2.03	0.57
1:B:764:ASP:HB2	1:B:782:ASN:HA	1.85	0.57
1:A:218:GLN:OE1	1:A:265:THR:HG21	2.03	0.57
1:B:560:ASN:O	1:B:562:THR:N	2.37	0.57
1:C:352:TYR:HD1	1:C:396:ARG:CB	2.16	0.57
1:A:394:TYR:CE1	1:A:422:GLY:HA3	2.40	0.57
1:A:540:THR:HG22	1:A:542:ASP:OD2	2.05	0.57
1:B:554:TYR:CD2	1:B:595:PRO:HG3	2.38	0.57
1:C:147:TYR:HA	1:C:173:THR:CG2	2.28	0.57
1:C:443:ILE:HG13	1:C:443:ILE:O	2.04	0.57
1:C:538:ASN:HB3	1:C:544:ASN:ND2	2.18	0.57
1:B:682:ALA:HB1	1:B:683:PRO:HD3	1.87	0.57
1:C:370:ASP:O	1:C:371:SER:C	2.42	0.57
1:A:401:ASN:HB3	1:A:415:GLN:HB3	1.86	0.57
1:B:619:GLY:HA3	1:B:634:ALA:HB2	1.87	0.57
1:C:434:TRP:CB	1:C:441:ALA:HB1	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ASN:HD21	1:B:261:SER:H	1.51	0.57
1:C:281:VAL:HG13	1:C:281:VAL:O	2.05	0.57
1:C:554:TYR:CE2	1:C:595:PRO:CG	2.88	0.57
1:A:543:LEU:HA	1:A:576:VAL:O	2.04	0.57
1:A:167:GLN:NE2	1:A:572:TYR:CE1	2.73	0.57
1:C:352:TYR:CE1	1:C:396:ARG:HG2	2.37	0.57
1:A:233:ALA:HA	1:A:393:GLN:OE1	2.05	0.56
1:B:698:ASP:O	1:B:699:ASP:C	2.43	0.56
1:A:540:THR:C	1:A:542:ASP:H	2.09	0.56
1:A:719:TYR:HE2	1:A:721:PHE:HD1	1.54	0.56
1:A:768:ARG:HG3	1:A:778:SER:CB	2.33	0.56
1:B:136:GLN:CG	1:B:413:LYS:HZ1	2.18	0.56
1:B:140:ILE:HG22	1:B:141:THR:H	1.68	0.56
1:B:404:HIS:O	1:B:411:VAL:HG23	2.05	0.56
1:B:506:TRP:CH2	1:B:508:GLY:HA2	2.39	0.56
1:B:596:GLN:HG2	1:B:600:TYR:CD2	2.40	0.56
1:B:631:THR:HG22	1:B:677:ILE:HG13	1.86	0.56
1:C:401:ASN:HB3	1:C:415:GLN:HB3	1.87	0.56
1:C:503:PHE:O	1:C:506:TRP:HB3	2.05	0.56
1:C:543:LEU:HA	1:C:576:VAL:O	2.05	0.56
1:C:698:ASP:O	1:C:699:ASP:C	2.43	0.56
1:A:145:GLY:CA	1:A:175:GLN:HG2	2.35	0.56
1:A:145:GLY:HA2	1:A:175:GLN:HG2	1.87	0.56
1:A:391:TRP:O	1:A:391:TRP:HD1	1.88	0.56
1:A:467:PHE:HE2	1:A:468:LEU:CD2	2.16	0.56
1:A:511:GLY:O	1:A:513:PRO:HD3	2.04	0.56
1:A:496:TYR:CE1	1:A:513:PRO:HB3	2.40	0.56
1:B:196:THR:HG21	1:B:709:PRO:HD2	1.87	0.56
1:C:540:THR:C	1:C:542:ASP:H	2.09	0.56
1:C:762:LEU:HD21	1:C:789:TYR:CE2	2.37	0.56
1:A:432:GLY:O	1:A:433:ASP:C	2.42	0.56
1:A:790:TYR:CE1	1:A:801:TYR:CE1	2.93	0.56
1:B:401:ASN:HB3	1:B:415:GLN:HB3	1.87	0.56
1:B:477:GLY:HA3	1:B:532:TYR:CE1	2.40	0.56
1:B:511:GLY:O	1:B:513:PRO:HD3	2.05	0.56
1:C:391:TRP:CZ3	1:C:427:LEU:HD11	2.40	0.56
1:C:707:TRP:O	1:C:709:PRO:HD3	2.05	0.56
1:A:467:PHE:HE2	1:A:468:LEU:HD23	1.67	0.56
1:A:255:LEU:O	1:A:550:ARG:HD2	2.06	0.56
1:A:683:PRO:HG2	1:A:684:GLY:N	2.21	0.56
1:B:191:HIS:CD2	1:B:716:TYR:CZ	2.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:VAL:HG13	1:C:246:VAL:O	2.05	0.56
1:C:538:ASN:HD22	1:C:538:ASN:H	1.51	0.56
1:A:185:ILE:HG23	1:A:186:ASP:N	2.20	0.56
1:A:631:THR:HG22	1:A:677:ILE:HG22	1.88	0.56
1:A:774:LYS:O	1:A:775:LEU:HB2	2.06	0.56
1:B:554:TYR:O	1:B:564:ARG:HB2	2.06	0.56
1:A:247:GLU:HG3	1:A:267:ASN:HB3	1.86	0.56
1:B:242:ILE:O	1:B:271:LYS:HG3	2.06	0.56
1:B:392:GLU:HB3	1:B:424:HIS:HB3	1.86	0.56
1:B:745:TYR:HE1	1:B:750:SER:O	1.86	0.56
1:A:140:ILE:HG22	1:A:141:THR:H	1.70	0.56
1:A:774:LYS:O	1:A:775:LEU:CB	2.53	0.56
1:B:358:LYS:HA	1:B:390:SER:HB3	1.88	0.56
1:B:538:ASN:N	1:B:538:ASN:HD22	2.02	0.56
1:C:280:HIS:O	1:C:295:LEU:HD12	2.05	0.56
1:C:568:ARG:HA	1:C:568:ARG:NE	2.20	0.56
1:B:540:THR:C	1:B:542:ASP:H	2.09	0.56
1:C:391:TRP:O	1:C:391:TRP:CD1	2.59	0.56
1:C:554:TYR:O	1:C:564:ARG:HB2	2.06	0.56
1:C:689:ALA:HB1	1:C:714:SER:O	2.05	0.56
1:A:190:ARG:NH1	1:A:197:VAL:CG1	2.69	0.56
1:A:220:ASP:OD2	1:A:270:ARG:HG3	2.05	0.56
1:A:560:ASN:O	1:A:562:THR:N	2.39	0.56
1:B:706:THR:OG1	1:B:741:TRP:CE2	2.58	0.56
1:C:653:LYS:O	1:C:655:THR:N	2.38	0.56
1:A:694:LYS:O	1:A:694:LYS:HD3	2.05	0.56
1:B:341:ASN:O	1:B:343:ASP:N	2.39	0.56
1:B:387:LYS:N	1:B:508:GLY:O	2.29	0.56
1:B:689:ALA:HB2	1:B:715:LEU:HA	1.88	0.56
1:C:394:TYR:OH	1:C:422:GLY:HA3	2.05	0.56
1:C:140:ILE:HG22	1:C:141:THR:H	1.70	0.55
1:C:233:ALA:HA	1:C:393:GLN:OE1	2.05	0.55
1:A:323:ASP:O	1:A:325:TYR:N	2.39	0.55
1:A:358:LYS:HA	1:A:390:SER:HB3	1.87	0.55
1:A:443:ILE:HG13	1:A:443:ILE:O	2.06	0.55
1:A:529:LEU:HB2	1:A:553:ASP:OD2	2.06	0.55
1:B:503:PHE:O	1:B:506:TRP:HB3	2.06	0.55
1:B:689:ALA:HB2	1:B:715:LEU:CD1	2.36	0.55
1:A:185:ILE:HD13	1:A:189:MSE:HG2	1.89	0.55
1:A:503:PHE:O	1:A:506:TRP:HB3	2.07	0.55
1:B:486:GLU:HA	1:B:522:ILE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:ARG:NH1	1:C:755:PHE:HE1	2.04	0.55
1:A:719:TYR:CE2	1:A:721:PHE:CD1	2.94	0.55
1:B:201:ASP:HB3	1:B:363:SER:N	2.22	0.55
1:B:653:LYS:H	1:B:653:LYS:CD	2.12	0.55
1:C:689:ALA:HB2	1:C:715:LEU:HA	1.88	0.55
1:A:648:ALA:O	1:A:649:LEU:C	2.44	0.55
1:B:253:THR:CG2	1:B:265:THR:OG1	2.54	0.55
1:B:394:TYR:CE1	1:B:422:GLY:HA3	2.41	0.55
1:C:391:TRP:O	1:C:391:TRP:HD1	1.88	0.55
1:C:526:THR:HG22	1:C:554:TYR:HE1	1.71	0.55
1:C:716:TYR:CD1	1:C:733:GLY:HA3	2.42	0.55
1:A:246:VAL:CG2	1:A:268:LEU:HD23	2.30	0.55
1:A:689:ALA:HB2	1:A:715:LEU:HA	1.89	0.55
1:B:538:ASN:CB	1:B:544:ASN:OD1	2.54	0.55
1:C:352:TYR:CD1	1:C:396:ARG:CD	2.89	0.55
1:C:694:LYS:HD3	1:C:710:GLN:HA	1.89	0.55
1:A:552:VAL:CG2	1:A:553:ASP:N	2.70	0.55
1:A:658:ALA:O	1:A:659:ILE:O	2.24	0.55
1:A:375:ARG:NH1	1:A:755:PHE:HE1	2.05	0.55
1:C:220:ASP:OD2	1:C:270:ARG:NE	2.40	0.55
1:C:552:VAL:CG2	1:C:553:ASP:N	2.69	0.55
1:C:560:ASN:O	1:C:562:THR:N	2.40	0.55
1:A:707:TRP:O	1:A:709:PRO:HD3	2.07	0.55
1:C:552:VAL:HG11	1:C:593:PHE:HZ	1.72	0.55
1:C:689:ALA:CB	1:C:715:LEU:HA	2.37	0.55
1:A:475:VAL:HG22	1:A:475:VAL:O	2.07	0.55
1:C:216:ASN:HA	1:C:227:ARG:NH2	2.22	0.55
1:C:357:PRO:HD2	1:C:392:GLU:HA	1.88	0.55
1:C:475:VAL:O	1:C:475:VAL:HG22	2.06	0.55
1:C:496:TYR:CE1	1:C:513:PRO:HB3	2.42	0.55
1:C:709:PRO:HG2	1:C:737:GLN:HB2	1.89	0.55
1:A:391:TRP:O	1:A:391:TRP:CD1	2.59	0.55
1:A:568:ARG:NE	1:A:568:ARG:HA	2.21	0.55
1:A:595:PRO:HA	1:A:610:PRO:HB3	1.89	0.55
1:B:370:ASP:O	1:B:371:SER:C	2.44	0.55
1:B:552:VAL:CG2	1:B:553:ASP:N	2.69	0.55
1:C:341:ASN:O	1:C:343:ASP:N	2.40	0.55
1:C:694:LYS:HE2	1:C:708:GLU:O	2.06	0.55
1:A:423:TYR:CD1	1:A:423:TYR:O	2.60	0.54
1:A:554:TYR:O	1:A:564:ARG:HB2	2.07	0.54
1:B:683:PRO:HG2	1:B:684:GLY:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:HIS:O	1:C:411:VAL:HG23	2.08	0.54
1:A:691:TYR:HA	1:A:712:GLN:O	2.07	0.54
1:B:721:PHE:HD2	1:B:725:LEU:HD12	1.72	0.54
1:B:375:ARG:NH1	1:B:755:PHE:HE1	2.05	0.54
1:C:386:ALA:O	1:C:389:SER:N	2.37	0.54
1:A:342:PRO:C	1:A:344:THR:N	2.61	0.54
1:A:341:ASN:O	1:A:343:ASP:N	2.40	0.54
1:A:348:VAL:HG12	1:A:400:ALA:HA	1.88	0.54
1:A:698:ASP:O	1:A:699:ASP:C	2.46	0.54
1:B:538:ASN:HA	1:B:544:ASN:HA	1.89	0.54
1:B:764:ASP:HA	1:B:784:VAL:HG23	1.88	0.54
1:B:766:MSE:SE	1:B:766:MSE:C	2.96	0.54
1:C:200:TYR:CE2	1:C:206:ASN:HB3	2.41	0.54
1:C:774:LYS:O	1:C:775:LEU:CB	2.56	0.54
1:C:812:ARG:HG3	1:C:813:TRP:N	2.15	0.54
1:A:510:ILE:CG2	1:A:511:GLY:N	2.70	0.54
1:A:769:TYR:HD2	1:A:771:ILE:HG22	1.73	0.54
1:B:348:VAL:HG12	1:B:400:ALA:HA	1.88	0.54
1:C:538:ASN:N	1:C:538:ASN:HD22	2.05	0.54
1:C:607:LEU:O	1:C:608:LEU:C	2.44	0.54
1:A:341:ASN:C	1:A:343:ASP:N	2.61	0.54
1:B:484:HIS:ND1	1:B:525:LYS:HG2	2.22	0.54
1:B:589:TYR:CE1	1:B:614:GLN:HB3	2.42	0.54
1:B:650:TYR:HE1	1:B:654:PRO:HD2	1.71	0.54
1:C:298:SER:HB2	1:C:310:ARG:HG3	1.90	0.54
1:C:350:ALA:CB	1:C:398:VAL:HG22	2.38	0.54
1:B:184:ASN:OD1	1:B:186:ASP:N	2.41	0.54
1:A:689:ALA:HB1	1:A:714:SER:O	2.08	0.54
1:B:173:THR:OG1	1:B:174:ARG:N	2.40	0.54
1:B:191:HIS:HD2	1:B:716:TYR:CZ	2.26	0.54
1:B:200:TYR:CE2	1:B:206:ASN:HB3	2.43	0.54
1:B:341:ASN:C	1:B:343:ASP:N	2.61	0.54
1:B:569:PHE:CE2	1:B:571:PRO:HB3	2.43	0.54
1:B:597:ASP:HB3	1:B:599:TRP:CE3	2.42	0.54
1:C:253:THR:OG1	1:C:257:THR:CG2	2.56	0.54
1:C:220:ASP:OD2	1:C:270:ARG:HG3	2.08	0.54
1:C:255:LEU:O	1:C:550:ARG:HD2	2.08	0.54
1:C:595:PRO:HA	1:C:610:PRO:HB3	1.90	0.54
1:C:484:HIS:ND1	1:C:525:LYS:HG2	2.22	0.54
1:C:631:THR:HG22	1:C:677:ILE:HG13	1.90	0.54
1:A:271:LYS:HB3	1:A:310:ARG:CZ	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:O	1:A:341:ASN:HB2	2.07	0.54
1:A:597:ASP:HB3	1:A:599:TRP:CE3	2.43	0.54
1:C:342:PRO:C	1:C:344:THR:N	2.61	0.54
1:C:769:TYR:HD2	1:C:771:ILE:HG22	1.73	0.54
1:A:689:ALA:CB	1:A:715:LEU:HA	2.38	0.54
1:B:607:LEU:O	1:B:608:LEU:C	2.47	0.54
1:B:755:PHE:HB3	1:B:793:ILE:HG21	1.89	0.54
1:C:167:GLN:NE2	1:C:572:TYR:CE1	2.76	0.54
1:C:271:LYS:HB3	1:C:310:ARG:CZ	2.38	0.54
1:C:746:ASN:HD21	1:C:749:ARG:HG2	1.71	0.54
1:A:446:GLN:HB3	1:A:448:TYR:HE1	1.73	0.53
1:A:607:LEU:O	1:A:608:LEU:C	2.46	0.53
1:B:220:ASP:OD2	1:B:270:ARG:NE	2.41	0.53
1:B:754:LYS:N	1:B:754:LYS:CD	2.71	0.53
1:C:442:LYS:HA	1:C:498:ASN:O	2.07	0.53
1:C:158:LEU:HD13	1:C:475:VAL:HB	1.89	0.53
1:C:592:ILE:HG12	1:C:593:PHE:N	2.23	0.53
1:A:366:PHE:HB3	1:A:382:PHE:HD2	1.73	0.53
1:A:447:LYS:HD2	1:A:515:TRP:CD1	2.43	0.53
1:A:681:LEU:HB2	1:A:687:VAL:HG12	1.91	0.53
1:C:170:THR:HG21	1:C:193:PRO:HG2	1.91	0.53
1:A:184:ASN:OD1	1:A:186:ASP:N	2.41	0.53
1:B:596:GLN:OE1	1:B:644:ALA:HB2	2.08	0.53
1:B:689:ALA:CB	1:B:715:LEU:HA	2.38	0.53
1:B:689:ALA:HB1	1:B:714:SER:O	2.07	0.53
1:C:324:HIS:CE1	1:C:383:ASN:HB3	2.33	0.53
1:A:651:ASN:O	1:A:653:LYS:HG3	2.09	0.53
1:B:218:GLN:OE1	1:B:265:THR:HG21	2.07	0.53
1:B:323:ASP:O	1:B:325:TYR:N	2.42	0.53
1:B:689:ALA:HB2	1:B:715:LEU:HD12	1.89	0.53
1:B:769:TYR:HD2	1:B:771:ILE:HG22	1.73	0.53
1:C:375:ARG:CZ	1:C:755:PHE:CE1	2.91	0.53
1:C:774:LYS:O	1:C:775:LEU:HB2	2.09	0.53
1:A:394:TYR:OH	1:A:422:GLY:HA3	2.07	0.53
1:A:592:ILE:HG12	1:A:593:PHE:N	2.22	0.53
1:A:689:ALA:HB2	1:A:715:LEU:CD1	2.38	0.53
1:A:740:SER:O	1:A:756:SER:HA	2.09	0.53
1:B:231:TYR:CE2	1:B:485:TRP:HH2	2.27	0.53
1:B:241:ALA:HB2	1:B:292:ARG:NH2	2.24	0.53
1:B:716:TYR:CD1	1:B:733:GLY:HA3	2.43	0.53
1:A:378:VAL:HG22	1:A:382:PHE:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LYS:N	1:A:508:GLY:O	2.30	0.53
1:B:296:ASP:OD2	1:B:310:ARG:NH2	2.42	0.53
1:B:446:GLN:HB3	1:B:448:TYR:HE1	1.74	0.53
1:B:707:TRP:O	1:B:709:PRO:HD3	2.08	0.53
1:C:281:VAL:HB	1:C:295:LEU:HD13	1.91	0.53
1:C:372:GLN:OE1	1:C:372:GLN:N	2.42	0.53
1:C:538:ASN:HA	1:C:544:ASN:HA	1.90	0.53
1:C:638:ILE:HD12	1:C:670:THR:HG21	1.91	0.53
1:A:152:ILE:HD13	1:A:169:ILE:HG21	1.91	0.53
1:A:375:ARG:CZ	1:A:755:PHE:CE1	2.91	0.53
1:A:366:PHE:HB3	1:A:382:PHE:CD2	2.44	0.53
1:A:655:THR:O	1:A:659:ILE:HB	2.09	0.53
1:B:342:PRO:C	1:B:344:THR:N	2.61	0.53
1:B:157:ARG:HD3	1:B:460:TYR:CD2	2.43	0.53
1:C:539:VAL:HB	1:C:543:LEU:CD2	2.39	0.53
1:A:201:ASP:N	1:A:201:ASP:OD1	2.41	0.53
1:B:266:ILE:HG22	1:B:267:ASN:N	2.24	0.53
1:C:538:ASN:CB	1:C:544:ASN:HD22	2.21	0.53
1:C:683:PRO:CG	1:C:684:GLY:H	2.21	0.53
1:C:740:SER:O	1:C:756:SER:HA	2.09	0.53
1:A:242:ILE:O	1:A:271:LYS:HG3	2.09	0.53
1:A:551:VAL:HG22	1:A:552:VAL:H	1.73	0.53
1:B:189:MSE:HE1	1:B:266:ILE:CD1	2.38	0.53
1:B:396:ARG:HG3	1:B:420:ILE:HD11	1.90	0.53
1:B:774:LYS:O	1:B:775:LEU:HB2	2.09	0.53
1:C:266:ILE:HG22	1:C:267:ASN:N	2.24	0.53
1:C:339:ASP:C	1:C:340:LEU:HG	2.28	0.53
1:C:506:TRP:CE2	1:C:508:GLY:HA2	2.44	0.53
1:A:484:HIS:ND1	1:A:525:LYS:HG2	2.24	0.53
1:A:477:GLY:HA3	1:A:532:TYR:CE1	2.44	0.53
1:B:247:GLU:CG	1:B:267:ASN:HD22	2.22	0.53
1:B:344:THR:HG21	1:B:405:ASN:ND2	2.24	0.53
1:B:625:LEU:HD13	1:B:628:ARG:NH1	2.23	0.53
1:C:246:VAL:CG2	1:C:268:LEU:HD23	2.39	0.53
1:C:596:GLN:OE1	1:C:644:ALA:HB2	2.08	0.53
1:A:372:GLN:N	1:A:372:GLN:OE1	2.42	0.52
1:A:670:THR:O	1:A:670:THR:HG22	2.08	0.52
1:B:496:TYR:CE1	1:B:513:PRO:HB3	2.43	0.52
1:B:738:GLY:O	1:B:739:LYS:O	2.28	0.52
1:C:201:ASP:OD2	1:C:204:ARG:NE	2.41	0.52
1:C:378:VAL:HG22	1:C:382:PHE:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ARG:NH1	1:C:532:TYR:OH	2.42	0.52
1:A:241:ALA:HB2	1:A:292:ARG:NH2	2.24	0.52
1:A:743:MSE:SE	1:A:753:GLU:O	2.77	0.52
1:B:372:GLN:OE1	1:B:372:GLN:N	2.41	0.52
1:B:619:GLY:HA3	1:B:634:ALA:CB	2.39	0.52
1:C:145:GLY:CA	1:C:175:GLN:HG2	2.38	0.52
1:C:186:ASP:C	1:C:188:VAL:H	2.13	0.52
1:C:211:GLY:N	1:C:708:GLU:OE1	2.43	0.52
1:A:404:HIS:O	1:A:411:VAL:HG23	2.10	0.52
1:A:599:TRP:HE1	2:I:4:DSN:HA	1.73	0.52
1:B:372:GLN:HA	1:B:748:PRO:HB3	1.91	0.52
1:B:658:ALA:O	1:B:659:ILE:O	2.27	0.52
1:B:706:THR:OG1	1:B:741:TRP:CG	2.62	0.52
1:C:446:GLN:HB3	1:C:448:TYR:CE1	2.45	0.52
1:A:470:ARG:NH1	1:A:470:ARG:HG2	2.23	0.52
1:B:158:LEU:HD13	1:B:475:VAL:HB	1.91	0.52
1:C:157:ARG:HD3	1:C:460:TYR:CD2	2.44	0.52
1:A:441:ALA:H	1:A:500:THR:HG22	1.75	0.52
1:A:590:THR:OG1	1:A:615:ASN:HB3	2.10	0.52
1:B:443:ILE:HG13	1:B:443:ILE:O	2.09	0.52
1:B:725:LEU:C	1:B:727:LYS:H	2.12	0.52
1:B:763:VAL:HG11	1:B:785:PHE:CD2	2.45	0.52
1:C:194:GLY:HA3	1:C:250:LYS:NZ	2.24	0.52
1:C:148:THR:HB	1:C:679:GLY:HA2	1.91	0.52
1:C:694:LYS:O	1:C:694:LYS:HD3	2.09	0.52
1:A:186:ASP:C	1:A:188:VAL:H	2.13	0.52
1:A:271:LYS:HD3	1:A:310:ARG:NH2	2.25	0.52
1:A:486:GLU:HA	1:A:522:ILE:O	2.10	0.52
1:A:619:GLY:HA3	1:A:634:ALA:CB	2.39	0.52
1:B:589:TYR:HE1	1:B:614:GLN:CB	2.23	0.52
1:B:745:TYR:HB2	1:B:752:TRP:HE1	1.74	0.52
1:C:185:ILE:O	1:C:188:VAL:HB	2.10	0.52
1:C:341:ASN:C	1:C:343:ASP:N	2.61	0.52
1:C:439:ASN:HD21	1:C:504:ILE:HG22	1.75	0.52
1:C:446:GLN:HG2	1:C:491:TRP:CB	2.39	0.52
1:C:527:ARG:HH11	1:C:529:LEU:CD1	2.23	0.52
1:A:201:ASP:HB3	1:A:363:SER:N	2.25	0.52
1:A:439:ASN:HD21	1:A:504:ILE:HG22	1.75	0.52
1:B:595:PRO:HA	1:B:610:PRO:HB3	1.91	0.52
1:B:740:SER:O	1:B:756:SER:HA	2.10	0.52
1:A:527:ARG:HH11	1:A:529:LEU:CD1	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:GLY:O	1:A:803:ASP:C	2.48	0.52
1:B:135:ASN:ND2	1:B:138:GLY:O	2.43	0.52
1:B:325:TYR:CE1	1:B:327:ARG:HB3	2.44	0.52
1:B:529:LEU:HB2	1:B:553:ASP:OD2	2.10	0.52
1:B:790:TYR:CE1	1:B:801:TYR:CE1	2.96	0.52
1:A:185:ILE:O	1:A:188:VAL:N	2.39	0.52
1:A:240:MSE:C	1:A:242:ILE:H	2.13	0.52
1:B:148:THR:HB	1:B:679:GLY:HA2	1.92	0.52
1:C:341:ASN:O	1:C:342:PRO:C	2.48	0.52
1:C:551:VAL:HG22	1:C:552:VAL:H	1.74	0.52
1:C:625:LEU:HD13	1:C:628:ARG:NH1	2.24	0.52
1:C:681:LEU:HB2	1:C:687:VAL:HG12	1.91	0.52
1:C:200:TYR:CD1	1:C:795:PHE:CZ	2.97	0.52
1:A:192:THR:CB	1:A:195:ILE:HD12	2.39	0.52
1:A:339:ASP:C	1:A:340:LEU:HG	2.29	0.52
1:A:506:TRP:CE2	1:A:508:GLY:HA2	2.45	0.52
1:B:247:GLU:HG3	1:B:267:ASN:HB3	1.91	0.52
1:B:357:PRO:HG2	1:B:391:TRP:H	1.75	0.52
1:B:446:GLN:HB3	1:B:448:TYR:CE1	2.45	0.52
1:B:681:LEU:HB2	1:B:687:VAL:HG12	1.92	0.52
1:A:152:ILE:CD1	1:A:169:ILE:HG21	2.40	0.51
1:A:189:MSE:CE	1:A:195:ILE:HG21	2.39	0.51
1:A:271:LYS:HZ3	1:A:310:ARG:NH2	2.06	0.51
1:A:812:ARG:CG	1:A:813:TRP:H	2.13	0.51
1:B:185:ILE:CG2	1:B:186:ASP:N	2.74	0.51
1:B:270:ARG:NH1	1:B:351:ASP:OD2	2.44	0.51
1:B:341:ASN:O	1:B:344:THR:N	2.43	0.51
1:B:357:PRO:HD2	1:B:392:GLU:HA	1.91	0.51
1:B:723:GLY:O	1:B:724:ALA:C	2.49	0.51
1:C:357:PRO:HG2	1:C:391:TRP:H	1.74	0.51
1:A:288:TRP:O	1:A:319:HIS:HB2	2.09	0.51
1:A:446:GLN:HG2	1:A:491:TRP:CB	2.40	0.51
1:A:211:GLY:N	1:A:708:GLU:OE1	2.41	0.51
1:A:726:ASP:N	1:A:726:ASP:OD1	2.41	0.51
1:A:762:LEU:HD21	1:A:789:TYR:CE2	2.38	0.51
1:B:709:PRO:HG2	1:B:737:GLN:HB2	1.92	0.51
1:C:152:ILE:CD1	1:C:169:ILE:HG21	2.41	0.51
1:C:185:ILE:CG2	1:C:186:ASP:N	2.73	0.51
1:C:624:TYR:N	1:C:624:TYR:CD1	2.79	0.51
1:C:372:GLN:HA	1:C:748:PRO:HB3	1.91	0.51
1:A:158:LEU:HD13	1:A:475:VAL:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:GLY:HA2	1:B:175:GLN:HG2	1.92	0.51
1:B:220:ASP:OD2	1:B:270:ARG:HG3	2.09	0.51
1:B:423:TYR:O	1:B:423:TYR:CD1	2.63	0.51
1:B:802:GLY:O	1:B:803:ASP:C	2.48	0.51
1:B:812:ARG:HG3	1:B:813:TRP:N	2.16	0.51
1:C:152:ILE:HD13	1:C:169:ILE:HG21	1.92	0.51
1:C:323:ASP:O	1:C:325:TYR:N	2.44	0.51
1:C:486:GLU:HA	1:C:522:ILE:O	2.09	0.51
1:C:518:PRO:HB2	1:C:521:TYR:CZ	2.45	0.51
1:A:281:VAL:HB	1:A:295:LEU:HD13	1.92	0.51
1:B:140:ILE:HG22	1:B:142:GLU:H	1.76	0.51
1:B:279:GLY:O	1:B:280:HIS:HB3	2.10	0.51
1:B:280:HIS:C	1:B:280:HIS:CD2	2.83	0.51
1:B:339:ASP:C	1:B:340:LEU:HG	2.31	0.51
1:B:510:ILE:CG2	1:B:511:GLY:N	2.73	0.51
1:B:774:LYS:O	1:B:775:LEU:CB	2.58	0.51
1:C:365:SER:CA	1:C:384:ASN:ND2	2.74	0.51
1:C:446:GLN:HB3	1:C:448:TYR:HE1	1.74	0.51
1:C:590:THR:OG1	1:C:615:ASN:HB3	2.11	0.51
1:A:228:ASN:OD1	1:A:230:GLY:N	2.43	0.51
1:A:253:THR:OG1	1:A:257:THR:CG2	2.59	0.51
1:A:360:SER:HB3	1:A:390:SER:CA	2.38	0.51
1:A:357:PRO:HG2	1:A:391:TRP:H	1.75	0.51
1:A:716:TYR:CD1	1:A:733:GLY:HA3	2.46	0.51
1:B:194:GLY:HA3	1:B:250:LYS:NZ	2.25	0.51
1:C:201:ASP:HB3	1:C:363:SER:N	2.26	0.51
1:C:618:ILE:O	1:C:618:ILE:CG2	2.57	0.51
1:A:396:ARG:HG3	1:A:420:ILE:HD11	1.91	0.51
1:A:624:TYR:CD1	1:A:624:TYR:N	2.79	0.51
1:A:640:GLU:OE2	1:A:643:ARG:HG3	2.10	0.51
1:B:375:ARG:CZ	1:B:755:PHE:CE1	2.93	0.51
1:C:192:THR:CB	1:C:195:ILE:HD12	2.40	0.51
1:C:510:ILE:CG2	1:C:511:GLY:N	2.73	0.51
1:C:725:LEU:C	1:C:727:LYS:H	2.13	0.51
1:A:387:LYS:HG3	1:A:509:ASP:CA	2.41	0.51
1:A:723:GLY:O	1:A:724:ALA:C	2.48	0.51
1:A:749:ARG:HH11	1:A:751:ARG:HH21	1.57	0.51
1:B:145:GLY:CA	1:B:175:GLN:HG2	2.40	0.51
1:B:646:GLU:O	1:B:646:GLU:HG3	2.09	0.51
1:B:734:ALA:HA	1:B:762:LEU:O	2.11	0.51
1:C:414:VAL:CB	1:C:459:ILE:HG22	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:ASN:ND2	1:C:435:PRO:HG2	2.25	0.51
1:C:802:GLY:O	1:C:803:ASP:C	2.48	0.51
1:A:220:ASP:OD2	1:A:270:ARG:NE	2.44	0.51
1:A:414:VAL:CB	1:A:459:ILE:HG22	2.41	0.51
1:B:170:THR:HG21	1:B:193:PRO:HG2	1.93	0.51
1:B:378:VAL:HG22	1:B:382:PHE:HB2	1.92	0.51
1:B:446:GLN:HG2	1:B:491:TRP:CB	2.39	0.51
1:B:657:PRO:C	1:B:659:ILE:H	2.14	0.51
1:B:655:THR:CG2	1:B:659:ILE:HD12	2.34	0.51
1:B:670:THR:O	1:B:670:THR:HG22	2.09	0.51
1:C:196:THR:HG21	1:C:709:PRO:HD2	1.91	0.51
1:A:218:GLN:HA	1:A:222:ILE:O	2.10	0.51
1:A:538:ASN:HA	1:A:544:ASN:HA	1.92	0.51
1:B:240:MSE:C	1:B:242:ILE:H	2.14	0.51
1:B:646:GLU:HA	1:B:663:TYR:CD2	2.46	0.51
1:C:185:ILE:C	1:C:185:ILE:HD13	2.31	0.51
1:C:790:TYR:CE1	1:C:801:TYR:CE1	2.98	0.51
1:A:140:ILE:HG22	1:A:142:GLU:H	1.74	0.51
1:A:372:GLN:HA	1:A:748:PRO:HB3	1.92	0.51
1:A:446:GLN:HB3	1:A:448:TYR:CE1	2.46	0.51
1:B:592:ILE:HG12	1:B:593:PHE:N	2.25	0.51
1:C:211:GLY:HA2	1:C:708:GLU:OE1	2.11	0.51
1:C:695:ILE:CD1	1:C:710:GLN:HE21	2.24	0.51
1:A:157:ARG:NH2	1:A:458:ASP:OD2	2.44	0.50
1:B:141:THR:C	1:B:143:ASP:H	2.15	0.50
1:B:277:PHE:CG	1:B:278:LYS:N	2.79	0.50
1:B:387:LYS:HG3	1:B:509:ASP:CA	2.41	0.50
1:C:766:MSE:SE	1:C:766:MSE:C	2.99	0.50
1:A:201:ASP:OD2	1:A:204:ARG:NE	2.42	0.50
1:A:446:GLN:HG2	1:A:491:TRP:HB3	1.93	0.50
1:B:157:ARG:NH1	1:B:532:TYR:OH	2.43	0.50
1:B:179:ASP:OD1	1:B:768:ARG:NH2	2.45	0.50
1:B:473:GLU:HG2	1:B:536:ARG:HB3	1.93	0.50
1:B:682:ALA:HB3	1:B:685:TRP:HB2	1.94	0.50
1:C:640:GLU:OE2	1:C:643:ARG:HG3	2.10	0.50
1:A:266:ILE:CG2	1:A:267:ASN:N	2.74	0.50
1:A:341:ASN:O	1:A:344:THR:N	2.45	0.50
1:A:527:ARG:HH11	1:A:529:LEU:HD11	1.77	0.50
1:A:553:ASP:HA	1:A:566:SER:HA	1.93	0.50
1:A:683:PRO:CG	1:A:684:GLY:H	2.24	0.50
1:B:185:ILE:C	1:B:185:ILE:HD13	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:TRP:O	1:B:441:ALA:HB2	2.12	0.50
1:B:647:ASP:OD1	1:B:648:ALA:N	2.45	0.50
1:B:653:LYS:HG2	1:B:659:ILE:HG13	1.92	0.50
1:B:706:THR:OG1	1:B:741:TRP:CD2	2.64	0.50
1:C:241:ALA:HB2	1:C:292:ARG:NH2	2.27	0.50
1:C:619:GLY:HA3	1:C:634:ALA:HB2	1.93	0.50
1:A:709:PRO:HG2	1:A:737:GLN:HB2	1.93	0.50
1:A:789:TYR:CE1	1:A:802:GLY:HA3	2.46	0.50
1:B:253:THR:OG1	1:B:257:THR:CG2	2.59	0.50
1:B:275:HIS:CE1	1:B:308:ARG:HH11	2.30	0.50
1:B:604:SER:O	1:B:605:ASN:HB2	2.11	0.50
1:B:650:TYR:CZ	1:B:653:LYS:HB2	2.46	0.50
1:C:168:SER:HB2	1:C:617:GLU:OE2	2.11	0.50
1:A:298:SER:HB2	1:A:310:ARG:HG3	1.94	0.50
1:A:341:ASN:CB	1:A:342:PRO:CD	2.86	0.50
1:A:388:TRP:CH2	1:A:428:GLY:HA3	2.46	0.50
1:A:725:LEU:C	1:A:727:LYS:H	2.15	0.50
1:A:749:ARG:NH1	1:A:751:ARG:HH21	2.08	0.50
1:B:255:LEU:O	1:B:550:ARG:HD2	2.11	0.50
1:B:551:VAL:HG22	1:B:552:VAL:H	1.76	0.50
1:C:240:MSE:C	1:C:242:ILE:H	2.13	0.50
1:A:467:PHE:CD2	1:A:468:LEU:CD2	2.94	0.50
1:A:569:PHE:CE2	1:A:571:PRO:HB3	2.47	0.50
1:A:653:LYS:O	1:A:653:LYS:HD2	2.12	0.50
1:B:201:ASP:OD2	1:B:204:ARG:NE	2.43	0.50
1:C:414:VAL:HB	1:C:459:ILE:HG22	1.93	0.50
1:C:412:GLY:CA	1:C:461:LEU:HD23	2.42	0.50
1:C:728:LEU:HB2	1:C:769:TYR:CD1	2.46	0.50
1:C:755:PHE:HB3	1:C:793:ILE:HG21	1.93	0.50
1:A:556:VAL:HG13	1:A:556:VAL:O	2.12	0.50
1:A:648:ALA:O	1:A:650:TYR:N	2.45	0.50
1:B:341:ASN:O	1:B:342:PRO:C	2.48	0.50
1:B:506:TRP:CE2	1:B:508:GLY:HA2	2.47	0.50
1:B:624:TYR:CD1	1:B:624:TYR:N	2.79	0.50
1:B:657:PRO:O	1:B:659:ILE:HG22	2.11	0.50
1:B:683:PRO:CG	1:B:684:GLY:H	2.25	0.50
1:C:218:GLN:HA	1:C:222:ILE:O	2.11	0.50
1:C:189:MSE:HE1	1:C:266:ILE:HD11	1.92	0.50
1:C:734:ALA:HA	1:C:762:LEU:O	2.12	0.50
1:A:148:THR:OG1	1:A:149:PRO:HD2	2.11	0.50
1:A:277:PHE:CG	1:A:278:LYS:N	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:LEU:HD12	1:A:575:ALA:HB2	1.93	0.50
1:A:625:LEU:C	1:A:627:GLY:N	2.65	0.50
1:A:596:GLN:OE1	1:A:644:ALA:HB2	2.11	0.50
1:A:783:ASN:C	1:A:783:ASN:HD22	2.15	0.50
1:B:192:THR:CB	1:B:195:ILE:HD12	2.39	0.50
1:B:553:ASP:HA	1:B:566:SER:HA	1.94	0.50
1:B:600:TYR:HD1	1:B:663:TYR:CD1	2.30	0.50
1:C:296:ASP:OD2	1:C:310:ARG:NH2	2.42	0.50
1:C:341:ASN:O	1:C:344:THR:N	2.45	0.50
1:C:441:ALA:H	1:C:500:THR:HG22	1.77	0.50
1:A:697:ARG:HH21	1:A:703:LYS:HZ2	1.59	0.50
1:B:442:LYS:HA	1:B:498:ASN:O	2.11	0.50
1:C:140:ILE:CG2	1:C:141:THR:N	2.75	0.50
1:C:145:GLY:HA2	1:C:175:GLN:HG2	1.92	0.50
1:C:247:GLU:CG	1:C:267:ASN:HD22	2.24	0.50
1:A:170:THR:HG21	1:A:193:PRO:HG2	1.94	0.49
1:A:812:ARG:HG3	1:A:813:TRP:N	2.15	0.49
1:B:247:GLU:HG3	1:B:267:ASN:HD22	1.76	0.49
1:B:346:LEU:HA	1:B:402:LEU:HB3	1.93	0.49
1:B:262:LEU:HD23	1:B:592:ILE:CG2	2.42	0.49
1:B:646:GLU:HA	1:B:663:TYR:HD2	1.76	0.49
1:C:141:THR:C	1:C:143:ASP:H	2.15	0.49
1:C:288:TRP:O	1:C:319:HIS:HB2	2.12	0.49
1:C:657:PRO:C	1:C:659:ILE:H	2.14	0.49
1:A:185:ILE:CG2	1:A:186:ASP:N	2.75	0.49
1:A:412:GLY:CA	1:A:461:LEU:HD23	2.42	0.49
1:A:414:VAL:HB	1:A:459:ILE:HG22	1.94	0.49
1:A:542:ASP:HA	1:A:578:ASP:CG	2.30	0.49
1:A:755:PHE:HB3	1:A:793:ILE:HG21	1.94	0.49
1:B:763:VAL:HG11	1:B:785:PHE:HE2	1.75	0.49
1:C:140:ILE:HG22	1:C:142:GLU:H	1.76	0.49
1:C:434:TRP:O	1:C:436:ALA:N	2.45	0.49
4:I:1:PVE:H202	4:I:1:PVE:H11	1.78	0.49
1:A:308:ARG:NH2	1:A:339:ASP:OD2	2.45	0.49
1:A:341:ASN:O	1:A:342:PRO:C	2.48	0.49
1:A:391:TRP:HD1	1:A:393:GLN:HG3	1.77	0.49
1:B:204:ARG:HD3	1:B:391:TRP:CH2	2.46	0.49
1:B:370:ASP:HB2	1:B:435:PRO:HB2	1.93	0.49
1:C:253:THR:OG1	1:C:257:THR:HG23	2.12	0.49
1:C:423:TYR:O	1:C:423:TYR:CD1	2.66	0.49
1:C:370:ASP:HB2	1:C:435:PRO:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:THR:O	1:A:256:LEU:HD12	2.12	0.49
1:A:392:GLU:HB3	1:A:424:HIS:HB3	1.93	0.49
1:A:396:ARG:HD3	1:A:420:ILE:HD11	1.95	0.49
1:B:288:TRP:O	1:B:319:HIS:HB2	2.12	0.49
1:B:388:TRP:CH2	1:B:428:GLY:HA3	2.47	0.49
1:C:470:ARG:NH1	1:C:470:ARG:HG2	2.25	0.49
1:C:569:PHE:CE2	1:C:571:PRO:HB3	2.47	0.49
1:C:738:GLY:O	1:C:739:LYS:O	2.31	0.49
1:A:694:LYS:HD3	1:A:710:GLN:HA	1.95	0.49
1:C:553:ASP:HA	1:C:566:SER:HA	1.94	0.49
1:C:751:ARG:O	1:C:751:ARG:HG3	2.12	0.49
1:B:230:GLY:HA2	4:J:1:PVE:O25	2.12	0.49
1:A:604:SER:O	1:A:605:ASN:HB2	2.13	0.49
1:A:196:THR:HG21	1:A:709:PRO:HD2	1.93	0.49
1:B:298:SER:HB2	1:B:310:ARG:HG3	1.94	0.49
1:B:386:ALA:O	1:B:389:SER:N	2.44	0.49
1:B:441:ALA:H	1:B:500:THR:HG22	1.76	0.49
1:B:628:ARG:HH11	1:B:628:ARG:HB2	1.78	0.49
1:C:387:LYS:N	1:C:508:GLY:O	2.34	0.49
1:C:604:SER:O	1:C:605:ASN:HB2	2.13	0.49
1:C:624:TYR:O	1:C:625:LEU:HB2	2.13	0.49
1:C:723:GLY:O	1:C:724:ALA:C	2.50	0.49
1:A:764:ASP:HA	1:A:784:VAL:HG23	1.94	0.49
1:B:140:ILE:CG2	1:B:141:THR:N	2.74	0.49
1:B:189:MSE:CE	1:B:266:ILE:HD12	2.41	0.49
1:B:590:THR:OG1	1:B:615:ASN:HB3	2.11	0.49
1:B:618:ILE:CG2	1:B:618:ILE:O	2.60	0.49
1:C:173:THR:OG1	1:C:174:ARG:N	2.46	0.49
1:A:292:ARG:HD2	1:A:316:GLN:OE1	2.12	0.49
1:B:182:LEU:HD22	1:B:187:ASP:O	2.13	0.49
1:C:434:TRP:C	1:C:436:ALA:H	2.16	0.49
1:C:670:THR:HG22	1:C:670:THR:O	2.11	0.49
1:A:598:SER:N	1:A:599:TRP:CE3	2.81	0.49
1:A:682:ALA:HB3	1:A:683:PRO:HD2	1.95	0.49
1:B:186:ASP:C	1:B:188:VAL:H	2.16	0.49
1:B:211:GLY:N	1:B:708:GLU:OE1	2.43	0.49
1:B:412:GLY:CA	1:B:461:LEU:HD23	2.43	0.49
1:B:556:VAL:HG13	1:B:556:VAL:O	2.11	0.49
1:B:546:PHE:N	1:B:574:GLY:O	2.43	0.49
1:B:698:ASP:O	1:B:699:ASP:O	2.30	0.49
1:C:179:ASP:OD1	1:C:768:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ASP:OD2	1:C:245:ARG:NH1	2.45	0.49
1:C:383:ASN:O	1:C:385:GLY:N	2.46	0.49
1:C:647:ASP:HB3	1:C:662:ALA:O	2.13	0.49
1:A:474:LEU:HD11	1:A:533:MSE:CG	2.31	0.49
1:B:152:ILE:HD13	1:B:169:ILE:HG21	1.94	0.49
1:B:605:ASN:ND2	1:B:605:ASN:O	2.46	0.49
1:C:538:ASN:HB2	1:C:544:ASN:HD22	1.78	0.49
1:C:698:ASP:O	1:C:699:ASP:O	2.31	0.49
1:A:599:TRP:NE1	2:I:4:DSN:HA	2.28	0.49
1:A:262:LEU:HD23	1:A:592:ILE:CG2	2.43	0.48
1:A:657:PRO:O	1:A:659:ILE:N	2.46	0.48
1:A:148:THR:HB	1:A:679:GLY:HA2	1.94	0.48
1:A:735:ARG:HG3	1:A:736:TRP:N	2.28	0.48
1:A:782:ASN:CB	1:A:806:ASN:HD22	2.25	0.48
1:B:147:TYR:HA	1:B:173:THR:CG2	2.29	0.48
1:B:325:TYR:C	1:B:326:GLU:HG3	2.34	0.48
1:B:394:TYR:OH	1:B:422:GLY:HA3	2.13	0.48
1:B:423:TYR:N	1:B:450:GLY:O	2.44	0.48
1:B:561:PRO:O	1:B:563:ILE:HG23	2.13	0.48
1:B:728:LEU:HB2	1:B:769:TYR:CD1	2.48	0.48
1:B:735:ARG:HG3	1:B:736:TRP:N	2.28	0.48
1:C:201:ASP:N	1:C:201:ASP:OD1	2.45	0.48
1:C:262:LEU:HD23	1:C:592:ILE:CG2	2.43	0.48
1:C:740:SER:O	1:C:757:GLN:N	2.38	0.48
1:A:561:PRO:O	1:A:563:ILE:HG23	2.13	0.48
1:A:659:ILE:CG1	1:A:660:THR:H	2.24	0.48
1:A:740:SER:O	1:A:757:GLN:N	2.37	0.48
1:B:418:HIS:HE1	1:B:453:LYS:HD3	1.78	0.48
1:B:537:PHE:O	1:B:545:LEU:N	2.39	0.48
1:C:185:ILE:O	1:C:188:VAL:N	2.41	0.48
1:C:370:ASP:OD2	1:C:373:GLY:HA3	2.13	0.48
1:C:545:LEU:HD12	1:C:575:ALA:HB2	1.95	0.48
1:A:434:TRP:C	1:A:436:ALA:H	2.16	0.48
1:A:442:LYS:HA	1:A:498:ASN:O	2.13	0.48
1:A:695:ILE:HD11	1:A:710:GLN:HE22	1.74	0.48
1:B:598:SER:N	1:B:599:TRP:CE3	2.81	0.48
1:C:277:PHE:CG	1:C:278:LYS:N	2.81	0.48
1:C:376:ASN:HD21	1:C:435:PRO:HG2	1.77	0.48
1:C:441:ALA:O	1:C:500:THR:HG22	2.13	0.48
1:C:527:ARG:HH11	1:C:529:LEU:HD11	1.77	0.48
1:C:561:PRO:O	1:C:563:ILE:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:764:ASP:HA	1:C:784:VAL:HG23	1.95	0.48
1:A:200:TYR:HB3	1:A:201:ASP:OD1	2.14	0.48
1:A:518:PRO:HB2	1:A:521:TYR:CZ	2.49	0.48
1:A:689:ALA:HB2	1:A:715:LEU:HD12	1.95	0.48
1:B:135:ASN:ND2	1:B:135:ASN:N	2.57	0.48
1:B:470:ARG:HH11	1:B:470:ARG:HG2	1.77	0.48
1:B:599:TRP:HE1	2:J:4:DSN:HA	1.78	0.48
1:C:646:GLU:HA	1:C:663:TYR:CD2	2.48	0.48
1:A:173:THR:OG1	1:A:174:ARG:N	2.46	0.48
1:A:624:TYR:O	1:A:625:LEU:HB2	2.12	0.48
1:B:370:ASP:OD2	1:B:373:GLY:HA3	2.14	0.48
1:B:391:TRP:CZ3	1:B:427:LEU:HD11	2.48	0.48
1:B:637:GLU:HG3	1:B:671:LYS:CB	2.38	0.48
1:C:200:TYR:HB3	1:C:201:ASP:OD1	2.13	0.48
1:C:298:SER:HB2	1:C:310:ARG:CG	2.43	0.48
1:C:352:TYR:HB2	1:C:396:ARG:HB3	1.95	0.48
1:C:789:TYR:CE1	1:C:802:GLY:HA3	2.49	0.48
1:A:140:ILE:CG2	1:A:141:THR:N	2.75	0.48
1:A:149:PRO:HB3	1:A:171:VAL:HG11	1.96	0.48
1:A:698:ASP:O	1:A:699:ASP:O	2.31	0.48
1:B:286:GLY:CA	1:B:808:MSE:HG3	2.43	0.48
1:B:341:ASN:HD22	1:B:342:PRO:HD3	1.78	0.48
1:C:149:PRO:HB3	1:C:171:VAL:HG11	1.95	0.48
1:C:529:LEU:O	1:C:552:VAL:HG23	2.13	0.48
1:A:418:HIS:HE1	1:A:453:LYS:HD3	1.78	0.48
1:A:687:VAL:HG23	1:A:717:THR:HB	1.96	0.48
1:B:185:ILE:O	1:B:188:VAL:HB	2.13	0.48
1:B:414:VAL:CB	1:B:459:ILE:HG22	2.43	0.48
1:B:518:PRO:HG2	1:B:521:TYR:CE2	2.46	0.48
1:C:681:LEU:HD22	1:C:687:VAL:CG1	2.43	0.48
1:A:375:ARG:CZ	1:A:755:PHE:HE1	2.27	0.48
1:B:200:TYR:CZ	1:B:206:ASN:HB3	2.49	0.48
1:B:434:TRP:C	1:B:436:ALA:H	2.17	0.48
1:B:694:LYS:HD3	1:B:710:GLN:HA	1.95	0.48
1:C:260:GLY:O	1:C:594:MSE:HB2	2.13	0.48
1:A:277:PHE:O	1:A:278:LYS:HB2	2.14	0.48
1:A:391:TRP:CD1	1:A:393:GLN:HG3	2.49	0.48
1:B:218:GLN:HA	1:B:222:ILE:O	2.14	0.48
1:C:233:ALA:HA	1:C:393:GLN:CG	2.44	0.48
1:C:270:ARG:NH1	1:C:351:ASP:OD2	2.47	0.48
1:A:158:LEU:O	1:A:160:LEU:HG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:O	1:A:255:LEU:N	2.47	0.48
1:A:535:ALA:HB1	1:A:537:PHE:CE1	2.49	0.48
1:B:152:ILE:CD1	1:B:169:ILE:HG21	2.44	0.48
1:B:271:LYS:HB3	1:B:310:ARG:CZ	2.44	0.48
1:B:763:VAL:CG1	1:B:785:PHE:CD2	2.96	0.48
1:C:154:THR:O	1:C:256:LEU:HD12	2.14	0.48
1:C:253:THR:CG2	1:C:265:THR:OG1	2.58	0.48
1:C:247:GLU:HG3	1:C:267:ASN:HB3	1.96	0.48
1:C:387:LYS:HG3	1:C:509:ASP:CA	2.44	0.48
1:C:434:TRP:HE3	1:C:434:TRP:HA	1.79	0.48
1:C:619:GLY:HA3	1:C:634:ALA:CB	2.44	0.48
1:C:683:PRO:CG	1:C:684:GLY:N	2.77	0.48
1:C:781:VAL:HB	1:C:807:LEU:CD2	2.44	0.48
1:A:200:TYR:CE2	1:A:206:ASN:HB3	2.49	0.47
1:A:227:ARG:NH1	1:A:260:GLY:HA2	2.29	0.47
1:A:253:THR:CG2	1:A:265:THR:OG1	2.57	0.47
1:A:319:HIS:HA	1:A:326:GLU:HA	1.95	0.47
1:B:148:THR:OG1	1:B:149:PRO:HD2	2.14	0.47
1:B:396:ARG:CG	1:B:420:ILE:HD11	2.44	0.47
1:B:418:HIS:CE1	1:B:453:LYS:HD3	2.48	0.47
1:B:740:SER:HB2	1:B:757:GLN:HB3	1.96	0.47
1:C:406:PHE:HB3	1:C:408:ASN:OD1	2.14	0.47
1:A:185:ILE:O	1:A:188:VAL:HB	2.14	0.47
1:A:376:ASN:HD21	1:A:435:PRO:CG	2.26	0.47
1:A:738:GLY:O	1:A:739:LYS:O	2.32	0.47
1:C:136:GLN:HG2	1:C:137:LEU:H	1.78	0.47
1:C:285:ALA:CB	1:C:291:TYR:HD1	2.27	0.47
1:C:526:THR:CG2	1:C:554:TYR:HE1	2.26	0.47
1:C:628:ARG:HG2	1:C:680:GLU:OE1	2.13	0.47
1:C:783:ASN:C	1:C:783:ASN:HD22	2.15	0.47
1:A:396:ARG:HG3	1:A:420:ILE:CG1	2.44	0.47
1:B:434:TRP:HE3	1:B:434:TRP:HA	1.77	0.47
1:B:625:LEU:C	1:B:627:GLY:N	2.65	0.47
1:C:230:GLY:HA2	4:K:1:PVE:O25	2.13	0.47
1:C:325:TYR:C	1:C:326:GLU:HG3	2.33	0.47
1:A:503:PHE:O	1:A:504:ILE:O	2.33	0.47
1:A:655:THR:O	1:A:656:ASN:O	2.31	0.47
1:A:728:LEU:HB2	1:A:769:TYR:CD1	2.50	0.47
1:B:286:GLY:HA2	1:B:808:MSE:HA	1.97	0.47
1:B:638:ILE:HD12	1:B:670:THR:HG21	1.95	0.47
1:C:279:GLY:O	1:C:280:HIS:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:HIS:CE1	1:C:525:LYS:HE2	2.48	0.47
1:A:745:TYR:HB2	1:A:752:TRP:NE1	2.29	0.47
1:A:779:VAL:HG23	1:A:809:PHE:HA	1.96	0.47
1:B:779:VAL:HG23	1:B:809:PHE:HA	1.96	0.47
1:C:259:ALA:HB1	1:C:595:PRO:HD2	1.95	0.47
1:C:552:VAL:CG1	1:C:593:PHE:CZ	2.95	0.47
1:A:209:ALA:HB2	1:A:214:ILE:CD1	2.43	0.47
1:A:396:ARG:CG	1:A:420:ILE:HD11	2.45	0.47
1:A:474:LEU:CD1	1:A:475:VAL:N	2.66	0.47
1:A:766:MSE:SE	1:A:766:MSE:C	3.03	0.47
1:B:239:ASP:OD2	1:B:292:ARG:NH2	2.40	0.47
1:B:376:ASN:HD21	1:B:435:PRO:CG	2.25	0.47
1:B:396:ARG:HG3	1:B:420:ILE:CG1	2.45	0.47
1:B:430:ILE:HD11	1:B:441:ALA:HB3	1.96	0.47
1:B:540:THR:HG22	1:B:542:ASP:OD1	2.15	0.47
1:B:545:LEU:HD12	1:B:575:ALA:HB2	1.96	0.47
1:C:375:ARG:HH11	1:C:375:ARG:HG3	1.79	0.47
1:A:185:ILE:O	1:A:186:ASP:C	2.51	0.47
1:A:273:PRO:HG2	1:A:337:GLU:OE1	2.14	0.47
1:A:434:TRP:O	1:A:436:ALA:N	2.47	0.47
1:A:517:THR:O	1:A:518:PRO:C	2.53	0.47
1:B:281:VAL:CG1	1:B:281:VAL:O	2.63	0.47
1:B:307:VAL:HG13	1:B:307:VAL:O	2.14	0.47
1:B:484:HIS:CE1	1:B:525:LYS:HE2	2.50	0.47
1:B:527:ARG:HH11	1:B:529:LEU:CD1	2.28	0.47
1:C:158:LEU:O	1:C:160:LEU:HG	2.15	0.47
1:C:182:LEU:HD22	1:C:187:ASP:O	2.14	0.47
1:C:194:GLY:HA3	1:C:250:LYS:HZ3	1.79	0.47
1:C:546:PHE:N	1:C:574:GLY:O	2.46	0.47
1:C:628:ARG:CB	1:C:628:ARG:HH11	2.28	0.47
1:C:646:GLU:HA	1:C:663:TYR:HD2	1.78	0.47
1:C:375:ARG:CZ	1:C:755:PHE:HE1	2.28	0.47
1:A:141:THR:C	1:A:143:ASP:H	2.18	0.47
1:A:281:VAL:O	1:A:281:VAL:CG1	2.62	0.47
1:A:346:LEU:HA	1:A:402:LEU:HB3	1.96	0.47
1:B:271:LYS:HD3	1:B:310:ARG:NH2	2.30	0.47
1:B:782:ASN:CB	1:B:806:ASN:HD22	2.28	0.47
1:C:410:TRP:CZ3	1:C:464:PRO:O	2.68	0.47
1:C:477:GLY:HA3	1:C:532:TYR:CE1	2.50	0.47
1:C:749:ARG:C	1:C:751:ARG:H	2.18	0.47
1:A:292:ARG:HG3	1:A:316:GLN:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ALA:O	1:A:389:SER:N	2.47	0.47
1:A:286:GLY:CA	1:A:808:MSE:HG3	2.44	0.47
1:B:158:LEU:O	1:B:160:LEU:HG	2.14	0.47
1:B:441:ALA:O	1:B:500:THR:HG22	2.15	0.47
1:B:527:ARG:HH21	1:B:555:ARG:HD2	1.80	0.47
1:B:601:ARG:HD3	1:B:607:LEU:N	2.30	0.47
1:B:628:ARG:HH11	1:B:628:ARG:CB	2.27	0.47
1:B:640:GLU:OE2	1:B:643:ARG:HG3	2.14	0.47
1:B:749:ARG:C	1:B:751:ARG:H	2.18	0.47
1:B:812:ARG:HH11	1:B:812:ARG:HG2	1.80	0.47
1:C:225:THR:C	1:C:227:ARG:H	2.17	0.47
1:C:360:SER:HB3	1:C:390:SER:CA	2.40	0.47
1:A:271:LYS:HZ3	1:A:310:ARG:HH22	1.63	0.47
1:A:296:ASP:OD2	1:A:310:ARG:NH2	2.48	0.47
1:A:375:ARG:HG3	1:A:375:ARG:HH11	1.79	0.47
1:A:370:ASP:HB2	1:A:435:PRO:HB2	1.97	0.47
1:B:781:VAL:HB	1:B:807:LEU:CD2	2.44	0.47
1:C:253:THR:O	1:C:255:LEU:N	2.48	0.47
1:C:318:LYS:HE2	1:C:327:ARG:HH21	1.80	0.47
1:C:625:LEU:C	1:C:627:GLY:N	2.66	0.47
1:C:814:ASP:HB3	1:C:815:PHE:H	1.62	0.47
1:B:280:HIS:O	1:B:295:LEU:HD12	2.15	0.47
1:B:387:LYS:HD2	1:B:509:ASP:HB3	1.97	0.47
1:A:335:ILE:O	1:A:336:LEU:HD12	2.15	0.46
1:A:430:ILE:HD11	1:A:441:ALA:HB3	1.97	0.46
1:A:423:TYR:N	1:A:450:GLY:O	2.40	0.46
1:A:465:PHE:CZ	1:A:467:PHE:HB2	2.50	0.46
1:A:658:ALA:C	1:A:659:ILE:O	2.53	0.46
1:B:233:ALA:HA	1:B:393:GLN:CG	2.44	0.46
1:B:633:LEU:O	1:B:633:LEU:HD23	2.15	0.46
1:B:211:GLY:HA2	1:B:708:GLU:OE1	2.15	0.46
1:B:687:VAL:HG23	1:B:717:THR:HB	1.97	0.46
1:B:766:MSE:HB2	1:B:780:ASN:ND2	2.30	0.46
1:C:391:TRP:HD1	1:C:393:GLN:HG3	1.79	0.46
1:C:600:TYR:HD1	1:C:663:TYR:CD1	2.32	0.46
1:C:737:GLN:HG2	1:C:760:TYR:CB	2.45	0.46
1:A:212:PHE:CD2	1:A:262:LEU:HB2	2.50	0.46
1:A:734:ALA:HA	1:A:762:LEU:O	2.16	0.46
1:B:253:THR:O	1:B:255:LEU:N	2.48	0.46
1:B:295:LEU:O	1:B:312:VAL:HG23	2.15	0.46
1:C:319:HIS:HA	1:C:326:GLU:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:SER:CB	1:C:390:SER:HA	2.40	0.46
1:C:344:THR:HB	1:C:403:GLU:HG3	1.97	0.46
1:A:434:TRP:O	1:A:441:ALA:HB2	2.16	0.46
1:A:418:HIS:CE1	1:A:453:LYS:HD3	2.50	0.46
1:A:484:HIS:CE1	1:A:525:LYS:HE2	2.50	0.46
1:A:546:PHE:N	1:A:574:GLY:O	2.45	0.46
1:A:618:ILE:CG2	1:A:618:ILE:O	2.64	0.46
1:A:749:ARG:C	1:A:751:ARG:H	2.19	0.46
1:B:209:ALA:HB2	1:B:214:ILE:CD1	2.45	0.46
1:B:246:VAL:O	1:B:246:VAL:CG1	2.63	0.46
1:B:308:ARG:NH2	1:B:339:ASP:OD2	2.49	0.46
1:B:375:ARG:CZ	1:B:755:PHE:HE1	2.29	0.46
1:B:396:ARG:HD3	1:B:420:ILE:HD11	1.95	0.46
1:B:713:LEU:O	1:B:735:ARG:HA	2.16	0.46
1:B:742:GLN:OE1	1:B:742:GLN:HA	2.16	0.46
1:C:220:ASP:OD2	1:C:270:ARG:CD	2.64	0.46
1:C:247:GLU:HG3	1:C:267:ASN:HD22	1.79	0.46
1:C:385:GLY:O	1:C:508:GLY:HA3	2.16	0.46
1:C:740:SER:HB2	1:C:757:GLN:HB3	1.97	0.46
1:C:757:GLN:O	1:C:758:GLU:O	2.33	0.46
1:A:135:ASN:ND2	1:A:138:GLY:O	2.49	0.46
1:A:225:THR:C	1:A:227:ARG:H	2.19	0.46
1:A:289:ASP:O	1:A:318:LYS:HA	2.15	0.46
1:A:396:ARG:CD	1:A:420:ILE:HD11	2.45	0.46
1:B:414:VAL:HB	1:B:459:ILE:HG22	1.97	0.46
1:B:385:GLY:O	1:B:508:GLY:HA3	2.15	0.46
1:B:796:TYR:O	1:B:797:THR:HB	2.15	0.46
1:C:392:GLU:HB3	1:C:424:HIS:HB3	1.97	0.46
1:C:687:VAL:HG23	1:C:717:THR:HB	1.97	0.46
1:C:812:ARG:HG2	1:C:812:ARG:HH11	1.81	0.46
1:A:179:ASP:HB3	1:A:766:MSE:HE3	1.98	0.46
1:A:694:LYS:HE2	1:A:708:GLU:O	2.16	0.46
1:B:324:HIS:CE1	1:B:383:ASN:HD22	2.33	0.46
1:B:527:ARG:HH11	1:B:529:LEU:HD11	1.81	0.46
1:C:209:ALA:HB2	1:C:214:ILE:CD1	2.43	0.46
1:C:289:ASP:O	1:C:318:LYS:HA	2.16	0.46
1:C:388:TRP:CH2	1:C:428:GLY:HA3	2.50	0.46
1:C:435:PRO:O	1:C:436:ALA:O	2.33	0.46
1:C:423:TYR:N	1:C:450:GLY:O	2.44	0.46
1:C:682:ALA:HB3	1:C:683:PRO:HD2	1.97	0.46
1:A:621:LYS:HG2	1:A:632:SER:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:ALA:HB3	1:A:685:TRP:HB2	1.98	0.46
1:B:434:TRP:O	1:B:436:ALA:N	2.49	0.46
1:C:335:ILE:O	1:C:336:LEU:HD12	2.15	0.46
1:C:670:THR:OG1	1:C:696:ILE:HD12	2.15	0.46
1:A:148:THR:HB	1:A:679:GLY:CA	2.46	0.46
1:A:152:ILE:O	1:A:152:ILE:HG13	2.14	0.46
1:A:185:ILE:C	1:A:185:ILE:HD13	2.35	0.46
1:A:783:ASN:C	1:A:783:ASN:ND2	2.69	0.46
1:A:812:ARG:HG2	1:A:812:ARG:HH11	1.81	0.46
1:B:319:HIS:HA	1:B:326:GLU:HA	1.98	0.46
1:C:526:THR:HG22	1:C:554:TYR:CE1	2.50	0.46
1:C:556:VAL:O	1:C:556:VAL:HG13	2.16	0.46
1:C:596:GLN:HB2	1:C:596:GLN:HE21	1.54	0.46
1:C:735:ARG:HG3	1:C:736:TRP:N	2.29	0.46
1:C:783:ASN:C	1:C:783:ASN:ND2	2.70	0.46
1:A:683:PRO:CG	1:A:684:GLY:N	2.79	0.46
1:A:772:THR:OG1	1:A:775:LEU:HB3	2.16	0.46
1:C:198:SER:HB3	1:C:206:ASN:ND2	2.31	0.46
1:C:305:GLY:C	1:C:307:VAL:N	2.68	0.46
1:C:628:ARG:HH11	1:C:628:ARG:HB2	1.80	0.46
1:A:441:ALA:O	1:A:500:THR:HG22	2.15	0.46
1:A:706:THR:HB	1:A:741:TRP:CE2	2.50	0.46
1:B:233:ALA:CA	1:B:393:GLN:OE1	2.63	0.46
1:C:464:PRO:HA	1:C:472:HIS:O	2.16	0.46
1:C:490:TYR:CD1	1:C:490:TYR:N	2.83	0.46
1:C:747:ASN:CB	1:C:748:PRO:HD3	2.42	0.46
1:B:185:ILE:O	1:B:186:ASP:C	2.54	0.46
1:B:490:TYR:CD1	1:B:490:TYR:N	2.84	0.46
1:B:633:LEU:HB2	1:B:675:ALA:HB2	1.98	0.46
1:B:754:LYS:C	1:B:754:LYS:CD	2.84	0.46
1:C:746:ASN:HD21	1:C:749:ARG:HG3	1.81	0.46
1:A:184:ASN:ND2	1:A:187:ASP:OD2	2.49	0.45
1:A:305:GLY:C	1:A:307:VAL:N	2.69	0.45
1:A:383:ASN:O	1:A:385:GLY:N	2.48	0.45
1:B:225:THR:C	1:B:227:ARG:H	2.18	0.45
1:B:216:ASN:OD1	1:B:227:ARG:NH2	2.48	0.45
1:B:475:VAL:O	1:B:476:VAL:C	2.53	0.45
1:B:591:ASP:OD1	1:B:614:GLN:HG3	2.16	0.45
1:C:317:ASP:C	1:C:317:ASP:OD1	2.54	0.45
1:C:661:TYR:HD1	1:C:662:ALA:N	2.01	0.45
2:I:7:FHO:HG1C	2:I:7:FHO:HZ	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ASP:OD2	1:A:397:THR:HG23	2.17	0.45
1:A:503:PHE:O	1:A:504:ILE:C	2.53	0.45
1:B:156:THR:C	1:B:158:LEU:H	2.18	0.45
1:B:305:GLY:C	1:B:307:VAL:N	2.68	0.45
1:B:368:LEU:HD21	1:B:799:ALA:HB2	1.97	0.45
1:B:372:GLN:CD	1:B:373:GLY:N	2.70	0.45
1:C:289:ASP:N	1:C:289:ASP:OD1	2.49	0.45
1:C:434:TRP:O	1:C:441:ALA:HB2	2.16	0.45
1:C:609:GLU:HB3	1:C:610:PRO:HD2	1.98	0.45
1:C:682:ALA:HB3	1:C:685:TRP:HB2	1.97	0.45
1:A:182:LEU:HD13	1:A:187:ASP:O	2.16	0.45
1:A:370:ASP:OD2	1:A:373:GLY:HA3	2.16	0.45
1:A:490:TYR:N	1:A:490:TYR:CD1	2.84	0.45
1:B:189:MSE:CE	1:B:195:ILE:HD13	2.45	0.45
1:B:288:TRP:CZ2	1:B:321:PHE:HB3	2.52	0.45
1:B:344:THR:HB	1:B:403:GLU:HG3	1.97	0.45
1:B:421:ASN:O	1:B:452:THR:CG2	2.63	0.45
1:B:474:LEU:HD12	1:B:534:THR:O	2.17	0.45
1:B:517:THR:O	1:B:518:PRO:C	2.53	0.45
1:C:142:GLU:HG2	1:C:142:GLU:O	2.16	0.45
1:C:169:ILE:CG2	1:C:170:THR:N	2.80	0.45
1:C:383:ASN:C	1:C:385:GLY:N	2.70	0.45
1:C:651:ASN:ND2	1:C:652:SER:H	2.15	0.45
1:C:745:TYR:HB2	1:C:752:TRP:NE1	2.30	0.45
1:A:275:HIS:CE1	1:A:308:ARG:HH11	2.34	0.45
1:A:537:PHE:CE2	1:A:547:LEU:HD12	2.42	0.45
1:A:601:ARG:CG	1:A:601:ARG:HH11	2.24	0.45
1:B:154:THR:O	1:B:256:LEU:HD12	2.16	0.45
1:B:281:VAL:HB	1:B:295:LEU:HD13	1.98	0.45
1:B:396:ARG:CD	1:B:420:ILE:HD11	2.46	0.45
1:B:601:ARG:HD3	1:B:607:LEU:CA	2.46	0.45
1:B:746:ASN:O	1:B:747:ASN:C	2.55	0.45
1:B:751:ARG:HG3	1:B:751:ARG:O	2.16	0.45
1:B:365:SER:N	1:B:799:ALA:O	2.48	0.45
1:C:169:ILE:CD1	1:C:249:LEU:HD12	2.45	0.45
1:C:216:ASN:ND2	1:C:261:SER:H	2.13	0.45
1:C:307:VAL:O	1:C:307:VAL:HG13	2.16	0.45
1:C:418:HIS:HE1	1:C:453:LYS:HD3	1.81	0.45
1:C:624:TYR:O	1:C:625:LEU:CB	2.64	0.45
1:A:169:ILE:HD11	1:A:249:LEU:HD13	1.96	0.45
1:A:344:THR:HB	1:A:403:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:TYR:C	1:A:789:TYR:CD1	2.90	0.45
1:B:292:ARG:HG3	1:B:316:GLN:HB2	1.98	0.45
1:B:509:ASP:O	1:B:509:ASP:CG	2.54	0.45
1:C:783:ASN:O	1:C:784:VAL:C	2.55	0.45
1:A:298:SER:HB2	1:A:310:ARG:CG	2.47	0.45
1:A:233:ALA:HA	1:A:393:GLN:CG	2.47	0.45
1:A:601:ARG:HD3	1:A:607:LEU:N	2.32	0.45
1:A:591:ASP:OD1	1:A:614:GLN:HG3	2.17	0.45
1:A:713:LEU:O	1:A:735:ARG:HA	2.17	0.45
1:A:740:SER:HB2	1:A:757:GLN:HB3	1.97	0.45
1:B:201:ASP:CG	1:B:204:ARG:HE	2.20	0.45
1:B:243:TYR:HB3	1:B:269:ILE:O	2.17	0.45
1:B:682:ALA:HB3	1:B:683:PRO:HD2	1.99	0.45
1:B:683:PRO:CG	1:B:684:GLY:N	2.79	0.45
1:A:325:TYR:C	1:A:326:GLU:HG3	2.36	0.45
1:A:628:ARG:HB2	1:A:628:ARG:HH11	1.82	0.45
1:A:772:THR:O	1:A:773:ASP:C	2.55	0.45
1:B:277:PHE:O	1:B:278:LYS:HB2	2.17	0.45
1:C:169:ILE:HD11	1:C:249:LEU:HD13	1.98	0.45
1:A:638:ILE:HD12	1:A:670:THR:HG21	1.99	0.45
1:B:231:TYR:CD2	1:B:485:TRP:CH2	3.05	0.45
1:C:633:LEU:O	1:C:633:LEU:HD23	2.17	0.45
1:C:681:LEU:HD23	1:C:685:TRP:CD2	2.52	0.45
1:A:351:ASP:OD2	1:A:397:THR:CG2	2.64	0.45
1:A:797:THR:HG22	1:A:797:THR:O	2.17	0.45
1:B:169:ILE:CG2	1:B:170:THR:N	2.79	0.45
1:C:148:THR:HB	1:C:679:GLY:CA	2.46	0.45
1:C:391:TRP:CD1	1:C:393:GLN:HG3	2.51	0.45
1:C:418:HIS:CE1	1:C:453:LYS:HD3	2.51	0.45
1:A:751:ARG:O	1:A:751:ARG:HG3	2.16	0.45
1:A:804:PRO:O	1:A:805:ARG:C	2.54	0.45
1:B:335:ILE:O	1:B:336:LEU:HD12	2.17	0.45
1:B:738:GLY:O	1:B:739:LYS:C	2.55	0.45
1:B:757:GLN:O	1:B:758:GLU:O	2.34	0.45
1:A:279:GLY:O	1:A:280:HIS:HB3	2.17	0.44
1:A:410:TRP:CZ3	1:A:464:PRO:O	2.69	0.44
1:A:601:ARG:HD3	1:A:607:LEU:CA	2.47	0.44
1:A:637:GLU:HG3	1:A:671:LYS:CB	2.35	0.44
1:B:212:PHE:CD2	1:B:262:LEU:HB2	2.52	0.44
1:B:649:LEU:O	1:B:651:ASN:N	2.45	0.44
1:B:783:ASN:O	1:B:784:VAL:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:PRO:HG2	1:C:337:GLU:OE1	2.17	0.44
1:C:728:LEU:HB2	1:C:769:TYR:CE1	2.52	0.44
1:A:255:LEU:HD22	1:A:572:TYR:CG	2.52	0.44
1:A:302:THR:O	1:A:303:GLU:C	2.55	0.44
1:A:546:PHE:HB2	1:A:574:GLY:O	2.18	0.44
1:A:628:ARG:CB	1:A:628:ARG:HH11	2.30	0.44
1:A:682:ALA:CB	1:A:683:PRO:HD2	2.48	0.44
1:B:383:ASN:O	1:B:385:GLY:N	2.50	0.44
1:B:707:TRP:CH2	1:B:793:ILE:HB	2.52	0.44
1:C:274:THR:HG22	1:C:298:SER:OG	2.16	0.44
1:C:706:THR:HB	1:C:741:TRP:CE2	2.53	0.44
1:A:169:ILE:CD1	1:A:249:LEU:HD12	2.45	0.44
1:A:280:HIS:CE1	1:A:296:ASP:HB3	2.52	0.44
1:A:628:ARG:HG2	1:A:680:GLU:OE1	2.17	0.44
1:B:156:THR:C	1:B:158:LEU:N	2.71	0.44
1:C:184:ASN:ND2	1:C:187:ASP:OD2	2.51	0.44
1:C:537:PHE:O	1:C:545:LEU:N	2.40	0.44
1:A:243:TYR:HA	1:A:270:ARG:HA	2.00	0.44
1:A:270:ARG:NH1	1:A:351:ASP:OD2	2.50	0.44
1:A:621:LYS:HG2	1:A:632:SER:CB	2.46	0.44
1:A:783:ASN:O	1:A:784:VAL:C	2.55	0.44
1:A:796:TYR:O	1:A:797:THR:HB	2.18	0.44
1:B:226:ALA:HB3	1:B:235:ASN:HD21	1.83	0.44
1:C:308:ARG:NH2	1:C:339:ASP:OD2	2.50	0.44
1:C:351:ASP:OD2	1:C:397:THR:CG2	2.66	0.44
1:C:504:ILE:O	1:C:505:ASN:C	2.56	0.44
1:C:180:PHE:HA	1:C:780:ASN:ND2	2.33	0.44
1:C:368:LEU:HD21	1:C:799:ALA:HB2	2.00	0.44
1:A:414:VAL:HG23	1:A:459:ILE:CG2	2.48	0.44
1:A:430:ILE:HB	1:A:443:ILE:HG22	2.00	0.44
1:B:275:HIS:CE1	1:B:308:ARG:NH1	2.86	0.44
1:B:740:SER:O	1:B:757:GLN:N	2.40	0.44
1:C:391:TRP:CE3	1:C:427:LEU:HD11	2.53	0.44
1:C:682:ALA:HB2	1:C:685:TRP:HE3	1.83	0.44
1:C:779:VAL:HG23	1:C:809:PHE:HA	1.98	0.44
1:A:616:TYR:HE2	1:A:639:HIS:ND1	2.16	0.44
1:B:148:THR:HB	1:B:679:GLY:CA	2.47	0.44
1:B:198:SER:HB3	1:B:206:ASN:ND2	2.33	0.44
1:B:220:ASP:OD2	1:B:270:ARG:CD	2.66	0.44
1:B:341:ASN:CB	1:B:342:PRO:CD	2.87	0.44
1:B:461:LEU:HB2	1:B:476:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:698:ASP:O	1:B:701:GLY:HA3	2.17	0.44
1:C:136:GLN:CD	1:C:136:GLN:H	2.21	0.44
1:C:189:MSE:CE	1:C:266:ILE:HD12	2.44	0.44
1:C:280:HIS:CE1	1:C:296:ASP:HB3	2.53	0.44
1:C:651:ASN:ND2	1:C:652:SER:N	2.65	0.44
1:A:204:ARG:HD3	1:A:391:TRP:CH2	2.53	0.44
1:A:216:ASN:ND2	1:A:261:SER:H	2.15	0.44
1:B:247:GLU:O	1:B:267:ASN:HB3	2.17	0.44
1:B:298:SER:HB2	1:B:310:ARG:CG	2.47	0.44
1:C:419:LYS:HG2	1:C:420:ILE:N	2.32	0.44
1:C:430:ILE:HD11	1:C:441:ALA:HB3	2.00	0.44
1:C:511:GLY:O	1:C:513:PRO:CD	2.65	0.44
1:C:637:GLU:HA	1:C:671:LYS:HA	2.00	0.44
1:A:434:TRP:CE3	1:A:434:TRP:CA	2.96	0.44
1:A:529:LEU:HB3	1:A:530:GLY:H	1.71	0.44
1:A:707:TRP:CH2	1:A:793:ILE:HB	2.53	0.44
1:B:302:THR:O	1:B:303:GLU:C	2.56	0.44
1:B:435:PRO:O	1:B:436:ALA:O	2.34	0.44
1:B:781:VAL:HB	1:B:807:LEU:HD21	1.99	0.44
1:C:290:ASN:HA	1:C:318:LYS:CB	2.48	0.44
1:C:372:GLN:CD	1:C:373:GLY:N	2.71	0.44
1:C:414:VAL:HG23	1:C:459:ILE:CG2	2.48	0.44
1:C:781:VAL:HB	1:C:807:LEU:HD21	2.00	0.44
1:B:366:PHE:HB3	1:B:382:PHE:CD2	2.53	0.44
1:B:674:GLU:HB2	1:B:692:THR:HG23	1.99	0.44
1:C:216:ASN:HD21	1:C:261:SER:N	2.11	0.44
1:C:237:LEU:HD23	1:C:237:LEU:N	2.32	0.44
1:C:601:ARG:HD3	1:C:607:LEU:N	2.33	0.44
1:C:804:PRO:O	1:C:805:ARG:C	2.56	0.44
1:B:149:PRO:HB3	1:B:171:VAL:HG11	1.99	0.43
1:B:185:ILE:O	1:B:188:VAL:N	2.44	0.43
1:B:682:ALA:HB2	1:B:685:TRP:HE3	1.82	0.43
1:B:781:VAL:HA	1:B:807:LEU:HD23	2.00	0.43
1:C:185:ILE:O	1:C:186:ASP:C	2.55	0.43
1:C:204:ARG:HD3	1:C:391:TRP:CH2	2.53	0.43
1:C:496:TYR:CZ	1:C:513:PRO:HD3	2.53	0.43
1:C:526:THR:HA	1:C:555:ARG:O	2.18	0.43
1:C:633:LEU:HB2	1:C:675:ALA:HB2	1.99	0.43
1:C:746:ASN:O	1:C:747:ASN:C	2.56	0.43
1:A:219:TYR:N	1:A:222:ILE:O	2.49	0.43
1:B:351:ASP:OD2	1:B:397:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:ARG:HG3	1:B:375:ARG:HH11	1.83	0.43
1:C:275:HIS:CE1	1:C:308:ARG:HH11	2.36	0.43
1:C:601:ARG:HD3	1:C:607:LEU:CA	2.49	0.43
1:C:591:ASP:OD1	1:C:614:GLN:HG3	2.18	0.43
1:C:709:PRO:CG	1:C:737:GLN:HB2	2.47	0.43
1:C:721:PHE:CD2	1:C:728:LEU:HD23	2.53	0.43
1:A:475:VAL:O	1:A:476:VAL:C	2.56	0.43
1:A:527:ARG:HH21	1:A:555:ARG:HD2	1.84	0.43
1:A:719:TYR:HE2	1:A:721:PHE:CD1	2.31	0.43
1:B:173:THR:CG2	1:B:176:ASN:HB2	2.48	0.43
1:B:327:ARG:HG3	1:B:328:LYS:N	2.33	0.43
1:B:461:LEU:HB2	1:B:476:VAL:CG1	2.48	0.43
1:B:578:ASP:HA	1:B:584:SER:OG	2.18	0.43
1:B:609:GLU:HB3	1:B:610:PRO:HD2	2.00	0.43
1:C:140:ILE:CG2	1:C:141:THR:H	2.31	0.43
1:C:247:GLU:O	1:C:267:ASN:HB3	2.18	0.43
1:C:262:LEU:HD21	1:C:613:GLY:HA3	2.00	0.43
1:C:774:LYS:HB3	1:C:814:ASP:OD2	2.18	0.43
1:A:156:THR:C	1:A:158:LEU:H	2.21	0.43
1:A:410:TRP:HE1	1:A:462:THR:N	2.16	0.43
1:A:721:PHE:CD2	1:A:728:LEU:HD23	2.54	0.43
1:B:482:PHE:CE1	1:B:527:ARG:CG	3.01	0.43
1:B:628:ARG:HG2	1:B:680:GLU:OE1	2.18	0.43
1:B:795:PHE:C	1:B:797:THR:N	2.72	0.43
1:C:576:VAL:HA	1:C:585:VAL:O	2.17	0.43
1:C:721:PHE:HD2	1:C:725:LEU:HD12	1.83	0.43
1:C:200:TYR:HD1	1:C:795:PHE:CE1	2.36	0.43
1:A:139:THR:CG2	1:A:150:GLY:HA3	2.49	0.43
1:A:271:LYS:NZ	1:A:310:ARG:HH22	2.14	0.43
1:A:345:MSE:HE3	1:A:403:GLU:CD	2.38	0.43
1:A:510:ILE:HG22	1:A:511:GLY:N	2.34	0.43
1:B:140:ILE:CG2	1:B:141:THR:H	2.29	0.43
1:B:419:LYS:HG2	1:B:420:ILE:N	2.33	0.43
1:B:435:PRO:HG3	1:B:503:PHE:CZ	2.53	0.43
1:B:616:TYR:HE2	1:B:639:HIS:ND1	2.17	0.43
1:C:243:TYR:CZ	1:C:268:LEU:HD13	2.53	0.43
1:C:421:ASN:O	1:C:452:THR:CG2	2.64	0.43
1:C:695:ILE:HD11	1:C:710:GLN:NE2	2.28	0.43
1:A:576:VAL:HA	1:A:585:VAL:O	2.17	0.43
1:A:659:ILE:CG1	1:A:660:THR:N	2.82	0.43
1:A:738:GLY:O	1:A:739:LYS:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:ASN:O	1:A:747:ASN:C	2.56	0.43
1:B:228:ASN:OD1	1:B:228:ASN:C	2.56	0.43
1:B:237:LEU:N	1:B:237:LEU:HD23	2.33	0.43
1:B:425:ALA:O	1:B:448:TYR:N	2.40	0.43
1:B:556:VAL:HG12	1:B:563:ILE:O	2.18	0.43
1:B:542:ASP:HB3	1:B:578:ASP:HB2	1.99	0.43
1:B:804:PRO:O	1:B:805:ARG:C	2.55	0.43
1:C:152:ILE:HB	1:C:154:THR:HG22	1.99	0.43
1:C:371:SER:HB3	1:C:372:GLN:OE1	2.19	0.43
1:C:386:ALA:O	1:C:387:LYS:C	2.55	0.43
1:C:621:LYS:HG2	1:C:632:SER:HB2	2.00	0.43
1:C:738:GLY:O	1:C:739:LYS:C	2.56	0.43
1:A:237:LEU:N	1:A:237:LEU:HD23	2.34	0.43
1:A:286:GLY:HA2	1:A:808:MSE:HA	2.01	0.43
1:A:342:PRO:HB3	1:A:405:ASN:O	2.19	0.43
1:A:386:ALA:O	1:A:387:LYS:C	2.57	0.43
1:A:419:LYS:HG2	1:A:420:ILE:N	2.33	0.43
1:A:385:GLY:O	1:A:508:GLY:HA3	2.17	0.43
1:A:596:GLN:HB2	1:A:596:GLN:HE21	1.54	0.43
1:A:682:ALA:HB2	1:A:685:TRP:HE3	1.84	0.43
1:A:719:TYR:CD2	1:A:721:PHE:CD1	3.06	0.43
1:A:365:SER:N	1:A:799:ALA:O	2.46	0.43
1:B:216:ASN:ND2	1:B:261:SER:H	2.17	0.43
1:B:365:SER:HB2	1:B:799:ALA:O	2.19	0.43
1:B:797:THR:HG22	1:B:797:THR:O	2.19	0.43
1:C:156:THR:C	1:C:158:LEU:H	2.22	0.43
1:C:475:VAL:O	1:C:476:VAL:C	2.55	0.43
1:C:674:GLU:HB2	1:C:692:THR:HG23	1.99	0.43
1:C:713:LEU:O	1:C:735:ARG:HA	2.18	0.43
1:C:781:VAL:HA	1:C:807:LEU:HD23	2.00	0.43
1:A:586:TYR:CD1	1:A:619:GLY:O	2.72	0.43
1:A:633:LEU:HB2	1:A:675:ALA:HB2	2.01	0.43
1:A:721:PHE:HD2	1:A:725:LEU:HD12	1.83	0.43
1:A:761:TRP:HA	1:A:761:TRP:CE3	2.54	0.43
1:B:695:ILE:HD13	1:B:695:ILE:HA	1.93	0.43
1:B:722:LYS:O	1:B:723:GLY:C	2.57	0.43
1:B:179:ASP:HB3	1:B:766:MSE:HE3	2.00	0.43
1:C:184:ASN:OD1	1:C:186:ASP:N	2.52	0.43
1:C:517:THR:O	1:C:518:PRO:C	2.57	0.43
1:C:682:ALA:CB	1:C:683:PRO:HD2	2.49	0.43
1:C:796:TYR:O	1:C:797:THR:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ASP:O	1:B:318:LYS:HA	2.19	0.43
1:B:430:ILE:HB	1:B:443:ILE:HG22	2.00	0.43
1:C:430:ILE:HB	1:C:443:ILE:HG22	2.01	0.43
1:C:446:GLN:HG2	1:C:491:TRP:HB3	2.00	0.43
1:C:602:ASP:O	1:C:604:SER:N	2.52	0.43
1:C:653:LYS:H	1:C:653:LYS:HG3	1.49	0.43
1:C:659:ILE:HG23	1:C:660:THR:N	2.23	0.43
1:C:695:ILE:HD13	1:C:695:ILE:HA	1.92	0.43
1:C:797:THR:HG22	1:C:797:THR:O	2.19	0.43
1:A:431:MSE:SE	1:A:444:VAL:HG21	2.68	0.43
1:B:189:MSE:HG3	1:B:207:TYR:CD2	2.54	0.43
1:B:386:ALA:O	1:B:387:LYS:C	2.56	0.43
1:B:410:TRP:HE1	1:B:462:THR:N	2.17	0.43
1:B:503:PHE:O	1:B:504:ILE:C	2.57	0.43
1:B:745:TYR:CE1	1:B:750:SER:HA	2.54	0.43
1:C:352:TYR:CE1	1:C:396:ARG:CD	3.01	0.43
1:A:169:ILE:CG2	1:A:170:THR:N	2.82	0.42
1:A:186:ASP:O	1:A:188:VAL:N	2.52	0.42
1:A:182:LEU:CD2	1:A:187:ASP:O	2.52	0.42
1:A:372:GLN:CD	1:A:373:GLY:N	2.72	0.42
1:A:435:PRO:HG3	1:A:503:PHE:CZ	2.54	0.42
1:A:472:HIS:CE1	1:A:538:ASN:ND2	2.87	0.42
1:B:374:ASN:HB3	1:B:375:ARG:H	1.56	0.42
1:B:410:TRP:CZ3	1:B:464:PRO:O	2.72	0.42
1:B:504:ILE:O	1:B:505:ASN:C	2.55	0.42
1:C:296:ASP:CG	1:C:310:ARG:HH21	2.22	0.42
1:C:295:LEU:O	1:C:312:VAL:HG23	2.19	0.42
1:C:749:ARG:O	1:C:751:ARG:N	2.52	0.42
1:A:189:MSE:HG3	1:A:207:TYR:CE2	2.54	0.42
1:A:243:TYR:HB3	1:A:269:ILE:O	2.19	0.42
1:A:307:VAL:O	1:A:307:VAL:HG13	2.19	0.42
1:A:399:PHE:C	1:A:399:PHE:CD1	2.92	0.42
1:A:500:THR:O	1:A:501:ASP:C	2.58	0.42
1:A:511:GLY:O	1:A:513:PRO:CD	2.67	0.42
1:A:728:LEU:HB2	1:A:769:TYR:CE1	2.54	0.42
1:B:342:PRO:HB3	1:B:405:ASN:O	2.19	0.42
1:B:599:TRP:NE1	2:J:4:DSN:HA	2.33	0.42
1:C:136:GLN:HG2	1:C:137:LEU:N	2.34	0.42
1:C:243:TYR:HA	1:C:270:ARG:HA	2.02	0.42
1:C:503:PHE:O	1:C:504:ILE:C	2.57	0.42
1:C:365:SER:N	1:C:799:ALA:O	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:GLY:HA2	1:C:808:MSE:HA	2.01	0.42
1:A:200:TYR:CZ	1:A:206:ASN:HB3	2.54	0.42
1:A:244:ASP:OD2	1:A:245:ARG:NH1	2.53	0.42
1:B:253:THR:OG1	1:B:257:THR:HG23	2.20	0.42
1:B:391:TRP:CD1	1:B:391:TRP:C	2.92	0.42
1:B:472:HIS:CE1	1:B:538:ASN:ND2	2.88	0.42
1:C:179:ASP:HB3	1:C:766:MSE:HE3	2.01	0.42
1:C:435:PRO:HG3	1:C:503:PHE:CZ	2.54	0.42
1:C:529:LEU:HB3	1:C:530:GLY:H	1.71	0.42
1:C:789:TYR:CD1	1:C:789:TYR:C	2.93	0.42
1:A:406:PHE:HB3	1:A:408:ASN:OD1	2.19	0.42
1:A:695:ILE:HD13	1:A:695:ILE:HA	1.86	0.42
1:A:180:PHE:HA	1:A:780:ASN:ND2	2.35	0.42
1:A:795:PHE:C	1:A:797:THR:N	2.73	0.42
1:B:589:TYR:CE1	1:B:614:GLN:HG2	2.54	0.42
1:B:694:LYS:HE2	1:B:708:GLU:O	2.19	0.42
1:C:212:PHE:CD2	1:C:262:LEU:HB2	2.54	0.42
1:C:399:PHE:C	1:C:399:PHE:CD1	2.92	0.42
1:C:722:LYS:O	1:C:723:GLY:C	2.58	0.42
1:A:551:VAL:HG22	1:A:552:VAL:N	2.35	0.42
1:A:757:GLN:O	1:A:758:GLU:O	2.38	0.42
1:A:782:ASN:HB3	1:A:806:ASN:HD22	1.84	0.42
1:B:180:PHE:HA	1:B:780:ASN:ND2	2.34	0.42
1:B:399:PHE:C	1:B:399:PHE:CD1	2.93	0.42
1:B:434:TRP:CE3	1:B:434:TRP:CA	3.01	0.42
1:B:640:GLU:HB3	1:B:668:ALA:HB3	2.02	0.42
1:B:783:ASN:HD22	1:B:783:ASN:C	2.20	0.42
1:B:807:LEU:HA	1:B:807:LEU:HD23	1.80	0.42
1:C:159:VAL:C	1:C:160:LEU:HG	2.40	0.42
1:C:219:TYR:N	1:C:222:ILE:O	2.50	0.42
1:C:556:VAL:HG12	1:C:563:ILE:O	2.19	0.42
1:A:655:THR:O	1:A:656:ASN:C	2.58	0.42
1:A:747:ASN:HB3	1:A:748:PRO:CD	2.40	0.42
1:B:141:THR:O	1:B:143:ASP:N	2.53	0.42
1:B:235:ASN:O	1:B:237:LEU:N	2.53	0.42
1:B:380:ARG:NH1	1:B:380:ARG:HG3	2.34	0.42
1:B:464:PRO:HA	1:B:472:HIS:O	2.19	0.42
1:B:259:ALA:HB1	1:B:595:PRO:HD2	2.02	0.42
1:B:596:GLN:HE21	1:B:596:GLN:HB2	1.54	0.42
1:C:434:TRP:CA	1:C:434:TRP:CE3	3.01	0.42
1:C:645:GLU:CG	1:C:664:LYS:HZ2	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:791:THR:HG23	1:C:800:SER:HB2	2.01	0.42
1:A:372:GLN:O	1:A:373:GLY:O	2.38	0.42
1:A:435:PRO:O	1:A:436:ALA:O	2.37	0.42
1:A:746:ASN:ND2	1:A:749:ARG:CB	2.82	0.42
1:B:202:THR:HG21	1:B:361:GLY:H	1.84	0.42
1:B:262:LEU:HD23	1:B:592:ILE:HG23	2.02	0.42
1:B:196:THR:OG1	1:B:708:GLU:HG3	2.20	0.42
1:B:757:GLN:HA	1:B:757:GLN:NE2	2.35	0.42
1:C:143:ASP:O	1:C:145:GLY:N	2.53	0.42
1:C:277:PHE:O	1:C:278:LYS:HB2	2.19	0.42
1:C:472:HIS:CE1	1:C:538:ASN:ND2	2.88	0.42
1:C:647:ASP:OD1	1:C:648:ALA:N	2.52	0.42
1:C:698:ASP:O	1:C:701:GLY:HA3	2.19	0.42
1:A:190:ARG:HG2	1:A:190:ARG:HH11	1.84	0.42
1:A:253:THR:OG1	1:A:257:THR:HG23	2.19	0.42
1:B:209:ALA:HB2	1:B:214:ILE:CG1	2.50	0.42
1:B:231:TYR:CD2	1:B:485:TRP:HH2	2.38	0.42
1:B:292:ARG:HD2	1:B:316:GLN:OE1	2.20	0.42
1:B:401:ASN:CB	1:B:415:GLN:HB3	2.49	0.42
1:B:692:THR:O	1:B:711:ASP:HA	2.20	0.42
1:B:791:THR:HG23	1:B:800:SER:HB2	2.02	0.42
1:C:262:LEU:HD23	1:C:592:ILE:HG23	2.01	0.42
1:C:492:ASN:HA	1:C:492:ASN:HD22	1.48	0.42
1:C:621:LYS:HG2	1:C:632:SER:CB	2.49	0.42
1:A:421:ASN:O	1:A:452:THR:CG2	2.66	0.42
1:A:526:THR:HA	1:A:555:ARG:O	2.18	0.42
1:A:614:GLN:HE21	1:A:614:GLN:HB2	1.62	0.42
1:A:807:LEU:HA	1:A:807:LEU:HD12	1.93	0.42
1:B:152:ILE:HB	1:B:154:THR:HG22	2.01	0.42
1:B:240:MSE:C	1:B:242:ILE:N	2.73	0.42
1:B:391:TRP:CD1	1:B:393:GLN:CG	3.02	0.42
1:B:447:LYS:HD2	1:B:515:TRP:CG	2.55	0.42
1:B:586:TYR:CD1	1:B:619:GLY:O	2.72	0.42
1:B:723:GLY:O	1:B:725:LEU:N	2.53	0.42
1:B:814:ASP:HB3	1:B:815:PHE:H	1.61	0.42
1:C:211:GLY:CA	1:C:708:GLU:OE1	2.68	0.42
1:C:302:THR:O	1:C:303:GLU:C	2.57	0.42
1:C:474:LEU:HD12	1:C:534:THR:O	2.20	0.42
1:C:163:ARG:NH2	1:C:584:SER:OG	2.49	0.42
1:C:639:HIS:CD2	1:C:669:LYS:HG3	2.55	0.42
1:C:368:LEU:HD21	1:C:798:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ILE:CG2	1:A:141:THR:H	2.31	0.42
1:A:177:MSE:HE2	1:A:245:ARG:HA	2.01	0.42
1:A:410:TRP:CE2	1:A:463:GLY:N	2.88	0.42
1:A:472:HIS:ND1	1:A:538:ASN:ND2	2.68	0.42
1:A:556:VAL:O	1:A:556:VAL:HG22	2.20	0.42
1:A:554:TYR:CD1	1:A:595:PRO:HG3	2.55	0.42
1:A:749:ARG:HH11	1:A:751:ARG:NH2	2.18	0.42
1:B:243:TYR:HA	1:B:270:ARG:HA	2.01	0.42
1:B:475:VAL:CG1	1:B:534:THR:HB	2.50	0.42
1:B:500:THR:O	1:B:501:ASP:C	2.58	0.42
1:B:749:ARG:O	1:B:751:ARG:N	2.50	0.42
1:C:351:ASP:OD2	1:C:397:THR:HG23	2.20	0.42
1:C:552:VAL:HG22	1:C:553:ASP:H	1.83	0.42
1:A:430:ILE:CD1	1:A:441:ALA:HB3	2.50	0.41
1:A:475:VAL:CG1	1:A:534:THR:HB	2.50	0.41
1:A:637:GLU:HA	1:A:671:LYS:HA	2.02	0.41
1:A:670:THR:OG1	1:A:696:ILE:HD12	2.19	0.41
1:B:262:LEU:HD21	1:B:613:GLY:HA3	2.01	0.41
1:B:351:ASP:OD2	1:B:397:THR:CG2	2.68	0.41
1:B:414:VAL:HG23	1:B:459:ILE:CG2	2.50	0.41
1:B:783:ASN:ND2	1:B:783:ASN:C	2.73	0.41
1:C:169:ILE:HA	1:C:169:ILE:HD13	1.84	0.41
1:C:342:PRO:HB3	1:C:405:ASN:O	2.20	0.41
1:C:807:LEU:HA	1:C:807:LEU:HD23	1.83	0.41
1:A:156:THR:C	1:A:158:LEU:N	2.74	0.41
1:A:161:THR:HB	1:A:162:PRO:CD	2.50	0.41
1:A:556:VAL:HG12	1:A:563:ILE:O	2.20	0.41
1:A:791:THR:HG23	1:A:800:SER:HB2	2.02	0.41
1:B:159:VAL:C	1:B:160:LEU:HG	2.40	0.41
1:B:280:HIS:ND1	1:B:812:ARG:NH2	2.68	0.41
1:B:445:ALA:HB3	1:B:493:LEU:HD11	2.02	0.41
1:B:624:TYR:O	1:B:625:LEU:HB2	2.20	0.41
1:C:243:TYR:CE2	1:C:268:LEU:CB	3.03	0.41
1:C:372:GLN:O	1:C:373:GLY:O	2.38	0.41
1:C:380:ARG:NH1	1:C:380:ARG:HG3	2.33	0.41
1:C:414:VAL:HG23	1:C:459:ILE:HG22	2.01	0.41
1:C:158:LEU:CD1	1:C:475:VAL:HB	2.50	0.41
1:A:159:VAL:C	1:A:160:LEU:HG	2.41	0.41
1:A:609:GLU:HB3	1:A:610:PRO:HD2	2.02	0.41
1:A:655:THR:CG2	1:A:656:ASN:H	2.26	0.41
1:B:401:ASN:HB3	1:B:415:GLN:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:TYR:HE1	1:B:614:GLN:HG2	1.84	0.41
1:B:693:HIS:HA	1:B:710:GLN:O	2.21	0.41
1:B:728:LEU:HB2	1:B:769:TYR:CE1	2.55	0.41
1:C:295:LEU:O	1:C:312:VAL:HA	2.19	0.41
1:C:500:THR:O	1:C:501:ASP:C	2.57	0.41
1:C:502:ASP:OD1	1:C:502:ASP:C	2.58	0.41
1:C:526:THR:CG2	1:C:554:TYR:CE1	3.02	0.41
1:A:288:TRP:CZ2	1:A:321:PHE:HB3	2.55	0.41
1:A:430:ILE:HD11	1:A:441:ALA:CB	2.50	0.41
1:A:368:LEU:HD21	1:A:799:ALA:HB2	2.01	0.41
1:B:637:GLU:HA	1:B:671:LYS:HA	2.03	0.41
1:B:655:THR:C	1:B:656:ASN:O	2.58	0.41
1:B:655:THR:CA	1:B:659:ILE:HD12	2.47	0.41
1:B:745:TYR:HB2	1:B:752:TRP:NE1	2.35	0.41
1:C:152:ILE:HG13	1:C:152:ILE:O	2.19	0.41
1:C:202:THR:HG21	1:C:361:GLY:H	1.85	0.41
1:C:383:ASN:C	1:C:385:GLY:H	2.23	0.41
1:C:352:TYR:HE1	1:C:396:ARG:HD2	1.81	0.41
1:A:341:ASN:C	1:A:343:ASP:H	2.23	0.41
1:A:698:ASP:O	1:A:701:GLY:HA3	2.21	0.41
1:A:814:ASP:HB3	1:A:815:PHE:H	1.61	0.41
1:B:295:LEU:O	1:B:312:VAL:HA	2.20	0.41
1:B:414:VAL:HG23	1:B:459:ILE:HG22	2.01	0.41
1:B:384:ASN:O	1:B:430:ILE:HG22	2.19	0.41
1:B:696:ILE:HG23	1:B:696:ILE:O	2.20	0.41
1:C:156:THR:C	1:C:158:LEU:N	2.74	0.41
1:C:313:ALA:HA	1:C:331:VAL:O	2.20	0.41
1:C:461:LEU:O	1:C:475:VAL:HA	2.20	0.41
1:C:461:LEU:HB2	1:C:476:VAL:CG1	2.51	0.41
1:C:503:PHE:O	1:C:504:ILE:O	2.38	0.41
1:C:668:ALA:HA	1:C:698:ASP:HA	2.03	0.41
1:C:766:MSE:HB2	1:C:780:ASN:ND2	2.35	0.41
1:A:246:VAL:O	1:A:246:VAL:CG1	2.67	0.41
1:A:378:VAL:CG2	1:A:382:PHE:HB2	2.51	0.41
1:A:414:VAL:HG23	1:A:459:ILE:HG22	2.01	0.41
1:A:537:PHE:O	1:A:545:LEU:N	2.42	0.41
1:A:262:LEU:HD23	1:A:592:ILE:HG23	2.02	0.41
1:A:602:ASP:O	1:A:604:SER:N	2.53	0.41
1:B:161:THR:HB	1:B:162:PRO:CD	2.50	0.41
1:B:235:ASN:C	1:B:237:LEU:H	2.24	0.41
1:B:502:ASP:C	1:B:502:ASP:OD1	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:PHE:CD2	1:B:504:ILE:N	2.89	0.41
1:B:682:ALA:CB	1:B:683:PRO:HD2	2.51	0.41
1:C:186:ASP:O	1:C:188:VAL:N	2.53	0.41
1:C:214:ILE:HG23	1:C:264:ALA:O	2.19	0.41
1:C:292:ARG:HD2	1:C:316:GLN:OE1	2.20	0.41
1:C:439:ASN:O	1:C:502:ASP:HA	2.21	0.41
1:C:532:TYR:HD2	1:C:550:ARG:NH1	2.19	0.41
1:C:795:PHE:C	1:C:797:THR:N	2.73	0.41
1:A:235:ASN:O	1:A:237:LEU:N	2.54	0.41
1:A:383:ASN:C	1:A:385:GLY:N	2.72	0.41
1:A:439:ASN:O	1:A:502:ASP:HA	2.20	0.41
1:A:640:GLU:HB3	1:A:668:ALA:HB3	2.03	0.41
1:B:526:THR:HA	1:B:555:ARG:O	2.20	0.41
1:B:529:LEU:O	1:B:552:VAL:HG23	2.20	0.41
1:B:532:TYR:HD2	1:B:550:ARG:NH1	2.18	0.41
1:B:639:HIS:CD2	1:B:669:LYS:HG3	2.56	0.41
1:B:682:ALA:HB3	1:B:685:TRP:CB	2.50	0.41
1:C:147:TYR:CD2	1:C:686:GLN:HB3	2.56	0.41
1:C:180:PHE:HA	1:C:780:ASN:HD21	1.86	0.41
1:C:235:ASN:C	1:C:237:LEU:H	2.24	0.41
1:C:582:THR:HG22	1:C:583:TYR:N	2.36	0.41
1:B:219:TYR:CD1	1:B:219:TYR:N	2.89	0.41
1:B:219:TYR:N	1:B:222:ILE:O	2.51	0.41
1:B:406:PHE:HB3	1:B:408:ASN:OD1	2.21	0.41
1:B:576:VAL:HA	1:B:585:VAL:O	2.20	0.41
1:B:211:GLY:CA	1:B:708:GLU:OE1	2.68	0.41
1:C:148:THR:OG1	1:C:149:PRO:HD2	2.19	0.41
1:C:281:VAL:O	1:C:281:VAL:CG1	2.68	0.41
1:C:323:ASP:O	1:C:324:HIS:ND1	2.54	0.41
1:C:443:ILE:CG1	1:C:443:ILE:O	2.68	0.41
1:C:772:THR:O	1:C:773:ASP:C	2.59	0.41
1:C:772:THR:OG1	1:C:775:LEU:HB3	2.20	0.41
1:A:209:ALA:HB2	1:A:214:ILE:CG1	2.51	0.41
1:A:226:ALA:HB3	1:A:235:ASN:HD21	1.86	0.41
1:A:361:GLY:HA2	1:A:385:GLY:CA	2.51	0.41
1:A:396:ARG:HG3	1:A:420:ILE:CD1	2.51	0.41
1:A:504:ILE:O	1:A:505:ASN:C	2.58	0.41
1:A:766:MSE:HG3	1:A:780:ASN:ND2	2.36	0.41
1:B:447:LYS:CE	3:B:2002:SO4:O4	2.65	0.41
1:B:214:ILE:HG23	1:B:264:ALA:O	2.21	0.41
1:B:430:ILE:HD11	1:B:441:ALA:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:LEU:O	1:B:475:VAL:HA	2.21	0.41
1:B:792:ASN:C	1:B:792:ASN:ND2	2.74	0.41
1:C:173:THR:CG2	1:C:176:ASN:HB2	2.50	0.41
1:C:186:ASP:C	1:C:188:VAL:N	2.74	0.41
1:C:341:ASN:C	1:C:343:ASP:H	2.24	0.41
1:C:472:HIS:ND1	1:C:538:ASN:ND2	2.69	0.41
1:A:255:LEU:HD22	1:A:572:TYR:CD2	2.55	0.41
1:A:290:ASN:HA	1:A:318:LYS:CB	2.50	0.41
1:A:561:PRO:O	1:A:562:THR:C	2.59	0.41
1:B:281:VAL:HB	1:B:295:LEU:CD1	2.50	0.41
1:B:510:ILE:HG22	1:B:511:GLY:N	2.36	0.41
1:C:235:ASN:O	1:C:237:LEU:N	2.53	0.41
1:C:539:VAL:HB	1:C:543:LEU:HD23	2.03	0.41
1:C:255:LEU:HD22	1:C:572:TYR:CG	2.56	0.41
1:C:593:PHE:C	1:C:593:PHE:CD1	2.94	0.41
1:A:260:GLY:C	1:A:592:ILE:HD11	2.41	0.41
1:A:275:HIS:CE1	1:A:308:ARG:NH1	2.89	0.41
1:A:357:PRO:O	1:A:390:SER:CB	2.61	0.41
1:A:582:THR:HG22	1:A:583:TYR:N	2.35	0.41
1:B:173:THR:HG23	1:B:176:ASN:HB2	2.02	0.41
1:B:178:ASP:O	1:B:179:ASP:C	2.59	0.41
1:B:699:ASP:O	1:B:700:SER:C	2.59	0.41
1:B:789:TYR:C	1:B:789:TYR:CD1	2.94	0.41
1:C:139:THR:CG2	1:C:150:GLY:HA3	2.50	0.41
1:C:503:PHE:CD2	1:C:504:ILE:N	2.89	0.41
1:C:761:TRP:HA	1:C:761:TRP:CE3	2.56	0.41
1:A:189:MSE:HE3	1:A:195:ILE:CD1	2.44	0.40
1:A:244:ASP:N	1:A:269:ILE:O	2.49	0.40
1:A:292:ARG:CG	1:A:316:GLN:HB2	2.50	0.40
1:A:202:THR:HG21	1:A:361:GLY:H	1.85	0.40
1:A:371:SER:HB3	1:A:372:GLN:OE1	2.21	0.40
1:A:647:ASP:HB3	1:A:662:ALA:O	2.22	0.40
1:A:674:GLU:HB2	1:A:692:THR:HG23	2.02	0.40
1:A:749:ARG:O	1:A:751:ARG:N	2.53	0.40
1:A:766:MSE:HB2	1:A:780:ASN:ND2	2.36	0.40
1:B:139:THR:CG2	1:B:150:GLY:HA3	2.51	0.40
1:B:143:ASP:O	1:B:145:GLY:N	2.55	0.40
1:B:169:ILE:HA	1:B:169:ILE:HD13	1.88	0.40
1:B:474:LEU:CG	1:B:475:VAL:N	2.84	0.40
1:B:670:THR:OG1	1:B:696:ILE:CG1	2.69	0.40
1:B:670:THR:OG1	1:B:696:ILE:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:725:LEU:C	1:B:727:LYS:N	2.74	0.40
1:C:681:LEU:HD23	1:C:685:TRP:CE2	2.57	0.40
1:C:764:ASP:HB3	1:C:782:ASN:C	2.38	0.40
1:A:699:ASP:O	1:A:700:SER:C	2.59	0.40
1:B:152:ILE:O	1:B:152:ILE:HG13	2.20	0.40
1:B:496:TYR:CZ	1:B:513:PRO:HD3	2.57	0.40
1:B:472:HIS:ND1	1:B:538:ASN:ND2	2.70	0.40
1:B:556:VAL:HG22	1:B:556:VAL:O	2.21	0.40
1:B:698:ASP:O	1:B:701:GLY:CA	2.70	0.40
1:C:365:SER:HB2	1:C:799:ALA:O	2.22	0.40
1:C:394:TYR:C	1:C:394:TYR:CD1	2.95	0.40
1:C:540:THR:HG22	1:C:542:ASP:OD1	2.21	0.40
1:C:651:ASN:O	1:C:653:LYS:HG3	2.21	0.40
1:C:725:LEU:C	1:C:727:LYS:N	2.74	0.40
1:A:158:LEU:O	1:A:160:LEU:CD1	2.70	0.40
1:A:235:ASN:C	1:A:237:LEU:H	2.25	0.40
1:A:295:LEU:O	1:A:312:VAL:HA	2.21	0.40
1:A:365:SER:HB2	1:A:799:ALA:O	2.21	0.40
1:A:401:ASN:CB	1:A:415:GLN:HB3	2.49	0.40
1:A:502:ASP:C	1:A:502:ASP:OD1	2.60	0.40
1:A:668:ALA:HA	1:A:698:ASP:HA	2.04	0.40
1:B:383:ASN:C	1:B:385:GLY:N	2.73	0.40
1:B:511:GLY:O	1:B:513:PRO:CD	2.68	0.40
1:B:552:VAL:HG22	1:B:553:ASP:H	1.86	0.40
1:B:772:THR:O	1:B:773:ASP:C	2.59	0.40
1:C:161:THR:HB	1:C:162:PRO:CD	2.52	0.40
1:C:174:ARG:HG3	1:C:178:ASP:OD2	2.21	0.40
1:C:288:TRP:CZ2	1:C:321:PHE:HB3	2.56	0.40
1:A:147:TYR:CE1	1:A:176:ASN:HA	2.56	0.40
1:A:259:ALA:HB1	1:A:595:PRO:HD2	2.04	0.40
1:A:323:ASP:O	1:A:324:HIS:ND1	2.54	0.40
1:B:209:ALA:CB	1:B:214:ILE:HG12	2.51	0.40
1:B:169:ILE:CD1	1:B:249:LEU:HD12	2.49	0.40
1:B:518:PRO:CG	1:B:521:TYR:CE2	3.05	0.40
1:B:762:LEU:CD2	1:B:789:TYR:HE2	2.23	0.40
1:C:430:ILE:CD1	1:C:441:ALA:HB3	2.52	0.40
1:B:207:TYR:O	1:B:214:ILE:HG13	2.22	0.40
1:B:244:ASP:OD2	1:B:245:ARG:NH1	2.55	0.40
1:B:170:THR:O	1:B:248:VAL:HG12	2.22	0.40
1:B:238:SER:HA	1:B:353:GLN:OE1	2.22	0.40
1:B:694:LYS:HD3	1:B:694:LYS:C	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:766:MSE:HG3	1:B:780:ASN:ND2	2.37	0.40
1:C:378:VAL:CG2	1:C:382:PHE:HB2	2.51	0.40
1:C:552:VAL:CG2	1:C:553:ASP:H	2.34	0.40
1:C:556:VAL:O	1:C:556:VAL:HG22	2.21	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	685/687 (100%)	521 (76%)	102 (15%)	62 (9%)	1	9
1	B	685/687 (100%)	519 (76%)	103 (15%)	63 (9%)	1	9
1	C	685/687 (100%)	518 (76%)	108 (16%)	59 (9%)	1	10
2	I	3/8 (38%)	1 (33%)	1 (33%)	1 (33%)	0	0
2	J	3/8 (38%)	1 (33%)	1 (33%)	1 (33%)	0	0
2	K	3/8 (38%)	1 (33%)	1 (33%)	1 (33%)	0	0
All	All	2064/2085 (99%)	1561 (76%)	316 (15%)	187 (9%)	1	9

All (187) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	241	ALA
1	A	324	HIS
1	A	341	ASN
1	A	345	MSE
1	A	371	SER
1	A	374	ASN
1	A	436	ALA

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Mol	Chain	Res	Type
1	A	561	PRO
1	A	605	ASN
1	A	626	ASP
1	A	650	TYR
1	A	655	THR
1	A	659	ILE
1	A	682	ALA
1	A	699	ASP
1	A	724	ALA
1	A	739	LYS
1	A	758	GLU
1	A	775	LEU
1	A	784	VAL
1	A	805	ARG
1	A	814	ASP
1	B	144	SER
1	B	241	ALA
1	B	324	HIS
1	B	341	ASN
1	B	345	MSE
1	B	371	SER
1	B	374	ASN
1	B	436	ALA
1	B	561	PRO
1	B	605	ASN
1	B	626	ASP
1	B	655	THR
1	B	659	ILE
1	B	682	ALA
1	B	699	ASP
1	B	724	ALA
1	B	739	LYS
1	B	758	GLU
1	B	775	LEU
1	B	784	VAL
1	B	805	ARG
1	B	814	ASP
1	C	144	SER
1	C	241	ALA
1	C	324	HIS
1	C	341	ASN
1	C	345	MSE

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Mol	Chain	Res	Type
1	C	371	SER
1	C	374	ASN
1	C	436	ALA
1	C	561	PRO
1	C	605	ASN
1	C	626	ASP
1	C	651	ASN
1	C	659	ILE
1	C	660	THR
1	C	682	ALA
1	C	699	ASP
1	C	724	ALA
1	C	739	LYS
1	C	758	GLU
1	C	775	LEU
1	C	784	VAL
1	C	805	ARG
1	C	814	ASP
2	I	6	LYS
2	J	6	LYS
2	K	6	LYS
1	A	187	ASP
1	A	202	THR
1	A	236	THR
1	A	254	GLY
1	A	340	LEU
1	A	363	SER
1	A	373	GLY
1	A	501	ASP
1	A	504	ILE
1	A	508	GLY
1	A	516	GLY
1	A	579	LEU
1	A	603	SER
1	A	656	ASN
1	A	723	GLY
1	B	202	THR
1	B	236	THR
1	B	254	GLY
1	B	340	LEU
1	B	363	SER
1	B	469	GLY

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Mol	Chain	Res	Type
1	B	501	ASP
1	B	504	ILE
1	B	508	GLY
1	B	516	GLY
1	B	579	LEU
1	B	603	SER
1	B	723	GLY
1	C	187	ASP
1	C	236	THR
1	C	254	GLY
1	C	340	LEU
1	C	363	SER
1	C	373	GLY
1	C	501	ASP
1	C	504	ILE
1	C	508	GLY
1	C	516	GLY
1	C	579	LEU
1	C	603	SER
1	C	723	GLY
1	A	379	SER
1	A	469	GLY
1	A	505	ASN
1	A	649	LEU
1	A	683	PRO
1	A	750	SER
1	B	142	GLU
1	B	145	GLY
1	B	187	ASP
1	B	373	GLY
1	B	379	SER
1	B	505	ASN
1	B	650	TYR
1	B	658	ALA
1	B	683	PRO
1	B	750	SER
1	C	145	GLY
1	C	202	THR
1	C	379	SER
1	C	505	ASN
1	C	683	PRO
1	C	750	SER

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Mol	Chain	Res	Type
1	A	541	ASP
1	A	658	ALA
1	A	660	THR
1	B	439	ASN
1	B	541	ASP
1	C	142	GLU
1	C	384	ASN
1	C	439	ASN
1	C	469	GLY
1	C	541	ASP
1	C	608	LEU
1	C	655	THR
1	A	303	GLU
1	A	384	ASN
1	A	439	ASN
1	A	608	LEU
1	A	744	VAL
1	B	303	GLU
1	B	384	ASN
1	B	426	PRO
1	B	433	ASP
1	B	608	LEU
1	B	744	VAL
1	C	303	GLU
1	C	592	ILE
1	C	625	LEU
1	C	744	VAL
1	A	145	GLY
1	A	426	PRO
1	A	433	ASP
1	A	435	PRO
1	A	475	VAL
1	A	592	ILE
1	B	475	VAL
1	B	592	ILE
1	B	625	LEU
1	C	426	PRO
1	C	435	PRO
1	C	475	VAL
1	C	512	LYS
1	C	513	PRO
1	B	656	ASN

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Mol	Chain	Res	Type
1	A	258	GLY
1	A	512	LYS
1	A	513	PRO
1	B	435	PRO
1	A	803	ASP
1	B	513	PRO
1	B	803	ASP
1	C	803	ASP
1	B	258	GLY
1	B	512	LYS
1	B	657	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	582/570 (102%)	509 (88%)	73 (12%)	4	25
1	B	582/570 (102%)	505 (87%)	77 (13%)	4	23
1	C	582/570 (102%)	505 (87%)	77 (13%)	4	23
2	I	4/4 (100%)	2 (50%)	2 (50%)	0	0
2	J	4/4 (100%)	2 (50%)	2 (50%)	0	0
2	K	4/4 (100%)	2 (50%)	2 (50%)	0	0
All	All	1758/1722 (102%)	1525 (87%)	233 (13%)	4	23

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	139	THR
1	A	143	ASP
1	A	157	ARG
1	A	160	LEU
1	A	174	ARG
1	A	178	ASP

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Mol	Chain	Res	Type
1	A	185	ILE
1	A	196	THR
1	A	201	ASP
1	A	213	SER
1	A	218	GLN
1	A	225	THR
1	A	227	ARG
1	A	236	THR
1	A	257	THR
1	A	282	GLU
1	A	330	SER
1	A	341	ASN
1	A	342	PRO
1	A	344	THR
1	A	354	ASP
1	A	399	PHE
1	A	408	ASN
1	A	410	TRP
1	A	415	GLN
1	A	433	ASP
1	A	434	TRP
1	A	452	THR
1	A	462	THR
1	A	473	GLU
1	A	490	TYR
1	A	492	ASN
1	A	497	ASP
1	A	501	ASP
1	A	502	ASP
1	A	506	TRP
1	A	507	ASP
1	A	515	TRP
1	A	526	THR
1	A	538	ASN
1	A	557	THR
1	A	560	ASN
1	A	561	PRO
1	A	578	ASP
1	A	593	PHE
1	A	596	GLN
1	A	599	TRP
1	A	607	LEU

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Mol	Chain	Res	Type
1	A	614	GLN
1	A	624	TYR
1	A	628	ARG
1	A	630	ASN
1	A	633	LEU
1	A	650	TYR
1	A	653	LYS
1	A	661	TYR
1	A	670	THR
1	A	694	LYS
1	A	710	GLN
1	A	725	LEU
1	A	736	TRP
1	A	742	GLN
1	A	743	MSE
1	A	752	TRP
1	A	761	TRP
1	A	766	MSE
1	A	778	SER
1	A	783	ASN
1	A	788	THR
1	A	792	ASN
1	A	814	ASP
1	A	815	PHE
1	B	135	ASN
1	B	139	THR
1	B	143	ASP
1	B	160	LEU
1	B	174	ARG
1	B	185	ILE
1	B	196	THR
1	B	201	ASP
1	B	213	SER
1	B	218	GLN
1	B	225	THR
1	B	239	ASP
1	B	257	THR
1	B	327	ARG
1	B	330	SER
1	B	341	ASN
1	B	342	PRO
1	B	344	THR

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Mol	Chain	Res	Type
1	B	354	ASP
1	B	376	ASN
1	B	399	PHE
1	B	408	ASN
1	B	410	TRP
1	B	415	GLN
1	B	417	ASP
1	B	433	ASP
1	B	434	TRP
1	B	439	ASN
1	B	452	THR
1	B	462	THR
1	B	473	GLU
1	B	490	TYR
1	B	492	ASN
1	B	497	ASP
1	B	501	ASP
1	B	502	ASP
1	B	506	TRP
1	B	507	ASP
1	B	509	ASP
1	B	538	ASN
1	B	541	ASP
1	B	557	THR
1	B	560	ASN
1	B	561	PRO
1	B	568	ARG
1	B	578	ASP
1	B	593	PHE
1	B	596	GLN
1	B	599	TRP
1	B	606	LYS
1	B	607	LEU
1	B	614	GLN
1	B	624	TYR
1	B	628	ARG
1	B	630	ASN
1	B	633	LEU
1	B	653	LYS
1	B	656	ASN
1	B	670	THR
1	B	694	LYS

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Mol	Chain	Res	Type
1	B	706	THR
1	B	725	LEU
1	B	742	GLN
1	B	743	MSE
1	B	752	TRP
1	B	754	LYS
1	B	761	TRP
1	B	766	MSE
1	B	768	ARG
1	B	778	SER
1	B	782	ASN
1	B	783	ASN
1	B	788	THR
1	B	789	TYR
1	B	792	ASN
1	B	814	ASP
1	B	815	PHE
1	C	139	THR
1	C	143	ASP
1	C	160	LEU
1	C	185	ILE
1	C	196	THR
1	C	201	ASP
1	C	213	SER
1	C	218	GLN
1	C	225	THR
1	C	227	ARG
1	C	257	THR
1	C	274	THR
1	C	289	ASP
1	C	342	PRO
1	C	344	THR
1	C	354	ASP
1	C	377	ASP
1	C	396	ARG
1	C	399	PHE
1	C	402	LEU
1	C	408	ASN
1	C	410	TRP
1	C	415	GLN
1	C	433	ASP
1	C	434	TRP

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Mol	Chain	Res	Type
1	C	449	THR
1	C	452	THR
1	C	462	THR
1	C	473	GLU
1	C	479	SER
1	C	490	TYR
1	C	492	ASN
1	C	497	ASP
1	C	501	ASP
1	C	502	ASP
1	C	506	TRP
1	C	507	ASP
1	C	526	THR
1	C	536	ARG
1	C	538	ASN
1	C	543	LEU
1	C	554	TYR
1	C	557	THR
1	C	560	ASN
1	C	561	PRO
1	C	593	PHE
1	C	596	GLN
1	C	599	TRP
1	C	607	LEU
1	C	614	GLN
1	C	624	TYR
1	C	628	ARG
1	C	630	ASN
1	C	633	LEU
1	C	645	GLU
1	C	650	TYR
1	C	651	ASN
1	C	653	LYS
1	C	661	TYR
1	C	670	THR
1	C	694	LYS
1	C	725	LEU
1	C	726	ASP
1	C	736	TRP
1	C	742	GLN
1	C	743	MSE
1	C	752	TRP

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Mol	Chain	Res	Type
1	C	760	TYR
1	C	761	TRP
1	C	766	MSE
1	C	778	SER
1	C	782	ASN
1	C	783	ASN
1	C	788	THR
1	C	792	ASN
1	C	814	ASP
1	C	815	PHE
2	I	6	LYS
2	I	8	THR
2	J	6	LYS
2	J	8	THR
2	K	6	LYS
2	K	8	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	205	ASN
1	A	206	ASN
1	A	235	ASN
1	A	275	HIS
1	A	280	HIS
1	A	324	HIS
1	A	341	ASN
1	A	353	GLN
1	A	376	ASN
1	A	405	ASN
1	A	415	GLN
1	A	418	HIS
1	A	492	ASN
1	A	538	ASN
1	A	560	ASN
1	A	596	GLN
1	A	614	GLN
1	A	630	ASN
1	A	710	GLN
1	A	746	ASN
1	A	780	ASN

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Mol	Chain	Res	Type
1	A	782	ASN
1	A	806	ASN
1	B	135	ASN
1	B	191	HIS
1	B	205	ASN
1	B	235	ASN
1	B	275	HIS
1	B	280	HIS
1	B	324	HIS
1	B	341	ASN
1	B	376	ASN
1	B	383	ASN
1	B	405	ASN
1	B	415	GLN
1	B	418	HIS
1	B	439	ASN
1	B	538	ASN
1	B	560	ASN
1	B	596	GLN
1	B	614	GLN
1	B	630	ASN
1	B	710	GLN
1	B	746	ASN
1	B	757	GLN
1	B	780	ASN
1	B	782	ASN
1	B	783	ASN
1	B	806	ASN
1	C	183	ASN
1	C	205	ASN
1	C	235	ASN
1	C	275	HIS
1	C	280	HIS
1	C	324	HIS
1	C	376	ASN
1	C	384	ASN
1	C	415	GLN
1	C	418	HIS
1	C	492	ASN
1	C	538	ASN
1	C	544	ASN
1	C	560	ASN

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Mol	Chain	Res	Type
1	C	596	GLN
1	C	614	GLN
1	C	630	ASN
1	C	651	ASN
1	C	710	GLN
1	C	746	ASN
1	C	770	GLN
1	C	780	ASN
1	C	782	ASN
1	C	783	ASN
1	C	806	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FHO	I	5	2	8,10,11	0.91	0	4,11,13	1.69	1 (25%)
2	FHO	I	7	2	8,10,11	1.70	2 (25%)	4,11,13	1.62	1 (25%)
2	FHO	J	5	2	8,10,11	0.94	0	4,11,13	1.78	1 (25%)
2	FHO	K	7	2	8,10,11	1.44	2 (25%)	4,11,13	1.09	0
2	FHO	K	5	2	8,10,11	0.93	0	4,11,13	1.58	1 (25%)
2	FHO	J	7	2	8,10,11	1.94	2 (25%)	4,11,13	1.62	1 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FHO	I	5	2	-	4/7/10/12	-
2	FHO	I	7	2	-	5/7/10/12	-
2	FHO	J	5	2	-	4/7/10/12	-
2	FHO	K	7	2	-	3/7/10/12	-
2	FHO	K	5	2	-	4/7/10/12	-
2	FHO	J	7	2	-	5/7/10/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	7	FHO	CB-CA	4.01	1.58	1.53
2	I	7	FHO	CB-CA	3.25	1.57	1.53
2	J	7	FHO	CD-NE	2.61	1.51	1.46
2	I	7	FHO	CZ-NE	-2.33	1.31	1.34
2	K	7	FHO	CZ-NE	-2.30	1.31	1.34
2	K	7	FHO	CB-CA	2.05	1.56	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	5	FHO	OZ-NE-CD	3.05	121.18	113.67
2	I	5	FHO	OZ-NE-CD	2.95	120.93	113.67
2	K	5	FHO	OZ-NE-CD	2.84	120.66	113.67
2	J	7	FHO	CG-CD-NE	2.48	116.18	111.07
2	I	7	FHO	CG-CD-NE	2.47	116.16	111.07

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	5	FHO	N-CA-CB-CG
2	I	5	FHO	C-CA-CB-CG
2	I	5	FHO	CG-CD-NE-OZ
2	I	5	FHO	CG-CD-NE-CZ
2	I	7	FHO	N-CA-CB-CG
2	I	7	FHO	C-CA-CB-CG
2	I	7	FHO	NE-CD-CG-CB
2	I	7	FHO	CG-CD-NE-OZ
2	I	7	FHO	CG-CD-NE-CZ
2	J	5	FHO	N-CA-CB-CG
2	J	5	FHO	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	J	5	FHO	CG-CD-NE-OZ
2	J	5	FHO	CG-CD-NE-CZ
2	K	7	FHO	C-CA-CB-CG
2	K	7	FHO	CG-CD-NE-OZ
2	K	5	FHO	N-CA-CB-CG
2	K	5	FHO	C-CA-CB-CG
2	K	5	FHO	CG-CD-NE-OZ
2	K	5	FHO	CG-CD-NE-CZ
2	J	7	FHO	NE-CD-CG-CB
2	J	7	FHO	CG-CD-NE-OZ
2	J	7	FHO	CG-CD-NE-CZ
2	K	7	FHO	CA-CB-CG-CD
2	J	7	FHO	N-CA-CB-CG
2	J	7	FHO	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	7	FHO	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	2001	-	4,4,4	0.31	0	6,6,6	0.13	0
4	PVE	J	1	2	23,28,29	2.65	9 (39%)	25,40,42	5.10	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	2003	-	4,4,4	0.34	0	6,6,6	0.10	0
4	PVE	I	1	2	23,28,29	2.52	8 (34%)	25,40,42	4.93	1 (4%)
3	SO4	B	2002	-	4,4,4	0.34	0	6,6,6	0.14	0
4	PVE	K	1	2	23,28,29	2.78	8 (34%)	25,40,42	4.89	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PVE	J	1	2	1/1/3/6	5/8/21/23	0/2/3/3
4	PVE	K	1	2	1/1/3/6	6/8/21/23	0/2/3/3
4	PVE	I	1	2	1/1/3/6	5/8/21/23	0/2/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1	PVE	C5-C6	6.60	1.43	1.37
4	J	1	PVE	C9-N1	6.41	1.46	1.39
4	J	1	PVE	C8-C7	6.24	1.43	1.37
4	K	1	PVE	C8-C7	6.18	1.43	1.37
4	K	1	PVE	C9-N1	5.96	1.45	1.39
4	I	1	PVE	C5-C6	5.81	1.43	1.37
4	I	1	PVE	C8-C7	5.72	1.43	1.37
4	I	1	PVE	C9-N1	4.94	1.44	1.39
4	J	1	PVE	C5-C6	4.87	1.42	1.37
4	K	1	PVE	C2-N1	3.57	1.44	1.36
4	J	1	PVE	C2-N1	3.42	1.43	1.36
4	I	1	PVE	C3-N17	-3.21	1.35	1.41
4	J	1	PVE	C3-N17	-3.08	1.35	1.41
4	K	1	PVE	C4-C3	2.98	1.43	1.37
4	K	1	PVE	C3-C2	2.97	1.44	1.41
4	K	1	PVE	C3-N17	-2.74	1.36	1.41
4	I	1	PVE	C2-N1	2.64	1.42	1.36
4	I	1	PVE	C4-C3	2.63	1.42	1.37
4	K	1	PVE	C8-C9	2.49	1.45	1.40
4	J	1	PVE	C8-C9	2.42	1.45	1.40
4	J	1	PVE	C3-C2	2.40	1.43	1.41
4	I	1	PVE	C3-C2	2.32	1.43	1.41
4	J	1	PVE	C4-C3	2.30	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1	PVE	O26-C7	-2.19	1.31	1.36
4	I	1	PVE	C8-C9	2.11	1.44	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1	PVE	C15-C14-N1	25.13	144.00	111.97
4	I	1	PVE	C15-C14-N1	24.28	142.91	111.97
4	K	1	PVE	C15-C14-N1	23.99	142.55	111.97

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	J	1	PVE	C14
4	I	1	PVE	C14
4	K	1	PVE	C14

All (16) torsion outliers are listed below:

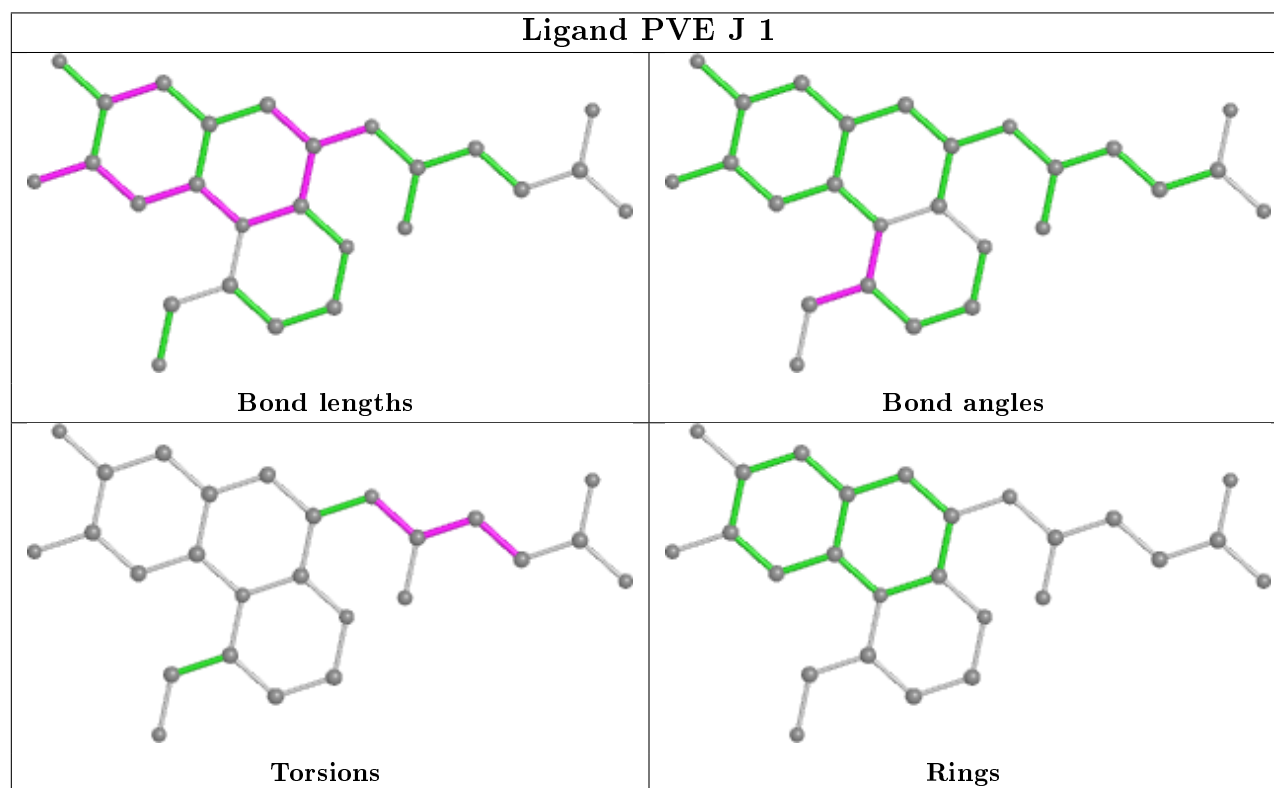
Mol	Chain	Res	Type	Atoms
4	J	1	PVE	C18-C20-C21-C22
4	J	1	PVE	C20-C18-N17-C3
4	I	1	PVE	C20-C18-N17-C3
4	K	1	PVE	C18-C20-C21-C22
4	K	1	PVE	C20-C18-N17-C3
4	K	1	PVE	C13-C14-C15-O16
4	I	1	PVE	O19-C18-N17-C3
4	K	1	PVE	O19-C18-N17-C3
4	J	1	PVE	O19-C18-N17-C3
4	J	1	PVE	O19-C18-C20-C21
4	I	1	PVE	C18-C20-C21-C22
4	J	1	PVE	N17-C18-C20-C21
4	I	1	PVE	O19-C18-C20-C21
4	I	1	PVE	N17-C18-C20-C21
4	K	1	PVE	O19-C18-C20-C21
4	K	1	PVE	N17-C18-C20-C21

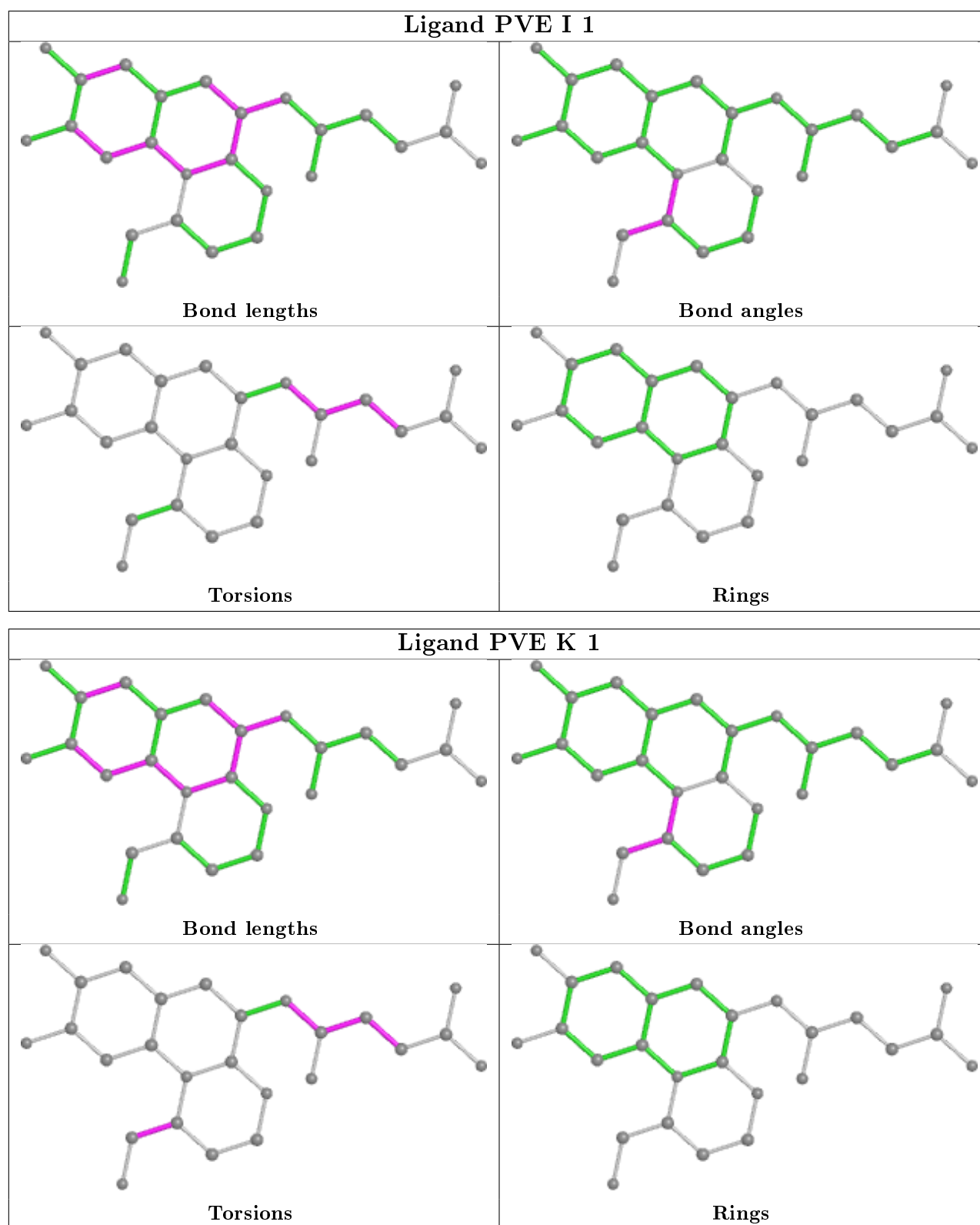
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1	PVE	3	0
4	I	1	PVE	1	0
3	B	2002	SO4	2	0
4	K	1	PVE	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 ⓘ

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	675/687 (98%)	-0.51	3 (0%) 92 86	9, 41, 69, 111	0
1	B	675/687 (98%)	-0.49	3 (0%) 92 86	9, 41, 70, 111	0
1	C	675/687 (98%)	-0.51	5 (0%) 87 78	9, 41, 70, 118	0
2	I	4/8 (50%)	0.07	0 100 100	56, 62, 63, 84	0
2	J	4/8 (50%)	-0.09	0 100 100	65, 71, 72, 83	0
2	K	4/8 (50%)	0.06	0 100 100	61, 66, 69, 95	0
All	All	2037/2085 (97%)	-0.50	11 (0%) 91 83	9, 41, 70, 118	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	ALA	3.7
1	C	130	THR	3.4
1	C	129	ALA	3.2
1	B	130	THR	2.9
1	C	132	ILE	2.8
1	A	557	THR	2.8
1	A	660	THR	2.6
1	C	660	THR	2.5
1	B	132	ILE	2.2
1	C	304	SER	2.2
1	B	557	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FHO	K	5	11/12	0.52	0.47	75,85,96,96	0
2	FHO	I	5	11/12	0.64	0.39	66,77,89,90	0
2	FHO	J	5	11/12	0.75	0.34	73,79,87,88	0
2	DSN	K	4	6/7	0.82	0.29	87,89,90,90	0
2	FHO	K	7	11/12	0.84	0.27	35,43,60,61	0
2	DSN	K	2	6/7	0.86	0.28	92,93,93,93	0
2	DSN	J	4	6/7	0.88	0.25	78,79,80,80	0
2	FHO	J	7	11/12	0.89	0.27	41,48,61,63	0
2	DSN	I	2	6/7	0.90	0.25	81,84,85,87	0
2	DSN	J	2	6/7	0.90	0.26	79,82,84,84	0
2	FHO	I	7	11/12	0.92	0.21	29,37,53,55	0
2	DSN	I	4	6/7	0.93	0.17	76,77,78,78	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

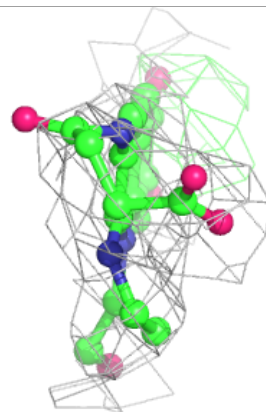
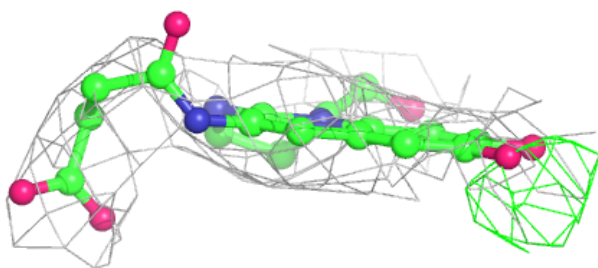
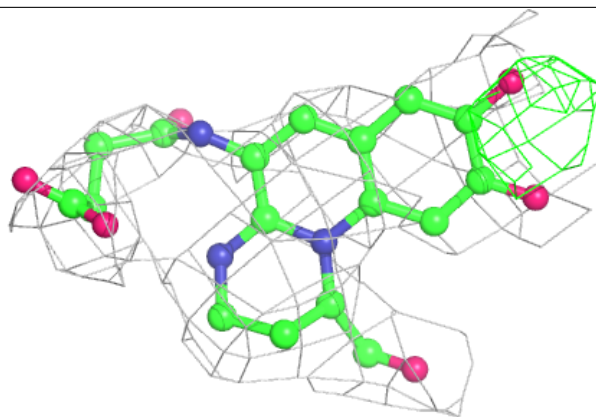
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PVE	J	1	26/27	0.78	0.32	81,86,92,92	0
4	PVE	I	1	26/27	0.79	0.33	82,85,91,91	0
4	PVE	K	1	26/27	0.81	0.33	86,88,91,92	0
3	SO4	B	2002	5/5	0.93	0.21	67,68,68,68	0
3	SO4	C	2003	5/5	0.94	0.26	97,98,98,98	0
3	SO4	A	2001	5/5	0.95	0.16	58,59,59,60	0

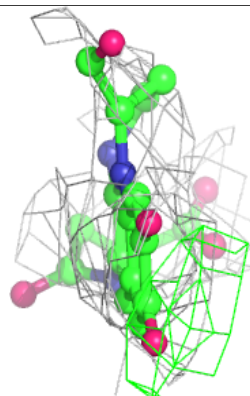
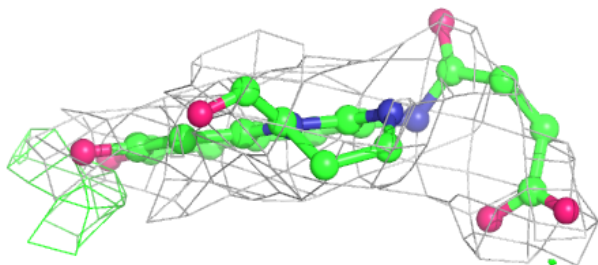
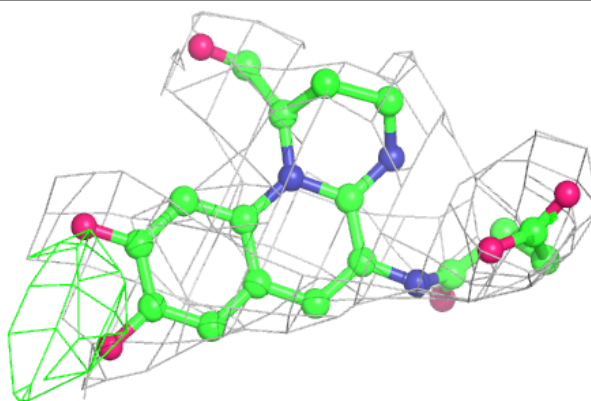
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

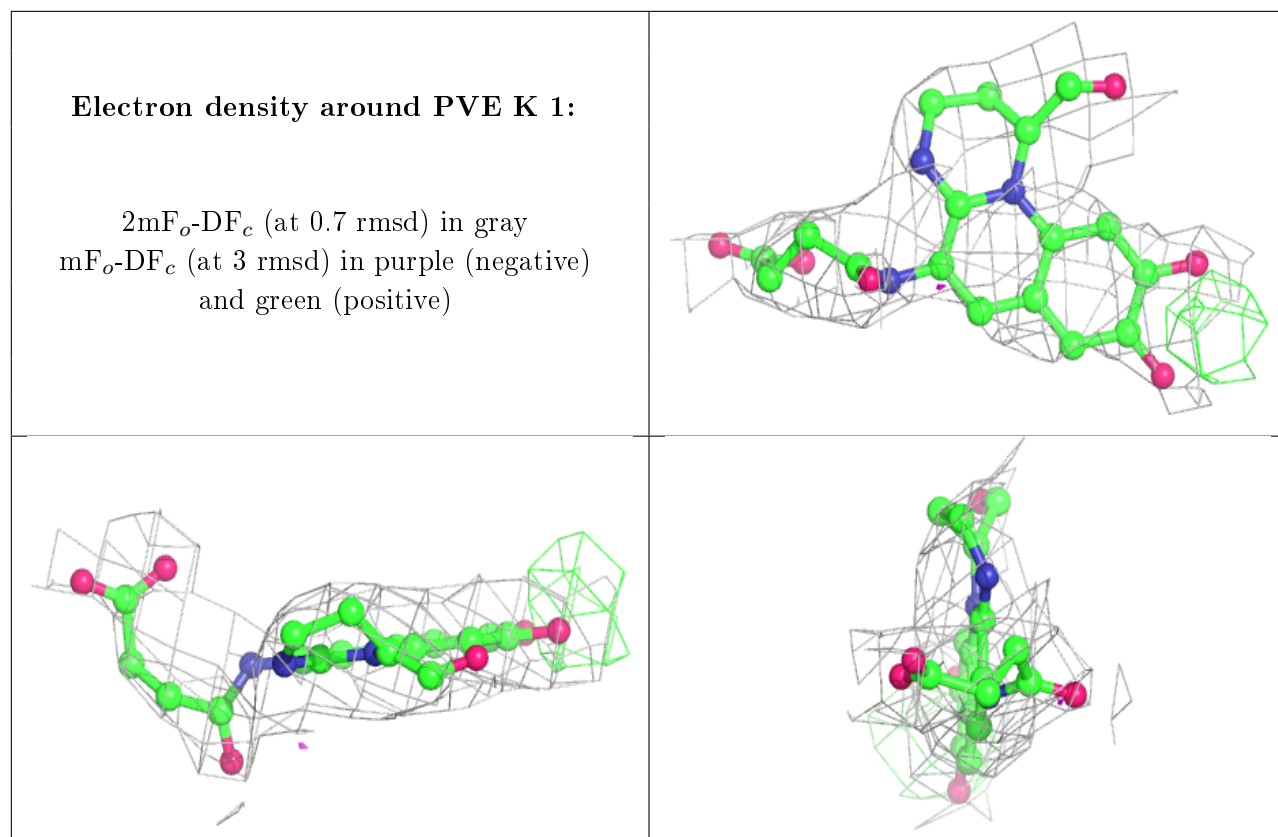
Electron density around PVE J 1:

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

**Electron density around PVE I 1:**

$2mF_o-DF_c$ (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.