



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:55 pm BST

PDB ID : 2ZZB
Title : Crystal structure of human thioredoxin reductase I and terpyridine platinum(II)
Authors : Lo, Y.C.; Ko, T.P.; Wang, A.H.J.
Deposited on : 2009-02-09
Resolution : 3.20 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

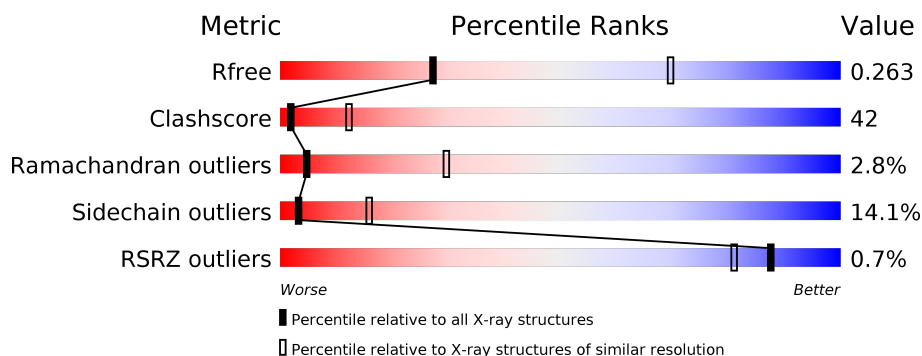
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	513	<div> <div>%</div> <div> <div></div> <div>39%</div> <div>45%</div> <div>10%</div> <div>• •</div> </div> </div>
1	B	513	<div> <div>37%</div> <div>46%</div> <div>11%</div> <div>• 5%</div> </div>
1	C	513	<div> <div>%</div> <div> <div></div> <div>38%</div> <div>47%</div> <div>12%</div> <div>•</div> </div> </div>
1	D	513	<div> <div>38%</div> <div>49%</div> <div>7%</div> <div>• 6%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15394 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 Thioredoxin reductase 1, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3776	2397	645	713	21			
1	B	485	Total	C	N	O	S	0	0	0
			3750	2385	640	706	19			
1	C	493	Total	C	N	O	S	0	0	0
			3800	2414	649	716	21			
1	D	484	Total	C	N	O	S	0	0	0
			3741	2379	638	705	19			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q16881
A	-12	ALA	-	EXPRESSION TAG	UNP Q16881
A	-11	HIS	-	EXPRESSION TAG	UNP Q16881
A	-10	HIS	-	EXPRESSION TAG	UNP Q16881
A	-9	HIS	-	EXPRESSION TAG	UNP Q16881
A	-8	HIS	-	EXPRESSION TAG	UNP Q16881
A	-7	HIS	-	EXPRESSION TAG	UNP Q16881
A	-6	HIS	-	EXPRESSION TAG	UNP Q16881
A	-5	VAL	-	EXPRESSION TAG	UNP Q16881
A	-4	ASP	-	EXPRESSION TAG	UNP Q16881
A	-3	ASP	-	EXPRESSION TAG	UNP Q16881
A	-2	ASP	-	EXPRESSION TAG	UNP Q16881
A	-1	ASP	-	EXPRESSION TAG	UNP Q16881
A	498	CYS	U	SEE REMARK 999	UNP Q16881
B	-13	MET	-	EXPRESSION TAG	UNP Q16881
B	-12	ALA	-	EXPRESSION TAG	UNP Q16881
B	-11	HIS	-	EXPRESSION TAG	UNP Q16881
B	-10	HIS	-	EXPRESSION TAG	UNP Q16881
B	-9	HIS	-	EXPRESSION TAG	UNP Q16881
B	-8	HIS	-	EXPRESSION TAG	UNP Q16881
B	-7	HIS	-	EXPRESSION TAG	UNP Q16881

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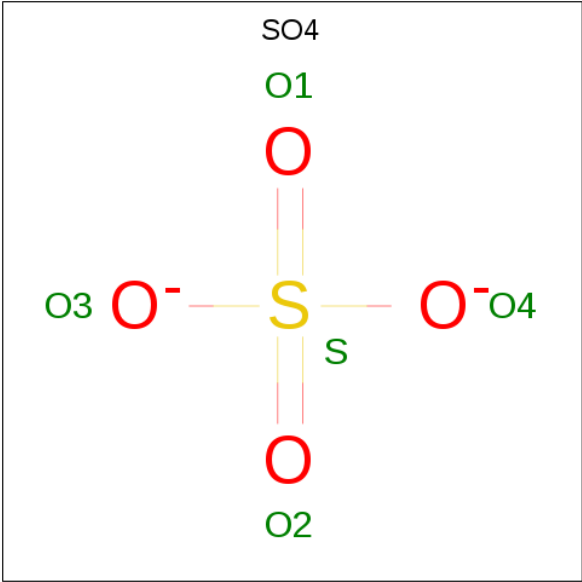
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	EXPRESSION TAG	UNP Q16881
B	-5	VAL	-	EXPRESSION TAG	UNP Q16881
B	-4	ASP	-	EXPRESSION TAG	UNP Q16881
B	-3	ASP	-	EXPRESSION TAG	UNP Q16881
B	-2	ASP	-	EXPRESSION TAG	UNP Q16881
B	-1	ASP	-	EXPRESSION TAG	UNP Q16881
B	498	CYS	U	SEE REMARK 999	UNP Q16881
C	-13	MET	-	EXPRESSION TAG	UNP Q16881
C	-12	ALA	-	EXPRESSION TAG	UNP Q16881
C	-11	HIS	-	EXPRESSION TAG	UNP Q16881
C	-10	HIS	-	EXPRESSION TAG	UNP Q16881
C	-9	HIS	-	EXPRESSION TAG	UNP Q16881
C	-8	HIS	-	EXPRESSION TAG	UNP Q16881
C	-7	HIS	-	EXPRESSION TAG	UNP Q16881
C	-6	HIS	-	EXPRESSION TAG	UNP Q16881
C	-5	VAL	-	EXPRESSION TAG	UNP Q16881
C	-4	ASP	-	EXPRESSION TAG	UNP Q16881
C	-3	ASP	-	EXPRESSION TAG	UNP Q16881
C	-2	ASP	-	EXPRESSION TAG	UNP Q16881
C	-1	ASP	-	EXPRESSION TAG	UNP Q16881
C	498	CYS	U	SEE REMARK 999	UNP Q16881
D	-13	MET	-	EXPRESSION TAG	UNP Q16881
D	-12	ALA	-	EXPRESSION TAG	UNP Q16881
D	-11	HIS	-	EXPRESSION TAG	UNP Q16881
D	-10	HIS	-	EXPRESSION TAG	UNP Q16881
D	-9	HIS	-	EXPRESSION TAG	UNP Q16881
D	-8	HIS	-	EXPRESSION TAG	UNP Q16881
D	-7	HIS	-	EXPRESSION TAG	UNP Q16881
D	-6	HIS	-	EXPRESSION TAG	UNP Q16881
D	-5	VAL	-	EXPRESSION TAG	UNP Q16881
D	-4	ASP	-	EXPRESSION TAG	UNP Q16881
D	-3	ASP	-	EXPRESSION TAG	UNP Q16881
D	-2	ASP	-	EXPRESSION TAG	UNP Q16881
D	-1	ASP	-	EXPRESSION TAG	UNP Q16881
D	498	CYS	U	SEE REMARK 999	UNP Q16881

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



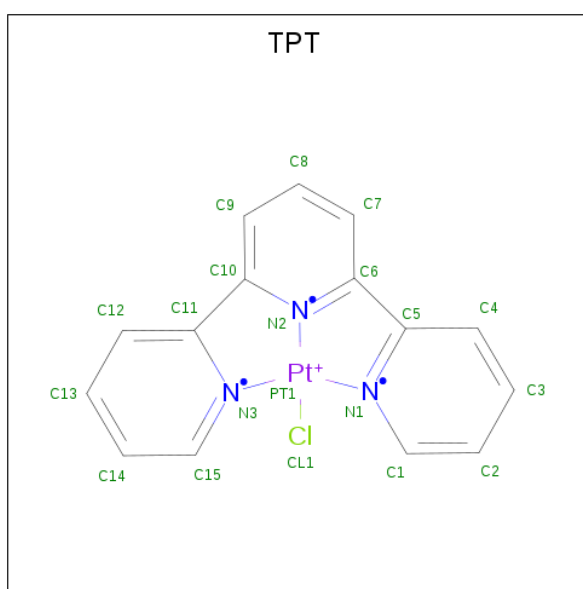
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



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

- Molecule 4 is 2,2':6',2''-TERPYRIDINE PLATINUM(II) Chloride (three-letter code: TPT) (formula: C₁₅H₁₁ClN₃Pt).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N Pt 19 15 3 1	0	0
4	D	1	Total C N Pt 19 15 3 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	19	Total O 19 19	0	0
5	B	17	Total O 17 17	0	0
5	C	13	Total O 13 13	0	0

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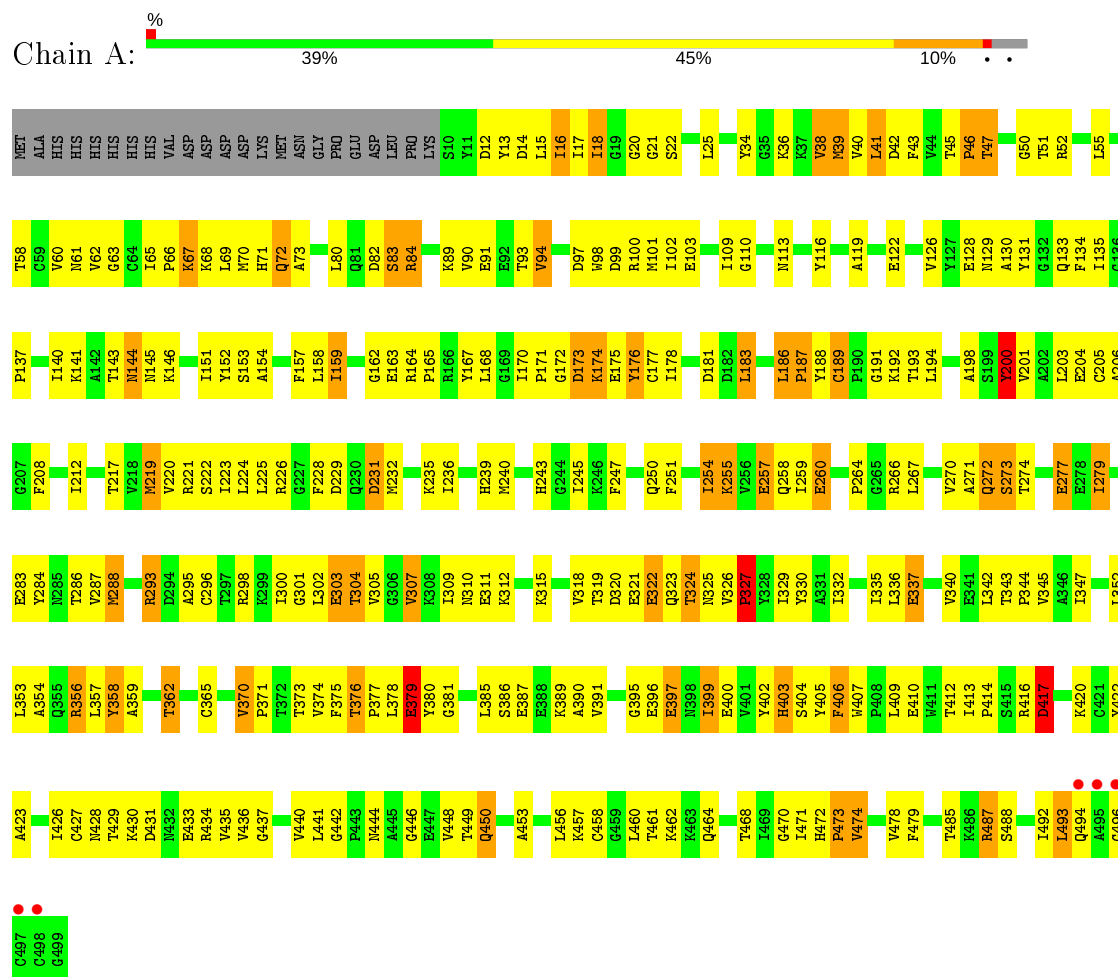
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	8	Total	O	0	0
			8	8		

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.

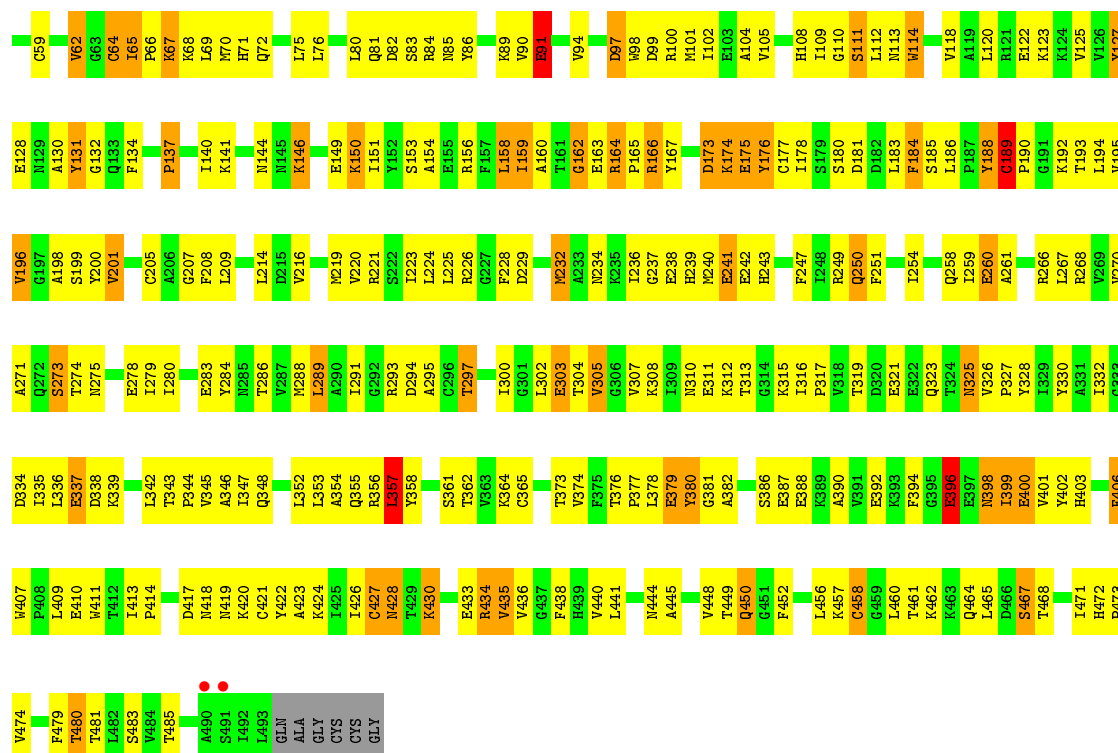
- Molecule 1: Thioredoxin reductase 1, cytoplasmic



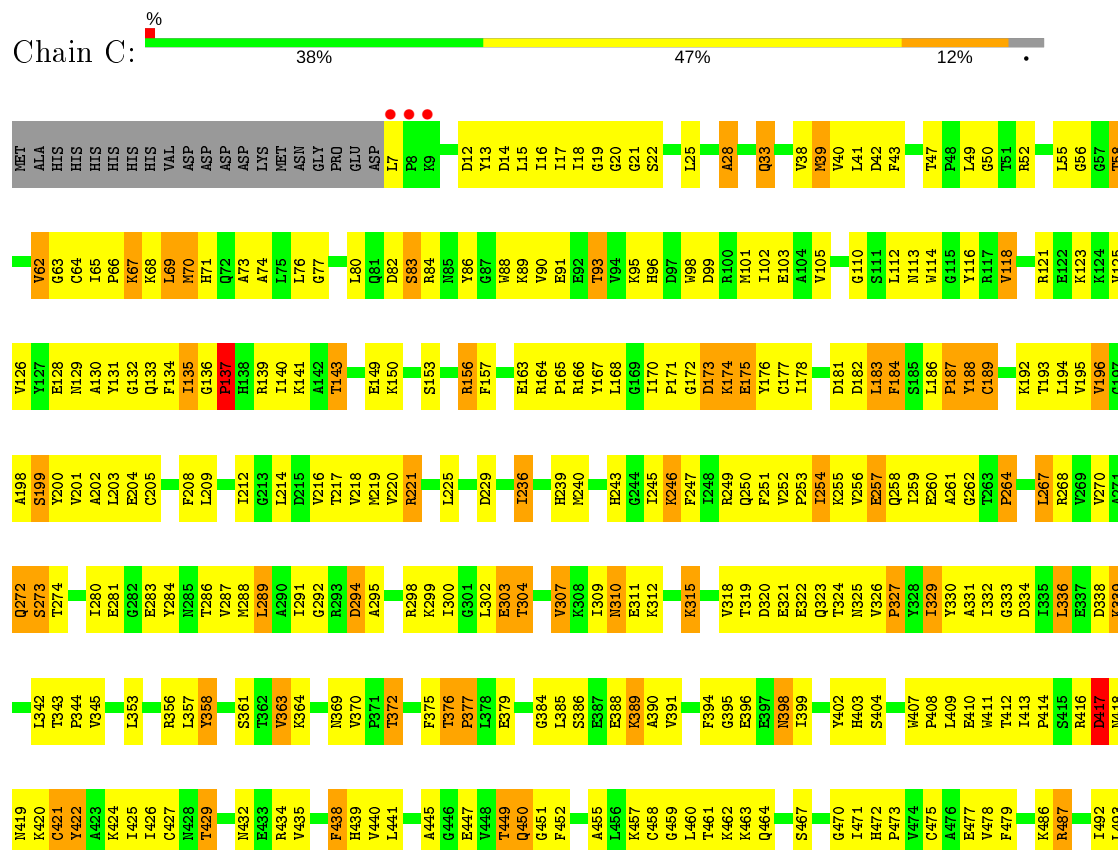
- Molecule 1: Thioredoxin reductase 1, cytoplasmic

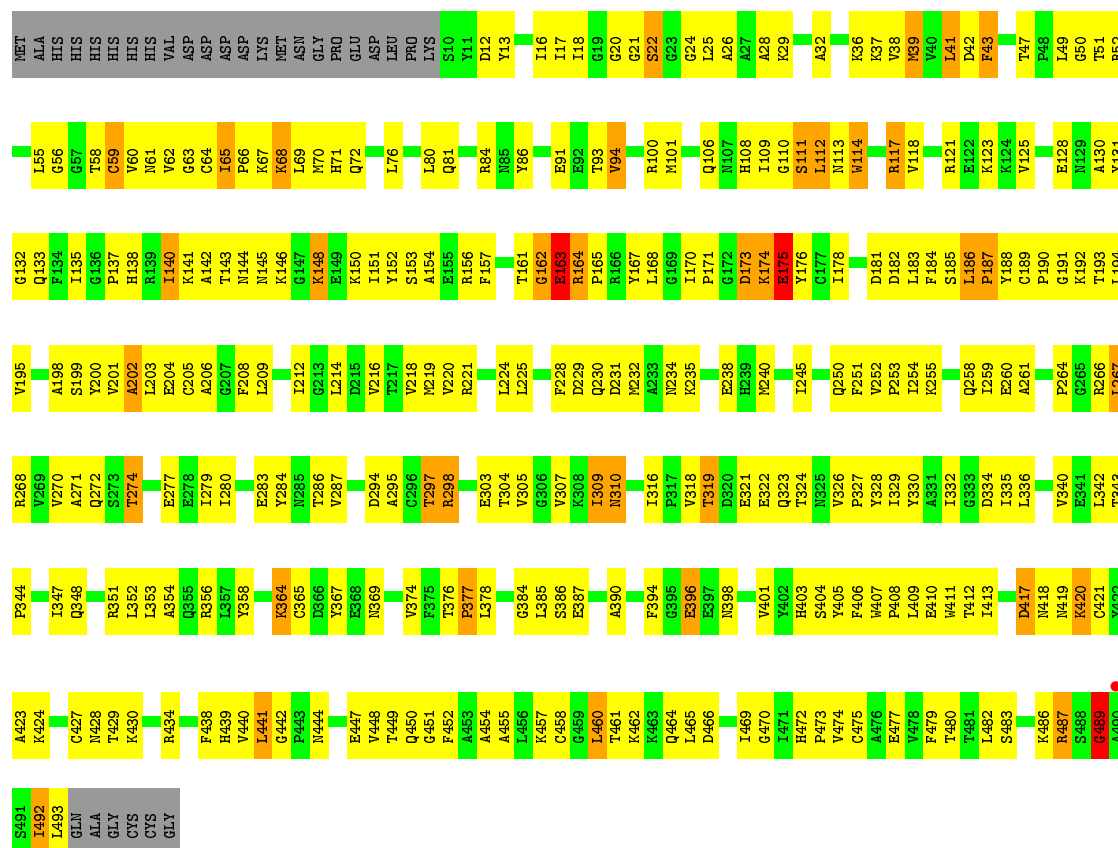
Chain B: 





• Molecule 1: Thioredoxin reductase 1, cytoplasmic





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	120.95Å 135.16Å 346.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 29.93 – 3.21	Depositor EDS
% Data completeness (in resolution range)	95.3 (30.00-3.20) 95.5 (29.93-3.21)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 3.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.305 0.209 , 0.263	Depositor DCC
R_{free} test set	2246 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	74.2	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15394	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: TPT, SO4, FAD

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	0.96	7/3850 (0.2%)	0.99	5/5211 (0.1%)
1	B	0.98	7/3824 (0.2%)	0.99	7/5177 (0.1%)
1	C	0.87	3/3875 (0.1%)	0.97	4/5245 (0.1%)
1	D	0.91	4/3815 (0.1%)	0.96	3/5166 (0.1%)
All	All	0.93	21/15364 (0.1%)	0.98	19/20799 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	3
1	C	0	2
1	D	0	1
All	All	0	10

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	CYS	CB-SG	13.15	2.04	1.82
1	C	189	CYS	CB-SG	10.57	2.00	1.82
1	C	421	CYS	CB-SG	-7.38	1.69	1.82
1	A	277	GLU	CG-CD	7.03	1.62	1.51
1	A	277	GLU	CB-CG	6.12	1.63	1.52
1	A	255	LYS	CD-CE	5.85	1.65	1.51
1	B	128	GLU	CG-CD	5.67	1.60	1.51
1	D	396	GLU	CG-CD	5.65	1.60	1.51
1	A	177	CYS	CB-SG	-5.57	1.72	1.81
1	B	91	GLU	CB-CG	5.50	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	175	GLU	CG-CD	5.48	1.60	1.51
1	D	114	TRP	CB-CG	5.47	1.60	1.50
1	B	17	ILE	CA-CB	5.42	1.67	1.54
1	D	175	GLU	CB-CG	5.39	1.62	1.52
1	B	91	GLU	CG-CD	5.26	1.59	1.51
1	B	303	GLU	CB-CG	-5.23	1.42	1.52
1	A	379	GLU	CG-CD	5.20	1.59	1.51
1	B	241	GLU	CG-CD	5.18	1.59	1.51
1	B	427	CYS	CB-SG	-5.17	1.73	1.81
1	C	88	TRP	CB-CG	-5.09	1.41	1.50
1	A	380	TYR	CD1-CE1	5.09	1.47	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	458	CYS	CA-CB-SG	10.36	132.66	114.00
1	A	189	CYS	CA-CB-SG	9.46	131.03	114.00
1	A	458	CYS	CA-CB-SG	8.79	129.82	114.00
1	C	189	CYS	CA-CB-SG	8.15	128.67	114.00
1	B	458	CYS	CA-CB-SG	8.00	128.41	114.00
1	A	41	LEU	CA-CB-CG	7.64	132.87	115.30
1	A	255	LYS	CD-CE-NZ	6.25	126.09	111.70
1	B	166	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	D	164	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	114	TRP	CA-CB-CG	-6.01	102.28	113.70
1	B	189	CYS	CA-CB-SG	5.91	124.64	114.00
1	D	351	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	421	CYS	CA-CB-SG	-5.54	104.02	114.00
1	B	201	VAL	CB-CA-C	-5.35	101.24	111.40
1	B	289	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	231	ASP	CB-CG-OD1	-5.17	113.64	118.30
1	C	336	LEU	CA-CB-CG	-5.10	103.58	115.30
1	B	357	LEU	CA-CB-CG	5.08	126.97	115.30
1	D	489	GLY	N-CA-C	5.05	125.73	113.10

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	TYR	Sidechain
1	A	176	TYR	Sidechain
1	A	200	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	406	PHE	Sidechain
1	B	127	TYR	Sidechain
1	B	176	TYR	Sidechain
1	B	43	PHE	Sidechain
1	C	167	TYR	Sidechain
1	C	402	TYR	Sidechain
1	D	43	PHE	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3776	0	3779	326	0
1	B	3750	0	3763	324	0
1	C	3800	0	3809	361	2
1	D	3741	0	3750	338	0
2	A	53	0	31	1	0
2	B	53	0	31	2	0
2	C	53	0	31	4	0
2	D	53	0	31	4	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	B	19	0	11	0	0
4	D	19	0	11	3	0
5	A	19	0	0	0	0
5	B	17	0	0	0	0
5	C	13	0	0	1	0
5	D	8	0	0	0	0
All	All	15394	0	15247	1282	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (1282) 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:A:189:CYS:SG	1:A:189:CYS:CB	2.04	1.42
1:A:84:ARG:HH11	1:A:84:ARG:HG3	1.11	1.16
1:C:163:GLU:HG2	1:C:295:ALA:HA	1.29	1.14
1:C:498:CYS:HB3	4:D:501:TPT:H15	1.27	1.12
1:A:163:GLU:HG2	1:A:295:ALA:HA	1.33	1.11
1:B:398:ASN:HD22	1:B:430:LYS:HG2	1.06	1.11
1:C:310:ASN:HD21	1:C:312:LYS:HB2	1.18	1.08
1:B:166:ARG:HB2	1:B:294:ASP:OD1	1.54	1.06
1:D:225:LEU:HB3	1:D:228:PHE:HD2	1.14	1.06
1:C:498:CYS:HB3	4:D:501:TPT:C15	1.86	1.05
1:D:55:LEU:HD12	1:D:56:GLY:H	1.23	1.04
1:B:378:LEU:HD21	1:B:441:LEU:HD21	1.39	1.01
1:C:135:ILE:HD11	1:C:141:LYS:HB2	1.42	1.00
1:B:55:LEU:HD12	1:B:56:GLY:H	1.25	0.99
1:C:302:LEU:HB3	1:C:307:VAL:HG12	1.43	0.99
1:D:254:ILE:HD11	1:D:270:VAL:HG12	1.43	0.98
1:C:498:CYS:CB	4:D:501:TPT:H15	1.94	0.97
1:B:259:ILE:HD11	1:B:268:ARG:HG3	1.45	0.96
1:B:64:CYS:HA	1:B:67:LYS:NZ	1.81	0.96
1:D:254:ILE:HD11	1:D:270:VAL:CG1	1.97	0.95
1:B:114:TRP:O	1:B:118:VAL:HG23	1.67	0.94
1:B:55:LEU:HD12	1:B:56:GLY:N	1.81	0.94
1:B:266:ARG:O	1:B:267:LEU:HD23	1.68	0.94
1:D:225:LEU:HB3	1:D:228:PHE:CD2	2.03	0.93
1:C:245:ILE:HG22	1:C:247:PHE:HE1	1.33	0.93
1:A:165:PRO:HG2	1:A:181:ASP:OD1	1.67	0.93
1:C:55:LEU:HD12	1:C:56:GLY:H	1.32	0.92
1:C:62:VAL:HG21	1:C:181:ASP:HA	1.52	0.92
1:D:245:ILE:HD12	1:D:245:ILE:H	1.33	0.92
1:D:150:LYS:HD2	1:D:151:ILE:H	1.33	0.92
1:D:67:LYS:HD3	1:D:204:GLU:OE1	1.70	0.91
1:C:332:ILE:HA	1:C:336:LEU:HD11	1.51	0.91
1:C:342:LEU:HD11	1:C:372:THR:HG23	1.52	0.90
1:C:166:ARG:HH21	1:C:292:GLY:HA3	1.32	0.90
1:C:319:THR:OG1	1:C:323:GLN:HB3	1.72	0.89
1:B:461:THR:H	1:B:464:GLN:HE21	1.18	0.89
1:A:323:GLN:HA	1:A:330:TYR:CD2	2.08	0.88
1:B:398:ASN:ND2	1:B:430:LYS:HG2	1.87	0.88
1:B:225:LEU:HB3	1:B:228:PHE:HD2	1.38	0.88
1:A:65:ILE:HB	1:A:66:PRO:HD3	1.54	0.88
1:B:109:ILE:HA	1:B:112:LEU:HD12	1.56	0.88
1:C:157:PHE:HB2	1:C:329:ILE:HG22	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:ARG:HG3	1:D:165:PRO:HD2	1.56	0.88
1:C:198:ALA:HB2	1:C:220:VAL:HG13	1.57	0.87
1:C:194:LEU:HD11	1:C:219:MET:HG3	1.57	0.87
1:D:148:LYS:HE3	1:D:148:LYS:HA	1.53	0.87
1:A:159:ILE:HG13	1:A:330:TYR:O	1.73	0.86
1:D:55:LEU:HD12	1:D:56:GLY:N	1.90	0.86
1:D:298:ARG:HG2	1:D:298:ARG:HH11	1.39	0.86
1:B:374:VAL:HG12	1:B:376:THR:HG23	1.58	0.86
1:B:398:ASN:HD22	1:B:430:LYS:CG	1.86	0.86
1:C:196:VAL:HG23	1:C:289:LEU:HA	1.57	0.86
1:A:323:GLN:HB2	1:A:330:TYR:HE2	1.41	0.86
1:C:245:ILE:HG22	1:C:247:PHE:CE1	2.11	0.86
1:C:251:PHE:CE2	1:C:280:ILE:HG12	2.10	0.86
1:A:99:ASP:O	1:A:103:GLU:HG3	1.75	0.85
1:C:250:GLN:O	1:C:251:PHE:HD1	1.59	0.85
1:C:67:LYS:HD3	1:C:204:GLU:OE1	1.77	0.85
1:C:101:MET:O	1:C:105:VAL:HG23	1.76	0.85
1:A:36:LYS:HG3	1:A:358:TYR:CD2	2.11	0.85
1:D:39:MET:HE2	1:D:41:LEU:HG	1.56	0.85
1:D:258:GLN:NE2	1:D:261:ALA:HA	1.90	0.84
1:A:157:PHE:HB2	1:A:329:ILE:HD13	1.59	0.84
1:B:188:TYR:HD1	1:B:188:TYR:O	1.61	0.83
1:C:461:THR:HB	1:C:464:GLN:HG3	1.59	0.83
1:D:423:ALA:HB1	1:D:479:PHE:CE1	2.14	0.83
1:D:401:VAL:HG11	1:D:486:LYS:HD2	1.59	0.83
1:C:196:VAL:HG21	1:C:289:LEU:HD22	1.59	0.83
1:A:323:GLN:HA	1:A:330:TYR:HD2	1.39	0.83
1:C:163:GLU:HG2	1:C:295:ALA:CA	2.09	0.83
1:A:200:TYR:HB2	1:A:374:VAL:HG13	1.61	0.82
1:C:80:LEU:CD2	1:D:80:LEU:HD23	2.09	0.82
1:D:65:ILE:HB	1:D:66:PRO:HD3	1.62	0.82
1:A:319:THR:CG2	1:A:323:GLN:HB3	2.10	0.82
1:C:55:LEU:HD12	1:C:56:GLY:N	1.93	0.81
1:A:485:THR:CG2	1:A:488:SER:HB3	2.10	0.81
1:B:461:THR:H	1:B:464:GLN:NE2	1.77	0.81
1:A:72:GLN:HB3	1:B:86:TYR:CE1	2.15	0.81
1:D:163:GLU:HG3	1:D:295:ALA:N	1.95	0.81
1:A:485:THR:HG23	1:A:488:SER:HB3	1.61	0.81
1:A:435:VAL:HG12	1:A:456:LEU:HD21	1.62	0.81
1:C:245:ILE:CG2	1:C:247:PHE:HE1	1.94	0.81
1:A:18:ILE:HD12	1:A:158:LEU:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLY:O	1:A:66:PRO:HD2	1.79	0.81
1:D:403:HIS:NE2	1:D:492:ILE:HD11	1.96	0.80
1:A:84:ARG:NH1	1:A:84:ARG:HG3	1.89	0.80
1:D:254:ILE:HD12	1:D:255:LYS:N	1.97	0.80
1:D:171:PRO:HG2	1:D:255:LYS:HG2	1.61	0.80
1:A:203:LEU:HD22	1:A:240:MET:SD	2.22	0.80
1:C:487:ARG:HB3	1:C:487:ARG:HH21	1.44	0.79
1:B:70:MET:HE1	1:B:184:PHE:HD1	1.47	0.79
1:C:302:LEU:HD22	1:C:307:VAL:HG11	1.63	0.79
1:D:444:ASN:O	1:D:448:VAL:HG23	1.83	0.78
1:A:428:ASN:OD1	1:A:430:LYS:HG2	1.84	0.78
1:C:62:VAL:CG2	1:C:181:ASP:HA	2.13	0.78
1:D:356:ARG:NH1	1:D:364:LYS:HA	1.99	0.78
1:A:163:GLU:HG2	1:A:295:ALA:CA	2.13	0.78
1:D:374:VAL:HG12	1:D:376:THR:HG23	1.66	0.78
1:A:471:ILE:HB	1:A:474:VAL:HG21	1.66	0.78
1:C:186:LEU:HD23	1:C:188:TYR:H	1.47	0.78
1:D:297:THR:HG21	1:D:316:ILE:HD11	1.66	0.77
1:A:47:THR:OG1	1:A:51:THR:HB	1.85	0.77
1:A:302:LEU:HD22	1:A:307:VAL:HG11	1.67	0.77
1:A:386:SER:OG	1:A:389:LYS:HB2	1.84	0.77
1:D:39:MET:CE	1:D:41:LEU:HG	2.14	0.76
1:B:158:LEU:HD12	1:B:159:ILE:N	2.00	0.76
1:C:318:VAL:HG11	1:C:336:LEU:HD22	1.67	0.76
1:D:188:TYR:O	1:D:188:TYR:CD1	2.38	0.76
1:A:193:THR:HG22	1:A:194:LEU:N	2.00	0.76
1:B:378:LEU:CD2	1:B:441:LEU:HD21	2.15	0.76
1:B:33:GLN:HG3	1:B:123:LYS:NZ	2.01	0.76
1:A:357:LEU:HB3	1:A:358:TYR:CD1	2.21	0.76
1:B:302:LEU:HD22	1:B:307:VAL:HG11	1.67	0.75
1:D:224:LEU:O	1:D:230:GLN:NE2	2.19	0.75
1:A:457:LYS:HD2	1:B:467:SER:OG	1.87	0.75
1:A:91:GLU:OE1	1:A:94:VAL:HA	1.86	0.75
1:B:266:ARG:C	1:B:267:LEU:HD23	2.06	0.75
1:A:47:THR:O	1:A:50:GLY:N	2.18	0.75
1:C:370:VAL:HG22	1:D:469:ILE:HD12	1.66	0.75
1:C:407:TRP:CZ2	1:C:412:THR:HA	2.21	0.74
1:C:80:LEU:HD22	1:D:80:LEU:HD23	1.67	0.74
1:B:338:ASP:O	1:B:339:LYS:HD3	1.86	0.74
1:C:353:LEU:HA	1:C:356:ARG:HH21	1.51	0.74
1:C:251:PHE:HE2	1:C:280:ILE:HG12	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LEU:HD23	1:B:68:LYS:HG2	1.70	0.74
1:D:272:GLN:HG3	1:D:279:ILE:HG22	1.68	0.74
1:A:302:LEU:HB3	1:A:307:VAL:HG12	1.69	0.73
1:A:402:TYR:CD1	1:A:462:LYS:HE2	2.23	0.73
1:D:297:THR:CG2	1:D:316:ILE:HD11	2.18	0.73
1:A:173:ASP:OD2	1:A:174:LYS:N	2.20	0.73
1:A:198:ALA:HB2	1:A:220:VAL:HG22	1.71	0.73
1:A:485:THR:HG23	1:A:488:SER:CB	2.17	0.73
1:C:193:THR:CG2	1:C:194:LEU:N	2.52	0.73
1:B:62:VAL:O	1:B:62:VAL:HG23	1.87	0.73
1:C:89:LYS:HG2	1:D:100:ARG:NH2	2.03	0.73
1:B:229:ASP:HA	1:B:386:SER:OG	1.89	0.73
1:D:188:TYR:O	1:D:188:TYR:HD1	1.70	0.73
1:C:135:ILE:CD1	1:C:141:LYS:HB2	2.17	0.72
1:D:66:PRO:HG3	1:D:109:ILE:HD11	1.70	0.72
1:B:461:THR:N	1:B:464:GLN:NE2	2.37	0.72
1:C:399:ILE:HD11	1:C:426:ILE:HG23	1.71	0.72
1:C:457:LYS:HA	1:C:457:LYS:HE2	1.70	0.72
1:A:397:GLU:CD	1:A:397:GLU:H	1.93	0.72
1:B:380:TYR:HE1	1:B:382:ALA:HB2	1.53	0.72
1:C:272:GLN:HG3	1:C:273:SER:O	1.89	0.72
1:B:348:GLN:HG3	1:B:352:LEU:HD12	1.72	0.72
1:B:423:ALA:HB1	1:B:479:PHE:CE1	2.25	0.71
1:C:251:PHE:CE1	1:C:273:SER:HB2	2.25	0.71
1:A:203:LEU:HD11	1:A:224:LEU:HD22	1.73	0.71
1:B:158:LEU:HD11	1:B:332:ILE:CG1	2.21	0.71
1:B:417:ASP:HB3	1:B:420:LYS:HG3	1.72	0.71
1:D:164:ARG:HG3	1:D:165:PRO:CD	2.19	0.71
1:A:46:PRO:HG3	1:A:52:ARG:HG2	1.72	0.71
1:B:192:LYS:HE2	1:B:284:TYR:CD2	2.25	0.71
1:C:333:GLY:H	1:C:336:LEU:HD12	1.55	0.71
1:D:163:GLU:HG3	1:D:295:ALA:HA	1.72	0.71
1:D:198:ALA:HB2	1:D:220:VAL:HG13	1.71	0.71
1:A:319:THR:HG22	1:A:323:GLN:HB3	1.72	0.71
1:B:70:MET:CE	1:B:184:PHE:HD1	2.04	0.71
1:C:353:LEU:CA	1:C:356:ARG:HH21	2.03	0.71
1:A:323:GLN:HB2	1:A:330:TYR:CE2	2.24	0.71
1:B:205:CYS:HA	1:B:208:PHE:CE2	2.26	0.71
1:C:302:LEU:HD22	1:C:307:VAL:CG1	2.21	0.71
1:A:68:LYS:HE3	1:A:375:PHE:CE2	2.26	0.70
1:B:239:HIS:CD2	1:B:378:LEU:HD22	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:GLU:HG3	1:D:295:ALA:CA	2.21	0.70
1:C:192:LYS:HE2	1:C:284:TYR:CD2	2.26	0.70
1:C:250:GLN:O	1:C:251:PHE:CD1	2.44	0.70
1:C:438:PHE:CE1	1:C:449:THR:HG23	2.26	0.70
1:A:385:LEU:HD12	1:A:390:ALA:HA	1.73	0.70
1:A:34:TYR:CE2	1:A:359:ALA:HB2	2.26	0.70
1:B:302:LEU:HD22	1:B:307:VAL:CG1	2.21	0.70
1:B:380:TYR:CE1	1:B:382:ALA:HB2	2.26	0.70
1:C:411:TRP:CH2	1:C:421:CYS:SG	2.84	0.70
1:D:298:ARG:HH11	1:D:298:ARG:CG	2.05	0.70
1:A:193:THR:CG2	1:A:194:LEU:N	2.54	0.70
1:B:13:TYR:CE2	1:B:39:MET:HB2	2.26	0.70
1:B:380:TYR:C	1:B:380:TYR:CD1	2.66	0.70
1:D:171:PRO:CG	1:D:255:LYS:HG2	2.21	0.69
1:D:487:ARG:HG3	1:D:487:ARG:HH21	1.55	0.69
1:C:473:PRO:HG2	1:D:68:LYS:HZ3	1.56	0.69
1:B:18:ILE:HD12	1:B:18:ILE:N	2.07	0.69
1:C:205:CYS:HA	1:C:208:PHE:CE2	2.27	0.69
1:C:199:SER:O	1:C:202:ALA:HB3	1.92	0.69
1:B:68:LYS:O	1:B:71:HIS:HB3	1.92	0.69
1:C:58:THR:OG1	2:C:500:FAD:O2A	2.10	0.69
1:C:89:LYS:HG2	1:D:100:ARG:HH22	1.57	0.69
1:D:117:ARG:NH2	1:D:117:ARG:HB3	2.07	0.69
1:B:131:TYR:CE2	2:B:500:FAD:N6A	2.61	0.69
1:B:232:MET:CE	1:B:232:MET:HA	2.23	0.69
1:C:25:LEU:HD21	1:C:55:LEU:HD11	1.74	0.69
1:D:462:LYS:O	1:D:466:ASP:OD2	2.09	0.69
1:A:358:TYR:CD1	1:A:358:TYR:N	2.60	0.69
1:B:398:ASN:HB3	1:B:430:LYS:HD3	1.73	0.69
1:D:267:LEU:HD12	1:D:284:TYR:O	1.93	0.69
1:D:328:TYR:CD2	1:D:329:ILE:HG13	2.27	0.69
1:A:60:VAL:O	1:A:109:ILE:HD13	1.93	0.68
1:A:402:TYR:CE1	1:A:462:LYS:HE2	2.28	0.68
1:D:62:VAL:HG11	1:D:181:ASP:OD1	1.92	0.68
1:D:203:LEU:HD12	1:D:225:LEU:HD21	1.75	0.68
1:C:192:LYS:HE2	1:C:284:TYR:HD2	1.59	0.68
1:C:86:TYR:CE1	1:C:413:ILE:HD12	2.29	0.68
1:D:209:LEU:HD22	1:D:214:LEU:HD12	1.75	0.68
1:B:342:LEU:O	1:B:345:VAL:HG12	1.92	0.68
1:B:400:GLU:HA	1:B:400:GLU:OE2	1.94	0.68
1:C:385:LEU:HD13	1:C:390:ALA:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:THR:HB	1:B:344:PRO:HD3	1.76	0.68
1:C:194:LEU:HD23	1:C:287:VAL:HG13	1.76	0.68
1:C:326:VAL:HB	1:C:329:ILE:HG13	1.75	0.68
1:A:15:LEU:HD13	1:A:358:TYR:OH	1.92	0.68
1:A:98:TRP:NE1	1:A:102:ILE:HG13	2.08	0.68
1:C:157:PHE:HB2	1:C:329:ILE:CG2	2.24	0.68
1:D:323:GLN:HE21	1:D:327:PRO:HA	1.58	0.68
1:A:159:ILE:HD11	1:A:329:ILE:HG22	1.73	0.67
1:A:353:LEU:CA	1:A:356:ARG:HH21	2.07	0.67
1:D:245:ILE:HD12	1:D:245:ILE:N	2.08	0.67
1:A:186:LEU:HD12	1:A:188:TYR:H	1.58	0.67
1:C:318:VAL:HG23	1:C:323:GLN:O	1.94	0.67
1:A:323:GLN:OE1	1:A:327:PRO:HA	1.95	0.67
1:B:399:ILE:HD12	1:B:428:ASN:HA	1.77	0.67
1:D:173:ASP:O	1:D:175:GLU:N	2.27	0.67
1:A:69:LEU:HD13	1:B:413:ILE:HD11	1.77	0.67
1:D:326:VAL:HG11	1:D:329:ILE:HD12	1.77	0.67
1:A:357:LEU:HB3	1:A:358:TYR:CE1	2.30	0.67
1:B:194:LEU:HD13	1:B:284:TYR:CE1	2.30	0.67
1:A:340:VAL:CG1	1:A:342:LEU:HD12	2.25	0.66
1:C:98:TRP:NE1	1:C:102:ILE:HG13	2.10	0.66
1:A:178:ILE:O	1:A:288:MET:HA	1.95	0.66
1:C:440:VAL:HB	1:C:479:PHE:HZ	1.61	0.66
1:B:177:CYS:HB3	1:B:289:LEU:HD13	1.77	0.66
1:B:435:VAL:HG21	1:B:460:LEU:HD23	1.78	0.66
1:C:333:GLY:H	1:C:336:LEU:CD1	2.07	0.66
1:B:323:GLN:HG3	1:B:330:TYR:CE2	2.30	0.66
1:C:196:VAL:CG2	1:C:289:LEU:HD22	2.25	0.66
1:A:84:ARG:HH11	1:A:84:ARG:CG	1.99	0.66
1:C:386:SER:OG	1:C:388:GLU:HG2	1.94	0.66
1:C:407:TRP:CH2	1:C:412:THR:HG22	2.31	0.66
1:D:200:TYR:CD2	1:D:201:VAL:N	2.63	0.66
1:D:67:LYS:HE2	2:D:500:FAD:H6	1.77	0.66
1:A:72:GLN:CG	1:B:410:GLU:HG3	2.26	0.66
1:B:302:LEU:HD22	1:B:307:VAL:CB	2.25	0.66
1:B:430:LYS:HD2	1:B:430:LYS:N	2.09	0.66
1:D:245:ILE:CD1	1:D:245:ILE:H	2.06	0.66
1:C:318:VAL:HG23	1:C:323:GLN:C	2.16	0.66
1:C:339:LYS:HA	1:C:339:LYS:HE3	1.76	0.66
1:D:80:LEU:HD13	1:D:94:VAL:HG21	1.78	0.66
1:A:200:TYR:HB2	1:A:374:VAL:CG1	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:LEU:HB3	1:B:228:PHE:CD2	2.27	0.66
1:B:353:LEU:HG	1:B:357:LEU:HD12	1.78	0.66
1:A:100:ARG:HD2	1:C:121:ARG:HG2	1.77	0.65
1:A:376:THR:HB	1:A:377:PRO:CD	2.26	0.65
1:C:251:PHE:CD2	1:C:280:ILE:HG12	2.31	0.65
1:D:195:VAL:HB	1:D:218:VAL:HG22	1.77	0.65
1:D:176:TYR:CE1	1:D:258:GLN:HB2	2.32	0.65
1:B:435:VAL:HG23	1:B:460:LEU:O	1.96	0.65
1:B:65:ILE:HB	1:B:66:PRO:HD3	1.79	0.65
1:D:174:LYS:HB2	1:D:175:GLU:OE1	1.96	0.65
1:C:403:HIS:ND1	1:C:492:ILE:HD13	2.10	0.65
1:A:426:ILE:O	1:A:436:VAL:HG22	1.96	0.65
1:D:258:GLN:NE2	1:D:260:GLU:O	2.30	0.65
1:B:241:GLU:CD	1:B:249:ARG:HH12	2.00	0.65
1:D:163:GLU:OE1	1:D:334:ASP:HB3	1.96	0.65
1:A:55:LEU:O	1:A:113:ASN:ND2	2.29	0.65
1:A:200:TYR:CD1	1:A:201:VAL:N	2.64	0.65
1:C:310:ASN:C	1:C:310:ASN:ND2	2.50	0.65
1:B:196:VAL:HG23	1:B:289:LEU:HA	1.78	0.65
1:C:20:GLY:N	1:C:42:ASP:HB2	2.12	0.65
1:C:219:MET:CE	1:C:251:PHE:HB3	2.26	0.65
1:C:309:ILE:HG13	1:C:310:ASN:N	2.10	0.64
1:C:494:GLN:O	1:C:495:ALA:HB2	1.96	0.64
1:A:163:GLU:OE2	1:A:315:LYS:NZ	2.30	0.64
1:A:464:GLN:NE2	1:B:458:CYS:HB3	2.11	0.64
1:C:47:THR:O	1:C:50:GLY:N	2.29	0.64
1:D:438:PHE:C	1:D:439:HIS:HD1	2.00	0.64
1:A:322:GLU:HG2	1:A:332:ILE:HG22	1.78	0.64
1:A:492:ILE:C	1:A:493:LEU:HG	2.16	0.64
1:D:460:LEU:HD12	1:D:461:THR:H	1.62	0.64
1:D:65:ILE:HB	1:D:66:PRO:CD	2.27	0.64
1:B:259:ILE:HD11	1:B:268:ARG:CG	2.22	0.64
1:A:72:GLN:HG2	1:B:410:GLU:HG3	1.79	0.64
1:D:258:GLN:HE22	1:D:261:ALA:HA	1.60	0.64
1:C:173:ASP:OD2	1:C:174:LYS:N	2.27	0.64
1:C:196:VAL:HG11	1:C:253:PRO:HG3	1.79	0.64
1:A:410:GLU:HG2	1:B:72:GLN:OE1	1.97	0.64
1:C:310:ASN:HD22	1:C:310:ASN:C	2.00	0.64
1:A:267:LEU:O	1:A:283:GLU:HA	1.98	0.64
1:B:406:PHE:CE2	1:B:421:CYS:HB3	2.32	0.64
1:C:336:LEU:CB	1:C:339:LYS:HG3	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:MET:SD	1:A:208:PHE:CE1	2.91	0.63
1:A:21:GLY:HA3	2:A:500:FAD:O5B	1.99	0.63
1:C:427:CYS:HA	1:C:434:ARG:O	1.99	0.63
1:A:98:TRP:CE2	1:A:102:ILE:HD11	2.32	0.63
1:C:203:LEU:HD12	1:C:225:LEU:HD21	1.80	0.63
1:D:254:ILE:HD11	1:D:270:VAL:CB	2.28	0.63
1:A:301:GLY:O	1:A:304:THR:HG23	1.98	0.63
1:B:108:HIS:O	1:B:111:SER:OG	2.14	0.63
1:B:158:LEU:HD11	1:B:332:ILE:HG13	1.79	0.63
1:D:163:GLU:HG3	1:D:294:ASP:C	2.19	0.63
1:D:423:ALA:HB1	1:D:479:PHE:HE1	1.60	0.63
1:B:188:TYR:CD1	1:B:188:TYR:O	2.49	0.63
1:C:245:ILE:CG2	1:C:247:PHE:CE1	2.77	0.63
1:C:432:ASN:O	1:C:461:THR:HG23	1.98	0.63
1:C:90:VAL:HG12	1:C:91:GLU:H	1.63	0.63
1:B:33:GLN:HG3	1:B:123:LYS:HZ2	1.62	0.63
1:C:259:ILE:HG22	1:C:259:ILE:O	1.99	0.63
1:C:62:VAL:HA	1:C:184:PHE:HD2	1.63	0.63
1:D:146:LYS:HZ2	1:D:148:LYS:HB2	1.64	0.63
1:D:418:ASN:O	1:D:419:ASN:HB2	1.98	0.63
1:A:173:ASP:O	1:A:175:GLU:N	2.32	0.62
1:D:309:ILE:HG13	1:D:310:ASN:N	2.14	0.62
1:D:460:LEU:HA	1:D:464:GLN:OE1	1.99	0.62
1:B:224:LEU:N	1:B:224:LEU:HD12	2.14	0.62
1:B:232:MET:HE2	1:B:232:MET:HA	1.80	0.62
1:C:114:TRP:O	1:C:118:VAL:HG23	1.98	0.62
1:C:41:LEU:HD23	1:C:128:GLU:HB3	1.80	0.62
1:C:173:ASP:O	1:C:175:GLU:N	2.31	0.62
1:C:411:TRP:O	1:C:414:PRO:HD2	1.98	0.62
1:A:135:ILE:CG2	1:A:141:LYS:HB2	2.30	0.62
1:D:460:LEU:HD12	1:D:461:THR:N	2.15	0.62
1:A:378:LEU:HG	1:A:441:LEU:CD1	2.29	0.62
1:B:64:CYS:HA	1:B:67:LYS:HZ2	1.61	0.62
1:C:200:TYR:O	1:C:204:GLU:HG3	2.00	0.62
1:B:198:ALA:HB2	1:B:220:VAL:HG13	1.80	0.62
1:B:378:LEU:HD21	1:B:441:LEU:CD2	2.22	0.62
1:D:378:LEU:CD2	1:D:441:LEU:HD21	2.29	0.62
1:A:325:ASN:OD1	1:A:326:VAL:HG23	1.99	0.62
1:D:267:LEU:HD13	1:D:287:VAL:HG23	1.80	0.62
1:D:332:ILE:O	1:D:332:ILE:HD12	2.00	0.62
1:A:163:GLU:OE1	1:A:293:ARG:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ILE:HG13	1:A:310:ASN:N	2.13	0.62
1:D:250:GLN:HB3	1:D:274:THR:HG23	1.82	0.62
1:D:130:ALA:HB1	1:D:143:THR:O	2.00	0.62
1:A:18:ILE:HD13	1:A:159:ILE:HG23	1.82	0.62
1:A:353:LEU:N	1:A:356:ARG:HH21	1.98	0.62
1:B:98:TRP:CZ2	1:B:102:ILE:HD11	2.34	0.62
1:A:110:GLY:O	1:A:113:ASN:HB2	1.99	0.61
1:A:245:ILE:HG22	1:A:247:PHE:CE2	2.34	0.61
1:C:249:ARG:HB3	1:C:250:GLN:NE2	2.15	0.61
1:C:461:THR:HG22	1:C:463:LYS:H	1.65	0.61
1:D:378:LEU:HG	1:D:441:LEU:CD2	2.30	0.61
1:B:149:GLU:C	1:B:150:LYS:HG2	2.20	0.61
1:C:177:CYS:SG	1:C:289:LEU:HD21	2.40	0.61
1:A:266:ARG:HG3	1:A:266:ARG:HH11	1.64	0.61
1:A:340:VAL:HG12	1:A:345:VAL:HG21	1.82	0.61
1:C:186:LEU:HD21	1:C:188:TYR:O	2.01	0.61
1:D:376:THR:O	1:D:377:PRO:C	2.39	0.61
1:C:156:ARG:HH11	1:C:156:ARG:HB2	1.65	0.61
1:C:178:ILE:O	1:C:288:MET:HA	2.00	0.61
1:C:473:PRO:O	1:C:473:PRO:HG2	2.00	0.61
1:B:65:ILE:HG22	1:B:66:PRO:N	2.15	0.61
1:C:408:PRO:HD2	1:C:411:TRP:CE3	2.35	0.61
1:D:319:THR:OG1	1:D:323:GLN:HB3	1.99	0.61
1:A:340:VAL:HG21	1:A:370:VAL:HG21	1.83	0.61
1:C:194:LEU:HG	1:C:195:VAL:N	2.16	0.60
1:D:13:TYR:CD1	1:D:39:MET:HB2	2.35	0.60
1:C:345:VAL:HG22	1:D:469:ILE:HD13	1.83	0.60
1:A:298:ARG:NH2	1:A:311:GLU:O	2.31	0.60
1:B:186:LEU:HD23	1:B:190:PRO:HG3	1.82	0.60
1:D:407:TRP:CD1	1:D:418:ASN:HA	2.36	0.60
1:A:378:LEU:O	1:A:379:GLU:O	2.19	0.60
1:C:168:LEU:HG	1:C:291:ILE:HD13	1.84	0.60
1:D:386:SER:OG	1:D:387:GLU:N	2.34	0.60
1:D:438:PHE:HE1	1:D:440:VAL:HG12	1.65	0.60
1:B:258:GLN:OE1	1:B:261:ALA:HB2	2.01	0.60
1:D:150:LYS:HD2	1:D:151:ILE:N	2.12	0.60
1:D:81:GLN:HG2	1:D:84:ARG:HH12	1.67	0.60
1:B:315:LYS:HE3	1:B:334:ASP:O	2.01	0.60
1:B:449:THR:O	1:B:450:GLN:C	2.37	0.60
1:C:194:LEU:HB2	1:C:284:TYR:CD1	2.37	0.60
1:C:163:GLU:OE1	1:C:315:LYS:NZ	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:VAL:HG22	1:C:319:THR:N	2.17	0.60
1:C:399:ILE:HD11	1:C:426:ILE:CG2	2.31	0.60
1:C:475:CYS:O	1:C:478:VAL:HG23	2.02	0.60
1:C:298:ARG:HH12	1:C:311:GLU:HA	1.66	0.60
1:D:140:ILE:HG13	1:D:141:LYS:N	2.17	0.60
1:B:13:TYR:CD2	1:B:39:MET:HB2	2.37	0.60
1:C:55:LEU:O	1:C:113:ASN:ND2	2.35	0.60
1:C:336:LEU:HB2	1:C:339:LYS:HG3	1.84	0.60
1:C:251:PHE:HE2	1:C:280:ILE:HG23	1.67	0.59
1:C:473:PRO:O	1:D:68:LYS:NZ	2.35	0.59
1:A:46:PRO:HG3	1:A:52:ARG:CG	2.31	0.59
1:C:69:LEU:HD22	1:D:413:ILE:HD12	1.83	0.59
1:D:208:PHE:CD1	1:D:209:LEU:N	2.70	0.59
1:A:25:LEU:HD13	1:A:116:TYR:CD1	2.38	0.59
1:B:131:TYR:HD2	1:B:132:GLY:N	2.00	0.59
1:C:68:LYS:O	1:C:71:HIS:HB3	2.02	0.59
1:D:492:ILE:O	1:D:493:LEU:C	2.41	0.59
1:B:315:LYS:HB2	1:B:337:GLU:HG2	1.85	0.59
1:C:178:ILE:HB	1:C:182:ASP:HB2	1.85	0.59
1:C:219:MET:HE1	1:C:251:PHE:O	2.01	0.59
1:C:80:LEU:HD22	1:D:80:LEU:CD2	2.33	0.59
1:A:168:LEU:HB3	1:A:170:ILE:HG23	1.83	0.59
1:A:405:TYR:CE2	1:A:422:TYR:HD1	2.20	0.59
1:C:229:ASP:HA	1:C:388:GLU:OE2	2.03	0.59
1:C:411:TRP:C	1:C:414:PRO:HD2	2.23	0.59
1:D:460:LEU:HD11	1:D:465:LEU:HB2	1.84	0.59
1:C:300:ILE:HD11	1:C:302:LEU:HD11	1.85	0.59
1:B:250:GLN:HE21	1:B:275:ASN:ND2	2.01	0.58
1:B:90:VAL:HG12	1:B:91:GLU:N	2.18	0.58
1:C:249:ARG:HB3	1:C:250:GLN:HE22	1.68	0.58
1:C:69:LEU:HD11	1:D:409:LEU:HD11	1.85	0.58
1:B:402:TYR:CE1	1:B:462:LYS:HD3	2.38	0.58
1:C:67:LYS:CD	1:C:204:GLU:OE1	2.50	0.58
1:D:67:LYS:CD	1:D:204:GLU:OE1	2.49	0.58
1:A:22:SER:OG	1:A:343:THR:HG23	2.03	0.58
1:A:80:LEU:HD23	1:B:80:LEU:HD22	1.86	0.58
1:B:173:ASP:OD1	1:B:174:LYS:N	2.33	0.58
1:A:72:GLN:HB3	1:B:86:TYR:HE1	1.65	0.58
1:C:467:SER:OG	1:D:457:LYS:HD2	2.03	0.58
1:C:90:VAL:HG12	1:C:91:GLU:N	2.18	0.58
1:D:70:MET:HG2	1:D:101:MET:SD	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:GLY:CA	1:D:140:ILE:HD11	2.33	0.58
1:A:236:ILE:HG21	1:A:376:THR:HG21	1.84	0.58
1:D:440:VAL:HB	1:D:479:PHE:HZ	1.68	0.58
1:C:356:ARG:HH11	1:C:364:LYS:HA	1.68	0.58
1:D:22:SER:OG	1:D:343:THR:HG23	2.04	0.58
1:D:254:ILE:HD12	1:D:255:LYS:H	1.67	0.58
1:D:323:GLN:NE2	1:D:327:PRO:HA	2.19	0.58
1:B:200:TYR:CD1	1:B:201:VAL:N	2.71	0.58
1:B:194:LEU:HD13	1:B:284:TYR:CZ	2.38	0.58
1:B:46:PRO:HG3	1:B:52:ARG:HG2	1.84	0.58
1:B:302:LEU:HD22	1:B:307:VAL:HB	1.84	0.58
1:C:69:LEU:CD2	1:D:413:ILE:HD12	2.34	0.58
1:D:13:TYR:HD2	1:D:37:LYS:HG2	1.69	0.58
1:A:303:GLU:OE1	1:A:304:THR:HG22	2.04	0.57
1:A:407:TRP:CZ2	1:A:412:THR:HA	2.39	0.57
1:A:286:THR:HG22	1:A:287:VAL:N	2.17	0.57
1:B:158:LEU:HD11	1:B:332:ILE:HG12	1.86	0.57
1:C:325:ASN:O	1:C:327:PRO:HD3	2.05	0.57
1:C:435:VAL:HG21	1:C:460:LEU:HD23	1.87	0.57
1:C:268:ARG:HH21	1:C:281:GLU:CD	2.07	0.57
1:B:158:LEU:C	1:B:158:LEU:HD12	2.25	0.57
1:C:201:VAL:HG13	2:C:500:FAD:HM73	1.86	0.57
1:C:76:LEU:O	1:C:80:LEU:HG	2.05	0.57
1:D:178:ILE:HB	1:D:182:ASP:HB2	1.87	0.57
1:A:203:LEU:HD11	1:A:224:LEU:CD2	2.34	0.57
1:A:17:ILE:HB	1:A:40:VAL:HG22	1.87	0.57
1:B:97:ASP:OD1	1:B:97:ASP:O	2.22	0.57
1:D:150:LYS:CD	1:D:151:ILE:H	2.12	0.57
1:A:254:ILE:HD12	1:A:270:VAL:HG23	1.86	0.57
1:B:141:LYS:HD2	1:B:149:GLU:OE1	2.05	0.57
1:B:62:VAL:HG21	1:B:181:ASP:OD1	2.05	0.57
1:D:423:ALA:O	1:D:424:LYS:HB3	2.05	0.57
1:A:18:ILE:HD12	1:A:159:ILE:HA	1.85	0.57
1:A:385:LEU:CD1	1:A:390:ALA:HA	2.35	0.57
1:D:38:VAL:CG1	1:D:39:MET:N	2.67	0.57
1:B:254:ILE:HD11	1:B:270:VAL:HG12	1.86	0.57
1:A:208:PHE:O	1:A:212:ILE:HG12	2.04	0.56
1:D:356:ARG:HH12	1:D:364:LYS:HA	1.69	0.56
1:A:165:PRO:CG	1:A:181:ASP:OD1	2.47	0.56
1:C:62:VAL:HA	1:C:184:PHE:CD2	2.40	0.56
1:D:318:VAL:HG11	1:D:336:LEU:HD22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:NH1	1:A:84:ARG:CG	2.64	0.56
1:C:168:LEU:HB3	1:C:170:ILE:HG23	1.86	0.56
1:D:135:ILE:O	1:D:304:THR:HB	2.05	0.56
1:A:173:ASP:OD2	1:A:174:LYS:HG3	2.04	0.56
1:A:172:GLY:O	1:A:173:ASP:O	2.22	0.56
1:B:195:VAL:O	1:B:195:VAL:HG12	2.03	0.56
1:C:194:LEU:HD13	1:C:284:TYR:CE1	2.40	0.56
1:D:378:LEU:HG	1:D:441:LEU:HD21	1.86	0.56
1:A:20:GLY:N	1:A:42:ASP:HB2	2.20	0.56
1:A:159:ILE:HD11	1:A:329:ILE:CG2	2.35	0.56
1:A:352:LEU:HD12	1:A:365:CYS:HB2	1.88	0.56
1:B:234:ASN:O	1:B:238:GLU:HG3	2.05	0.56
1:C:98:TRP:HZ3	1:C:209:LEU:CD2	2.19	0.56
1:D:190:PRO:HD2	1:D:214:LEU:HD11	1.87	0.56
1:A:318:VAL:CG1	1:A:336:LEU:HD22	2.36	0.56
1:C:409:LEU:HD23	1:D:68:LYS:HE2	1.87	0.56
1:B:178:ILE:HD12	1:B:288:MET:HG3	1.87	0.56
1:B:356:ARG:HH11	1:B:364:LYS:HA	1.70	0.56
1:C:193:THR:HG22	1:C:194:LEU:N	2.19	0.56
1:D:470:GLY:N	1:D:480:THR:HG21	2.20	0.56
1:A:342:LEU:HB2	1:A:345:VAL:CG2	2.36	0.56
1:C:310:ASN:ND2	1:C:312:LYS:HB2	2.02	0.56
1:D:221:ARG:HH11	1:D:252:VAL:HG13	1.70	0.56
1:A:387:GLU:O	1:A:391:VAL:HG23	2.05	0.55
1:D:374:VAL:CG1	1:D:376:THR:HG23	2.35	0.55
1:D:462:LYS:NZ	1:D:466:ASP:OD1	2.38	0.55
1:D:58:THR:O	1:D:63:GLY:N	2.40	0.55
1:A:413:ILE:HD12	1:B:104:ALA:HB1	1.88	0.55
1:C:417:ASP:HB3	1:C:420:LYS:HG3	1.89	0.55
1:C:356:ARG:NH1	1:C:364:LYS:HA	2.22	0.55
1:D:259:ILE:HD11	1:D:268:ARG:HB2	1.86	0.55
1:A:20:GLY:H	1:A:42:ASP:HB2	1.71	0.55
1:A:163:GLU:CG	1:A:295:ALA:HA	2.23	0.55
1:B:386:SER:O	1:B:390:ALA:HB2	2.07	0.55
1:D:322:GLU:OE1	1:D:356:ARG:NH2	2.40	0.55
1:C:409:LEU:CD2	1:D:68:LYS:HB3	2.36	0.55
1:A:203:LEU:HD12	1:A:225:LEU:HD21	1.87	0.55
1:A:473:PRO:HG2	1:A:473:PRO:O	2.06	0.55
1:B:427:CYS:HA	1:B:434:ARG:O	2.06	0.55
1:C:131:TYR:CD2	1:C:132:GLY:N	2.75	0.55
1:D:144:ASN:OD1	1:D:146:LYS:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLN:HG3	1:A:273:SER:O	2.07	0.55
1:C:236:ILE:O	1:C:240:MET:HG3	2.06	0.55
1:C:342:LEU:HD11	1:C:372:THR:CG2	2.32	0.55
1:C:20:GLY:H	1:C:42:ASP:HB2	1.71	0.55
1:C:68:LYS:HG2	1:D:473:PRO:HG2	1.88	0.55
1:C:473:PRO:HG2	1:D:68:LYS:NZ	2.22	0.55
1:C:172:GLY:C	1:C:175:GLU:HG2	2.27	0.55
1:A:18:ILE:CD1	1:A:159:ILE:HA	2.37	0.55
1:C:302:LEU:HB2	5:C:514:HOH:O	2.07	0.55
1:D:332:ILE:HD12	1:D:332:ILE:C	2.27	0.55
1:B:97:ASP:OD1	1:B:97:ASP:C	2.44	0.55
1:C:319:THR:C	1:C:321:GLU:H	2.10	0.55
1:D:132:GLY:HA3	1:D:140:ILE:HD11	1.89	0.55
1:C:186:LEU:HD23	1:C:186:LEU:C	2.28	0.54
1:C:407:TRP:CZ3	1:C:412:THR:HG22	2.42	0.54
1:A:133:GLN:O	1:A:140:ILE:HG13	2.07	0.54
1:C:267:LEU:HD12	1:C:267:LEU:N	2.22	0.54
1:D:229:ASP:OD2	1:D:232:MET:HG2	2.07	0.54
1:A:171:PRO:HD2	1:A:254:ILE:O	2.07	0.54
1:A:318:VAL:HG11	1:A:336:LEU:CD2	2.38	0.54
1:C:20:GLY:H	1:C:42:ASP:CB	2.21	0.54
1:C:214:LEU:O	1:C:216:VAL:HG23	2.07	0.54
1:A:157:PHE:HB2	1:A:329:ILE:CD1	2.32	0.54
1:A:164:ARG:NH1	1:A:164:ARG:HG3	2.22	0.54
1:A:413:ILE:N	1:A:414:PRO:HD2	2.22	0.54
1:B:402:TYR:CD1	1:B:462:LYS:HE2	2.42	0.54
1:D:297:THR:HG21	1:D:316:ILE:CD1	2.36	0.54
1:B:250:GLN:HG2	1:D:250:GLN:NE2	2.22	0.54
1:B:259:ILE:O	1:B:260:GLU:HB2	2.08	0.54
1:B:259:ILE:CD1	1:B:268:ARG:HG3	2.29	0.54
1:C:19:GLY:N	1:C:41:LEU:O	2.25	0.54
1:D:219:MET:CE	1:D:253:PRO:HD3	2.38	0.54
1:B:394:PHE:HB2	1:B:399:ILE:HD13	1.89	0.54
1:C:102:ILE:HG22	1:C:103:GLU:N	2.22	0.54
1:C:33:GLN:OE1	1:C:123:LYS:HD2	2.07	0.54
1:C:361:SER:OG	1:C:363:VAL:HG23	2.07	0.54
1:D:188:TYR:O	1:D:189:CYS:C	2.44	0.54
1:D:451:GLY:O	1:D:454:ALA:HB3	2.08	0.54
1:A:219:MET:HG2	1:A:251:PHE:O	2.07	0.54
1:A:231:ASP:O	1:A:235:LYS:HG3	2.08	0.54
1:A:460:LEU:HD12	1:A:461:THR:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ASP:CA	1:B:386:SER:OG	2.55	0.54
1:B:20:GLY:N	1:B:42:ASP:HB2	2.23	0.54
1:C:258:GLN:OE1	1:C:261:ALA:HB2	2.08	0.54
1:C:344:PRO:CG	1:D:472:HIS:HB2	2.38	0.54
1:D:487:ARG:C	1:D:489:GLY:N	2.61	0.54
1:D:487:ARG:HH21	1:D:487:ARG:CG	2.20	0.54
1:B:62:VAL:CG2	1:B:62:VAL:O	2.56	0.54
1:C:418:ASN:ND2	1:C:419:ASN:ND2	2.55	0.54
1:A:397:GLU:CD	1:A:397:GLU:N	2.59	0.54
1:B:214:LEU:O	1:B:216:VAL:HG23	2.07	0.54
1:C:171:PRO:HD2	1:C:254:ILE:O	2.08	0.54
1:A:342:LEU:HB2	1:A:345:VAL:HG23	1.89	0.53
1:B:163:GLU:HG2	1:B:295:ALA:HA	1.90	0.53
1:C:435:VAL:O	1:C:435:VAL:HG23	2.08	0.53
1:D:318:VAL:CG2	1:D:323:GLN:O	2.56	0.53
1:A:43:PHE:HB2	1:A:130:ALA:C	2.29	0.53
1:A:188:TYR:O	1:A:189:CYS:C	2.46	0.53
1:A:323:GLN:CA	1:A:330:TYR:CD2	2.89	0.53
1:C:98:TRP:HE1	1:C:102:ILE:HG13	1.73	0.53
1:C:494:GLN:O	1:C:495:ALA:CB	2.56	0.53
1:A:321:GLU:O	1:A:322:GLU:HB2	2.08	0.53
1:A:83:SER:HA	1:B:76:LEU:HD13	1.90	0.53
1:B:110:GLY:HA2	1:B:113:ASN:ND2	2.22	0.53
1:A:80:LEU:HD23	1:B:80:LEU:CD2	2.39	0.53
1:C:250:GLN:HB3	1:C:274:THR:HG22	1.90	0.53
1:C:403:HIS:CD2	1:C:486:LYS:HG3	2.43	0.53
1:D:343:THR:HB	1:D:344:PRO:CD	2.39	0.53
1:C:69:LEU:HD22	1:D:413:ILE:CD1	2.38	0.53
1:A:236:ILE:O	1:A:240:MET:HG3	2.09	0.53
1:A:259:ILE:O	1:A:260:GLU:HB2	2.08	0.53
1:A:323:GLN:CA	1:A:330:TYR:HD2	2.17	0.53
1:A:464:GLN:NE2	1:B:458:CYS:CB	2.71	0.53
1:A:471:ILE:HB	1:A:474:VAL:CG2	2.37	0.53
1:B:398:ASN:HB3	1:B:430:LYS:HG2	1.91	0.53
1:A:98:TRP:CZ2	1:A:102:ILE:HD11	2.43	0.53
1:A:300:ILE:HG13	1:A:302:LEU:HG	1.89	0.53
1:A:378:LEU:HG	1:A:441:LEU:HD11	1.90	0.53
1:C:407:TRP:CZ2	1:C:412:THR:HG22	2.44	0.53
1:C:65:ILE:HB	1:C:66:PRO:CD	2.39	0.53
1:A:171:PRO:CB	1:A:255:LYS:HE3	2.39	0.53
1:A:378:LEU:HD11	1:A:442:GLY:HA2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ILE:HB	1:A:66:PRO:CD	2.35	0.53
1:B:141:LYS:HD2	1:B:149:GLU:CD	2.30	0.53
1:C:125:VAL:HG12	1:C:126:VAL:N	2.23	0.53
1:D:254:ILE:HD11	1:D:270:VAL:HB	1.91	0.53
1:B:472:HIS:CD2	1:B:473:PRO:HB3	2.44	0.52
1:C:65:ILE:N	1:C:65:ILE:HD12	2.24	0.52
1:A:404:SER:OG	1:A:405:TYR:N	2.43	0.52
1:B:236:ILE:HD11	1:B:380:TYR:HD2	1.74	0.52
1:B:98:TRP:O	1:B:99:ASP:C	2.48	0.52
1:C:18:ILE:HD11	1:C:140:ILE:HD12	1.90	0.52
1:B:380:TYR:HD1	1:B:381:GLY:N	2.07	0.52
1:C:336:LEU:HB3	1:C:339:LYS:HG3	1.92	0.52
1:C:493:LEU:O	1:C:494:GLN:HG3	2.09	0.52
1:A:310:ASN:OD1	1:A:312:LYS:HB3	2.09	0.52
1:C:193:THR:HG23	1:C:194:LEU:N	2.24	0.52
1:C:39:MET:HE1	1:C:41:LEU:HD21	1.91	0.52
1:C:62:VAL:O	1:C:62:VAL:HG22	2.09	0.52
1:C:300:ILE:HG13	1:C:302:LEU:HG	1.92	0.52
1:D:378:LEU:HD11	1:D:442:GLY:HA2	1.92	0.52
1:D:487:ARG:C	1:D:489:GLY:H	2.13	0.52
1:A:94:VAL:HG11	1:B:90:VAL:HG22	1.92	0.52
1:B:450:GLN:OE1	1:B:450:GLN:HA	2.10	0.52
1:D:12:ASP:HB2	1:D:153:SER:O	2.08	0.52
1:D:258:GLN:HG3	1:D:260:GLU:H	1.75	0.52
1:A:16:ILE:HG12	1:A:39:MET:HB3	1.90	0.52
1:B:188:TYR:O	1:B:189:CYS:C	2.48	0.52
1:B:97:ASP:OD1	1:B:100:ARG:N	2.27	0.52
1:C:326:VAL:HB	1:C:329:ILE:CG1	2.40	0.52
1:D:60:VAL:HG12	1:D:109:ILE:HG23	1.92	0.52
1:D:438:PHE:HE1	1:D:440:VAL:CG1	2.22	0.52
1:A:66:PRO:HG3	1:A:109:ILE:HD11	1.91	0.52
1:B:131:TYR:CD2	1:B:132:GLY:N	2.77	0.52
1:B:423:ALA:O	1:B:424:LYS:CB	2.57	0.52
1:B:444:ASN:O	1:B:448:VAL:HG23	2.09	0.52
1:B:462:LYS:O	1:B:462:LYS:HG3	2.09	0.52
1:C:110:GLY:O	1:C:113:ASN:HB2	2.09	0.52
1:D:441:LEU:C	1:D:441:LEU:HD23	2.30	0.52
1:A:144:ASN:OD1	1:A:146:LYS:N	2.43	0.52
1:B:20:GLY:HA3	1:B:42:ASP:HB2	1.91	0.52
1:B:440:VAL:HB	1:B:479:PHE:HZ	1.75	0.52
1:A:191:GLY:O	1:A:192:LYS:C	2.47	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:GLU:H	1:B:303:GLU:CD	2.14	0.51
1:C:259:ILE:O	1:C:260:GLU:HB2	2.11	0.51
1:A:325:ASN:O	1:A:327:PRO:HD3	2.10	0.51
1:A:193:THR:CG2	1:A:194:LEU:H	2.23	0.51
1:A:332:ILE:HA	1:A:336:LEU:HD11	1.92	0.51
1:A:409:LEU:HG	1:B:69:LEU:CD1	2.40	0.51
1:C:413:ILE:HB	1:C:414:PRO:HD3	1.92	0.51
1:C:438:PHE:C	1:C:438:PHE:CD1	2.82	0.51
1:C:440:VAL:HB	1:C:479:PHE:CZ	2.42	0.51
1:C:164:ARG:HB3	1:C:165:PRO:HD2	1.91	0.51
1:C:239:HIS:CE1	1:C:243:HIS:HD2	2.29	0.51
1:C:388:GLU:HG2	1:C:389:LYS:H	1.76	0.51
1:D:146:LYS:NZ	1:D:148:LYS:CB	2.73	0.51
1:B:271:ALA:HB3	1:B:280:ILE:HD11	1.93	0.51
1:C:176:TYR:CE1	1:C:258:GLN:NE2	2.77	0.51
1:D:170:ILE:HB	1:D:254:ILE:O	2.10	0.51
1:D:18:ILE:N	1:D:18:ILE:HD12	2.26	0.51
1:A:254:ILE:HD11	1:A:279:ILE:HD13	1.92	0.51
1:A:315:LYS:HB3	1:A:337:GLU:HA	1.92	0.51
1:B:32:ALA:HB2	1:B:125:VAL:CG2	2.41	0.51
1:D:410:GLU:OE1	1:D:410:GLU:N	2.40	0.51
1:A:386:SER:HG	1:A:389:LYS:HB2	1.75	0.51
1:B:398:ASN:CB	1:B:430:LYS:HD3	2.40	0.51
1:C:394:PHE:O	1:C:398:ASN:ND2	2.44	0.51
1:D:208:PHE:HD1	1:D:209:LEU:N	2.08	0.51
1:D:20:GLY:HA3	1:D:42:ASP:HB2	1.93	0.51
1:A:164:ARG:CG	1:A:164:ARG:HH11	2.23	0.51
1:A:340:VAL:HG13	1:A:342:LEU:HD12	1.91	0.51
1:B:162:GLY:HA2	1:B:335:ILE:HG23	1.93	0.51
1:B:267:LEU:O	1:B:283:GLU:HA	2.10	0.51
1:C:385:LEU:HB3	1:C:390:ALA:HB2	1.92	0.51
1:D:110:GLY:O	1:D:111:SER:C	2.46	0.51
1:D:117:ARG:HB3	1:D:117:ARG:CZ	2.40	0.51
1:D:168:LEU:CD1	1:D:253:PRO:HG2	2.40	0.51
1:A:73:ALA:HB2	1:B:86:TYR:HD1	1.74	0.51
1:C:188:TYR:O	1:C:189:CYS:C	2.50	0.51
1:C:403:HIS:CE1	1:C:492:ILE:HD13	2.46	0.51
1:D:254:ILE:CD1	1:D:270:VAL:HB	2.41	0.51
1:D:43:PHE:HB2	1:D:130:ALA:C	2.31	0.51
1:B:480:THR:CG2	1:B:481:THR:HG23	2.41	0.51
1:C:96:HIS:CE1	1:C:212:ILE:HG21	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:THR:O	1:D:162:GLY:O	2.29	0.51
1:B:192:LYS:HG2	1:B:284:TYR:HD2	1.75	0.50
1:B:45:THR:O	1:B:164:ARG:NH2	2.37	0.50
1:D:385:LEU:HD13	1:D:390:ALA:HA	1.93	0.50
1:A:375:PHE:CD1	1:A:375:PHE:N	2.79	0.50
1:A:63:GLY:C	1:A:66:PRO:HD2	2.30	0.50
1:B:398:ASN:HB3	1:B:430:LYS:CD	2.40	0.50
1:C:134:PHE:N	1:C:300:ILE:O	2.38	0.50
1:D:21:GLY:HA3	2:D:500:FAD:O5B	2.11	0.50
1:A:318:VAL:HG11	1:A:336:LEU:HD22	1.93	0.50
1:C:96:HIS:ND1	1:C:212:ILE:HB	2.26	0.50
1:C:303:GLU:OE1	1:C:304:THR:HG23	2.11	0.50
1:C:332:ILE:CA	1:C:336:LEU:HD11	2.33	0.50
1:C:410:GLU:OE2	1:C:410:GLU:N	2.30	0.50
1:C:70:MET:CE	1:C:105:VAL:HG21	2.41	0.50
1:D:173:ASP:C	1:D:175:GLU:N	2.64	0.50
1:D:138:HIS:CD2	1:D:328:TYR:CZ	2.99	0.50
1:A:245:ILE:CG2	1:A:247:PHE:HE2	2.24	0.50
1:A:399:ILE:HD12	1:A:426:ILE:HG22	1.93	0.50
1:A:449:THR:O	1:A:450:GLN:C	2.49	0.50
1:B:319:THR:C	1:B:321:GLU:H	2.14	0.50
1:B:406:PHE:CE2	1:B:421:CYS:CB	2.94	0.50
1:C:17:ILE:HD12	1:C:28:ALA:HB2	1.93	0.50
1:B:373:THR:HG22	1:B:374:VAL:N	2.27	0.50
1:B:438:PHE:C	1:B:438:PHE:CD1	2.85	0.50
1:C:195:VAL:HB	1:C:218:VAL:HG22	1.93	0.50
1:C:471:ILE:HG22	1:C:472:HIS:N	2.27	0.50
1:D:295:ALA:HB1	1:D:335:ILE:HG22	1.94	0.50
1:D:144:ASN:OD1	1:D:145:ASN:N	2.44	0.50
1:B:134:PHE:CG	1:B:305:VAL:HG21	2.47	0.50
1:B:36:LYS:HE3	1:B:358:TYR:CD1	2.47	0.50
1:D:404:SER:OG	1:D:405:TYR:N	2.45	0.50
1:A:68:LYS:HE3	1:A:375:PHE:HE2	1.74	0.50
1:A:440:VAL:O	1:A:440:VAL:HG13	2.11	0.50
1:B:323:GLN:HE21	1:B:327:PRO:HA	1.76	0.50
1:C:131:TYR:HB3	1:C:143:THR:HG23	1.94	0.50
1:C:163:GLU:CG	1:C:295:ALA:HA	2.21	0.50
1:A:39:MET:HE2	1:A:128:GLU:HB2	1.94	0.50
1:A:70:MET:SD	1:A:208:PHE:CZ	3.05	0.50
1:A:34:TYR:N	1:A:34:TYR:CD1	2.79	0.50
1:C:369:ASN:HD22	1:C:384:GLY:HA2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:TRP:HH2	1:C:421:CYS:SG	2.34	0.50
1:D:401:VAL:CG1	1:D:486:LYS:HD2	2.36	0.50
1:B:173:ASP:O	1:B:175:GLU:N	2.45	0.49
1:C:43:PHE:HD2	1:C:131:TYR:CD1	2.30	0.49
1:C:298:ARG:C	1:C:299:LYS:HD2	2.32	0.49
1:C:43:PHE:CD2	1:C:131:TYR:HD1	2.29	0.49
1:D:110:GLY:O	1:D:113:ASN:N	2.45	0.49
1:D:156:ARG:HG3	1:D:156:ARG:HH11	1.76	0.49
1:D:219:MET:HE3	1:D:251:PHE:O	2.11	0.49
1:B:193:THR:HG22	1:B:194:LEU:N	2.26	0.49
1:B:221:ARG:O	1:B:250:GLN:HA	2.11	0.49
1:D:142:ALA:CB	1:D:152:TYR:HE1	2.25	0.49
1:C:370:VAL:CG2	1:D:469:ILE:HD12	2.39	0.49
1:C:251:PHE:CE2	1:C:280:ILE:HG23	2.47	0.49
1:C:333:GLY:N	1:C:336:LEU:CD1	2.76	0.49
1:C:99:ASP:O	1:C:103:GLU:HG3	2.12	0.49
1:A:220:VAL:O	1:A:220:VAL:HG12	2.13	0.49
1:B:47:THR:CG2	1:B:51:THR:OG1	2.60	0.49
1:A:245:ILE:HG22	1:A:247:PHE:HE2	1.76	0.49
1:A:450:GLN:O	1:A:453:ALA:HB3	2.13	0.49
1:B:232:MET:HE1	1:B:422:TYR:HD2	1.78	0.49
1:C:186:LEU:HD21	1:C:188:TYR:CD1	2.48	0.49
1:C:318:VAL:CG2	1:C:319:THR:N	2.75	0.49
1:C:63:GLY:O	1:C:66:PRO:HG2	2.11	0.49
1:D:438:PHE:C	1:D:438:PHE:CD1	2.85	0.49
1:B:164:ARG:HD2	1:B:165:PRO:HD3	1.94	0.49
1:B:175:GLU:HG3	1:B:176:TYR:CE2	2.48	0.49
1:C:186:LEU:CD2	1:C:188:TYR:H	2.21	0.49
1:A:47:THR:HG1	1:A:51:THR:HB	1.77	0.49
1:B:185:SER:O	1:B:186:LEU:C	2.49	0.49
1:B:387:GLU:OE1	1:B:401:VAL:HG21	2.13	0.49
1:C:16:ILE:HD13	1:C:39:MET:HB3	1.95	0.49
1:D:150:LYS:HE3	1:D:151:ILE:O	2.12	0.49
1:A:223:ILE:HD11	1:A:226:ARG:HG3	1.94	0.49
1:A:58:THR:HG23	1:A:62:VAL:HG23	1.94	0.49
1:B:402:TYR:CD2	1:B:485:THR:HG22	2.47	0.49
1:D:68:LYS:O	1:D:71:HIS:HB3	2.13	0.49
1:A:315:LYS:HG2	1:A:336:LEU:O	2.11	0.49
1:A:36:LYS:HG3	1:A:358:TYR:CE2	2.46	0.49
1:A:470:GLY:HA2	1:B:450:GLN:HE22	1.77	0.49
1:B:15:LEU:HD12	1:B:16:ILE:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ASN:HB3	1:B:430:LYS:CG	2.43	0.49
1:C:221:ARG:O	1:C:250:GLN:HA	2.12	0.49
1:C:251:PHE:CD1	1:C:273:SER:HA	2.48	0.49
1:A:219:MET:CG	1:A:251:PHE:O	2.61	0.49
1:B:278:GLU:HG2	1:B:279:ILE:N	2.28	0.49
1:C:307:VAL:O	1:C:307:VAL:CG1	2.60	0.49
1:C:398:ASN:C	1:C:429:THR:HG1	2.16	0.49
1:D:16:ILE:HG13	1:D:154:ALA:CB	2.43	0.49
1:D:328:TYR:CE2	1:D:329:ILE:HD11	2.48	0.49
1:A:225:LEU:HB3	1:A:228:PHE:CD2	2.47	0.48
1:A:274:THR:HG22	1:A:274:THR:O	2.12	0.48
1:C:302:LEU:HD13	1:C:307:VAL:HG11	1.95	0.48
1:C:413:ILE:HG13	1:D:69:LEU:HD22	1.95	0.48
1:D:146:LYS:NZ	1:D:148:LYS:HB2	2.28	0.48
1:A:435:VAL:HG12	1:A:456:LEU:CD2	2.37	0.48
1:A:478:VAL:HG22	1:A:478:VAL:O	2.13	0.48
1:B:430:LYS:N	1:B:430:LYS:CD	2.74	0.48
1:B:146:LYS:HD2	1:B:146:LYS:O	2.13	0.48
1:C:447:GLU:OE2	1:D:475:CYS:HB2	2.13	0.48
1:D:378:LEU:CG	1:D:441:LEU:HD21	2.43	0.48
1:A:98:TRP:O	1:A:102:ILE:HG12	2.14	0.48
1:B:134:PHE:CD1	1:B:305:VAL:HG21	2.49	0.48
1:B:426:ILE:O	1:B:436:VAL:HG22	2.12	0.48
1:C:411:TRP:CZ3	1:C:421:CYS:SG	3.06	0.48
1:C:43:PHE:HB2	1:C:130:ALA:C	2.34	0.48
1:C:487:ARG:CB	1:C:487:ARG:HH21	2.21	0.48
1:D:318:VAL:HG23	1:D:323:GLN:C	2.34	0.48
1:D:13:TYR:CD2	1:D:37:LYS:HG2	2.47	0.48
1:A:12:ASP:HB2	1:A:153:SER:O	2.13	0.48
1:A:15:LEU:HB3	1:A:38:VAL:CG1	2.43	0.48
1:B:12:ASP:HB2	1:B:153:SER:O	2.12	0.48
1:B:379:GLU:HB3	1:B:445:ALA:HB3	1.94	0.48
1:C:70:MET:HB3	1:C:208:PHE:CD1	2.49	0.48
1:C:80:LEU:HD23	1:C:80:LEU:HA	1.51	0.48
1:A:323:GLN:CB	1:A:330:TYR:CE2	2.94	0.48
1:D:17:ILE:HD12	1:D:17:ILE:N	2.29	0.48
1:D:36:LYS:HE2	1:D:358:TYR:CD1	2.49	0.48
1:D:59:CYS:SG	1:D:343:THR:OG1	2.57	0.48
1:B:20:GLY:CA	1:B:42:ASP:HB2	2.44	0.48
1:B:345:VAL:HG13	1:B:346:ALA:N	2.29	0.48
1:C:166:ARG:HB2	1:C:294:ASP:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:ASN:ND2	1:C:326:VAL:HG23	2.28	0.48
1:D:193:THR:HG22	1:D:194:LEU:N	2.28	0.48
1:A:39:MET:HG3	1:A:126:VAL:CG1	2.43	0.48
1:A:43:PHE:CD1	1:A:131:TYR:HB2	2.48	0.48
1:C:219:MET:HE3	1:C:251:PHE:HB3	1.93	0.48
1:D:173:ASP:C	1:D:175:GLU:H	2.16	0.48
1:D:449:THR:O	1:D:450:GLN:C	2.52	0.48
1:A:404:SER:HA	1:A:492:ILE:HD13	1.96	0.48
1:B:25:LEU:CD2	1:B:120:LEU:HD11	2.43	0.48
1:C:20:GLY:H	1:C:42:ASP:CG	2.18	0.48
1:C:416:ARG:O	1:C:417:ASP:C	2.51	0.48
1:B:178:ILE:O	1:B:288:MET:HA	2.14	0.48
1:B:396:GLU:HG3	1:B:396:GLU:O	2.14	0.48
1:B:70:MET:HE1	1:B:184:PHE:CD1	2.37	0.48
1:C:21:GLY:HA3	2:C:500:FAD:O5B	2.13	0.48
1:D:394:PHE:O	1:D:398:ASN:ND2	2.45	0.48
1:A:353:LEU:HA	1:A:356:ARG:HH21	1.78	0.47
1:B:441:LEU:O	1:B:441:LEU:HD23	2.14	0.47
1:D:138:HIS:HD2	1:D:328:TYR:CZ	2.31	0.47
1:D:208:PHE:CE1	1:D:209:LEU:HG	2.48	0.47
1:A:97:ASP:HB2	1:B:89:LYS:HE3	1.96	0.47
1:C:254:ILE:HG13	1:C:270:VAL:O	2.14	0.47
1:A:340:VAL:CG1	1:A:345:VAL:HG21	2.43	0.47
1:C:17:ILE:HD11	1:C:28:ALA:HA	1.95	0.47
1:C:425:ILE:O	1:C:425:ILE:HG13	2.14	0.47
1:D:427:CYS:HA	1:D:434:ARG:O	2.14	0.47
1:A:315:LYS:HB3	1:A:337:GLU:CA	2.43	0.47
1:B:325:ASN:ND2	1:B:325:ASN:C	2.67	0.47
1:C:251:PHE:HE2	1:C:280:ILE:CG2	2.28	0.47
1:C:289:LEU:HD23	1:C:289:LEU:N	2.30	0.47
1:D:319:THR:C	1:D:321:GLU:H	2.17	0.47
1:A:220:VAL:CG1	1:A:222:SER:O	2.63	0.47
1:A:435:VAL:CG1	1:A:456:LEU:HD21	2.38	0.47
1:A:402:TYR:HD1	1:A:462:LYS:HE2	1.76	0.47
1:B:12:ASP:HB3	1:B:13:TYR:CD1	2.50	0.47
1:B:380:TYR:C	1:B:380:TYR:HD1	2.17	0.47
1:C:303:GLU:CD	1:C:303:GLU:H	2.16	0.47
1:D:297:THR:HG22	1:D:316:ILE:HD11	1.96	0.47
1:D:386:SER:O	1:D:390:ALA:HB2	2.14	0.47
1:D:403:HIS:CE1	1:D:492:ILE:HD11	2.48	0.47
1:A:293:ARG:HB3	1:A:293:ARG:HH11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:GLN:HE22	1:C:123:LYS:NZ	2.12	0.47
1:C:217:THR:HG23	1:C:246:LYS:HB3	1.97	0.47
1:C:424:LYS:HG3	1:C:439:HIS:HB2	1.97	0.47
1:D:200:TYR:CE2	1:D:201:VAL:HG23	2.49	0.47
1:A:302:LEU:HD22	1:A:307:VAL:CG1	2.41	0.47
1:B:392:GLU:O	1:B:392:GLU:HG2	2.15	0.47
1:B:411:TRP:O	1:B:414:PRO:HG2	2.14	0.47
1:C:445:ALA:O	1:C:449:THR:OG1	2.33	0.47
1:D:200:TYR:O	1:D:204:GLU:HG3	2.15	0.47
1:D:352:LEU:HA	1:D:352:LEU:HD23	1.71	0.47
1:D:407:TRP:CZ3	1:D:412:THR:HG22	2.49	0.47
1:D:461:THR:N	1:D:464:GLN:OE1	2.47	0.47
1:A:144:ASN:OD1	1:A:144:ASN:C	2.52	0.47
1:A:164:ARG:NH1	1:A:164:ARG:CG	2.77	0.47
1:A:409:LEU:HG	1:B:69:LEU:HD12	1.95	0.47
1:C:166:ARG:HH21	1:C:292:GLY:CA	2.16	0.47
1:D:258:GLN:NE2	1:D:261:ALA:CA	2.72	0.47
1:D:32:ALA:HB2	1:D:125:VAL:HG22	1.96	0.47
1:D:39:MET:HE3	1:D:128:GLU:HB2	1.96	0.47
1:A:293:ARG:NH1	1:A:293:ARG:HB3	2.29	0.47
1:A:342:LEU:O	1:A:345:VAL:HG23	2.15	0.47
1:B:100:ARG:O	1:B:100:ARG:HG3	2.15	0.47
1:B:297:THR:HG21	1:B:316:ILE:HD11	1.95	0.47
1:B:353:LEU:O	1:B:354:ALA:C	2.53	0.47
1:C:259:ILE:CG2	1:C:259:ILE:O	2.63	0.47
1:D:25:LEU:O	1:D:28:ALA:HB3	2.14	0.47
1:D:38:VAL:HG12	1:D:39:MET:N	2.30	0.47
1:A:116:TYR:O	1:A:119:ALA:HB3	2.14	0.47
1:A:352:LEU:HD12	1:A:365:CYS:CA	2.45	0.47
1:B:16:ILE:HD13	1:B:39:MET:HB3	1.97	0.47
1:D:188:TYR:CE1	1:D:264:PRO:HB3	2.50	0.47
1:D:259:ILE:O	1:D:260:GLU:HB2	2.14	0.47
1:D:259:ILE:HG21	1:D:266:ARG:HH21	1.80	0.47
1:D:342:LEU:HD23	1:D:342:LEU:HA	1.68	0.47
1:A:250:GLN:O	1:A:251:PHE:CD1	2.69	0.46
1:A:378:LEU:HG	1:A:441:LEU:HD12	1.98	0.46
1:B:131:TYR:C	1:B:131:TYR:CD2	2.87	0.46
1:C:176:TYR:CD1	1:C:258:GLN:NE2	2.81	0.46
1:C:319:THR:HG1	1:C:323:GLN:HB3	1.74	0.46
1:D:305:VAL:HG21	1:D:329:ILE:HD11	1.97	0.46
1:D:343:THR:HB	1:D:344:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:LEU:HA	1:B:464:GLN:NE2	2.30	0.46
1:B:465:LEU:O	1:B:468:THR:HB	2.15	0.46
1:D:209:LEU:HD23	1:D:209:LEU:HA	1.67	0.46
1:A:298:ARG:HG2	1:A:298:ARG:HH11	1.79	0.46
1:B:85:ASN:HB3	1:B:413:ILE:HG22	1.97	0.46
1:B:427:CYS:HB3	1:B:433:GLU:O	2.14	0.46
1:C:438:PHE:CE2	1:C:452:PHE:CG	3.03	0.46
1:C:77:GLY:O	1:C:80:LEU:HB2	2.15	0.46
1:D:208:PHE:O	1:D:212:ILE:HG23	2.16	0.46
1:D:318:VAL:HG23	1:D:323:GLN:O	2.16	0.46
1:D:438:PHE:CZ	1:D:479:PHE:CE2	3.03	0.46
1:D:487:ARG:CG	1:D:487:ARG:NH2	2.78	0.46
1:B:243:HIS:NE2	1:D:493:LEU:HD21	2.30	0.46
1:A:245:ILE:CG2	1:A:247:PHE:CE2	2.97	0.46
1:A:323:GLN:NE2	1:A:330:TYR:HE2	2.14	0.46
1:A:405:TYR:CD2	1:A:422:TYR:HD1	2.34	0.46
1:D:307:VAL:HG23	1:D:326:VAL:HG21	1.96	0.46
1:D:72:GLN:HG3	1:D:76:LEU:HD11	1.96	0.46
1:A:172:GLY:HA2	1:A:176:TYR:CE2	2.50	0.46
1:A:420:LYS:HD2	1:A:420:LYS:HA	1.69	0.46
1:B:250:GLN:O	1:B:251:PHE:CD1	2.68	0.46
1:B:297:THR:CG2	1:B:316:ILE:HD11	2.45	0.46
1:B:343:THR:O	1:B:347:ILE:HG13	2.16	0.46
1:B:38:VAL:CG1	1:B:39:MET:N	2.78	0.46
1:C:257:GLU:OE2	1:C:268:ARG:NH1	2.49	0.46
1:D:219:MET:HE1	1:D:253:PRO:HD3	1.96	0.46
1:D:258:GLN:CG	1:D:260:GLU:H	2.28	0.46
1:D:157:PHE:HB2	1:D:329:ILE:HG12	1.98	0.46
1:B:98:TRP:CE2	1:B:102:ILE:HD11	2.50	0.46
1:B:38:VAL:HG12	1:B:39:MET:N	2.30	0.46
1:B:413:ILE:N	1:B:414:PRO:HD2	2.31	0.46
1:B:42:ASP:OD1	2:B:500:FAD:H1B	2.16	0.46
1:C:25:LEU:HD13	1:C:116:TYR:CD1	2.50	0.46
1:C:398:ASN:C	1:C:429:THR:OG1	2.53	0.46
1:C:438:PHE:HE1	1:C:440:VAL:HG12	1.81	0.46
1:A:357:LEU:CB	1:A:358:TYR:CD1	2.98	0.46
1:A:371:PRO:HB2	1:B:471:ILE:HD11	1.97	0.46
1:C:219:MET:CE	1:C:251:PHE:O	2.63	0.46
1:C:166:ARG:NH2	1:C:292:GLY:HA3	2.15	0.46
1:C:399:ILE:CD1	1:C:426:ILE:HG23	2.44	0.46
1:D:199:SER:O	1:D:202:ALA:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:TYR:N	1:A:358:TYR:HD1	2.09	0.46
1:B:376:THR:O	1:B:377:PRO:C	2.52	0.46
1:B:75:LEU:HA	1:B:75:LEU:HD23	1.76	0.46
1:C:136:GLY:O	1:C:137:PRO:C	2.54	0.46
1:D:38:VAL:HG12	1:D:125:VAL:HG13	1.98	0.46
1:D:47:THR:OG1	1:D:51:THR:HB	2.16	0.46
1:A:266:ARG:HG3	1:A:266:ARG:NH1	2.30	0.46
1:A:323:GLN:CB	1:A:330:TYR:HE2	2.20	0.46
1:B:196:VAL:HG23	1:B:288:MET:O	2.16	0.46
1:C:193:THR:HG23	1:C:194:LEU:H	1.79	0.46
1:C:68:LYS:HE3	1:C:375:PHE:CE2	2.51	0.46
1:D:163:GLU:CG	1:D:294:ASP:C	2.85	0.46
1:D:231:ASP:OD2	1:D:424:LYS:NZ	2.48	0.46
1:D:65:ILE:CB	1:D:66:PRO:CD	2.94	0.46
1:A:164:ARG:HA	1:A:164:ARG:HD2	1.60	0.46
1:A:183:LEU:O	1:A:183:LEU:HD12	2.15	0.46
1:A:67:LYS:NZ	1:A:204:GLU:OE2	2.48	0.46
1:B:16:ILE:HG12	1:B:154:ALA:HB2	1.98	0.46
1:B:250:GLN:NE2	1:B:275:ASN:ND2	2.63	0.46
1:D:229:ASP:OD2	1:D:231:ASP:HB3	2.16	0.46
1:A:39:MET:CG	1:A:126:VAL:HG12	2.45	0.45
1:A:159:ILE:O	1:A:335:ILE:HD11	2.16	0.45
1:B:70:MET:CE	1:B:184:PHE:CD1	2.92	0.45
1:C:407:TRP:HB2	1:C:418:ASN:OD1	2.16	0.45
1:D:462:LYS:HG3	1:D:466:ASP:OD2	2.16	0.45
1:A:321:GLU:HA	1:A:356:ARG:NH1	2.32	0.45
1:A:158:LEU:HD11	1:A:332:ILE:HG12	1.97	0.45
1:B:13:TYR:CZ	1:B:39:MET:HE2	2.52	0.45
1:C:150:LYS:HB2	1:C:150:LYS:HE2	1.74	0.45
1:B:273:SER:OG	1:B:274:THR:N	2.49	0.45
1:B:312:LYS:HE2	1:B:313:THR:HG23	1.98	0.45
1:D:142:ALA:HB3	1:D:152:TYR:HE1	1.81	0.45
1:D:234:ASN:O	1:D:238:GLU:HG3	2.16	0.45
1:B:65:ILE:O	1:B:66:PRO:C	2.54	0.45
1:C:422:TYR:CD2	1:C:422:TYR:C	2.90	0.45
1:A:194:LEU:HD21	1:A:219:MET:CE	2.46	0.45
1:B:464:GLN:HB2	1:B:464:GLN:HE21	1.59	0.45
1:C:20:GLY:CA	1:C:42:ASP:HB2	2.47	0.45
1:C:343:THR:HB	1:C:344:PRO:HD3	1.99	0.45
1:C:391:VAL:O	1:C:395:GLY:N	2.45	0.45
1:A:162:GLY:O	1:A:296:CYS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLU:HA	1:A:356:ARG:HH11	1.80	0.45
1:B:144:ASN:OD1	1:B:144:ASN:C	2.54	0.45
1:B:278:GLU:HG2	1:B:279:ILE:H	1.81	0.45
1:D:39:MET:HE2	1:D:41:LEU:CG	2.39	0.45
1:A:194:LEU:HD12	1:A:217:THR:O	2.16	0.45
1:A:302:LEU:HD13	1:A:307:VAL:HG11	1.99	0.45
1:A:324:THR:OG1	1:A:329:ILE:O	2.23	0.45
1:A:444:ASN:O	1:A:448:VAL:HG23	2.16	0.45
1:A:344:PRO:HD3	1:B:472:HIS:HB2	1.99	0.45
1:C:357:LEU:HD13	1:C:358:TYR:CZ	2.51	0.45
1:D:452:PHE:O	1:D:455:ALA:HB3	2.17	0.45
1:A:239:HIS:NE2	1:A:243:HIS:CE1	2.85	0.45
1:A:423:ALA:HB1	1:A:479:PHE:CZ	2.52	0.45
1:A:47:THR:HG21	1:A:181:ASP:HB2	1.98	0.45
1:B:198:ALA:HB1	1:B:224:LEU:HA	1.99	0.45
1:B:21:GLY:O	1:B:24:GLY:N	2.49	0.45
1:D:81:GLN:HA	1:D:84:ARG:NH1	2.31	0.45
1:A:221:ARG:O	1:A:250:GLN:HA	2.17	0.45
1:A:357:LEU:HD13	1:A:358:TYR:HE1	1.82	0.45
1:A:82:ASP:OD2	1:A:416:ARG:NH1	2.32	0.45
1:B:310:ASN:OD1	1:B:312:LYS:HB3	2.17	0.45
1:A:151:ILE:HG22	1:A:152:TYR:N	2.32	0.45
1:A:186:LEU:HD12	1:A:188:TYR:N	2.27	0.45
1:A:70:MET:SD	1:A:101:MET:HE3	2.57	0.45
1:B:183:LEU:O	1:B:185:SER:N	2.50	0.45
1:C:422:TYR:HE2	1:C:424:LYS:HG2	1.82	0.45
1:D:183:LEU:O	1:D:185:SER:N	2.50	0.45
1:A:151:ILE:N	1:A:151:ILE:HD12	2.32	0.44
1:B:214:LEU:HD23	1:B:214:LEU:HA	1.78	0.44
1:B:295:ALA:HB1	1:B:335:ILE:HG22	1.99	0.44
1:B:480:THR:HG22	1:B:481:THR:HG23	1.98	0.44
1:C:125:VAL:CG1	1:C:126:VAL:N	2.80	0.44
1:A:186:LEU:CD1	1:A:186:LEU:C	2.86	0.44
1:B:110:GLY:HA2	1:B:113:ASN:HD22	1.82	0.44
1:B:18:ILE:N	1:B:18:ILE:CD1	2.78	0.44
1:B:241:GLU:OE2	1:B:249:ARG:NH2	2.43	0.44
1:B:471:ILE:CG2	1:B:474:VAL:HG21	2.46	0.44
1:B:440:VAL:HB	1:B:479:PHE:CZ	2.52	0.44
1:C:452:PHE:O	1:C:455:ALA:HB3	2.17	0.44
1:D:173:ASP:O	1:D:174:LYS:C	2.53	0.44
1:D:231:ASP:O	1:D:235:LYS:HG2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:GLU:OE1	1:D:424:LYS:NZ	2.46	0.44
1:D:411:TRP:CH2	1:D:421:CYS:SG	3.11	0.44
1:D:438:PHE:C	1:D:439:HIS:ND1	2.69	0.44
1:A:80:LEU:HD21	1:B:90:VAL:HG21	1.98	0.44
1:B:14:ASP:HB2	1:B:37:LYS:O	2.16	0.44
1:B:237:GLY:O	1:B:240:MET:N	2.50	0.44
1:B:13:TYR:CZ	1:B:39:MET:CE	3.00	0.44
1:C:200:TYR:CD1	1:C:201:VAL:N	2.85	0.44
1:C:319:THR:C	1:C:321:GLU:N	2.70	0.44
1:A:134:PHE:N	1:A:300:ILE:O	2.38	0.44
1:B:457:LYS:HA	1:B:457:LYS:HD3	1.84	0.44
1:C:302:LEU:CB	1:C:307:VAL:HG12	2.31	0.44
1:D:194:LEU:HB2	1:D:284:TYR:CD1	2.52	0.44
1:D:385:LEU:HD11	1:D:394:PHE:HE1	1.82	0.44
1:D:479:PHE:HA	1:D:482:LEU:HD11	2.00	0.44
1:B:19:GLY:HA3	1:B:160:ALA:O	2.17	0.44
1:B:65:ILE:HD12	1:B:65:ILE:N	2.32	0.44
1:A:101:MET:HB2	1:B:86:TYR:O	2.18	0.44
1:D:267:LEU:O	1:D:283:GLU:HA	2.17	0.44
1:D:438:PHE:CE2	1:D:452:PHE:CD2	3.06	0.44
1:C:39:MET:HE1	1:C:41:LEU:CD2	2.47	0.44
1:C:449:THR:O	1:C:450:GLN:C	2.55	0.44
1:D:148:LYS:HE3	1:D:148:LYS:CA	2.37	0.44
1:A:319:THR:C	1:A:321:GLU:H	2.21	0.44
1:A:403:HIS:CE1	1:A:492:ILE:HD11	2.53	0.44
1:B:105:VAL:O	1:B:109:ILE:HG13	2.18	0.44
1:B:167:TYR:CE2	1:B:174:LYS:HA	2.52	0.44
1:B:192:LYS:HE2	1:B:284:TYR:CE2	2.51	0.44
1:B:229:ASP:HA	1:B:386:SER:HG	1.80	0.44
1:D:62:VAL:CG2	1:D:181:ASP:HA	2.48	0.44
1:A:362:THR:O	1:A:362:THR:OG1	2.28	0.44
1:A:436:VAL:HG23	1:A:437:GLY:N	2.32	0.44
1:B:406:PHE:C	1:B:406:PHE:CD2	2.91	0.44
1:B:460:LEU:HA	1:B:464:GLN:HE22	1.83	0.44
1:D:131:TYR:CD2	1:D:132:GLY:N	2.86	0.44
1:B:418:ASN:O	1:B:419:ASN:HB2	2.18	0.44
1:C:43:PHE:HD2	1:C:131:TYR:HD1	1.65	0.44
1:D:318:VAL:HG22	1:D:323:GLN:N	2.33	0.44
1:D:26:ALA:HB2	1:D:347:ILE:HD13	2.00	0.44
1:B:199:SER:O	1:B:200:TYR:C	2.55	0.43
1:C:12:ASP:HB2	1:C:153:SER:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:PRO:CB	1:C:255:LYS:HE3	2.48	0.43
1:D:175:GLU:N	1:D:175:GLU:OE1	2.51	0.43
1:A:271:ALA:O	1:A:279:ILE:HA	2.17	0.43
1:A:405:TYR:O	1:A:406:PHE:HB3	2.17	0.43
1:B:400:GLU:OE2	1:B:400:GLU:CA	2.64	0.43
1:C:240:MET:HE3	1:C:245:ILE:HD13	1.99	0.43
1:C:262:GLY:O	1:C:264:PRO:HA	2.18	0.43
1:C:67:LYS:HE2	1:C:67:LYS:HB3	1.85	0.43
1:D:163:GLU:HA	1:D:295:ALA:HA	2.00	0.43
1:C:464:GLN:HE22	1:D:458:CYS:HA	1.83	0.43
1:A:410:GLU:OE1	1:B:68:LYS:HE2	2.19	0.43
1:D:205:CYS:HA	1:D:208:PHE:CE2	2.54	0.43
1:C:344:PRO:HG3	1:D:472:HIS:HB2	2.01	0.43
1:A:376:THR:HB	1:A:377:PRO:HD3	2.00	0.43
1:A:416:ARG:O	1:A:417:ASP:C	2.56	0.43
1:B:336:LEU:HD12	1:B:336:LEU:HA	1.69	0.43
1:B:438:PHE:CE2	1:B:452:PHE:CD2	3.07	0.43
1:C:413:ILE:N	1:C:414:PRO:CD	2.82	0.43
1:C:461:THR:HG22	1:C:462:LYS:N	2.34	0.43
1:D:146:LYS:HZ1	1:D:148:LYS:HB3	1.83	0.43
1:D:298:ARG:NH1	1:D:298:ARG:CG	2.71	0.43
1:D:417:ASP:HA	1:D:420:LYS:HD3	2.00	0.43
1:D:65:ILE:O	1:D:66:PRO:C	2.54	0.43
1:A:172:GLY:C	1:A:175:GLU:HG2	2.39	0.43
1:A:89:LYS:O	1:B:94:VAL:HG13	2.18	0.43
1:C:246:LYS:HB2	1:C:246:LYS:HE3	1.64	0.43
1:C:183:LEU:HD23	1:C:288:MET:SD	2.58	0.43
1:D:186:LEU:HD21	1:D:188:TYR:CE1	2.54	0.43
1:C:477:GLU:HA	1:D:450:GLN:NE2	2.34	0.43
1:C:90:VAL:HG22	1:D:94:VAL:HG11	2.00	0.43
1:D:109:ILE:O	1:D:112:LEU:HB2	2.18	0.43
1:B:250:GLN:HG2	1:D:250:GLN:HE21	1.83	0.43
1:B:98:TRP:O	1:B:101:MET:N	2.51	0.43
1:C:170:ILE:O	1:C:170:ILE:HG13	2.18	0.43
1:C:65:ILE:N	1:C:65:ILE:CD1	2.82	0.43
1:C:447:GLU:OE1	1:D:474:VAL:HG12	2.18	0.43
1:A:259:ILE:O	1:A:259:ILE:CG2	2.66	0.43
1:B:113:ASN:HB2	1:B:114:TRP:CD1	2.54	0.43
1:B:122:GLU:O	1:B:122:GLU:HG2	2.19	0.43
1:B:315:LYS:HB3	1:B:337:GLU:CA	2.49	0.43
1:C:310:ASN:ND2	1:C:312:LYS:H	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:PHE:CD1	1:D:208:PHE:C	2.92	0.43
1:D:219:MET:HE1	1:D:253:PRO:CD	2.49	0.43
1:D:440:VAL:HB	1:D:479:PHE:CZ	2.52	0.43
1:D:408:PRO:HG3	1:D:475:CYS:SG	2.58	0.43
1:A:257:GLU:O	1:A:257:GLU:CG	2.66	0.43
1:A:61:ASN:HA	1:A:109:ILE:HD13	2.00	0.43
1:B:223:ILE:HG12	1:B:226:ARG:NH2	2.34	0.43
1:B:456:LEU:HD23	1:B:456:LEU:N	2.33	0.43
1:C:331:ALA:O	1:C:336:LEU:HD21	2.19	0.43
1:C:39:MET:CE	1:C:41:LEU:HG	2.49	0.43
1:D:133:GLN:NE2	1:D:141:LYS:NZ	2.66	0.43
1:A:66:PRO:O	1:A:70:MET:HG3	2.19	0.43
1:B:12:ASP:HB3	1:B:13:TYR:HD1	1.83	0.43
1:B:300:ILE:CG1	1:B:302:LEU:HG	2.49	0.43
1:B:49:LEU:HA	1:B:49:LEU:HD23	1.83	0.43
1:B:65:ILE:CD1	1:B:65:ILE:N	2.81	0.43
1:C:131:TYR:HD2	1:C:132:GLY:N	2.17	0.43
1:C:71:HIS:O	1:C:74:ALA:HB3	2.18	0.43
1:A:205:CYS:O	1:A:206:ALA:C	2.56	0.42
1:B:186:LEU:HD12	1:B:186:LEU:HA	1.74	0.42
1:B:387:GLU:O	1:B:390:ALA:HB3	2.18	0.42
1:B:407:TRP:CD1	1:B:418:ASN:HA	2.53	0.42
1:D:114:TRP:O	1:D:118:VAL:HG23	2.18	0.42
1:D:61:ASN:HA	1:D:109:ILE:HD13	2.00	0.42
1:B:209:LEU:HD23	1:B:209:LEU:HA	1.78	0.42
1:B:388:GLU:H	1:B:388:GLU:CD	2.23	0.42
1:B:403:HIS:N	1:B:403:HIS:CD2	2.86	0.42
1:C:173:ASP:CG	1:C:174:LYS:H	2.21	0.42
1:C:172:GLY:O	1:C:175:GLU:HG2	2.19	0.42
1:C:413:ILE:CD1	1:D:69:LEU:HD22	2.49	0.42
1:C:426:ILE:N	1:C:426:ILE:HD12	2.34	0.42
1:D:219:MET:HE1	1:D:253:PRO:N	2.34	0.42
1:D:438:PHE:CE1	1:D:440:VAL:HG12	2.50	0.42
1:A:239:HIS:CE1	1:A:378:LEU:HB2	2.54	0.42
1:A:302:LEU:HD13	1:A:309:ILE:CG2	2.49	0.42
1:C:434:ARG:NH1	1:C:459:GLY:O	2.53	0.42
1:D:106:GLN:HE21	1:D:185:SER:CB	2.32	0.42
1:A:178:ILE:O	1:A:178:ILE:HG13	2.19	0.42
1:B:163:GLU:OE1	1:B:293:ARG:HB2	2.19	0.42
1:B:33:GLN:HG3	1:B:123:LYS:CE	2.48	0.42
1:C:251:PHE:HE1	1:C:273:SER:HB2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:TYR:CE2	1:D:174:LYS:HA	2.55	0.42
1:D:487:ARG:CZ	1:D:487:ARG:HB2	2.50	0.42
1:D:66:PRO:HG3	1:D:109:ILE:CD1	2.45	0.42
1:A:168:LEU:HA	1:A:168:LEU:HD23	1.74	0.42
1:A:186:LEU:HD12	1:A:186:LEU:C	2.39	0.42
1:B:355:GLN:C	1:B:361:SER:HB3	2.40	0.42
1:C:188:TYR:O	1:C:188:TYR:HD1	2.01	0.42
1:C:84:ARG:HG3	1:C:84:ARG:HH11	1.84	0.42
1:A:68:LYS:O	1:A:71:HIS:HB3	2.19	0.42
1:B:137:PRO:HA	1:B:328:TYR:OH	2.20	0.42
1:B:254:ILE:HG12	1:B:270:VAL:O	2.19	0.42
1:B:47:THR:HG21	1:B:51:THR:OG1	2.19	0.42
1:A:90:VAL:HG21	1:B:80:LEU:HD11	2.01	0.42
1:C:62:VAL:HG21	1:C:181:ASP:OD2	2.19	0.42
1:C:342:LEU:CD1	1:C:372:THR:HG23	2.35	0.42
1:C:93:THR:CG2	1:C:93:THR:O	2.68	0.42
1:D:232:MET:CE	1:D:441:LEU:HB2	2.50	0.42
1:A:332:ILE:HG13	1:A:332:ILE:O	2.19	0.42
1:A:487:ARG:HE	1:A:487:ARG:HB3	1.41	0.42
1:A:222:SER:OG	3:A:502:SO4:O1	2.35	0.42
1:C:98:TRP:NE1	1:C:102:ILE:CG1	2.80	0.42
1:D:156:ARG:HG3	1:D:156:ARG:NH1	2.35	0.42
1:D:205:CYS:O	1:D:206:ALA:C	2.58	0.42
1:D:318:VAL:HG22	1:D:323:GLN:O	2.19	0.42
1:C:409:LEU:HD21	1:D:68:LYS:HB3	2.00	0.42
1:B:224:LEU:N	1:B:224:LEU:CD1	2.82	0.42
1:B:232:MET:HE3	1:B:232:MET:HA	1.99	0.42
1:B:15:LEU:HB3	1:B:38:VAL:HG22	2.01	0.42
1:A:68:LYS:HG2	1:B:409:LEU:HD23	2.01	0.42
1:C:252:VAL:HG12	1:C:253:PRO:O	2.20	0.42
1:C:334:ASP:OD1	2:C:500:FAD:H5'2	2.19	0.42
1:D:109:ILE:O	1:D:110:GLY:C	2.55	0.42
1:D:140:ILE:CG2	1:D:157:PHE:HE2	2.32	0.42
1:D:194:LEU:HD23	1:D:287:VAL:HG13	2.01	0.42
1:A:352:LEU:HA	1:A:352:LEU:HD23	1.89	0.42
1:A:353:LEU:HA	1:A:356:ARG:HE	1.85	0.42
1:B:163:GLU:O	1:B:164:ARG:HG2	2.20	0.42
1:C:473:PRO:HA	1:C:477:GLU:OE2	2.19	0.42
1:A:16:ILE:HB	1:A:157:PHE:CE2	2.54	0.42
1:A:203:LEU:HA	1:A:203:LEU:HD23	1.70	0.42
1:A:228:PHE:O	1:A:229:ASP:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:TYR:HE1	1:A:258:GLN:NE2	2.18	0.42
1:B:311:GLU:H	1:B:311:GLU:HG2	1.66	0.42
1:B:348:GLN:HA	1:B:348:GLN:OE1	2.19	0.42
1:C:172:GLY:HA3	1:C:256:VAL:O	2.20	0.42
1:D:16:ILE:HD12	1:D:157:PHE:CZ	2.55	0.42
1:D:20:GLY:O	1:D:25:LEU:HD11	2.20	0.42
1:C:470:GLY:O	1:D:344:PRO:HG3	2.20	0.42
1:A:176:TYR:CE1	1:A:258:GLN:NE2	2.87	0.41
1:A:194:LEU:HB2	1:A:284:TYR:CD2	2.55	0.41
1:B:428:ASN:ND2	1:B:428:ASN:C	2.73	0.41
1:B:65:ILE:CB	1:B:66:PRO:HD3	2.48	0.41
1:C:251:PHE:CE1	1:C:273:SER:CB	3.01	0.41
1:C:76:LEU:HD23	1:C:76:LEU:HA	1.83	0.41
1:A:187:PRO:O	1:A:188:TYR:HB3	2.20	0.41
1:A:472:HIS:CD2	1:A:473:PRO:HB3	2.54	0.41
1:A:472:HIS:HB2	1:B:344:PRO:CG	2.49	0.41
1:C:17:ILE:HB	1:C:40:VAL:HG22	2.02	0.41
1:C:417:ASP:CB	1:C:420:LYS:HG3	2.48	0.41
1:D:203:LEU:HB3	1:D:240:MET:CE	2.51	0.41
1:D:343:THR:N	1:D:344:PRO:HD2	2.35	0.41
1:D:438:PHE:HZ	1:D:479:PHE:CE2	2.38	0.41
1:A:399:ILE:CD1	1:A:426:ILE:HG22	2.50	0.41
1:B:144:ASN:OD1	1:B:146:LYS:N	2.53	0.41
1:B:247:PHE:N	1:B:247:PHE:CD2	2.87	0.41
1:B:356:ARG:NH1	1:B:364:LYS:HA	2.33	0.41
1:B:438:PHE:HE1	1:B:440:VAL:HG12	1.86	0.41
1:D:369:ASN:OD1	1:D:384:GLY:HA2	2.20	0.41
1:A:200:TYR:HD1	1:A:201:VAL:N	2.18	0.41
1:A:319:THR:O	1:A:321:GLU:N	2.53	0.41
1:A:391:VAL:O	1:A:395:GLY:N	2.42	0.41
1:A:399:ILE:HA	1:A:427:CYS:O	2.20	0.41
1:B:300:ILE:HD11	1:B:302:LEU:HG	2.03	0.41
1:C:66:PRO:HB2	1:C:184:PHE:CG	2.55	0.41
1:D:131:TYR:CE2	2:D:500:FAD:N6A	2.89	0.41
1:D:176:TYR:HB3	1:D:267:LEU:CD2	2.51	0.41
1:D:353:LEU:O	1:D:354:ALA:C	2.58	0.41
1:D:401:VAL:O	1:D:401:VAL:HG12	2.19	0.41
1:A:254:ILE:HD11	1:A:279:ILE:CD1	2.50	0.41
1:A:347:ILE:HG22	1:A:347:ILE:O	2.19	0.41
1:B:219:MET:HG2	1:B:251:PHE:O	2.21	0.41
1:C:272:GLN:HB2	1:C:272:GLN:HE21	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:TYR:CD2	1:C:39:MET:HB2	2.55	0.41
1:C:20:GLY:HA3	1:C:42:ASP:HB2	2.01	0.41
1:D:188:TYR:C	1:D:188:TYR:CD1	2.93	0.41
1:D:221:ARG:O	1:D:250:GLN:HA	2.20	0.41
1:D:253:PRO:HA	1:D:271:ALA:HA	2.01	0.41
1:D:219:MET:HE2	1:D:253:PRO:HD3	2.02	0.41
1:D:356:ARG:HH11	1:D:364:LYS:HA	1.83	0.41
1:A:39:MET:HG3	1:A:126:VAL:HG12	2.01	0.41
1:A:404:SER:HA	1:A:492:ILE:HG21	2.02	0.41
1:C:16:ILE:HB	1:C:157:PHE:CD2	2.56	0.41
1:C:173:ASP:C	1:C:175:GLU:N	2.72	0.41
1:C:286:THR:HG22	1:C:287:VAL:N	2.35	0.41
1:C:70:MET:SD	1:C:101:MET:HE3	2.61	0.41
1:D:106:GLN:HA	1:D:106:GLN:OE1	2.20	0.41
1:D:47:THR:O	1:D:50:GLY:N	2.45	0.41
1:D:470:GLY:H	1:D:480:THR:HG21	1.83	0.41
1:A:22:SER:CB	1:A:343:THR:HG23	2.49	0.41
1:A:446:GLY:C	1:B:474:VAL:HG11	2.41	0.41
1:A:402:TYR:HE1	1:A:462:LYS:HG2	1.85	0.41
1:B:173:ASP:CG	1:B:174:LYS:H	2.22	0.41
1:B:293:ARG:HH11	1:B:293:ARG:HG2	1.86	0.41
1:B:207:GLY:HA3	1:B:377:PRO:HD3	2.02	0.41
1:C:196:VAL:HG23	1:C:288:MET:O	2.20	0.41
1:D:29:LYS:HB3	1:D:123:LYS:HE2	2.03	0.41
1:D:20:GLY:CA	1:D:42:ASP:HB2	2.50	0.41
1:A:395:GLY:O	1:A:397:GLU:N	2.54	0.41
1:B:166:ARG:HG2	1:B:291:ILE:HD11	2.02	0.41
1:B:472:HIS:HD2	1:B:473:PRO:HB3	1.84	0.41
1:C:156:ARG:HD3	1:C:330:TYR:HE1	1.85	0.41
1:C:353:LEU:HA	1:C:356:ARG:NH2	2.28	0.41
1:C:86:TYR:HE2	1:C:414:PRO:HG3	1.86	0.41
1:D:176:TYR:CZ	1:D:258:GLN:CB	3.03	0.41
1:D:307:VAL:CG2	1:D:326:VAL:HG21	2.50	0.41
1:A:353:LEU:O	1:A:354:ALA:C	2.58	0.41
1:B:229:ASP:CB	1:B:386:SER:OG	2.69	0.41
1:C:408:PRO:O	1:C:411:TRP:N	2.45	0.41
1:D:117:ARG:NH2	1:D:117:ARG:CB	2.82	0.41
1:D:176:TYR:CZ	1:D:258:GLN:HB2	2.56	0.41
1:D:330:TYR:N	1:D:330:TYR:CD1	2.89	0.41
1:D:405:TYR:O	1:D:406:PHE:HB3	2.21	0.41
1:A:323:GLN:NE2	1:A:330:TYR:CE2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LEU:HD22	1:B:125:VAL:HG11	2.03	0.41
1:B:243:HIS:CE1	1:D:493:LEU:HD21	2.56	0.41
1:B:162:GLY:CA	1:B:335:ILE:HG23	2.51	0.41
1:B:402:TYR:CE1	1:B:462:LYS:CE	3.04	0.41
1:C:302:LEU:HD13	1:C:307:VAL:CG1	2.51	0.41
1:D:328:TYR:CE2	1:D:329:ILE:HG13	2.54	0.41
1:A:13:TYR:O	1:A:154:ALA:HA	2.20	0.41
1:A:186:LEU:CD1	1:A:187:PRO:N	2.84	0.41
1:B:326:VAL:HA	1:B:327:PRO:HD3	1.86	0.41
1:C:17:ILE:HD12	1:C:40:VAL:HG22	2.02	0.41
1:C:376:THR:O	1:C:377:PRO:C	2.58	0.41
1:C:447:GLU:CD	1:D:474:VAL:HG12	2.42	0.41
1:D:447:GLU:HG2	1:D:447:GLU:H	1.68	0.41
1:A:431:ASP:O	1:A:431:ASP:OD1	2.39	0.40
1:B:46:PRO:HG3	1:B:52:ARG:CG	2.50	0.40
1:B:90:VAL:CG1	1:B:91:GLU:N	2.83	0.40
1:C:112:LEU:HA	1:C:112:LEU:HD23	1.75	0.40
1:C:15:LEU:HD13	1:C:358:TYR:OH	2.21	0.40
1:C:192:LYS:HE2	1:C:284:TYR:CE2	2.56	0.40
1:C:440:VAL:HG22	1:C:441:LEU:N	2.36	0.40
1:D:108:HIS:O	1:D:109:ILE:C	2.59	0.40
1:D:191:GLY:O	1:D:192:LYS:C	2.59	0.40
1:B:166:ARG:HG2	1:B:167:TYR:N	2.37	0.40
1:B:315:LYS:HB3	1:B:337:GLU:HA	2.02	0.40
1:C:67:LYS:NZ	1:C:204:GLU:OE1	2.50	0.40
1:C:323:GLN:HA	1:C:330:TYR:CD2	2.55	0.40
1:C:457:LYS:HE2	1:C:457:LYS:CA	2.46	0.40
1:D:324:THR:OG1	1:D:329:ILE:O	2.34	0.40
1:D:161:THR:HG22	2:D:500:FAD:C5A	2.52	0.40
1:A:47:THR:O	1:A:50:GLY:CA	2.68	0.40
1:C:302:LEU:HB3	1:C:307:VAL:CG1	2.32	0.40
1:C:321:GLU:O	1:C:322:GLU:HB2	2.20	0.40
1:D:68:LYS:HZ2	1:D:68:LYS:HG3	1.61	0.40
1:A:321:GLU:CG	1:A:321:GLU:O	2.69	0.40
1:A:356:ARG:HB2	1:A:356:ARG:HE	1.60	0.40
1:A:373:THR:HA	1:A:381:GLY:HA2	2.04	0.40
1:B:471:ILE:HG22	1:B:474:VAL:CG2	2.51	0.40
1:C:188:TYR:O	1:C:188:TYR:CD1	2.75	0.40
1:C:73:ALA:HB2	1:D:86:TYR:HD1	1.87	0.40
1:D:110:GLY:O	1:D:113:ASN:HB2	2.21	0.40
1:D:318:VAL:CG2	1:D:323:GLN:C	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:474:VAL:O	1:D:477:GLU:HG2	2.21	0.40
1:A:232:MET:O	1:A:236:ILE:HG13	2.22	0.40
1:A:413:ILE:N	1:A:414:PRO:CD	2.84	0.40
1:B:183:LEU:C	1:B:185:SER:H	2.24	0.40
1:B:25:LEU:HD23	1:B:25:LEU:HA	1.83	0.40
1:B:43:PHE:HB2	1:B:130:ALA:C	2.42	0.40
1:B:82:ASP:O	1:B:84:ARG:N	2.54	0.40
1:C:82:ASP:O	1:C:83:SER:C	2.60	0.40
1:D:203:LEU:HD12	1:D:225:LEU:CD2	2.48	0.40
1:D:20:GLY:N	1:D:42:ASP:HB2	2.37	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:CYS:O	1:C:497:CYS:O[3_554]	1.59	0.61
1:C:498:CYS:SG	1:C:498:CYS:SG[3_554]	1.70	0.50

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	488/513 (95%)	418 (86%)	57 (12%)	13 (3%)	5	30
1	B	483/513 (94%)	409 (85%)	64 (13%)	10 (2%)	7	37
1	C	491/513 (96%)	404 (82%)	67 (14%)	20 (4%)	3	21
1	D	482/513 (94%)	407 (84%)	63 (13%)	12 (2%)	5	32
All	All	1944/2052 (95%)	1638 (84%)	251 (13%)	55 (3%)	5	29

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	ASP
1	A	174	LYS
1	A	379	GLU
1	B	184	PHE
1	C	173	ASP
1	C	174	LYS
1	C	495	ALA
1	D	184	PHE
1	A	187	PRO
1	A	320	ASP
1	A	396	GLU
1	A	417	ASP
1	B	174	LYS
1	B	379	GLU
1	B	396	GLU
1	B	450	GLN
1	C	379	GLU
1	C	417	ASP
1	D	22	SER
1	D	162	GLY
1	D	173	ASP
1	D	174	LYS
1	D	489	GLY
1	A	83	SER
1	A	260	GLU
1	A	327	PRO
1	A	450	GLN
1	B	83	SER
1	B	173	ASP
1	C	22	SER
1	C	184	PHE
1	C	221	ARG
1	C	304	THR
1	D	202	ALA
1	A	324	THR
1	B	260	GLU
1	C	315	LYS
1	C	450	GLN
1	D	163	GLU
1	D	396	GLU
1	C	28	ALA
1	C	320	ASP
1	C	327	PRO

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Mol	Chain	Res	Type
1	D	187	PRO
1	A	496	GLY
1	C	187	PRO
1	C	324	THR
1	C	396	GLU
1	B	65	ILE
1	B	162	GLY
1	C	62	VAL
1	D	65	ILE
1	C	451	GLY
1	D	24	GLY
1	C	137	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	401/422 (95%)	341 (85%)	60 (15%)	3	14
1	B	399/422 (94%)	343 (86%)	56 (14%)	3	16
1	C	404/422 (96%)	343 (85%)	61 (15%)	3	14
1	D	398/422 (94%)	349 (88%)	49 (12%)	4	21
All	All	1602/1688 (95%)	1376 (86%)	226 (14%)	3	16

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	16	ILE
1	A	18	ILE
1	A	38	VAL
1	A	39	MET
1	A	41	LEU
1	A	45	THR
1	A	46	PRO
1	A	47	THR

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Mol	Chain	Res	Type
1	A	67	LYS
1	A	72	GLN
1	A	84	ARG
1	A	93	THR
1	A	94	VAL
1	A	122	GLU
1	A	129	ASN
1	A	137	PRO
1	A	143	THR
1	A	144	ASN
1	A	145	ASN
1	A	159	ILE
1	A	183	LEU
1	A	186	LEU
1	A	200	TYR
1	A	219	MET
1	A	254	ILE
1	A	257	GLU
1	A	264	PRO
1	A	272	GLN
1	A	273	SER
1	A	277	GLU
1	A	279	ILE
1	A	288	MET
1	A	293	ARG
1	A	303	GLU
1	A	304	THR
1	A	305	VAL
1	A	307	VAL
1	A	322	GLU
1	A	327	PRO
1	A	337	GLU
1	A	356	ARG
1	A	358	TYR
1	A	362	THR
1	A	370	VAL
1	A	376	THR
1	A	397	GLU
1	A	399	ILE
1	A	400	GLU
1	A	403	HIS
1	A	417	ASP

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Mol	Chain	Res	Type
1	A	429	THR
1	A	433	GLU
1	A	434	ARG
1	A	468	THR
1	A	473	PRO
1	A	474	VAL
1	A	487	ARG
1	A	493	LEU
1	A	494	GLN
1	B	14	ASP
1	B	18	ILE
1	B	33	GLN
1	B	45	THR
1	B	59	CYS
1	B	62	VAL
1	B	64	CYS
1	B	67	LYS
1	B	81	GLN
1	B	91	GLU
1	B	97	ASP
1	B	111	SER
1	B	127	TYR
1	B	131	TYR
1	B	137	PRO
1	B	140	ILE
1	B	146	LYS
1	B	150	LYS
1	B	151	ILE
1	B	156	ARG
1	B	158	LEU
1	B	159	ILE
1	B	164	ARG
1	B	175	GLU
1	B	180	SER
1	B	188	TYR
1	B	189	CYS
1	B	196	VAL
1	B	232	MET
1	B	242	GLU
1	B	250	GLN
1	B	273	SER
1	B	286	THR

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Mol	Chain	Res	Type
1	B	297	THR
1	B	304	THR
1	B	305	VAL
1	B	308	LYS
1	B	317	PRO
1	B	325	ASN
1	B	337	GLU
1	B	357	LEU
1	B	362	THR
1	B	365	CYS
1	B	380	TYR
1	B	396	GLU
1	B	398	ASN
1	B	399	ILE
1	B	400	GLU
1	B	406	PHE
1	B	428	ASN
1	B	430	LYS
1	B	434	ARG
1	B	435	VAL
1	B	467	SER
1	B	480	THR
1	B	483	SER
1	C	7	LEU
1	C	14	ASP
1	C	33	GLN
1	C	38	VAL
1	C	39	MET
1	C	49	LEU
1	C	52	ARG
1	C	58	THR
1	C	64	CYS
1	C	67	LYS
1	C	69	LEU
1	C	70	MET
1	C	83	SER
1	C	93	THR
1	C	95	LYS
1	C	118	VAL
1	C	129	ASN
1	C	133	GLN
1	C	135	ILE

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Mol	Chain	Res	Type
1	C	137	PRO
1	C	139	ARG
1	C	143	THR
1	C	149	GLU
1	C	156	ARG
1	C	175	GLU
1	C	183	LEU
1	C	187	PRO
1	C	188	TYR
1	C	196	VAL
1	C	199	SER
1	C	236	ILE
1	C	246	LYS
1	C	254	ILE
1	C	257	GLU
1	C	264	PRO
1	C	267	LEU
1	C	272	GLN
1	C	273	SER
1	C	283	GLU
1	C	289	LEU
1	C	294	ASP
1	C	303	GLU
1	C	307	VAL
1	C	310	ASN
1	C	329	ILE
1	C	338	ASP
1	C	339	LYS
1	C	358	TYR
1	C	363	VAL
1	C	372	THR
1	C	376	THR
1	C	377	PRO
1	C	389	LYS
1	C	398	ASN
1	C	404	SER
1	C	417	ASP
1	C	422	TYR
1	C	429	THR
1	C	438	PHE
1	C	449	THR
1	C	487	ARG

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Mol	Chain	Res	Type
1	D	39	MET
1	D	41	LEU
1	D	49	LEU
1	D	52	ARG
1	D	59	CYS
1	D	64	CYS
1	D	68	LYS
1	D	91	GLU
1	D	93	THR
1	D	94	VAL
1	D	111	SER
1	D	112	LEU
1	D	117	ARG
1	D	121	ARG
1	D	137	PRO
1	D	140	ILE
1	D	148	LYS
1	D	163	GLU
1	D	175	GLU
1	D	186	LEU
1	D	187	PRO
1	D	216	VAL
1	D	267	LEU
1	D	274	THR
1	D	277	GLU
1	D	280	ILE
1	D	286	THR
1	D	297	THR
1	D	298	ARG
1	D	303	GLU
1	D	309	ILE
1	D	310	ASN
1	D	319	THR
1	D	340	VAL
1	D	348	GLN
1	D	364	LYS
1	D	365	CYS
1	D	367	TYR
1	D	377	PRO
1	D	417	ASP
1	D	420	LYS
1	D	428	ASN

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Mol	Chain	Res	Type
1	D	429	THR
1	D	430	LYS
1	D	441	LEU
1	D	460	LEU
1	D	483	SER
1	D	487	ARG
1	D	492	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	129	ASN
1	A	145	ASN
1	A	243	HIS
1	A	272	GLN
1	A	285	ASN
1	A	323	GLN
1	A	355	GLN
1	A	398	ASN
1	A	418	ASN
1	A	432	ASN
1	A	444	ASN
1	A	472	HIS
1	A	494	GLN
1	B	71	HIS
1	B	107	ASN
1	B	113	ASN
1	B	129	ASN
1	B	133	GLN
1	B	250	GLN
1	B	323	GLN
1	B	398	ASN
1	B	428	ASN
1	B	432	ASN
1	B	444	ASN
1	B	464	GLN
1	B	472	HIS
1	C	33	GLN
1	C	129	ASN
1	C	138	HIS
1	C	234	ASN

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Mol	Chain	Res	Type
1	C	243	HIS
1	C	250	GLN
1	C	272	GLN
1	C	310	ASN
1	C	355	GLN
1	C	369	ASN
1	C	398	ASN
1	C	418	ASN
1	C	419	ASN
1	C	472	HIS
1	C	494	GLN
1	D	106	GLN
1	D	107	ASN
1	D	113	ASN
1	D	129	ASN
1	D	133	GLN
1	D	258	GLN
1	D	323	GLN
1	D	419	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

10 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	$\# Z > 2$
4	TPT	D	501	-	16,23,24	4.73	12 (75%)	13,35,38	3.58	11 (84%)
3	SO4	C	502	-	4,4,4	0.31	0	6,6,6	0.19	0
3	SO4	A	502	-	4,4,4	0.35	0	6,6,6	0.35	0
3	SO4	D	502	-	4,4,4	0.26	0	6,6,6	0.37	0
2	FAD	A	500	-	51,58,58	1.98	9 (17%)	60,89,89	2.10	14 (23%)
2	FAD	C	500	-	51,58,58	2.29	6 (11%)	60,89,89	2.25	13 (21%)
3	SO4	B	502	-	4,4,4	0.30	0	6,6,6	0.23	0
4	TPT	B	501	-	16,23,24	4.73	12 (75%)	13,35,38	3.60	11 (84%)
2	FAD	D	500	-	51,58,58	2.11	6 (11%)	60,89,89	2.15	12 (20%)
2	FAD	B	500	-	51,58,58	1.93	8 (15%)	60,89,89	2.16	13 (21%)

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	TPT	D	501	-	-	-	0/5/5/5
2	FAD	B	500	-	-	3/30/50/50	0/6/6/6
2	FAD	A	500	-	-	3/30/50/50	0/6/6/6
2	FAD	C	500	-	-	4/30/50/50	0/6/6/6
4	TPT	B	501	-	-	-	0/5/5/5
2	FAD	D	500	-	-	4/30/50/50	0/6/6/6

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	FAD	C4X-C10	12.21	1.51	1.38
2	A	500	FAD	C4X-C10	10.84	1.49	1.38
2	D	500	FAD	C4X-C10	10.78	1.49	1.38
2	B	500	FAD	C4X-C10	8.54	1.47	1.38
4	D	501	TPT	C7-C6	-6.90	1.38	1.53
4	B	501	TPT	C7-C6	-6.86	1.38	1.53
4	B	501	TPT	C3-C4	-6.66	1.35	1.53
4	D	501	TPT	C3-C4	-6.63	1.35	1.53
4	D	501	TPT	C9-C10	-6.56	1.39	1.53
4	B	501	TPT	C9-C10	-6.50	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	501	TPT	C12-C11	-6.35	1.39	1.53
4	B	501	TPT	C12-C11	-6.31	1.39	1.53
4	B	501	TPT	C8-C9	-6.00	1.37	1.53
4	D	501	TPT	C8-C9	-5.98	1.37	1.53
4	B	501	TPT	C8-C7	-5.86	1.37	1.53
4	D	501	TPT	C8-C7	-5.84	1.37	1.53
4	D	501	TPT	C4-C5	-5.79	1.40	1.53
4	B	501	TPT	C4-C5	-5.78	1.40	1.53
4	B	501	TPT	C13-C12	-5.61	1.38	1.53
4	D	501	TPT	C13-C12	-5.56	1.38	1.53
2	D	500	FAD	C9A-N10	5.39	1.45	1.38
2	B	500	FAD	C4-C4X	5.17	1.50	1.41
2	C	500	FAD	O4B-C1B	5.06	1.48	1.41
2	D	500	FAD	O4B-C1B	4.31	1.47	1.41
2	C	500	FAD	C4-C4X	4.19	1.48	1.41
2	C	500	FAD	C9A-N10	3.83	1.43	1.38
2	C	500	FAD	C8A-N7A	-3.74	1.28	1.34
4	D	501	TPT	C1-C2	-3.72	1.38	1.51
4	B	501	TPT	C1-C2	-3.71	1.38	1.51
2	D	500	FAD	C8A-N7A	-3.54	1.28	1.34
2	B	500	FAD	C9A-N10	3.49	1.43	1.38
4	D	501	TPT	C15-C14	-3.29	1.39	1.51
2	A	500	FAD	C9A-N10	3.28	1.42	1.38
4	B	501	TPT	C15-C14	-3.25	1.39	1.51
2	A	500	FAD	C8A-N7A	-2.92	1.29	1.34
2	A	500	FAD	O4B-C1B	2.88	1.45	1.41
4	B	501	TPT	C3-C2	-2.80	1.40	1.51
4	D	501	TPT	C3-C2	-2.78	1.40	1.51
2	B	500	FAD	P-O2P	2.63	1.67	1.55
2	B	500	FAD	C8A-N7A	-2.52	1.30	1.34
2	A	500	FAD	O4-C4	-2.52	1.18	1.24
2	A	500	FAD	C4-C4X	2.49	1.45	1.41
2	B	500	FAD	O4B-C1B	2.39	1.44	1.41
2	B	500	FAD	C10-N1	2.37	1.36	1.33
2	D	500	FAD	O4-C4	-2.37	1.18	1.24
2	D	500	FAD	C8-C7	2.35	1.46	1.40
2	C	500	FAD	C2-N1	-2.25	1.33	1.38
2	A	500	FAD	C10-N1	2.21	1.36	1.33
4	B	501	TPT	C14-C13	-2.19	1.42	1.51
4	D	501	TPT	C14-C13	-2.18	1.42	1.51
2	A	500	FAD	C4-N3	2.02	1.36	1.33
2	B	500	FAD	C4-N3	2.02	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	FAD	C5'-C4'	2.00	1.54	1.51

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	FAD	C4-N3-C2	8.58	122.39	115.14
2	D	500	FAD	C4-N3-C2	8.43	122.26	115.14
2	A	500	FAD	C4-N3-C2	7.84	121.76	115.14
2	B	500	FAD	C4-N3-C2	7.50	121.47	115.14
2	B	500	FAD	C4X-N5-C5X	6.72	123.49	116.77
2	D	500	FAD	C4X-N5-C5X	6.05	122.81	116.77
2	C	500	FAD	C4X-N5-C5X	5.80	122.56	116.77
2	A	500	FAD	P-O3P-PA	-5.59	113.64	132.83
2	D	500	FAD	C1'-N10-C9A	5.52	122.64	118.29
2	A	500	FAD	C4X-N5-C5X	5.42	122.18	116.77
2	C	500	FAD	P-O3P-PA	-5.39	114.33	132.83
4	B	501	TPT	C3-C4-C5	5.38	120.91	111.22
4	D	501	TPT	C3-C4-C5	5.36	120.88	111.22
2	C	500	FAD	N3A-C2A-N1A	-5.21	120.54	128.68
2	A	500	FAD	N3A-C2A-N1A	-5.13	120.67	128.68
2	B	500	FAD	P-O3P-PA	-5.08	115.38	132.83
2	B	500	FAD	N3A-C2A-N1A	-4.91	121.00	128.68
2	C	500	FAD	C1'-N10-C9A	4.88	122.13	118.29
4	B	501	TPT	C13-C12-C11	4.76	119.79	111.22
4	D	501	TPT	C13-C12-C11	4.75	119.78	111.22
2	D	500	FAD	N3A-C2A-N1A	-4.73	121.29	128.68
4	B	501	TPT	C14-C13-C12	4.69	120.98	111.42
2	C	500	FAD	C4X-C4-N3	-4.69	117.02	123.43
2	D	500	FAD	P-O3P-PA	-4.68	116.75	132.83
4	D	501	TPT	C14-C13-C12	4.65	120.90	111.42
2	A	500	FAD	C1'-N10-C9A	4.46	121.80	118.29
2	B	500	FAD	C1'-N10-C9A	4.38	121.74	118.29
4	B	501	TPT	C8-C9-C10	4.31	118.99	111.22
4	D	501	TPT	C8-C9-C10	4.22	118.82	111.22
4	B	501	TPT	C1-C2-C3	4.22	118.58	111.44
2	C	500	FAD	C4-C4X-C10	-4.14	117.21	119.95
4	D	501	TPT	C1-C2-C3	4.12	118.41	111.44
2	B	500	FAD	C4X-C4-N3	-4.03	117.92	123.43
4	D	501	TPT	C2-C3-C4	3.97	119.51	111.42
4	B	501	TPT	C2-C3-C4	3.92	119.41	111.42
2	A	500	FAD	C4-C4X-C10	-3.90	117.37	119.95
2	B	500	FAD	C4-C4X-C10	-3.80	117.44	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	TPT	C8-C7-C6	3.62	117.74	111.22
2	D	500	FAD	C4X-C4-N3	-3.60	118.50	123.43
2	A	500	FAD	C4X-C4-N3	-3.59	118.52	123.43
4	B	501	TPT	C8-C7-C6	3.56	117.65	111.22
2	B	500	FAD	C4-C4X-N5	3.38	122.46	118.60
2	D	500	FAD	C4-C4X-C10	-3.28	117.78	119.95
2	C	500	FAD	C9A-N10-C10	-2.99	117.99	121.91
2	C	500	FAD	C4-C4X-N5	2.98	122.01	118.60
4	B	501	TPT	C6-C5-N1	2.91	115.33	109.19
4	D	501	TPT	C6-C5-N1	2.88	115.27	109.19
2	A	500	FAD	C9A-N10-C10	-2.85	118.18	121.91
4	B	501	TPT	C10-C11-N3	2.78	115.08	109.19
4	D	501	TPT	C10-C11-N3	2.73	114.96	109.19
2	C	500	FAD	C5X-C9A-N10	2.68	119.66	117.72
4	B	501	TPT	C9-C8-C7	2.59	120.43	112.87
4	D	501	TPT	C9-C8-C7	2.55	120.31	112.87
2	A	500	FAD	C4-C4X-N5	2.54	121.50	118.60
2	D	500	FAD	C9A-N10-C10	-2.53	118.60	121.91
2	B	500	FAD	C4X-C10-N10	-2.46	117.77	120.30
2	D	500	FAD	P-O5'-C5'	-2.45	107.32	121.68
2	B	500	FAD	P-O5'-C5'	-2.40	107.60	121.68
2	C	500	FAD	C4X-C10-N10	-2.38	117.85	120.30
2	A	500	FAD	C2A-N1A-C6A	2.36	122.80	118.75
2	B	500	FAD	C9A-N10-C10	-2.36	118.82	121.91
2	D	500	FAD	C4X-C10-N10	-2.35	117.88	120.30
4	D	501	TPT	C15-C14-C13	2.32	115.37	111.44
4	B	501	TPT	C15-C14-C13	2.31	115.35	111.44
2	C	500	FAD	P-O5'-C5'	-2.26	108.42	121.68
2	A	500	FAD	P-O5'-C5'	-2.25	108.50	121.68
2	D	500	FAD	PA-O5B-C5B	-2.19	108.82	121.68
2	A	500	FAD	C5X-C9A-N10	2.13	119.26	117.72
2	A	500	FAD	PA-O5B-C5B	-2.10	109.37	121.68
2	D	500	FAD	C2A-N1A-C6A	2.09	122.33	118.75
2	B	500	FAD	C3B-C2B-C1B	2.06	104.07	100.98
2	B	500	FAD	C2A-N1A-C6A	2.05	122.27	118.75
2	C	500	FAD	PA-O5B-C5B	-2.05	109.68	121.68
2	A	500	FAD	C4X-C10-N10	-2.02	118.22	120.30

There are no chirality outliers.

All (14) torsion outliers are listed below:

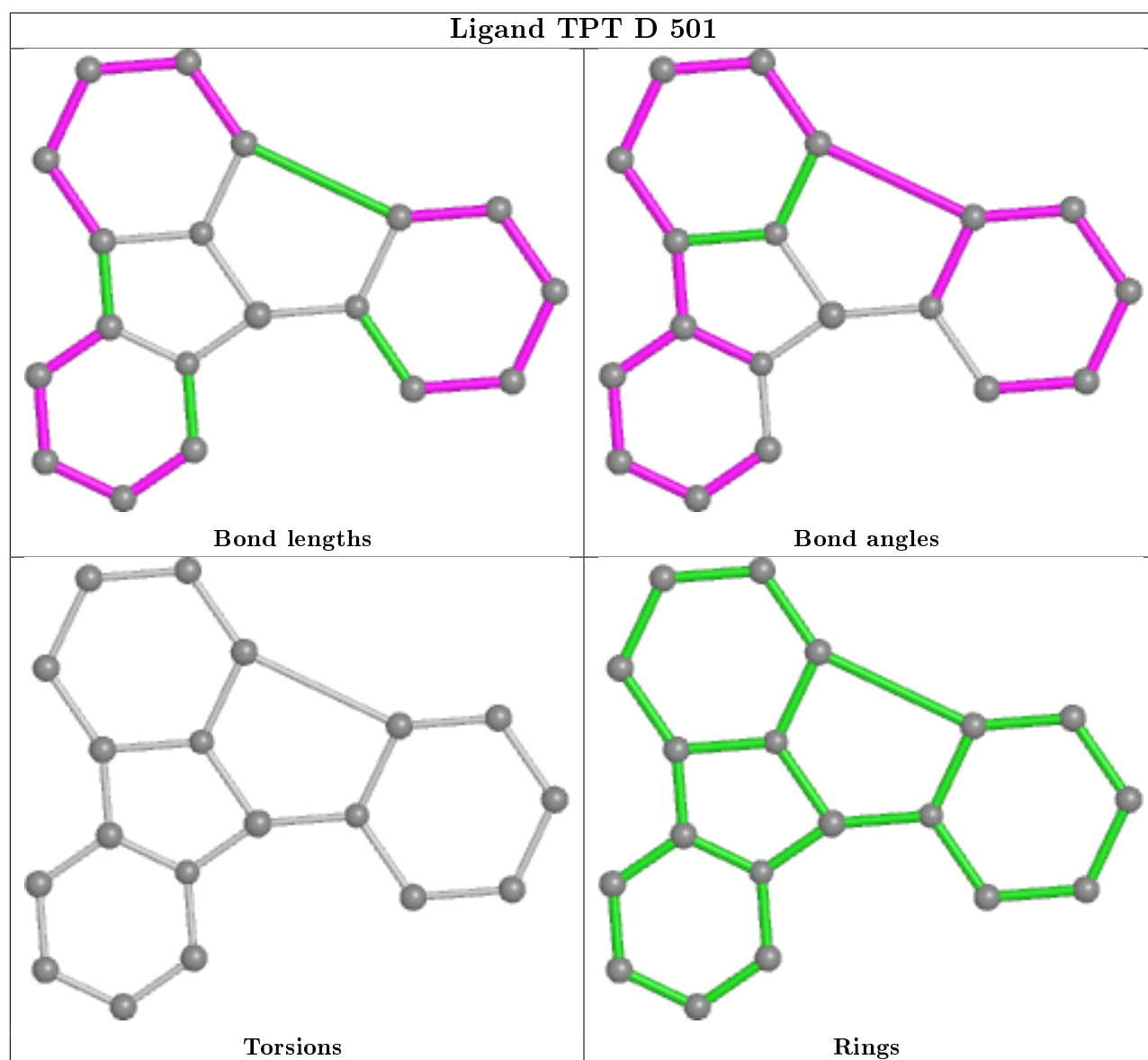
Mol	Chain	Res	Type	Atoms
2	A	500	FAD	C3B-C4B-C5B-O5B
2	C	500	FAD	C3B-C4B-C5B-O5B
2	D	500	FAD	C3B-C4B-C5B-O5B
2	B	500	FAD	C3B-C4B-C5B-O5B
2	A	500	FAD	O4B-C4B-C5B-O5B
2	C	500	FAD	O4B-C4B-C5B-O5B
2	D	500	FAD	O4B-C4B-C5B-O5B
2	B	500	FAD	O4B-C4B-C5B-O5B
2	C	500	FAD	C5'-O5'-P-O3P
2	D	500	FAD	C5'-O5'-P-O3P
2	D	500	FAD	C5B-O5B-PA-O1A
2	A	500	FAD	C5B-O5B-PA-O1A
2	C	500	FAD	C5B-O5B-PA-O1A
2	B	500	FAD	C5B-O5B-PA-O1A

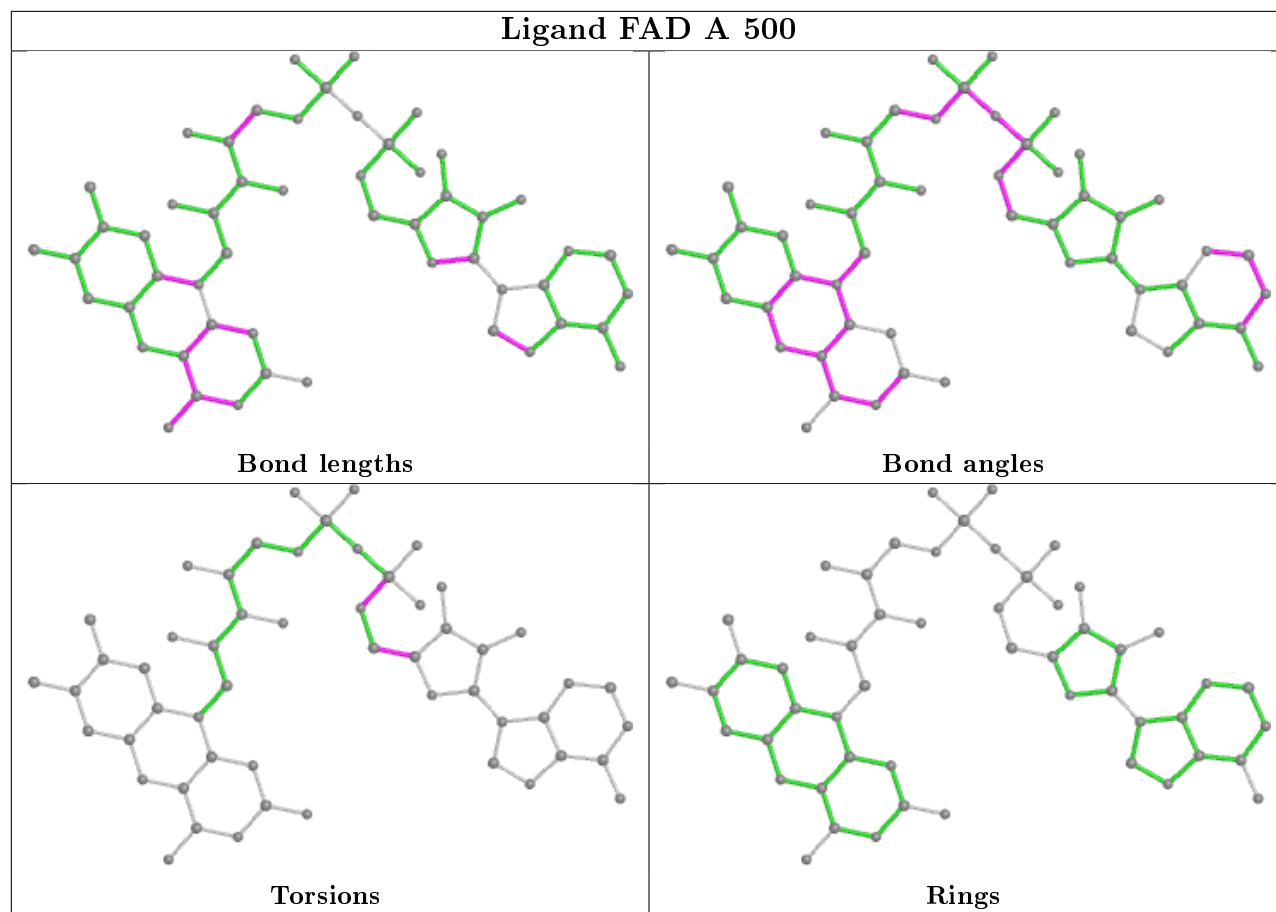
There are no ring outliers.

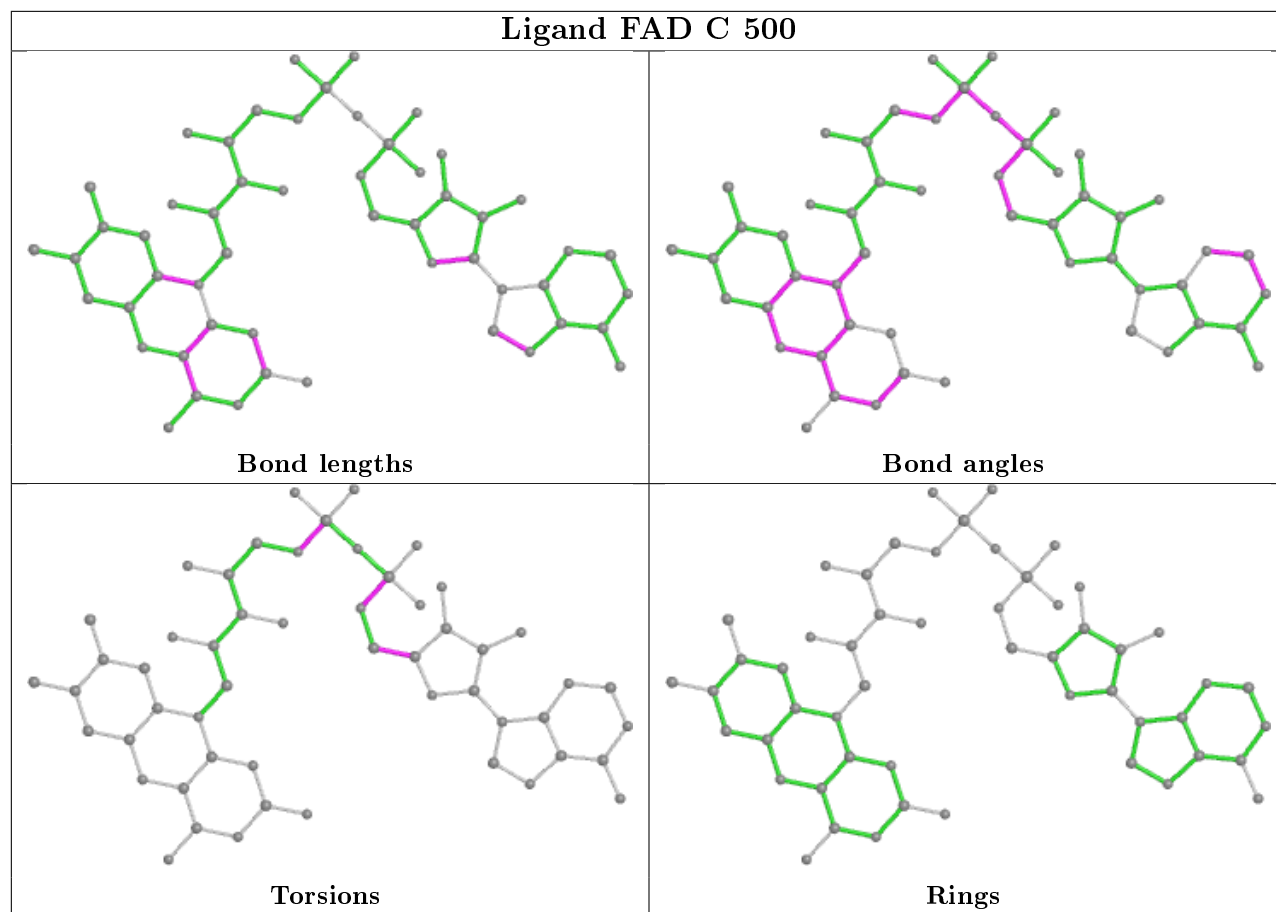
6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	501	TPT	3	0
3	A	502	SO4	1	0
2	A	500	FAD	1	0
2	C	500	FAD	4	0
2	D	500	FAD	4	0
2	B	500	FAD	2	0

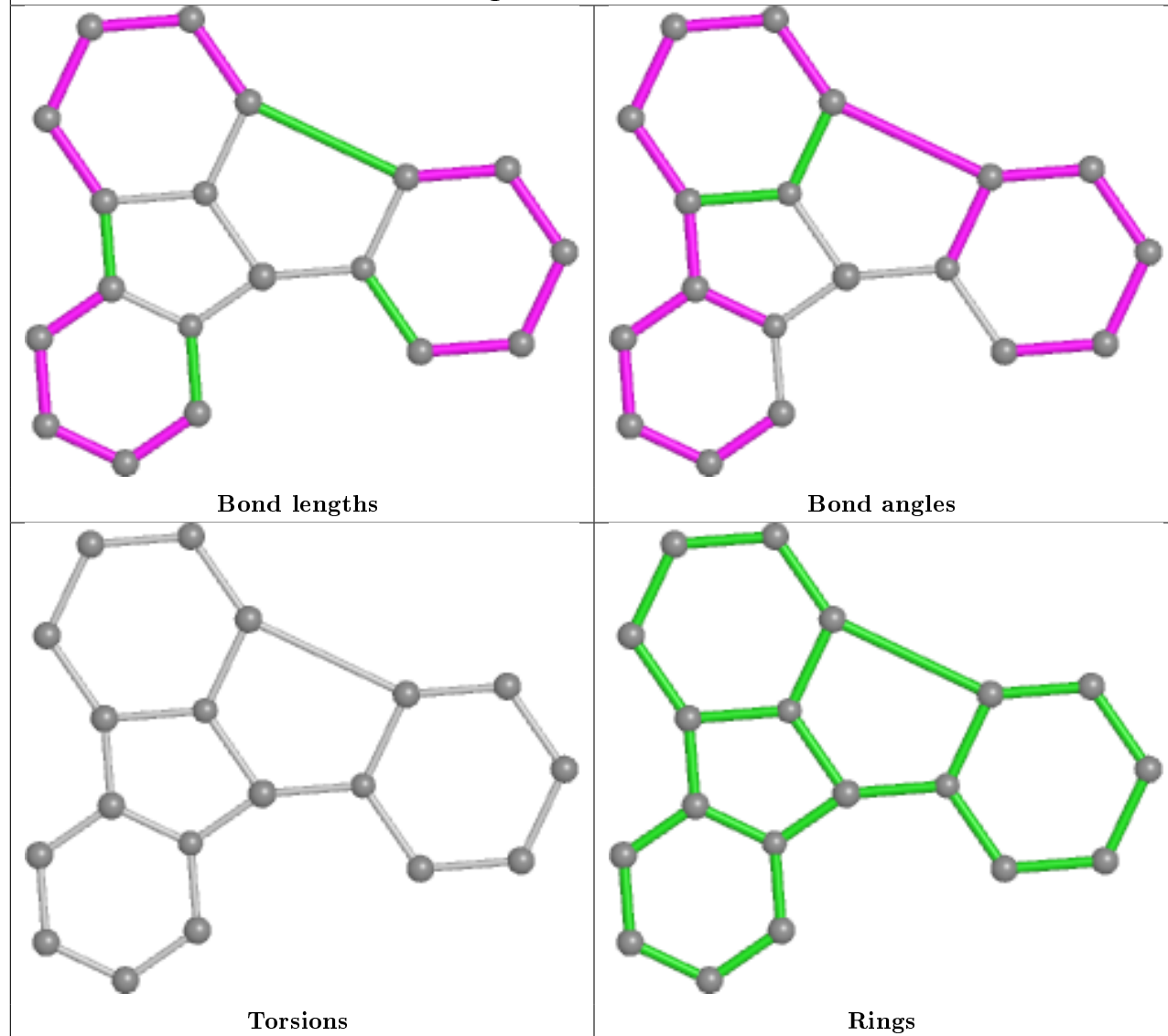
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

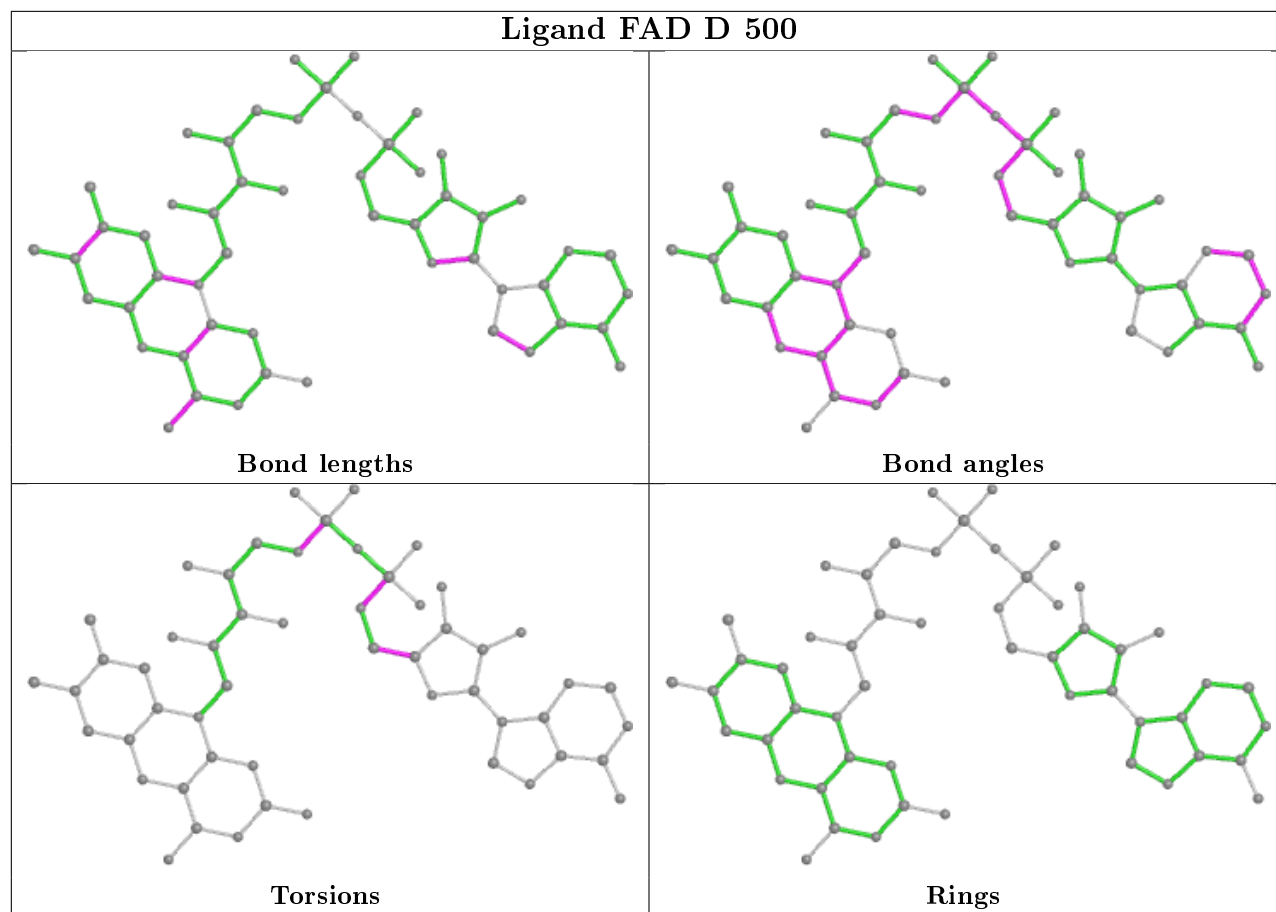


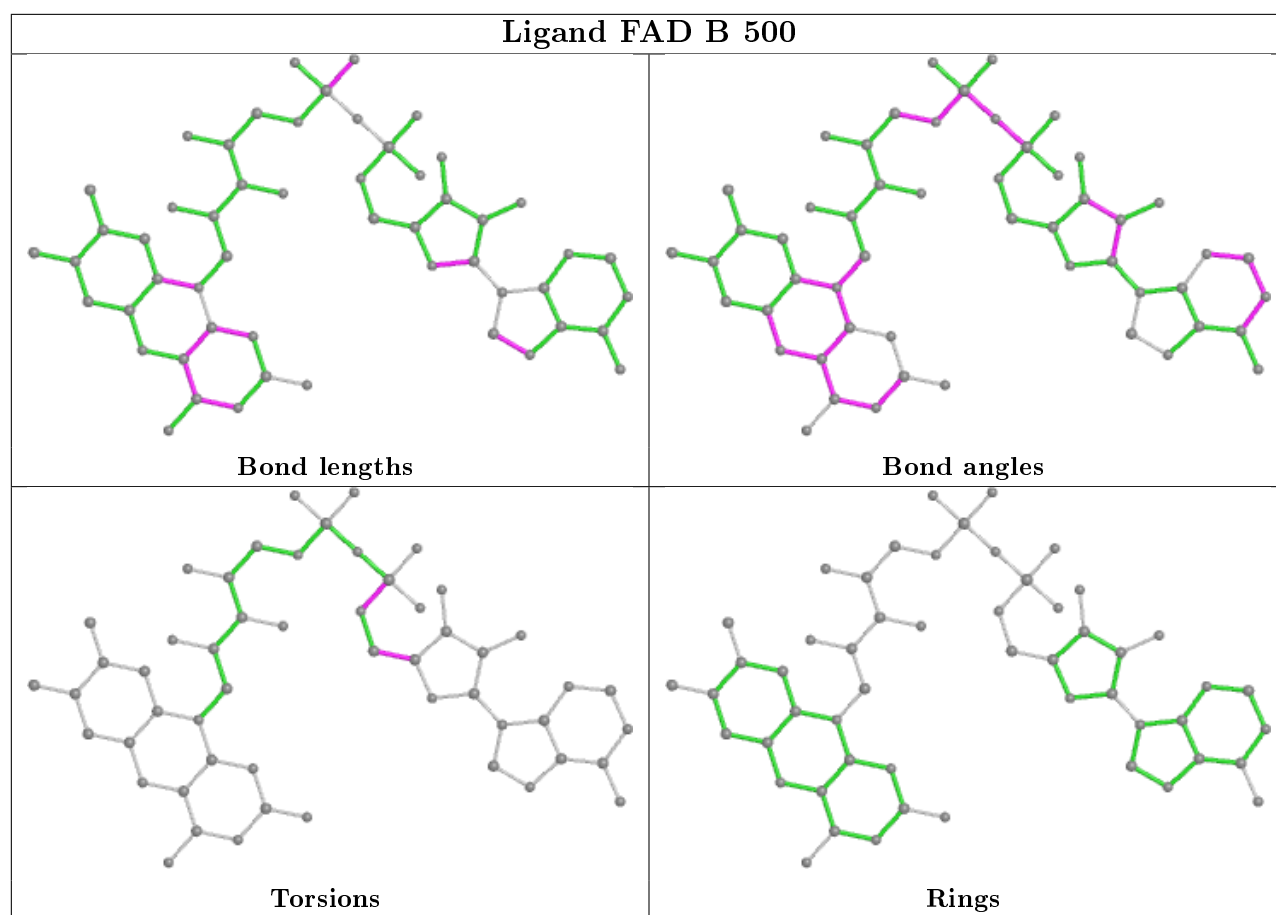




Ligand TPT B 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	490/513 (95%)	-0.41	5 (1%) 82 72	15, 50, 81, 128	0
1	B	485/513 (94%)	-0.47	2 (0%) 92 89	18, 45, 76, 107	0
1	C	493/513 (96%)	-0.36	6 (1%) 79 67	21, 58, 85, 137	0
1	D	484/513 (94%)	-0.39	1 (0%) 95 94	23, 53, 83, 104	0
All	All	1952/2052 (95%)	-0.41	14 (0%) 87 81	15, 51, 83, 137	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	497	CYS	5.9
1	C	499	GLY	5.1
1	A	496	GLY	4.8
1	C	8	PRO	4.5
1	A	498	CYS	3.8
1	A	495	ALA	3.5
1	C	9	LYS	2.5
1	B	491	SER	2.4
1	A	494	GLN	2.3
1	C	497	CYS	2.3
1	C	494	GLN	2.3
1	B	490	ALA	2.2
1	D	490	ALA	2.2
1	C	7	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

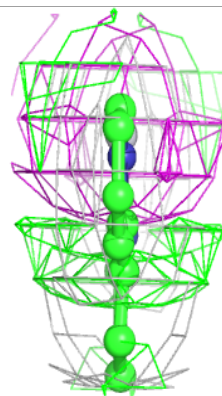
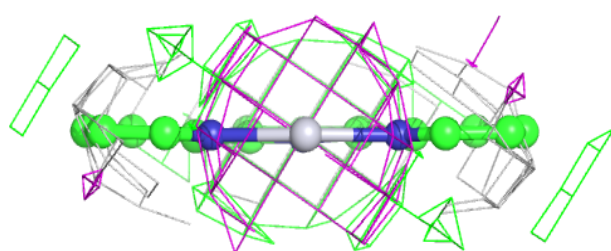
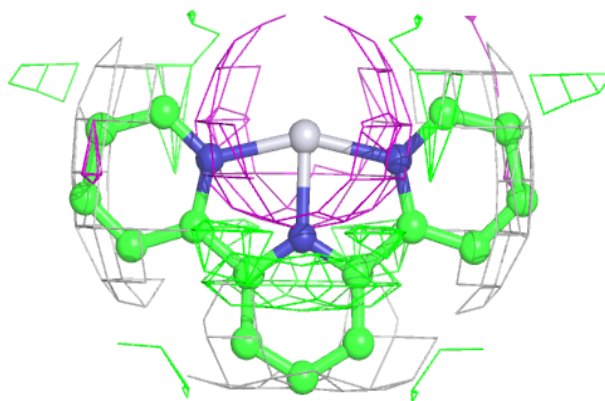
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	TPT	D	501	19/20	0.91	0.23	42,46,48,48	19
3	SO4	A	502	5/5	0.92	0.15	72,73,75,75	0
4	TPT	B	501	19/20	0.92	0.25	29,36,38,39	19
3	SO4	C	502	5/5	0.93	0.10	83,83,83,83	0
2	FAD	C	500	53/53	0.94	0.20	43,58,61,62	0
3	SO4	D	502	5/5	0.94	0.14	71,73,74,75	0
3	SO4	B	502	5/5	0.95	0.10	81,81,82,82	0
2	FAD	A	500	53/53	0.95	0.22	42,56,69,70	0
2	FAD	D	500	53/53	0.95	0.17	33,41,57,58	0
2	FAD	B	500	53/53	0.96	0.17	24,32,44,45	0

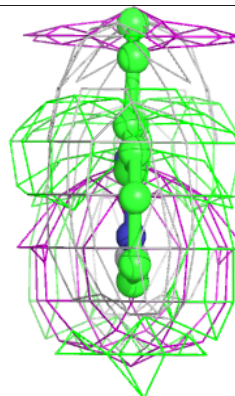
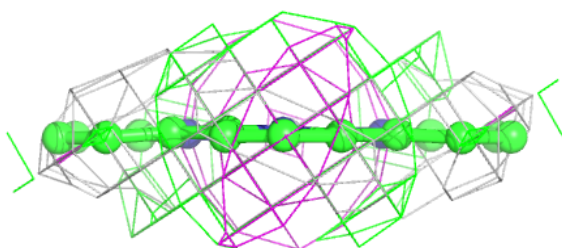
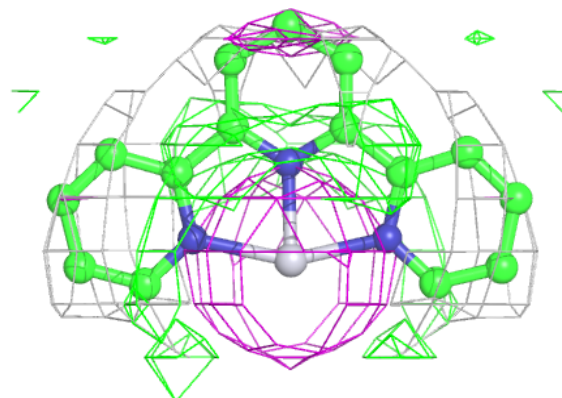
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPT D 501:

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

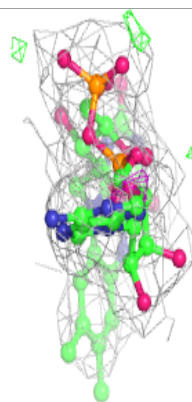
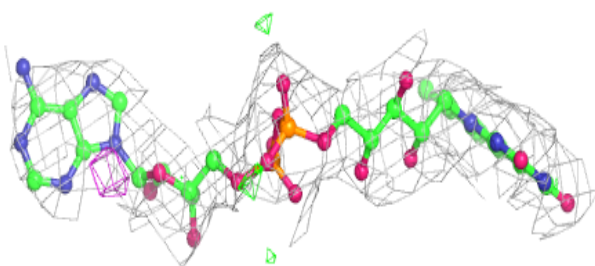
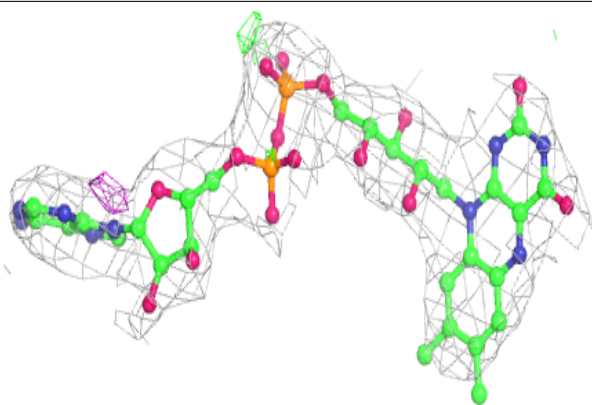
**Electron density around TPT B 501:**

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

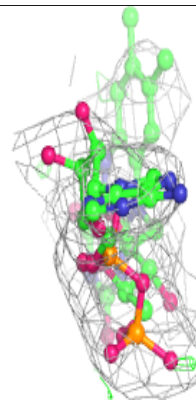
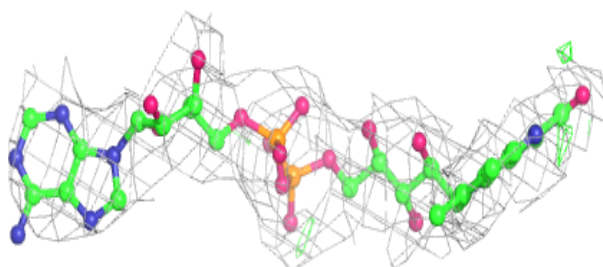
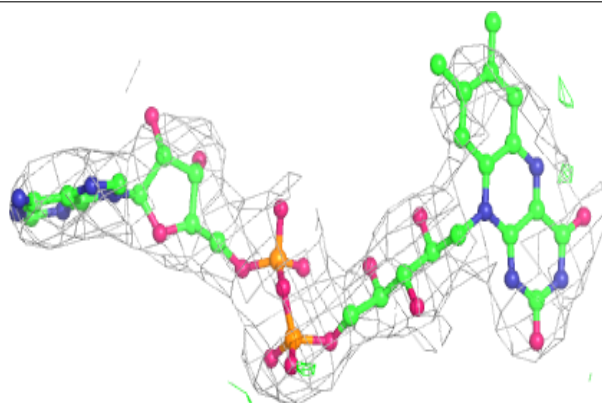


Electron density around FAD C 500:

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

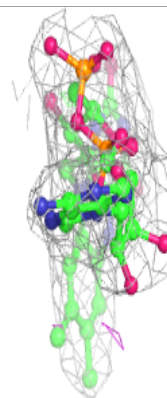
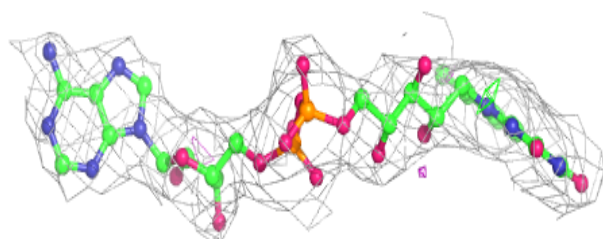
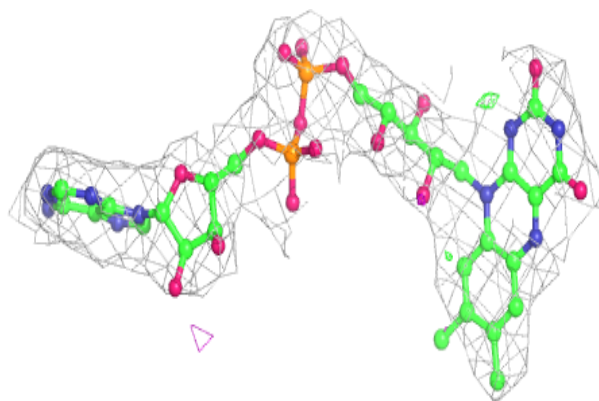
**Electron density around FAD A 500:**

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

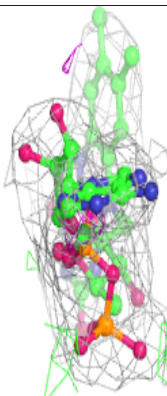
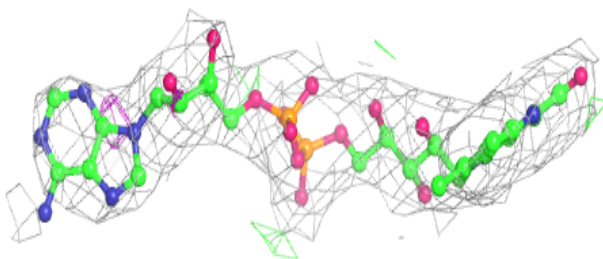
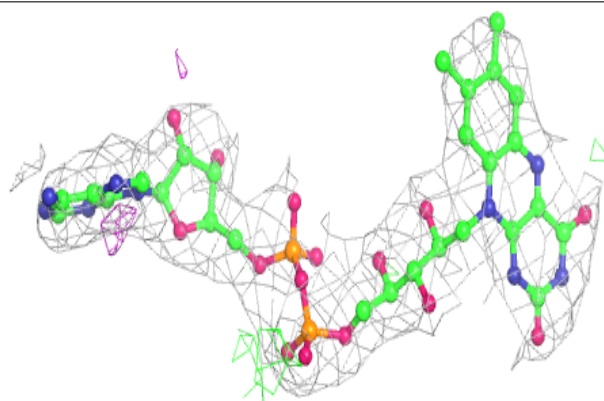


Electron density around FAD D 500:

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

**Electron density around FAD B 500:**

$2mF_o-DF_c$ (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.