



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:10 AM UTC

PDB ID : 2ZZ0 / pdb_00002zz0
Title : Crystal structure of human thioredoxin reductase I (SeCys 498 Cys)
Authors : Lo, Y.C.; Ko, T.P.; Wang, A.H.J.
Deposited on : 2009-02-02
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

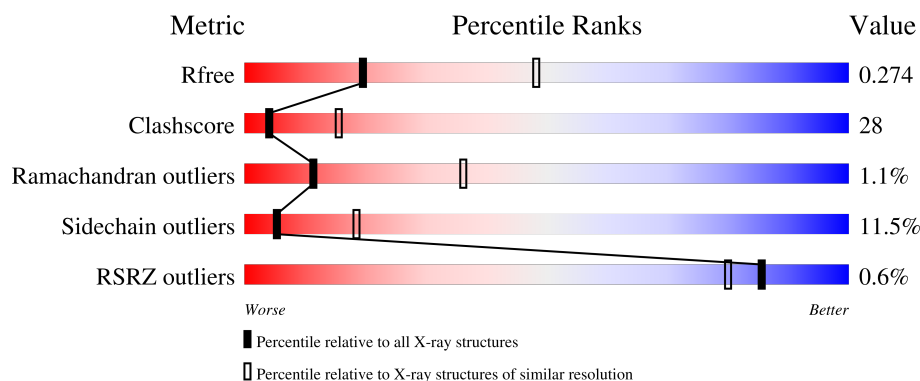
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	513	% 47% 39% 8% • •
1	B	513	% 50% 37% 8% 5%
1	C	513	% 47% 38% 8% • 5%
1	D	513	48% 39% 7% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15818 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	491	Total	C	N	O	S	0	0	0
			3785	2403	647	714	21			
1	B	487	Total	C	N	O	S	0	0	0
			3765	2396	642	708	19			
1	C	487	Total	C	N	O	S	0	0	0
			3765	2396	642	708	19			
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:

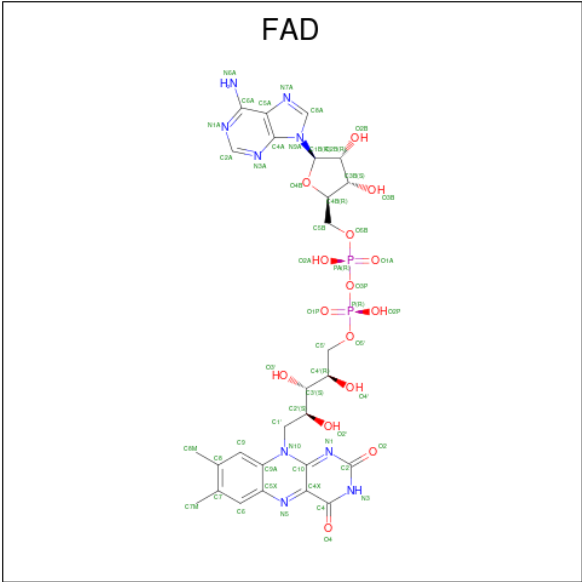
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q16881
A	-12	ALA	-	expression tag	UNP Q16881
A	-11	HIS	-	expression tag	UNP Q16881
A	-10	HIS	-	expression tag	UNP Q16881
A	-9	HIS	-	expression tag	UNP Q16881
A	-8	HIS	-	expression tag	UNP Q16881
A	-7	HIS	-	expression tag	UNP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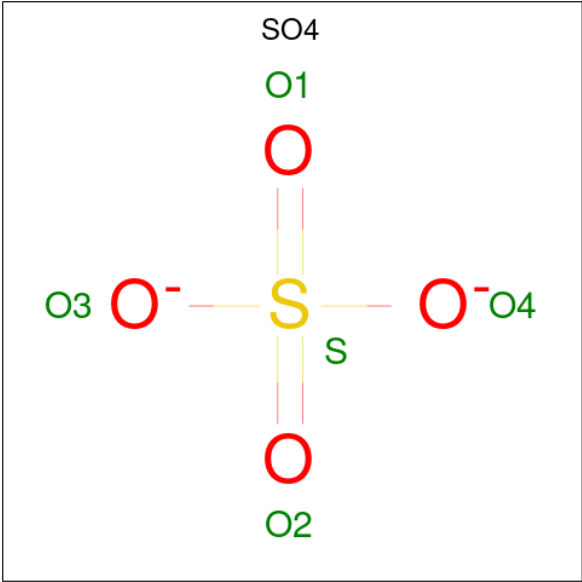
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP Q16881
B	-5	VAL	-	expression tag	UNP Q16881
B	-4	ASP	-	expression tag	UNP Q16881
B	-3	ASP	-	expression tag	UNP Q16881
B	-2	ASP	-	expression tag	UNP Q16881
B	-1	ASP	-	expression tag	UNP Q16881
B	498	CYS	SEC	SEE REMARK 999	UNP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

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: 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 (CCD ID: SO4) (formula: O₄S).



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

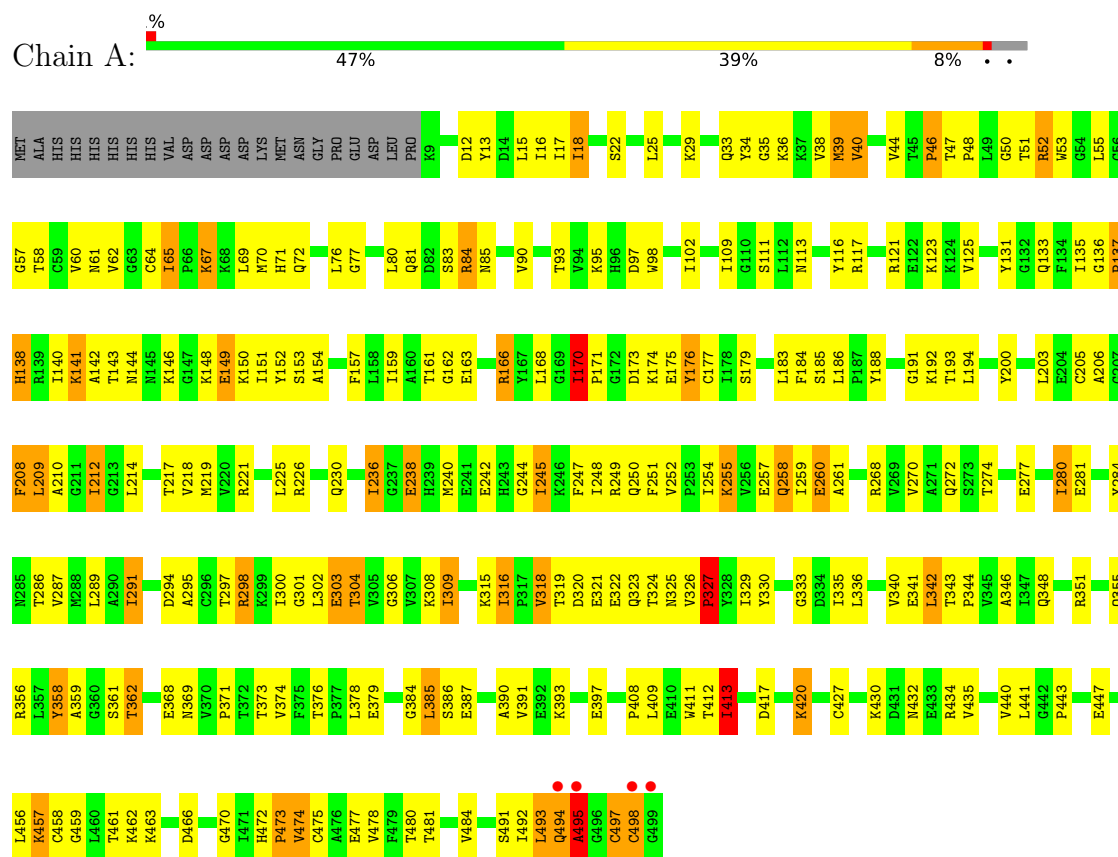
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	162	Total	O	0	0
			162	162		
4	B	137	Total	O	0	0
			137	137		
4	C	123	Total	O	0	0
			123	123		
4	D	108	Total	O	0	0
			108	108		

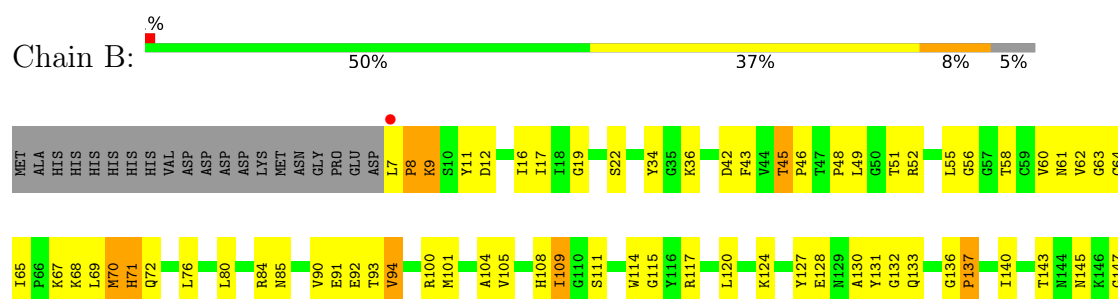
3 Residue-property plots

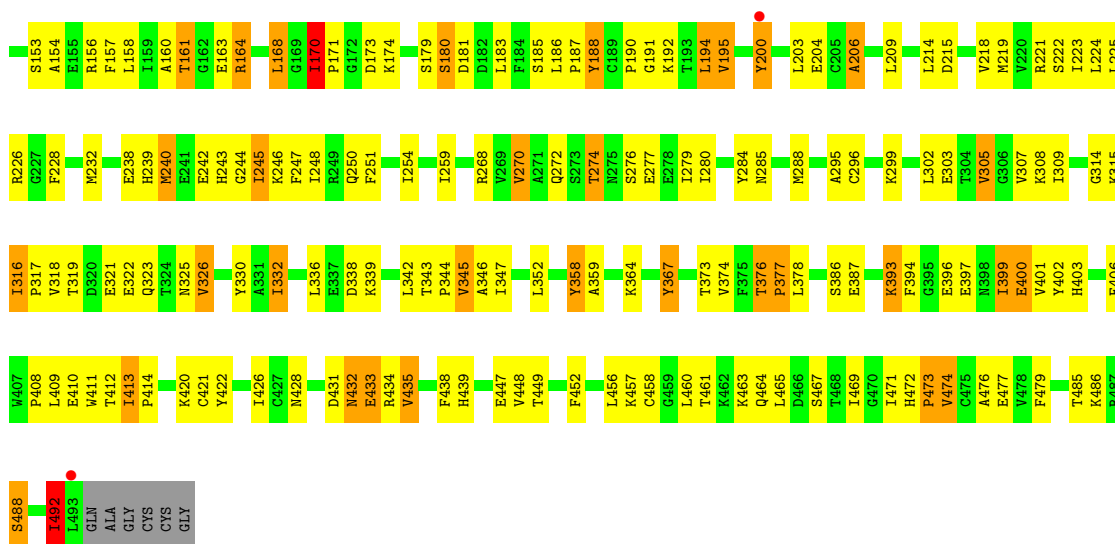
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Thioredoxin reductase 1, cytoplasmic

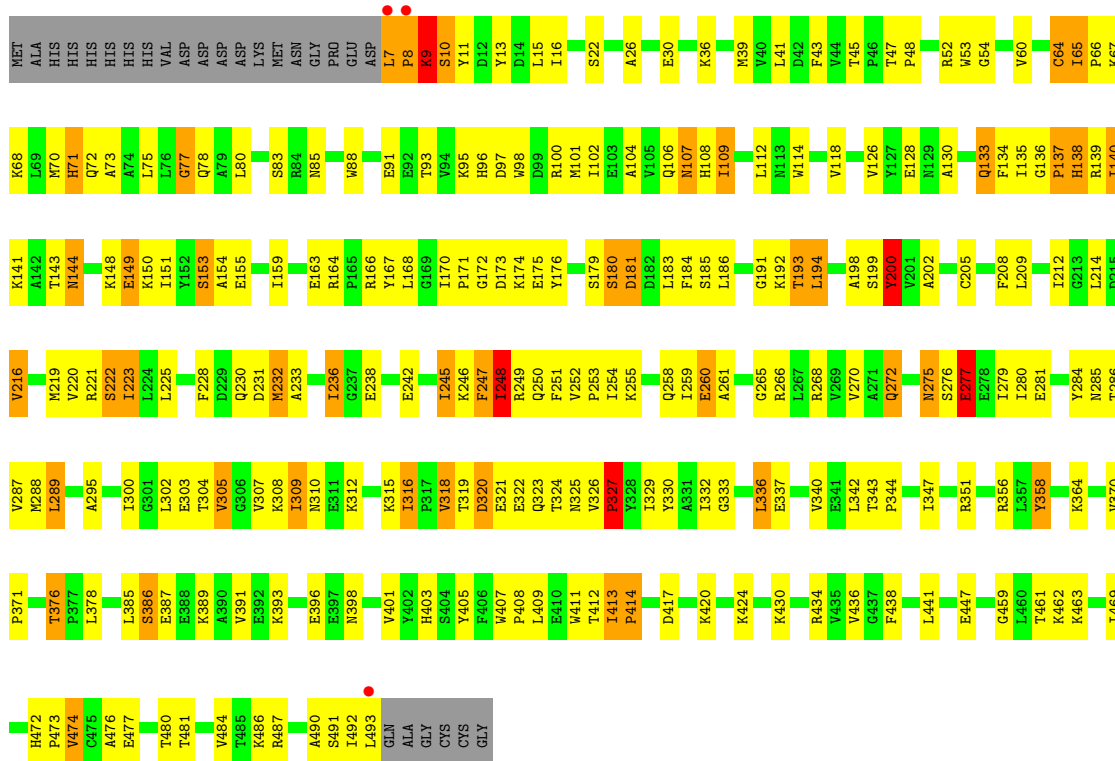


- Molecule 1: Thioredoxin reductase 1, cytoplasmic

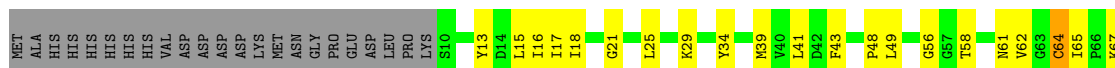




- Molecule 1: Thioredoxin reductase 1, cytoplasmic



- 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	121.09Å 135.41Å 345.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.0 (30.00-2.80) 90.9 (30.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.277 0.217 , 0.274	Depositor DCC
R_{free} test set	3233 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.8	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	0.93	EDS
Total number of atoms	15818	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: FAD, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.13	3/3859 (0.1%)	1.32	35/5222 (0.7%)
1	B	1.15	7/3840 (0.2%)	1.34	29/5200 (0.6%)
1	C	1.10	3/3840 (0.1%)	1.34	35/5200 (0.7%)
1	D	1.09	3/3815 (0.1%)	1.29	27/5166 (0.5%)
All	All	1.12	16/15354 (0.1%)	1.32	126/20788 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	1
All	All	0	5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	413	ILE	CA-CB	-10.93	1.48	1.54
1	B	65	ILE	CA-C	-6.54	1.46	1.52
1	D	65	ILE	CA-CB	-6.43	1.45	1.54
1	B	164	ARG	CA-CB	-6.12	1.45	1.53
1	C	232	MET	SD-CE	6.02	1.94	1.79
1	B	219	MET	SD-CE	5.94	1.94	1.79
1	B	51	THR	CA-CB	5.87	1.62	1.53
1	D	413	ILE	CA-CB	-5.70	1.51	1.54
1	D	135	ILE	CA-CB	-5.62	1.47	1.55
1	B	8	PRO	CA-C	5.53	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	231	ASP	C-O	5.45	1.30	1.24
1	C	401	VAL	CA-CB	5.29	1.60	1.53
1	A	440	VAL	CA-CB	5.17	1.61	1.54
1	A	412	THR	CA-CB	-5.16	1.45	1.53
1	B	373	THR	CA-CB	5.14	1.62	1.53
1	B	104	ALA	CA-CB	-5.01	1.45	1.53

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	316	ILE	N-CA-C	8.76	115.53	107.56
1	C	170	ILE	N-CA-C	8.23	115.94	109.19
1	B	386	SER	N-CA-C	-7.92	99.42	110.35
1	A	170	ILE	N-CA-C	7.88	115.66	109.19
1	B	200	TYR	CA-CB-CG	7.86	128.04	113.90
1	D	449	THR	N-CA-C	7.74	119.71	111.28
1	C	420	LYS	N-CA-C	-7.69	103.74	113.43
1	B	420	LYS	N-CA-C	-7.52	103.96	113.43
1	C	358	TYR	N-CA-C	7.33	121.64	113.21
1	B	316	ILE	N-CA-C	7.10	114.02	107.56
1	B	170	ILE	N-CA-C	7.01	114.94	109.19
1	D	420	LYS	N-CA-C	-6.99	104.75	113.55
1	A	495	ALA	CA-C-N	-6.97	107.74	121.41
1	A	495	ALA	C-N-CA	-6.97	107.74	121.41
1	C	10	SER	N-CA-C	6.97	121.48	112.41
1	C	370	VAL	N-CA-C	-6.97	102.63	108.63
1	B	65	ILE	CA-C-N	-6.92	111.86	119.19
1	B	65	ILE	C-N-CA	-6.92	111.86	119.19
1	A	316	ILE	N-CA-C	6.86	113.81	107.56
1	A	358	TYR	N-CA-C	6.85	121.09	113.21
1	C	393	LYS	N-CA-C	6.83	119.74	111.82
1	B	326	VAL	CA-C-N	6.80	128.34	119.84
1	B	326	VAL	C-N-CA	6.80	128.34	119.84
1	A	77	GLY	N-CA-C	-6.77	104.30	112.49
1	B	248	ILE	N-CA-C	-6.75	95.90	107.24
1	C	386	SER	N-CA-C	-6.74	101.84	110.53
1	C	277	GLU	N-CA-C	-6.72	104.83	113.16
1	C	230	GLN	N-CA-C	6.67	119.38	111.71
1	A	386	SER	N-CA-C	-6.65	101.17	110.35
1	B	206	ALA	N-CA-C	-6.60	104.08	111.28
1	A	417	ASP	N-CA-C	6.60	120.50	111.39
1	B	200	TYR	N-CA-CB	-6.60	98.50	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	358	TYR	N-CA-C	6.55	120.94	113.15
1	D	71	HIS	N-CA-C	-6.54	104.16	111.28
1	B	492	ILE	N-CA-C	-6.38	107.08	113.20
1	C	83	SER	N-CA-C	6.37	120.15	112.38
1	A	60	VAL	CB-CA-C	-6.33	103.48	112.22
1	B	277	GLU	N-CA-C	-6.26	105.21	112.92
1	A	497	CYS	N-CA-C	-6.26	106.28	114.04
1	D	393	LYS	N-CA-C	6.25	119.08	111.82
1	B	449	THR	N-CA-C	6.24	118.16	111.36
1	C	231	ASP	N-CA-C	-6.22	104.41	111.07
1	C	222	SER	O-C-N	6.18	125.40	120.83
1	C	417	ASP	N-CA-C	6.18	119.92	111.39
1	A	420	LYS	N-CA-C	-6.18	105.77	113.55
1	A	494	GLN	N-CA-C	6.17	118.84	107.99
1	A	206	ALA	N-CA-C	-6.16	104.57	111.28
1	A	65	ILE	CA-C-N	-6.12	112.70	119.19
1	A	65	ILE	C-N-CA	-6.12	112.70	119.19
1	C	181	ASP	N-CA-C	6.10	117.93	111.28
1	D	417	ASP	N-CA-C	6.05	119.74	111.39
1	B	168	LEU	N-CA-C	-6.03	99.88	109.76
1	C	77	GLY	N-CA-C	-6.02	105.52	112.50
1	C	65	ILE	CA-C-N	-5.95	112.88	119.19
1	C	65	ILE	C-N-CA	-5.95	112.88	119.19
1	B	60	VAL	N-CA-C	5.88	116.66	110.72
1	A	258	GLN	N-CA-C	5.86	118.31	108.23
1	B	9	LYS	CA-C-N	-5.85	110.37	121.54
1	B	9	LYS	C-N-CA	-5.85	110.37	121.54
1	D	370	VAL	N-CA-C	-5.84	103.60	108.63
1	C	60	VAL	CB-CA-C	-5.84	104.16	112.22
1	C	53	TRP	N-CA-C	5.79	116.19	108.38
1	C	236	ILE	CB-CA-C	-5.77	104.36	112.14
1	A	342	LEU	N-CA-C	5.72	118.80	109.24
1	D	83	SER	N-CA-C	5.72	118.29	111.71
1	D	77	GLY	N-CA-C	-5.70	105.47	112.77
1	D	386	SER	N-CA-C	-5.70	102.49	110.35
1	A	346	ALA	N-CA-C	-5.69	104.98	111.07
1	A	208	PHE	N-CA-C	5.67	118.23	111.71
1	B	412	THR	CA-C-N	-5.65	116.68	120.24
1	B	412	THR	C-N-CA	-5.65	116.68	120.24
1	D	248	ILE	N-CA-C	-5.65	97.75	107.24
1	A	457	LYS	N-CA-C	-5.62	106.27	113.01
1	A	71	HIS	N-CA-C	-5.58	105.19	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	VAL	CB-CA-C	-5.58	104.70	112.02
1	B	448	VAL	CB-CA-C	-5.57	104.73	112.02
1	C	60	VAL	N-CA-C	5.54	116.31	110.72
1	D	304	THR	CA-C-N	-5.54	115.94	122.36
1	D	304	THR	C-N-CA	-5.54	115.94	122.36
1	B	147	GLY	N-CA-C	-5.48	107.72	113.58
1	B	71	HIS	N-CA-C	-5.46	105.33	111.28
1	D	419	ASN	N-CA-C	5.45	118.76	111.24
1	B	393	LYS	N-CA-C	5.45	118.14	111.82
1	C	9	LYS	N-CA-C	5.44	122.39	110.80
1	A	230	GLN	N-CA-C	5.42	118.11	111.82
1	D	298	ARG	N-CA-C	5.42	118.01	111.40
1	A	209	LEU	N-CA-C	-5.40	105.29	111.07
1	C	71	HIS	N-CA-C	-5.40	105.40	111.28
1	C	248	ILE	N-CA-C	-5.36	97.91	107.18
1	A	97	ASP	N-CA-CB	-5.33	101.45	110.46
1	D	326	VAL	CA-C-N	5.33	126.50	119.84
1	D	326	VAL	C-N-CA	5.33	126.50	119.84
1	D	468	THR	CA-C-N	-5.28	115.36	122.91
1	D	468	THR	C-N-CA	-5.28	115.36	122.91
1	B	276	SER	N-CA-C	-5.26	101.42	109.41
1	C	413	ILE	CB-CA-C	-5.23	107.15	114.00
1	C	54	GLY	N-CA-C	5.23	120.50	111.98
1	C	216	VAL	N-CA-C	5.22	116.24	108.46
1	C	304	THR	CA-C-N	-5.22	116.31	122.36
1	C	304	THR	C-N-CA	-5.22	116.31	122.36
1	D	61	ASN	N-CA-C	5.21	120.29	113.88
1	A	298	ARG	N-CA-C	5.21	117.75	111.40
1	A	326	VAL	CA-C-N	5.20	126.34	119.84
1	A	326	VAL	C-N-CA	5.20	126.34	119.84
1	A	60	VAL	N-CA-C	5.18	115.95	110.72
1	A	83	SER	N-CA-C	5.18	118.70	112.38
1	B	358	TYR	N-CA-C	5.18	119.31	113.15
1	D	387	GLU	N-CA-C	-5.17	105.56	111.14
1	A	248	ILE	N-CA-C	-5.16	98.56	107.24
1	C	326	VAL	CA-C-N	5.16	126.29	119.84
1	C	326	VAL	C-N-CA	5.16	126.29	119.84
1	D	135	ILE	CB-CA-C	-5.16	105.78	110.63
1	D	225	LEU	N-CA-C	5.16	118.31	111.30
1	A	277	GLU	N-CA-C	-5.16	106.83	113.02
1	A	385	LEU	N-CA-C	5.14	117.74	110.50
1	D	65	ILE	CA-C-N	-5.13	113.64	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	65	ILE	C-N-CA	-5.13	113.64	119.28
1	C	414	PRO	N-CA-C	-5.11	107.74	114.03
1	B	314	GLY	N-CA-C	-5.11	107.49	114.64
1	A	15	LEU	N-CA-C	5.10	116.68	108.32
1	D	222	SER	O-C-N	5.09	124.60	120.83
1	A	393	LYS	N-CA-C	5.07	117.54	111.71
1	A	484	VAL	CB-CA-C	-5.07	104.83	110.96
1	C	45	THR	CB-CA-C	-5.01	101.78	109.85
1	C	320	ASP	N-CA-C	-5.01	107.14	113.20
1	D	314	GLY	N-CA-C	-5.00	107.63	114.64

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	TYR	Sidechain
1	B	188	TYR	Sidechain
1	B	402	TYR	Sidechain
1	C	200	TYR	Sidechain
1	D	176	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3785	0	3793	206	0
1	B	3765	0	3782	207	0
1	C	3765	0	3782	244	0
1	D	3741	0	3751	219	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	0	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	162	0	0	6	0
4	B	137	0	0	2	0
4	C	123	0	0	2	0
4	D	108	0	0	3	0
All	All	15818	0	15232	841	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (841) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:LYS:N	1:B:325:ASN:HD21	1.40	1.18
1:B:308:LYS:H	1:B:325:ASN:ND2	1.45	1.15
1:D:270:VAL:HG22	1:D:281:GLU:HG2	1.31	1.13
1:D:461:THR:HG22	1:D:464:GLN:H	1.07	1.13
1:D:70:MET:HG2	1:D:101:MET:HE3	1.15	1.11
1:B:308:LYS:HB2	1:B:325:ASN:HD22	1.07	1.07
1:B:308:LYS:HB2	1:B:325:ASN:ND2	1.69	1.06
1:D:277:GLU:OE2	1:D:277:GLU:HA	1.63	0.98
1:B:203:LEU:HD22	1:B:240:MET:HE1	1.45	0.97
1:D:461:THR:CG2	1:D:464:GLN:H	1.80	0.94
1:D:162:GLY:O	1:D:335:ILE:HD11	1.65	0.94
1:C:386:SER:H	1:C:389:LYS:HE3	1.34	0.93
1:C:70:MET:HE3	1:C:208:PHE:CE1	2.05	0.92
1:C:461:THR:HG22	1:C:463:LYS:H	1.32	0.90
1:B:7:LEU:HB3	1:B:8:PRO:HD3	1.53	0.90
1:C:232:MET:O	1:C:236:ILE:HD12	1.72	0.89
1:D:258:GLN:NE2	1:D:261:ALA:HA	1.88	0.89
1:D:70:MET:HG2	1:D:101:MET:CE	2.01	0.88
1:A:183:LEU:O	1:A:183:LEU:HD12	1.73	0.87
1:C:36:LYS:HZ2	1:C:358:TYR:HD1	1.22	0.87
1:C:332:ILE:HA	1:C:336:LEU:HD11	1.54	0.87
1:A:38:VAL:HG13	1:A:125:VAL:HG13	1.55	0.87
1:D:461:THR:H	1:D:464:GLN:HE21	1.22	0.87
1:B:401:VAL:HG11	1:B:486:LYS:HD2	1.55	0.87
1:C:205:CYS:HA	1:C:208:PHE:CE2	2.10	0.86
1:C:107:ASN:C	1:C:107:ASN:HD22	1.84	0.85
1:C:258:GLN:NE2	1:C:261:ALA:HA	1.92	0.85
1:B:195:VAL:HG13	1:B:218:VAL:HG22	1.58	0.85
1:C:308:LYS:HB2	1:C:325:ASN:ND2	1.90	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:HD13	1:A:39:MET:HB3	1.59	0.84
1:B:308:LYS:CB	1:B:325:ASN:ND2	2.41	0.83
1:C:192:LYS:N	1:C:285:ASN:HD22	1.76	0.82
1:C:378:LEU:HD23	1:C:441:LEU:HD11	1.58	0.82
1:B:254:ILE:CG1	1:B:270:VAL:HG12	2.10	0.82
1:C:192:LYS:H	1:C:285:ASN:HD22	1.27	0.81
1:D:461:THR:HG22	1:D:464:GLN:N	1.92	0.81
1:B:163:GLU:O	1:B:164:ARG:HG2	1.80	0.81
1:B:36:LYS:HE3	1:B:358:TYR:HD1	1.47	0.80
1:B:338:ASP:O	1:B:339:LYS:HD3	1.81	0.80
1:B:461:THR:HB	1:B:464:GLN:HG3	1.63	0.79
1:C:245:ILE:HG22	1:C:247:PHE:CE2	2.17	0.79
1:C:461:THR:HG22	1:C:463:LYS:N	1.97	0.79
1:C:67:LYS:HD2	1:C:68:LYS:N	1.97	0.79
1:A:238:GLU:O	1:A:242:GLU:HG3	1.82	0.79
1:C:233:ALA:HA	1:C:236:ILE:HD13	1.65	0.79
1:B:161:THR:HG21	1:B:296:CYS:O	1.84	0.78
1:D:203:LEU:HB3	1:D:240:MET:HE1	1.65	0.78
1:A:371:PRO:HB2	1:B:471:ILE:HD11	1.66	0.78
1:D:98:TRP:CZ2	1:D:102:ILE:HD11	2.19	0.77
1:B:158:LEU:HD11	1:B:332:ILE:HD13	1.65	0.77
1:B:403:HIS:CE1	1:B:492:ILE:HD11	2.19	0.77
1:C:137:PRO:O	1:C:139:ARG:HG3	1.83	0.77
1:D:302:LEU:HD22	1:D:307:VAL:HG11	1.65	0.77
1:B:485:THR:HG23	1:B:488:SER:H	1.50	0.77
1:B:325:ASN:OD1	1:B:326:VAL:HG23	1.84	0.76
1:B:259:ILE:HD11	1:B:268:ARG:HB2	1.67	0.76
1:C:474:VAL:O	1:C:477:GLU:HG2	1.86	0.76
1:C:183:LEU:HD22	1:C:288:MET:HE1	1.67	0.75
1:A:209:LEU:O	1:A:212:ILE:HG22	1.87	0.75
1:D:15:LEU:CD2	1:D:17:ILE:HD11	2.17	0.75
1:C:168:LEU:O	1:C:173:ASP:OD2	2.03	0.75
1:D:41:LEU:HD23	1:D:128:GLU:HB2	1.68	0.75
1:B:55:LEU:HD12	1:B:56:GLY:H	1.52	0.75
1:B:161:THR:CG2	1:B:296:CYS:HB2	2.17	0.75
1:C:39:MET:HE2	1:C:128:GLU:HB2	1.69	0.74
1:D:461:THR:HG23	1:D:463:LYS:H	1.51	0.74
1:A:33:GLN:HB2	1:A:123:LYS:HZ3	1.52	0.74
1:D:297:THR:HG22	1:D:316:ILE:HD11	1.69	0.74
1:B:45:THR:O	1:B:164:ARG:NH2	2.18	0.74
1:D:144:ASN:ND2	1:D:146:LYS:H	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:ARG:HH11	1:D:298:ARG:HG2	1.51	0.74
1:C:191:GLY:O	1:C:193:THR:CG2	2.36	0.73
1:A:205:CYS:HA	1:A:208:PHE:CE2	2.24	0.73
1:C:183:LEU:HD22	1:C:288:MET:CE	2.19	0.73
1:A:162:GLY:O	1:A:335:ILE:HD11	1.87	0.73
1:B:432:ASN:O	1:B:461:THR:HG23	1.89	0.73
1:C:447:GLU:HA	1:C:447:GLU:OE1	1.88	0.73
1:B:332:ILE:HA	1:B:336:LEU:HD11	1.69	0.73
1:C:236:ILE:HG21	1:C:376:THR:HG21	1.72	0.72
1:C:385:LEU:HA	1:C:389:LYS:HE3	1.71	0.72
1:D:58:THR:HG23	1:D:62:VAL:HG23	1.71	0.72
1:D:221:ARG:CZ	1:D:252:VAL:HG21	2.19	0.72
1:D:461:THR:N	1:D:464:GLN:HE21	1.87	0.72
1:C:144:ASN:ND2	1:C:148:LYS:HB2	2.04	0.72
1:D:219:MET:HE3	1:D:251:PHE:O	1.89	0.72
1:C:386:SER:N	1:C:389:LYS:HE3	2.03	0.72
1:C:70:MET:HE2	1:C:184:PHE:CE1	2.25	0.72
1:D:69:LEU:HD12	1:D:105:VAL:HG13	1.69	0.72
1:D:229:ASP:HA	1:D:386:SER:OG	1.90	0.71
1:A:39:MET:HE1	1:A:152:TYR:CZ	2.25	0.71
1:A:322:GLU:OE1	4:A:650:HOH:O	2.07	0.71
1:A:98:TRP:CZ2	1:A:102:ILE:HD11	2.26	0.71
1:D:400:GLU:OE1	4:D:590:HOH:O	2.08	0.71
1:A:80:LEU:HD23	1:B:80:LEU:CD2	2.21	0.71
1:C:254:ILE:HD11	1:C:270:VAL:HG12	1.73	0.71
1:B:251:PHE:CE2	1:B:280:ILE:HG12	2.25	0.71
1:A:432:ASN:O	1:A:461:THR:HG23	1.91	0.70
1:D:168:LEU:O	1:D:173:ASP:OD2	2.09	0.70
1:D:266:ARG:HB3	1:D:283:GLU:OE1	1.90	0.70
1:A:301:GLY:O	1:A:304:THR:HG23	1.91	0.70
1:D:461:THR:HG23	1:D:463:LYS:N	2.06	0.70
1:A:52:ARG:HG3	1:A:52:ARG:HH11	1.56	0.70
1:C:259:ILE:O	1:C:260:GLU:HB2	1.89	0.70
1:C:386:SER:H	1:C:389:LYS:CE	2.02	0.70
1:D:338:ASP:O	1:D:339:LYS:HD3	1.92	0.70
1:A:140:ILE:HG12	1:A:141:LYS:N	2.07	0.70
1:C:134:PHE:HA	1:C:140:ILE:HG13	1.72	0.70
1:B:36:LYS:HE3	1:B:358:TYR:CD1	2.26	0.69
1:C:275:ASN:HD22	1:C:275:ASN:C	2.01	0.69
1:C:77:GLY:HA2	1:C:80:LEU:HD12	1.74	0.69
1:C:411:TRP:C	1:C:414:PRO:HD2	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:ASN:C	1:C:107:ASN:ND2	2.49	0.69
1:C:245:ILE:HD12	1:C:245:ILE:H	1.58	0.69
1:D:258:GLN:NE2	1:D:261:ALA:CA	2.56	0.69
1:A:176:TYR:CD1	1:A:258:GLN:NE2	2.61	0.69
1:D:229:ASP:CA	1:D:386:SER:OG	2.41	0.69
1:C:221:ARG:HG3	1:C:252:VAL:HG22	1.75	0.68
1:C:491:SER:HB3	1:C:493:LEU:HG	1.75	0.68
1:B:194:LEU:HB2	1:B:284:TYR:CD2	2.28	0.68
1:A:70:MET:CE	1:A:184:PHE:HD1	2.07	0.68
1:A:250:GLN:O	1:A:274:THR:HG22	1.93	0.68
1:B:194:LEU:HD13	1:B:284:TYR:CZ	2.28	0.68
1:C:70:MET:HE2	1:C:184:PHE:HE1	1.57	0.68
1:D:15:LEU:HD21	1:D:17:ILE:HD11	1.75	0.68
1:B:432:ASN:C	1:B:433:GLU:HG2	2.17	0.67
1:A:183:LEU:HD12	1:A:183:LEU:C	2.16	0.67
1:B:80:LEU:HD12	1:B:94:VAL:HG21	1.75	0.67
1:A:258:GLN:OE1	1:A:261:ALA:HB2	1.95	0.67
1:A:173:ASP:OD2	1:A:174:LYS:N	2.26	0.67
1:C:378:LEU:HG	1:C:441:LEU:HD12	1.76	0.67
1:D:456:LEU:HD23	1:D:456:LEU:N	2.10	0.67
1:C:233:ALA:HA	1:C:236:ILE:CD1	2.25	0.67
1:A:166:ARG:HG2	1:A:291:ILE:HD11	1.75	0.67
1:C:378:LEU:HD23	1:C:441:LEU:CD1	2.25	0.67
1:C:403:HIS:CE1	1:C:486:LYS:HG3	2.30	0.67
1:A:148:LYS:HD3	1:A:148:LYS:N	2.09	0.67
1:D:239:HIS:CE1	1:D:378:LEU:HB2	2.29	0.67
1:B:428:ASN:ND2	1:B:431:ASP:HB2	2.10	0.67
1:B:163:GLU:HG2	1:B:295:ALA:HA	1.77	0.66
1:B:161:THR:HG22	1:B:296:CYS:HB2	1.78	0.66
1:A:133:GLN:O	1:A:140:ILE:HG13	1.95	0.66
1:B:186:LEU:HD23	1:B:190:PRO:HG3	1.77	0.66
1:A:33:GLN:HB2	1:A:123:LYS:NZ	2.11	0.65
1:A:36:LYS:HE2	1:A:36:LYS:HA	1.77	0.65
1:D:258:GLN:HE21	1:D:261:ALA:HA	1.60	0.65
1:C:305:VAL:O	1:C:305:VAL:HG22	1.97	0.65
1:B:8:PRO:O	1:B:9:LYS:HB3	1.94	0.65
1:B:195:VAL:CG1	1:B:218:VAL:HG22	2.27	0.65
1:C:144:ASN:HD21	1:C:148:LYS:HB2	1.61	0.65
1:D:254:ILE:HG13	1:D:270:VAL:HG12	1.78	0.65
1:A:245:ILE:HD12	1:A:245:ILE:H	1.62	0.64
1:C:191:GLY:O	1:C:193:THR:HG23	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ARG:HG2	3:B:901:SO4:O1	1.97	0.64
1:A:47:THR:O	1:A:50:GLY:N	2.24	0.64
1:A:461:THR:HG22	1:A:463:LYS:H	1.62	0.64
1:B:7:LEU:HB3	1:B:8:PRO:CD	2.24	0.64
1:C:191:GLY:O	1:C:193:THR:HG22	1.98	0.64
1:C:141:LYS:HD2	1:C:149:GLU:OE2	1.97	0.64
1:B:254:ILE:HG12	1:B:270:VAL:HG12	1.80	0.64
1:C:332:ILE:CA	1:C:336:LEU:HD11	2.28	0.64
1:D:41:LEU:CD2	1:D:128:GLU:HB2	2.27	0.64
1:B:154:ALA:HB3	1:B:157:PHE:CE1	2.33	0.64
1:C:163:GLU:O	1:C:164:ARG:HD2	1.96	0.64
1:C:319:THR:OG1	1:C:323:GLN:HB3	1.98	0.64
1:B:403:HIS:ND1	1:B:492:ILE:HD11	2.13	0.63
1:C:343:THR:HB	1:C:344:PRO:HD3	1.79	0.63
1:D:277:GLU:OE2	1:D:277:GLU:CA	2.40	0.63
1:B:62:VAL:HG12	1:B:62:VAL:O	1.99	0.63
1:C:198:ALA:HB2	1:C:220:VAL:HG22	1.79	0.63
1:C:447:GLU:OE2	1:D:475:CYS:HB2	1.97	0.63
1:D:194:LEU:HD12	1:D:194:LEU:C	2.24	0.63
1:D:305:VAL:CG2	1:D:328:TYR:OH	2.46	0.63
1:A:168:LEU:O	1:A:173:ASP:OD1	2.16	0.63
1:A:176:TYR:HD1	1:A:258:GLN:NE2	1.96	0.63
1:C:108:HIS:CD2	1:C:112:LEU:HD11	2.34	0.63
1:B:161:THR:CG2	1:B:296:CYS:O	2.46	0.63
1:B:238:GLU:O	1:B:242:GLU:HG3	1.98	0.63
1:D:205:CYS:HA	1:D:208:PHE:CE2	2.34	0.63
1:B:435:VAL:HG23	1:B:460:LEU:O	1.98	0.62
1:C:171:PRO:HB2	1:C:255:LYS:HG3	1.81	0.62
1:C:409:LEU:HD23	1:D:68:LYS:HG2	1.80	0.62
1:C:135:ILE:CD1	1:C:151:ILE:HD13	2.29	0.62
1:C:7:LEU:HB2	1:C:9:LYS:CE	2.29	0.62
1:A:18:ILE:HD12	1:A:159:ILE:HA	1.80	0.62
1:D:70:MET:HE3	1:D:101:MET:CE	2.29	0.62
1:A:462:LYS:HE2	1:A:466:ASP:OD1	1.99	0.62
1:C:30:GLU:HA	1:C:30:GLU:OE1	1.98	0.62
1:D:144:ASN:HD21	1:D:146:LYS:H	1.48	0.62
1:D:67:LYS:HD2	1:D:68:LYS:N	2.15	0.62
1:C:321:GLU:O	1:C:322:GLU:HB2	1.99	0.61
1:B:364:LYS:HD2	4:B:594:HOH:O	2.00	0.61
1:A:475:CYS:O	1:A:478:VAL:HG12	1.99	0.61
1:D:98:TRP:CE2	1:D:102:ILE:HD11	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ILE:HG13	1:B:270:VAL:HG12	1.82	0.61
1:D:316:ILE:HD12	1:D:335:ILE:CG2	2.30	0.61
1:A:498:CYS:HB2	1:B:115:GLY:HA3	1.80	0.61
1:C:67:LYS:HD2	1:C:67:LYS:C	2.26	0.61
1:B:223:ILE:HD11	1:B:226:ARG:HB2	1.83	0.61
1:B:400:GLU:OE1	1:B:400:GLU:HA	2.00	0.61
1:B:168:LEU:O	1:B:173:ASP:OD2	2.19	0.60
1:C:385:LEU:HD12	1:C:436:VAL:HB	1.83	0.60
1:D:315:LYS:HD3	1:D:336:LEU:O	1.99	0.60
1:D:492:ILE:HD13	1:D:492:ILE:N	2.16	0.60
1:B:62:VAL:HG11	1:B:181:ASP:OD1	2.01	0.60
1:C:236:ILE:HD12	1:C:236:ILE:H	1.65	0.60
1:C:487:ARG:HH21	1:C:487:ARG:HG3	1.65	0.60
1:B:406:PHE:CZ	1:B:421:CYS:HB3	2.36	0.60
1:C:258:GLN:NE2	1:C:261:ALA:CA	2.63	0.60
1:B:9:LYS:O	1:B:11:TYR:N	2.31	0.60
1:D:166:ARG:HG2	1:D:167:TYR:N	2.16	0.60
1:A:80:LEU:HD23	1:B:80:LEU:HD22	1.83	0.60
1:B:55:LEU:HD12	1:B:56:GLY:N	2.16	0.60
1:B:173:ASP:OD1	1:B:174:LYS:N	2.34	0.60
1:B:485:THR:HG23	1:B:488:SER:HB3	1.82	0.60
1:C:75:LEU:O	1:C:78:GLN:HB3	2.02	0.60
1:A:203:LEU:HD12	1:A:225:LEU:HD21	1.83	0.60
1:C:275:ASN:HD22	1:C:276:SER:N	1.98	0.60
1:D:250:GLN:HB3	1:D:274:THR:CG2	2.32	0.60
1:D:340:VAL:HB	1:D:345:VAL:HG21	1.82	0.60
1:B:232:MET:CE	1:B:439:HIS:HB3	2.32	0.60
1:B:240:MET:HE2	1:B:247:PHE:HZ	1.67	0.60
1:B:250:GLN:O	1:B:274:THR:HG23	2.02	0.60
1:A:245:ILE:HG22	1:A:247:PHE:CE2	2.37	0.59
1:A:254:ILE:CG1	1:A:270:VAL:HG12	2.32	0.59
1:C:411:TRP:O	1:C:414:PRO:HD2	2.02	0.59
1:A:210:ALA:HB3	1:A:245:ILE:HD11	1.84	0.59
1:D:423:ALA:HB1	1:D:479:PHE:CE1	2.37	0.59
1:A:362:THR:O	1:A:362:THR:OG1	2.18	0.59
1:C:70:MET:CE	1:C:208:PHE:CE1	2.81	0.59
1:C:251:PHE:CE2	1:C:280:ILE:HG12	2.37	0.59
1:C:332:ILE:HA	1:C:336:LEU:CD1	2.27	0.59
1:C:343:THR:O	1:C:347:ILE:HG13	2.03	0.59
1:C:258:GLN:HE21	1:C:261:ALA:HA	1.68	0.59
1:C:173:ASP:OD1	1:C:174:LYS:N	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:GLU:OE2	1:B:128:GLU:HA	2.03	0.59
1:D:17:ILE:HD12	1:D:158:LEU:HB3	1.85	0.59
1:A:159:ILE:HD11	1:A:329:ILE:CG2	2.33	0.59
1:C:438:PHE:CD1	1:C:438:PHE:C	2.81	0.59
1:B:232:MET:HE2	1:B:439:HIS:CB	2.33	0.58
1:C:168:LEU:HD12	1:C:289:LEU:HD11	1.83	0.58
1:C:192:LYS:H	1:C:285:ASN:ND2	1.99	0.58
1:A:98:TRP:NE1	1:A:102:ILE:HG13	2.18	0.58
1:C:391:VAL:HG13	1:C:396:GLU:HA	1.84	0.58
1:A:221:ARG:NH2	1:A:252:VAL:HG21	2.17	0.58
1:C:70:MET:SD	1:C:101:MET:HE3	2.43	0.58
1:C:41:LEU:HD23	1:C:128:GLU:HB3	1.85	0.58
1:D:203:LEU:CB	1:D:240:MET:HE1	2.32	0.58
1:B:209:LEU:HD22	1:B:214:LEU:HD12	1.84	0.58
1:B:67:LYS:HD2	1:B:68:LYS:N	2.19	0.58
1:B:225:LEU:HB3	1:B:228:PHE:CD2	2.37	0.58
1:B:250:GLN:C	1:B:274:THR:HG23	2.29	0.58
1:D:156:ARG:HG3	1:D:156:ARG:HH11	1.69	0.58
1:B:161:THR:CG2	1:B:296:CYS:CB	2.82	0.58
1:B:62:VAL:O	1:B:62:VAL:CG1	2.51	0.57
1:D:166:ARG:HG3	1:D:294:ASP:OD2	2.04	0.57
1:A:494:GLN:O	1:A:495:ALA:CB	2.52	0.57
1:C:7:LEU:HB2	1:C:9:LYS:HE3	1.86	0.57
1:C:91:GLU:CD	1:C:91:GLU:N	2.62	0.57
1:D:191:GLY:O	1:D:192:LYS:C	2.46	0.57
1:D:318:VAL:HG11	1:D:336:LEU:HD22	1.85	0.57
1:B:67:LYS:HD2	1:B:67:LYS:C	2.29	0.57
1:B:156:ARG:HG3	1:B:156:ARG:HH11	1.69	0.57
1:B:232:MET:HE2	1:B:439:HIS:HB2	1.85	0.57
1:B:411:TRP:C	1:B:414:PRO:HD2	2.30	0.57
1:B:461:THR:HG22	1:B:463:LYS:H	1.69	0.57
1:B:194:LEU:HB2	1:B:284:TYR:CE2	2.40	0.57
1:C:219:MET:HG2	1:C:251:PHE:O	2.04	0.57
1:C:222:SER:OG	1:C:223:ILE:HG23	2.04	0.57
1:D:154:ALA:HB3	1:D:157:PHE:CE1	2.40	0.57
1:D:302:LEU:HD22	1:D:307:VAL:CG1	2.33	0.57
1:C:159:ILE:HG13	1:C:330:TYR:O	2.05	0.57
1:D:297:THR:HG21	1:D:316:ILE:HG13	1.87	0.57
1:B:223:ILE:HD11	1:B:226:ARG:CB	2.34	0.57
1:C:36:LYS:NZ	1:C:358:TYR:HD1	2.00	0.57
1:C:320:ASP:OD2	1:C:364:LYS:HD3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:ASN:OD1	1:C:312:LYS:HG3	2.05	0.56
1:D:461:THR:CG2	1:D:464:GLN:HG3	2.35	0.56
1:A:210:ALA:CB	1:A:245:ILE:HD11	2.35	0.56
1:B:67:LYS:NZ	1:B:204:GLU:OE1	2.36	0.56
1:C:356:ARG:NH1	1:C:364:LYS:HA	2.20	0.56
1:D:70:MET:HE3	1:D:101:MET:HE2	1.86	0.56
1:D:254:ILE:CG1	1:D:270:VAL:HG12	2.35	0.56
1:B:232:MET:HE3	1:B:439:HIS:HB3	1.87	0.56
1:C:22:SER:OG	1:C:343:THR:HG23	2.05	0.56
1:C:305:VAL:HG21	1:C:329:ILE:HD11	1.87	0.56
1:C:405:TYR:HD1	1:C:492:ILE:HG13	1.71	0.56
1:C:474:VAL:HG21	1:D:446:GLY:HA3	1.86	0.56
1:C:221:ARG:HG3	1:C:252:VAL:CG2	2.35	0.56
1:C:391:VAL:HG13	1:C:396:GLU:CA	2.35	0.56
1:D:492:ILE:HD13	1:D:492:ILE:H	1.71	0.56
1:A:46:PRO:HG3	1:A:52:ARG:HB3	1.87	0.56
1:A:70:MET:SD	1:A:208:PHE:CE1	2.99	0.56
1:C:254:ILE:CD1	1:C:270:VAL:HG12	2.36	0.56
1:A:200:TYR:HB2	1:A:374:VAL:HG13	1.88	0.56
1:B:403:HIS:CE1	1:B:492:ILE:CD1	2.89	0.56
1:B:403:HIS:ND1	1:B:492:ILE:CD1	2.69	0.56
1:A:186:LEU:HD21	1:A:188:TYR:CE1	2.41	0.56
1:A:166:ARG:HB2	1:A:294:ASP:OD2	2.06	0.55
1:D:461:THR:HG22	1:D:464:GLN:HG3	1.88	0.55
1:A:52:ARG:HG3	1:A:52:ARG:NH1	2.21	0.55
1:C:387:GLU:O	1:C:391:VAL:HG23	2.05	0.55
1:C:96:HIS:CD2	1:C:212:ILE:HD11	2.40	0.55
1:C:163:GLU:HG2	1:C:295:ALA:HA	1.87	0.55
1:A:70:MET:HE1	1:A:184:PHE:HD1	1.70	0.55
1:A:80:LEU:HD23	1:B:80:LEU:HD23	1.88	0.55
1:C:11:TYR:HD1	1:C:153:SER:HG	1.54	0.55
1:B:200:TYR:HD1	1:B:374:VAL:HG22	1.70	0.55
1:A:55:LEU:O	1:A:113:ASN:ND2	2.40	0.55
1:A:474:VAL:HG13	1:B:447:GLU:CD	2.32	0.55
1:C:134:PHE:CD1	1:C:305:VAL:HG11	2.41	0.55
1:A:25:LEU:HD13	1:A:116:TYR:CD1	2.41	0.55
1:C:155:GLU:O	1:C:155:GLU:HG2	2.06	0.55
1:D:144:ASN:ND2	1:D:145:ASN:N	2.54	0.54
1:D:162:GLY:O	1:D:335:ILE:CD1	2.48	0.54
1:A:80:LEU:CD2	1:B:80:LEU:HD22	2.37	0.54
1:A:141:LYS:HD2	1:A:149:GLU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:TYR:CE2	1:D:424:LYS:HG2	2.42	0.54
1:B:85:ASN:HB3	1:B:413:ILE:HG22	1.89	0.54
1:B:403:HIS:ND1	1:B:422:TYR:OH	2.36	0.54
1:C:265:GLY:C	1:C:266:ARG:HG3	2.32	0.54
1:C:305:VAL:O	1:C:305:VAL:CG2	2.55	0.54
1:C:324:THR:HG23	1:C:329:ILE:O	2.07	0.54
1:C:371:PRO:HB2	1:D:471:ILE:HD11	1.88	0.54
1:A:458:CYS:HB3	1:B:458:CYS:HB3	1.88	0.54
1:B:240:MET:HG2	1:B:245:ILE:CD1	2.38	0.54
1:C:405:TYR:CD1	1:C:492:ILE:HG13	2.43	0.54
1:D:401:VAL:HG11	1:D:486:LYS:HD2	1.88	0.54
1:B:222:SER:OG	1:B:226:ARG:NH2	2.40	0.54
1:B:195:VAL:HG11	1:B:206:ALA:HB2	1.90	0.54
1:C:340:VAL:CG1	1:C:342:LEU:HD12	2.37	0.54
1:D:187:PRO:HG2	1:D:188:TYR:CD2	2.43	0.54
1:A:472:HIS:HB2	1:B:344:PRO:HG3	1.90	0.54
1:B:240:MET:HG2	1:B:245:ILE:HD12	1.90	0.54
1:B:325:ASN:OD1	1:B:326:VAL:N	2.41	0.54
1:C:209:LEU:O	1:C:212:ILE:HG22	2.08	0.54
1:C:238:GLU:O	1:C:242:GLU:HG3	2.06	0.54
1:C:247:PHE:N	1:C:247:PHE:CD2	2.74	0.54
1:C:88:TRP:HE3	1:D:94:VAL:HG13	1.73	0.54
1:D:114:TRP:HZ3	1:D:117:ARG:NH1	2.06	0.54
1:B:34:TYR:CE2	1:B:359:ALA:HB2	2.42	0.54
1:C:222:SER:OG	1:C:223:ILE:N	2.40	0.54
1:C:407:TRP:CH2	1:C:412:THR:HG22	2.44	0.53
1:D:229:ASP:CB	1:D:386:SER:OG	2.56	0.53
1:B:406:PHE:CE1	1:B:421:CYS:HB3	2.43	0.53
1:C:378:LEU:CD2	1:C:441:LEU:CD1	2.87	0.53
1:B:156:ARG:HG3	1:B:156:ARG:NH1	2.24	0.53
1:C:91:GLU:CD	1:C:91:GLU:H	2.16	0.53
1:D:62:VAL:HA	1:D:184:PHE:HD2	1.72	0.53
1:D:225:LEU:HB3	1:D:228:PHE:HD2	1.73	0.53
1:A:70:MET:HE3	1:A:184:PHE:HD1	1.73	0.53
1:D:396:GLU:OE2	1:D:396:GLU:C	2.51	0.53
1:B:376:THR:O	1:B:377:PRO:C	2.51	0.53
1:C:302:LEU:CD1	1:C:309:ILE:HG21	2.39	0.53
1:C:378:LEU:CD2	1:C:441:LEU:HD11	2.34	0.53
1:A:325:ASN:O	1:A:327:PRO:HD3	2.08	0.53
1:A:344:PRO:HB2	1:B:469:ILE:HG22	1.91	0.53
1:C:88:TRP:CE3	1:D:94:VAL:HG13	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:HIS:HB2	1:D:344:PRO:HG3	1.91	0.53
1:A:324:THR:OG1	1:A:329:ILE:O	2.22	0.53
1:B:225:LEU:HD22	1:B:228:PHE:CE2	2.44	0.53
1:B:318:VAL:HG11	1:B:336:LEU:HD22	1.91	0.52
1:D:176:TYR:CZ	1:D:258:GLN:HB2	2.44	0.52
1:D:194:LEU:HD12	1:D:195:VAL:N	2.24	0.52
1:D:310:ASN:OD1	1:D:312:LYS:HB3	2.08	0.52
1:B:461:THR:N	1:B:464:GLN:OE1	2.42	0.52
1:D:170:ILE:O	1:D:173:ASP:OD1	2.26	0.52
1:D:461:THR:CG2	1:D:463:LYS:HB3	2.40	0.52
1:D:474:VAL:O	1:D:477:GLU:HG2	2.09	0.52
1:B:240:MET:HE2	1:B:247:PHE:CZ	2.44	0.52
1:C:286:THR:HG22	1:C:287:VAL:N	2.22	0.52
1:D:297:THR:O	1:D:302:LEU:HD12	2.08	0.52
1:A:306:GLY:O	1:A:325:ASN:ND2	2.42	0.52
1:C:9:LYS:HD2	1:C:10:SER:H	1.75	0.52
1:D:306:GLY:O	1:D:325:ASN:ND2	2.36	0.52
1:A:133:GLN:C	1:A:140:ILE:HG13	2.34	0.52
1:A:157:PHE:HB2	1:A:329:ILE:HG12	1.92	0.52
1:A:191:GLY:O	1:A:192:LYS:C	2.53	0.52
1:C:245:ILE:HG22	1:C:247:PHE:HE2	1.74	0.52
1:D:250:GLN:O	1:D:274:THR:HG22	2.08	0.52
1:A:254:ILE:HD11	1:A:270:VAL:HG12	1.91	0.52
1:C:219:MET:SD	1:C:253:PRO:HG3	2.50	0.52
1:C:236:ILE:CG2	1:C:376:THR:HG21	2.39	0.52
1:A:379:GLU:O	1:A:441:LEU:HD12	2.08	0.51
1:A:209:LEU:HD22	1:A:214:LEU:CD1	2.40	0.51
1:B:68:LYS:O	1:B:71:HIS:HB3	2.09	0.51
1:B:319:THR:OG1	1:B:323:GLN:HB3	2.10	0.51
1:B:465:LEU:HD21	1:B:479:PHE:O	2.10	0.51
1:C:225:LEU:HB3	1:C:228:PHE:HD2	1.75	0.51
1:D:232:MET:HE2	1:D:439:HIS:HB3	1.92	0.51
1:D:297:THR:CG2	1:D:316:ILE:HD11	2.39	0.51
1:D:413:ILE:HB	1:D:414:PRO:HD3	1.92	0.51
1:A:144:ASN:HD21	1:A:148:LYS:HB2	1.75	0.51
1:A:166:ARG:CG	1:A:291:ILE:HD11	2.38	0.51
1:A:236:ILE:O	1:A:240:MET:HG3	2.11	0.51
1:B:225:LEU:HB3	1:B:228:PHE:HD2	1.75	0.51
1:C:65:ILE:HD12	1:C:65:ILE:N	2.26	0.51
1:A:62:VAL:HA	1:A:184:PHE:HD2	1.76	0.51
1:C:104:ALA:HB1	1:D:413:ILE:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LEU:HD12	1:B:187:PRO:HD2	1.91	0.51
1:D:207:GLY:HA3	1:D:377:PRO:HD3	1.92	0.51
1:D:298:ARG:HG2	1:D:298:ARG:NH1	2.25	0.51
1:C:300:ILE:HD11	1:C:302:LEU:HD21	1.91	0.51
1:D:144:ASN:CG	1:D:145:ASN:N	2.67	0.51
1:A:194:LEU:HD22	1:A:284:TYR:CE1	2.46	0.51
1:B:191:GLY:O	1:B:192:LYS:C	2.52	0.51
1:C:480:THR:HG22	1:C:481:THR:HG23	1.93	0.51
1:A:205:CYS:HA	1:A:208:PHE:CD2	2.46	0.50
1:B:432:ASN:O	1:B:433:GLU:HG2	2.11	0.50
1:C:176:TYR:CE1	1:C:258:GLN:HB2	2.46	0.50
1:C:472:HIS:ND1	1:C:473:PRO:HA	2.26	0.50
1:D:239:HIS:ND1	1:D:378:LEU:HB2	2.26	0.50
1:D:286:THR:HG22	1:D:287:VAL:N	2.27	0.50
1:A:150:LYS:HE2	4:A:519:HOH:O	2.11	0.50
1:C:104:ALA:HB1	1:D:413:ILE:HD13	1.93	0.50
1:D:376:THR:O	1:D:377:PRO:C	2.55	0.50
1:A:254:ILE:HG13	1:A:270:VAL:HG12	1.93	0.50
1:B:438:PHE:CD1	1:B:438:PHE:C	2.89	0.50
1:B:438:PHE:CE2	1:B:452:PHE:CG	2.99	0.50
1:C:16:ILE:CD1	1:C:154:ALA:HB2	2.41	0.50
1:C:487:ARG:HG3	1:C:487:ARG:NH2	2.27	0.50
1:D:424:LYS:HE3	1:D:426:ILE:HD11	1.93	0.50
1:A:159:ILE:HD12	1:A:330:TYR:O	2.12	0.50
1:C:474:VAL:HG13	1:D:447:GLU:OE1	2.12	0.50
1:D:176:TYR:CZ	1:D:258:GLN:CB	2.95	0.50
1:A:323:GLN:HA	1:A:330:TYR:CD2	2.47	0.50
1:A:472:HIS:ND1	1:A:473:PRO:HA	2.26	0.50
1:D:232:MET:O	1:D:236:ILE:HG13	2.12	0.50
1:D:114:TRP:HZ3	1:D:117:ARG:HH11	1.58	0.50
1:A:131:TYR:C	1:A:131:TYR:CD2	2.90	0.50
1:A:250:GLN:HB3	1:A:274:THR:CG2	2.41	0.50
1:B:410:GLU:H	1:B:410:GLU:CD	2.17	0.50
1:D:408:PRO:O	1:D:409:LEU:C	2.53	0.50
1:B:408:PRO:O	1:B:409:LEU:C	2.54	0.50
1:C:43:PHE:HB2	1:C:130:ALA:C	2.37	0.50
1:C:148:LYS:H	1:C:148:LYS:HD2	1.77	0.50
1:D:49:LEU:N	1:D:49:LEU:HD12	2.27	0.50
1:D:172:GLY:HA2	1:D:175:GLU:HG2	1.93	0.50
1:A:131:TYR:HE2	1:A:133:GLN:HG3	1.77	0.49
1:A:141:LYS:HD2	1:A:149:GLU:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ILE:HG23	1:B:158:LEU:HD23	1.94	0.49
1:C:70:MET:CG	1:C:101:MET:HE3	2.42	0.49
1:C:149:GLU:HG3	4:C:614:HOH:O	2.10	0.49
1:A:325:ASN:HB2	4:A:567:HOH:O	2.12	0.49
1:B:183:LEU:HD22	1:B:288:MET:SD	2.52	0.49
1:C:322:GLU:HG2	1:C:332:ILE:HG22	1.95	0.49
1:C:107:ASN:ND2	1:C:107:ASN:O	2.46	0.49
1:A:13:TYR:O	1:A:154:ALA:HA	2.11	0.49
1:A:72:GLN:HE21	1:A:76:LEU:HD11	1.76	0.49
1:A:84:ARG:HH11	1:A:84:ARG:HG3	1.77	0.49
1:C:138:HIS:O	1:C:153:SER:HA	2.13	0.49
1:C:247:PHE:N	1:C:247:PHE:HD2	2.10	0.49
1:A:135:ILE:CD1	1:A:151:ILE:HD13	2.43	0.49
1:C:378:LEU:HG	1:C:441:LEU:CD1	2.43	0.49
1:D:144:ASN:ND2	1:D:145:ASN:H	2.10	0.49
1:A:250:GLN:C	1:A:274:THR:HG22	2.36	0.49
1:C:70:MET:HE3	1:C:208:PHE:CZ	2.47	0.49
1:D:133:GLN:O	1:D:140:ILE:HG13	2.13	0.49
1:D:219:MET:HE1	1:D:253:PRO:CD	2.43	0.49
1:B:80:LEU:CD1	1:B:94:VAL:HG21	2.41	0.49
1:B:232:MET:CE	1:B:439:HIS:CB	2.91	0.49
1:B:393:LYS:HD3	1:B:394:PHE:CE1	2.47	0.49
1:B:90:VAL:HG12	1:B:91:GLU:N	2.28	0.48
1:A:255:LYS:HE3	1:A:257:GLU:HB3	1.94	0.48
1:B:411:TRP:O	1:B:414:PRO:HD2	2.13	0.48
1:C:64:CYS:HA	1:C:67:LYS:HE2	1.94	0.48
1:D:316:ILE:HD12	1:D:335:ILE:HG21	1.95	0.48
1:D:343:THR:HB	1:D:344:PRO:HD3	1.94	0.48
1:A:297:THR:HG21	1:A:316:ILE:HG13	1.96	0.48
1:D:408:PRO:HD2	1:D:411:TRP:CE3	2.48	0.48
1:A:369:ASN:HD22	1:A:384:GLY:HA2	1.79	0.48
1:B:42:ASP:HB3	1:B:127:TYR:HE1	1.78	0.48
1:B:244:GLY:O	1:B:245:ILE:C	2.56	0.48
1:C:98:TRP:CZ2	1:C:102:ILE:HD11	2.48	0.48
1:C:325:ASN:O	1:C:327:PRO:HD3	2.13	0.48
1:D:34:TYR:CE2	1:D:359:ALA:HB2	2.48	0.48
1:A:39:MET:HE1	1:A:152:TYR:CE2	2.48	0.48
1:A:62:VAL:HA	1:A:184:PHE:CD2	2.48	0.48
1:B:36:LYS:HG3	1:B:358:TYR:CD1	2.49	0.48
1:C:26:ALA:HB2	1:C:347:ILE:HG23	1.96	0.48
1:C:68:LYS:HD3	1:D:473:PRO:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:ASN:OD1	1:C:430:LYS:HD3	2.13	0.48
1:B:43:PHE:HB2	1:B:130:ALA:C	2.39	0.48
1:B:186:LEU:HD12	1:B:186:LEU:HA	1.53	0.48
1:D:193:THR:HG22	1:D:194:LEU:N	2.27	0.48
1:D:461:THR:HG21	1:D:463:LYS:HB3	1.96	0.48
1:A:219:MET:HG2	1:A:251:PHE:O	2.14	0.48
1:B:254:ILE:HD11	1:B:270:VAL:CG1	2.44	0.48
1:C:171:PRO:CB	1:C:255:LYS:HE2	2.44	0.48
1:A:249:ARG:NH2	4:A:642:HOH:O	2.47	0.48
1:D:97:ASP:OD1	1:D:100:ARG:HB2	2.14	0.48
1:D:366:ASP:OD2	1:D:457:LYS:HE3	2.14	0.48
1:A:268:ARG:HH11	1:A:281:GLU:CD	2.22	0.48
1:B:315:LYS:HD2	1:B:336:LEU:O	2.14	0.48
1:D:229:ASP:HB2	1:D:386:SER:OG	2.14	0.48
1:A:141:LYS:HE3	1:A:149:GLU:OE1	2.14	0.47
1:A:298:ARG:NH1	4:A:648:HOH:O	2.25	0.47
1:A:193:THR:HG22	1:A:194:LEU:N	2.29	0.47
1:B:72:GLN:O	1:B:76:LEU:HG	2.13	0.47
1:D:425:ILE:C	1:D:426:ILE:HD12	2.39	0.47
1:B:61:ASN:HA	1:B:109:ILE:HD13	1.96	0.47
1:B:163:GLU:C	1:B:164:ARG:HG2	2.39	0.47
1:C:315:LYS:HD3	1:C:337:GLU:HA	1.95	0.47
1:C:318:VAL:HG21	1:C:336:LEU:HD21	1.96	0.47
1:D:21:GLY:HA2	1:D:56:GLY:O	2.15	0.47
1:A:378:LEU:HD23	1:A:441:LEU:HD11	1.96	0.47
1:A:480:THR:OG1	1:A:481:THR:HG23	2.13	0.47
1:D:229:ASP:OD1	1:D:231:ASP:HB3	2.14	0.47
1:D:259:ILE:HD11	1:D:268:ARG:HE	1.80	0.47
1:D:305:VAL:HG22	1:D:305:VAL:O	2.15	0.47
1:C:205:CYS:HA	1:C:208:PHE:CD2	2.49	0.47
1:C:332:ILE:CA	1:C:336:LEU:CD1	2.91	0.47
1:A:39:MET:HE1	1:A:152:TYR:CE1	2.49	0.47
1:A:325:ASN:CB	4:A:567:HOH:O	2.61	0.47
1:A:409:LEU:HG	1:B:69:LEU:CD2	2.45	0.47
1:B:308:LYS:CA	1:B:325:ASN:HD21	2.21	0.47
1:C:172:GLY:HA2	1:C:175:GLU:HG2	1.97	0.47
1:C:247:PHE:C	1:C:248:ILE:HG12	2.38	0.47
1:C:385:LEU:HD22	1:C:389:LYS:HG2	1.95	0.47
1:D:156:ARG:HG3	1:D:156:ARG:NH1	2.30	0.47
1:D:283:GLU:HG2	4:D:539:HOH:O	2.15	0.47
1:D:475:CYS:O	1:D:477:GLU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:THR:HG22	1:A:462:LYS:N	2.29	0.47
1:B:472:HIS:ND1	1:B:473:PRO:HA	2.29	0.47
1:B:485:THR:HG23	1:B:488:SER:CB	2.45	0.47
1:D:200:TYR:O	1:D:201:VAL:C	2.57	0.47
1:B:168:LEU:HB3	1:B:170:ILE:HG23	1.97	0.47
1:B:308:LYS:N	1:B:325:ASN:ND2	2.24	0.47
1:B:408:PRO:HD2	1:B:411:TRP:CE3	2.49	0.47
1:C:97:ASP:OD1	1:C:100:ARG:HB2	2.14	0.47
1:C:315:LYS:HD3	1:C:336:LEU:O	2.15	0.47
1:D:137:PRO:HA	1:D:305:VAL:HG23	1.97	0.47
1:A:303:GLU:OE1	1:A:304:THR:N	2.45	0.47
1:B:49:LEU:HA	1:B:49:LEU:HD23	1.55	0.47
1:B:393:LYS:HD3	1:B:394:PHE:CZ	2.50	0.47
1:C:281:GLU:O	1:C:281:GLU:CG	2.62	0.47
1:A:171:PRO:HG2	1:A:255:LYS:HB2	1.96	0.46
1:B:72:GLN:NE2	1:B:76:LEU:HD21	2.29	0.46
1:C:136:GLY:O	1:C:137:PRO:C	2.57	0.46
1:C:232:MET:O	1:C:236:ILE:CD1	2.55	0.46
1:D:200:TYR:CD2	1:D:201:VAL:N	2.83	0.46
1:B:105:VAL:O	1:B:109:ILE:HG13	2.15	0.46
1:B:485:THR:CG2	1:B:488:SER:HB3	2.43	0.46
1:A:144:ASN:ND2	1:A:148:LYS:HB2	2.31	0.46
1:A:408:PRO:O	1:A:409:LEU:C	2.59	0.46
1:B:215:ASP:OD1	1:B:246:LYS:NZ	2.42	0.46
1:B:272:GLN:HG3	1:B:279:ILE:CG1	2.45	0.46
1:C:194:LEU:HD22	1:C:284:TYR:CE1	2.50	0.46
1:D:43:PHE:HB2	1:D:130:ALA:C	2.40	0.46
1:B:254:ILE:HG12	1:B:270:VAL:O	2.16	0.46
1:B:367:TYR:CD1	1:B:367:TYR:N	2.84	0.46
1:C:85:ASN:OD1	1:C:414:PRO:HA	2.15	0.46
1:C:385:LEU:CA	1:C:389:LYS:HE3	2.43	0.46
1:D:305:VAL:HG21	1:D:328:TYR:OH	2.15	0.46
1:A:55:LEU:HD23	1:A:117:ARG:HG2	1.97	0.46
1:A:409:LEU:HD23	1:B:68:LYS:HG2	1.98	0.46
1:B:158:LEU:HD21	1:B:332:ILE:CD1	2.46	0.46
1:C:114:TRP:O	1:C:118:VAL:HG23	2.16	0.46
1:C:413:ILE:HD12	1:D:104:ALA:HB1	1.98	0.46
1:A:286:THR:HG22	1:A:287:VAL:N	2.31	0.46
1:B:200:TYR:CD1	1:B:374:VAL:HG22	2.50	0.46
1:D:270:VAL:HG22	1:D:281:GLU:CG	2.22	0.46
1:D:407:TRP:CZ3	1:D:412:THR:HG22	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLU:OE1	1:A:420:LYS:HE3	2.16	0.46
1:D:25:LEU:O	1:D:29:LYS:HG3	2.15	0.46
1:D:225:LEU:O	1:D:226:ARG:C	2.59	0.46
1:A:135:ILE:HD11	1:A:151:ILE:CG2	2.45	0.46
1:D:192:LYS:HG2	1:D:284:TYR:HD2	1.80	0.46
1:D:422:TYR:HE2	1:D:424:LYS:HG2	1.79	0.46
1:A:84:ARG:HD2	1:A:90:VAL:HB	1.98	0.46
1:A:303:GLU:OE1	1:A:304:THR:CG2	2.64	0.46
1:B:9:LYS:O	1:B:9:LYS:CG	2.64	0.46
1:C:135:ILE:HD11	1:C:151:ILE:HD13	1.97	0.46
1:C:191:GLY:O	1:C:192:LYS:C	2.59	0.46
1:A:210:ALA:CB	1:A:245:ILE:CD1	2.94	0.45
1:A:318:VAL:HG13	1:A:319:THR:O	2.16	0.45
1:B:272:GLN:HG3	1:B:279:ILE:HG12	1.97	0.45
1:C:300:ILE:CD1	1:C:302:LEU:HD21	2.46	0.45
1:C:398:ASN:HB3	1:C:430:LYS:HG2	1.97	0.45
1:A:343:THR:HB	1:A:344:PRO:HD2	1.98	0.45
1:D:465:LEU:HD21	1:D:479:PHE:O	2.16	0.45
1:A:44:VAL:HG11	1:A:53:TRP:H	1.81	0.45
1:B:250:GLN:C	1:B:274:THR:CG2	2.90	0.45
1:B:251:PHE:HE2	1:B:280:ILE:HG12	1.76	0.45
1:C:183:LEU:HD22	1:C:288:MET:HE2	1.97	0.45
1:B:435:VAL:HG21	1:B:460:LEU:HD23	1.99	0.45
1:C:13:TYR:O	1:C:154:ALA:HA	2.16	0.45
1:C:484:VAL:HG13	1:C:490:ALA:HB3	1.98	0.45
1:A:95:LYS:HB2	1:A:95:LYS:HE3	1.74	0.45
1:A:474:VAL:O	1:A:477:GLU:HG2	2.16	0.45
1:D:106:GLN:OE1	1:D:106:GLN:HA	2.17	0.45
1:A:34:TYR:HD1	1:A:358:TYR:HB2	1.81	0.45
1:B:168:LEU:CB	1:B:170:ILE:HG23	2.46	0.45
1:C:106:GLN:NE2	1:C:184:PHE:O	2.50	0.45
1:D:402:TYR:CE2	1:D:462:LYS:HE3	2.52	0.45
1:B:250:GLN:O	1:B:251:PHE:CD1	2.70	0.45
1:C:351:ARG:NH1	4:C:530:HOH:O	2.43	0.45
1:A:22:SER:OG	1:A:343:THR:HG23	2.16	0.45
1:A:138:HIS:O	1:A:153:SER:HA	2.17	0.45
1:A:249:ARG:HA	1:A:249:ARG:HD2	1.77	0.45
1:A:333:GLY:HA3	2:A:900:FAD:O2P	2.17	0.45
1:C:8:PRO:HG2	1:C:9:LYS:H	1.81	0.45
1:D:245:ILE:H	1:D:245:ILE:HG13	1.62	0.45
1:A:163:GLU:OE2	1:A:315:LYS:NZ	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ILE:CD1	1:A:270:VAL:HG12	2.47	0.44
1:A:321:GLU:O	1:A:322:GLU:HB2	2.17	0.44
1:B:342:LEU:HB2	1:B:345:VAL:HG23	1.99	0.44
1:B:474:VAL:O	1:B:477:GLU:HG2	2.17	0.44
1:C:68:LYS:O	1:C:71:HIS:HB3	2.17	0.44
1:C:106:GLN:HA	1:C:109:ILE:HG13	1.99	0.44
1:D:236:ILE:HD11	1:D:380:TYR:CD2	2.51	0.44
1:D:403:HIS:CE1	1:D:492:ILE:HD12	2.50	0.44
1:A:70:MET:HE3	1:A:184:PHE:CD1	2.51	0.44
1:A:447:GLU:OE1	1:B:474:VAL:HG23	2.17	0.44
1:D:167:TYR:CE2	1:D:174:LYS:HA	2.52	0.44
1:D:423:ALA:HB1	1:D:479:PHE:CZ	2.53	0.44
1:D:461:THR:HB	1:D:464:GLN:NE2	2.32	0.44
1:A:166:ARG:HG2	1:A:291:ILE:CD1	2.43	0.44
1:B:70:MET:SD	1:B:101:MET:HE3	2.58	0.44
1:B:179:SER:O	1:B:180:SER:C	2.60	0.44
1:A:340:VAL:CG1	1:A:342:LEU:HD12	2.48	0.44
1:A:144:ASN:OD1	1:A:146:LYS:N	2.50	0.44
1:A:140:ILE:CG1	1:A:141:LYS:N	2.79	0.44
1:A:387:GLU:O	1:A:391:VAL:HG23	2.18	0.44
1:C:36:LYS:HG3	1:C:358:TYR:CD1	2.53	0.44
1:C:70:MET:SD	1:C:101:MET:CE	3.05	0.44
1:D:187:PRO:HG2	1:D:188:TYR:HD2	1.80	0.44
1:A:315:LYS:HD3	1:A:336:LEU:O	2.18	0.44
1:B:136:GLY:O	1:B:137:PRO:C	2.61	0.44
1:C:26:ALA:CB	1:C:347:ILE:HG23	2.48	0.44
1:C:65:ILE:N	1:C:65:ILE:CD1	2.81	0.44
1:C:199:SER:O	1:C:202:ALA:HB3	2.18	0.44
1:A:336:LEU:HD23	1:A:336:LEU:HA	1.77	0.44
1:A:411:TRP:CZ2	1:A:443:PRO:HG3	2.53	0.44
1:B:343:THR:HB	1:B:344:PRO:HD3	2.00	0.44
1:C:302:LEU:HD22	1:C:307:VAL:HG11	1.99	0.44
1:D:300:ILE:O	1:D:300:ILE:HG13	2.17	0.44
1:A:348:GLN:HA	1:A:348:GLN:OE1	2.18	0.44
1:B:221:ARG:HG3	1:B:222:SER:N	2.33	0.44
1:D:170:ILE:HB	1:D:171:PRO:CD	2.48	0.44
1:D:193:THR:CG2	1:D:194:LEU:N	2.81	0.44
1:A:141:LYS:HG3	1:A:142:ALA:N	2.31	0.43
1:B:302:LEU:HD13	1:B:307:VAL:HB	2.00	0.43
1:B:318:VAL:CG2	1:B:322:GLU:C	2.90	0.43
1:D:173:ASP:OD1	1:D:173:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:GLN:C	1:D:274:THR:HG22	2.42	0.43
1:D:411:TRP:C	1:D:414:PRO:HD2	2.43	0.43
1:A:70:MET:HE1	1:A:184:PHE:HA	1.99	0.43
1:A:492:ILE:O	1:A:494:GLN:N	2.52	0.43
1:B:185:SER:O	1:B:186:LEU:C	2.61	0.43
1:C:11:TYR:HD1	1:C:153:SER:OG	2.00	0.43
1:C:413:ILE:N	1:C:414:PRO:HD2	2.33	0.43
1:A:25:LEU:O	1:A:29:LYS:HD3	2.18	0.43
1:A:166:ARG:HH11	1:A:291:ILE:CD1	2.31	0.43
1:A:303:GLU:OE1	1:A:304:THR:HG22	2.18	0.43
1:C:47:THR:HG21	1:C:181:ASP:HB3	2.00	0.43
1:D:266:ARG:C	1:D:267:LEU:HD23	2.43	0.43
1:B:239:HIS:O	1:B:243:HIS:ND1	2.27	0.43
1:A:65:ILE:O	1:A:69:LEU:HD12	2.19	0.43
1:D:170:ILE:HB	1:D:171:PRO:HD2	1.99	0.43
1:A:161:THR:HG23	1:A:335:ILE:HG13	2.00	0.43
1:A:250:GLN:HB3	1:A:274:THR:HG22	1.99	0.43
1:B:192:LYS:H	1:B:285:ASN:HD22	1.67	0.43
1:B:345:VAL:O	1:B:346:ALA:C	2.62	0.43
1:C:95:LYS:O	1:D:89:LYS:HG3	2.18	0.43
1:C:246:LYS:C	1:C:247:PHE:CD2	2.96	0.43
1:C:302:LEU:HD13	1:C:309:ILE:CG2	2.48	0.43
1:D:399:ILE:HD12	1:D:428:ASN:HA	2.00	0.43
1:C:85:ASN:HB3	1:C:413:ILE:HG22	1.99	0.43
1:D:254:ILE:CD1	1:D:270:VAL:HG12	2.49	0.43
1:A:177:CYS:HB3	1:A:289:LEU:HD23	2.00	0.43
1:A:245:ILE:H	1:A:245:ILE:CD1	2.29	0.43
1:B:309:ILE:HG22	1:B:316:ILE:HG12	2.00	0.43
1:C:199:SER:O	1:C:200:TYR:C	2.60	0.43
1:A:193:THR:CG2	1:A:194:LEU:N	2.82	0.43
1:A:493:LEU:H	1:A:493:LEU:HG	1.51	0.43
1:B:321:GLU:O	1:B:322:GLU:HB2	2.17	0.43
1:C:409:LEU:HG	1:D:69:LEU:CD2	2.49	0.43
1:D:16:ILE:HD12	1:D:157:PHE:CZ	2.54	0.43
1:A:161:THR:CG2	1:A:335:ILE:HG13	2.49	0.43
1:A:168:LEU:HB3	1:A:170:ILE:HG23	2.00	0.43
1:A:427:CYS:HA	1:A:434:ARG:O	2.19	0.43
1:A:435:VAL:O	1:A:456:LEU:HD22	2.19	0.43
1:B:387:GLU:HG3	1:B:426:ILE:HD12	2.01	0.43
1:C:8:PRO:CG	1:C:9:LYS:H	2.32	0.43
1:D:488:SER:OG	1:D:489:GLY:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLY:O	1:A:137:PRO:C	2.61	0.42
1:A:225:LEU:O	1:A:226:ARG:C	2.61	0.42
1:A:259:ILE:O	1:A:259:ILE:HG22	2.19	0.42
1:B:120:LEU:HD23	1:B:120:LEU:HA	1.74	0.42
1:B:352:LEU:HD23	1:B:352:LEU:HA	1.87	0.42
1:C:70:MET:CE	1:C:208:PHE:CZ	3.01	0.42
1:C:186:LEU:HD12	1:C:186:LEU:HA	1.82	0.42
1:C:214:LEU:O	1:C:216:VAL:HG23	2.19	0.42
1:C:430:LYS:HB3	1:C:430:LYS:HE3	1.84	0.42
1:D:254:ILE:HD11	1:D:270:VAL:HG12	2.01	0.42
1:D:259:ILE:O	1:D:260:GLU:HB2	2.19	0.42
1:D:318:VAL:HG22	1:D:322:GLU:C	2.44	0.42
1:A:34:TYR:CE1	1:A:359:ALA:HB2	2.54	0.42
1:B:124:LYS:HE3	4:B:625:HOH:O	2.18	0.42
1:B:158:LEU:HA	1:B:330:TYR:O	2.19	0.42
1:C:36:LYS:HA	1:C:36:LYS:HD3	1.89	0.42
1:C:333:GLY:HA3	2:C:900:FAD:O2P	2.20	0.42
1:D:380:TYR:CD1	1:D:380:TYR:C	2.93	0.42
1:B:318:VAL:HG22	1:B:322:GLU:C	2.43	0.42
1:D:68:LYS:O	1:D:71:HIS:HB3	2.19	0.42
1:A:300:ILE:HG13	1:A:302:LEU:HG	2.01	0.42
1:B:16:ILE:HG13	1:B:154:ALA:HB2	1.99	0.42
1:C:408:PRO:O	1:C:409:LEU:C	2.61	0.42
1:D:158:LEU:HD21	1:D:332:ILE:CD1	2.50	0.42
1:D:325:ASN:ND2	1:D:326:VAL:HG23	2.35	0.42
1:D:431:ASP:CG	1:D:434:ARG:HH21	2.28	0.42
1:D:434:ARG:HE	1:D:434:ARG:HB2	1.62	0.42
1:C:65:ILE:HB	1:C:66:PRO:HD3	2.01	0.42
1:D:13:TYR:CE1	1:D:39:MET:HE2	2.54	0.42
1:D:136:GLY:O	1:D:137:PRO:C	2.61	0.42
1:D:403:HIS:CE1	1:D:492:ILE:CD1	3.02	0.42
1:A:409:LEU:HG	1:B:69:LEU:HD21	2.02	0.42
1:C:259:ILE:O	1:C:259:ILE:HG22	2.19	0.42
1:D:25:LEU:CD2	1:D:120:LEU:HD11	2.49	0.42
1:D:461:THR:H	1:D:464:GLN:NE2	2.03	0.42
1:A:434:ARG:NH1	1:A:459:GLY:O	2.53	0.42
1:C:7:LEU:HB2	1:C:9:LYS:NZ	2.34	0.42
1:C:72:GLN:HA	1:C:72:GLN:OE1	2.20	0.42
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.84	0.42
1:B:305:VAL:CG1	1:B:307:VAL:HG23	2.49	0.42
1:C:148:LYS:H	1:C:148:LYS:CD	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:GLU:CD	1:D:474:VAL:HG13	2.45	0.42
1:D:219:MET:HE1	1:D:253:PRO:HD3	2.02	0.42
1:D:230:GLN:HB2	1:D:388:GLU:OE2	2.19	0.42
1:A:62:VAL:O	1:A:184:PHE:HE2	2.03	0.42
1:A:244:GLY:O	1:A:245:ILE:C	2.60	0.42
1:C:183:LEU:CD2	1:C:288:MET:HE1	2.44	0.42
1:C:245:ILE:CG2	1:C:247:PHE:CE2	2.97	0.42
1:D:188:TYR:CE1	1:D:264:PRO:HB3	2.54	0.42
1:D:320:ASP:OD2	1:D:321:GLU:HG3	2.20	0.42
1:D:422:TYR:HE2	1:D:424:LYS:HD3	1.85	0.42
1:A:35:GLY:O	1:A:36:LYS:HE2	2.19	0.42
1:A:161:THR:HG23	1:A:335:ILE:CD1	2.49	0.42
1:A:355:GLN:HB3	1:A:361:SER:CB	2.50	0.42
1:A:470:GLY:HA2	1:A:480:THR:HG21	2.02	0.42
1:B:9:LYS:C	1:B:11:TYR:H	2.25	0.42
1:C:97:ASP:OD2	1:C:97:ASP:C	2.62	0.42
1:C:461:THR:CG2	1:C:463:LYS:H	2.17	0.42
1:D:64:CYS:HA	1:D:67:LYS:HE2	2.01	0.42
1:D:95:LYS:HB3	1:D:95:LYS:HE2	1.85	0.42
1:D:318:VAL:HG22	1:D:323:GLN:O	2.19	0.42
1:D:318:VAL:CG1	1:D:336:LEU:HD22	2.49	0.42
1:A:162:GLY:O	1:A:335:ILE:CD1	2.64	0.41
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.70	0.41
1:A:251:PHE:CE2	1:A:280:ILE:HD13	2.55	0.41
1:A:254:ILE:HD11	1:A:270:VAL:CG1	2.50	0.41
1:A:355:GLN:HB3	1:A:361:SER:HB3	2.02	0.41
1:D:80:LEU:HD13	1:D:94:VAL:HG11	2.01	0.41
1:D:176:TYR:CZ	1:D:258:GLN:HB3	2.55	0.41
1:A:217:THR:HG22	1:A:218:VAL:N	2.34	0.41
1:A:344:PRO:HD3	1:B:472:HIS:HB2	2.01	0.41
1:B:16:ILE:HG13	1:B:154:ALA:CB	2.50	0.41
1:C:472:HIS:HD1	1:C:473:PRO:HA	1.86	0.41
1:D:258:GLN:NE2	1:D:261:ALA:CB	2.83	0.41
1:B:224:LEU:O	1:B:225:LEU:C	2.64	0.41
1:C:66:PRO:CG	1:C:109:ILE:HD11	2.50	0.41
1:C:70:MET:HG2	1:C:101:MET:HE3	2.01	0.41
1:D:138:HIS:O	1:D:153:SER:HA	2.20	0.41
1:D:158:LEU:HD21	1:D:332:ILE:HD13	2.03	0.41
1:D:170:ILE:HD12	1:D:254:ILE:C	2.46	0.41
1:A:302:LEU:CD1	1:A:309:ILE:HG21	2.50	0.41
1:A:351:ARG:HE	1:A:351:ARG:HB3	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:LYS:HD3	1:A:430:LYS:HA	1.79	0.41
1:B:12:ASP:HB2	1:B:153:SER:O	2.20	0.41
1:B:399:ILE:O	1:B:399:ILE:HG22	2.20	0.41
1:C:272:GLN:HE21	1:C:272:GLN:HB3	1.57	0.41
1:D:250:GLN:HB3	1:D:274:THR:HG22	2.01	0.41
1:B:19:GLY:HA3	1:B:160:ALA:O	2.21	0.41
1:C:316:ILE:O	1:C:318:VAL:HG13	2.21	0.41
1:C:434:ARG:NH1	1:C:459:GLY:O	2.46	0.41
1:C:473:PRO:O	1:D:68:LYS:NZ	2.46	0.41
1:D:224:LEU:O	1:D:225:LEU:C	2.60	0.41
1:A:17:ILE:HB	1:A:40:VAL:HG13	2.02	0.41
1:B:378:LEU:HD12	1:B:378:LEU:HA	1.81	0.41
1:C:72:GLN:HG2	1:D:410:GLU:HG3	2.02	0.41
1:C:179:SER:O	1:C:180:SER:C	2.63	0.41
1:D:225:LEU:HB3	1:D:228:PHE:CD2	2.53	0.41
1:D:251:PHE:CD2	1:D:280:ILE:HD11	2.55	0.41
1:A:135:ILE:HD11	1:A:151:ILE:HG23	2.02	0.41
1:A:209:LEU:HD23	1:A:209:LEU:HA	1.94	0.41
1:A:457:LYS:HD2	1:B:467:SER:OG	2.21	0.41
1:B:188:TYR:CD1	1:B:188:TYR:C	2.99	0.41
1:C:73:ALA:HB2	1:D:86:TYR:HD1	1.86	0.41
1:C:133:GLN:O	1:C:140:ILE:HG12	2.21	0.41
1:A:67:LYS:HD2	1:A:67:LYS:C	2.46	0.41
1:B:131:TYR:CE2	1:B:132:GLY:O	2.74	0.41
1:B:158:LEU:HD21	1:B:332:ILE:HD11	2.02	0.41
1:C:155:GLU:O	1:C:155:GLU:CG	2.69	0.41
1:C:461:THR:CG2	1:C:462:LYS:N	2.84	0.41
1:C:469:ILE:HD13	1:C:469:ILE:HA	1.83	0.41
1:D:135:ILE:HG13	1:D:136:GLY:N	2.36	0.41
1:A:16:ILE:HB	1:A:157:PHE:CE2	2.56	0.41
1:A:85:ASN:HB2	1:A:413:ILE:HG22	2.03	0.41
1:A:258:GLN:OE1	1:A:261:ALA:CB	2.66	0.41
1:A:342:LEU:O	1:A:343:THR:C	2.63	0.41
1:B:117:ARG:HE	1:B:117:ARG:HB2	1.43	0.41
1:D:67:LYS:NZ	1:D:204:GLU:OE1	2.45	0.41
1:A:316:ILE:HD12	1:A:335:ILE:HG21	2.03	0.41
1:B:401:VAL:CG1	1:B:486:LYS:HD2	2.40	0.41
1:C:166:ARG:HG2	1:C:167:TYR:N	2.36	0.41
1:C:396:GLU:C	1:C:396:GLU:CD	2.88	0.41
1:D:249:ARG:NH1	4:D:505:HOH:O	2.54	0.41
1:A:323:GLN:HG3	1:A:330:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LEU:HD23	1:B:336:LEU:HA	1.75	0.40
1:B:434:ARG:HE	1:B:434:ARG:HB2	1.71	0.40
1:D:322:GLU:HG2	1:D:332:ILE:HG22	2.02	0.40
1:D:459:GLY:O	1:D:460:LEU:C	2.64	0.40
1:A:344:PRO:HB2	1:B:469:ILE:CG2	2.49	0.40
1:B:108:HIS:O	1:B:111:SER:HB3	2.21	0.40
1:D:48:PRO:HB2	1:D:49:LEU:HD12	2.02	0.40
1:D:62:VAL:HA	1:D:184:PHE:CD2	2.55	0.40
1:D:331:ALA:O	1:D:336:LEU:HD21	2.21	0.40
1:D:427:CYS:HA	1:D:434:ARG:O	2.21	0.40
1:A:57:GLY:O	1:A:61:ASN:ND2	2.45	0.40
1:A:308:LYS:H	1:A:325:ASN:CG	2.28	0.40
1:A:385:LEU:HD12	1:A:390:ALA:HA	2.03	0.40
1:B:316:ILE:O	1:B:317:PRO:C	2.64	0.40
1:C:137:PRO:O	1:C:139:ARG:N	2.54	0.40
1:C:171:PRO:CB	1:C:255:LYS:HG3	2.49	0.40
1:C:268:ARG:NH1	1:C:270:VAL:CG2	2.84	0.40
1:D:116:TYR:O	1:D:117:ARG:C	2.63	0.40
1:B:302:LEU:HD13	1:B:307:VAL:CG1	2.51	0.40
1:B:318:VAL:HG22	1:B:323:GLN:N	2.36	0.40
1:C:67:LYS:HD2	1:C:68:LYS:CA	2.52	0.40
1:C:277:GLU:H	1:C:277:GLU:HG3	1.33	0.40
1:C:281:GLU:O	1:C:281:GLU:HG3	2.21	0.40
1:C:463:LYS:HE2	1:C:463:LYS:HB3	1.87	0.40
1:D:293:ARG:HG2	1:D:293:ARG:NH1	2.36	0.40
1:D:461:THR:N	1:D:464:GLN:NE2	2.61	0.40
1:A:163:GLU:HG2	1:A:295:ALA:HA	2.03	0.40
1:A:259:ILE:O	1:A:260:GLU:CB	2.66	0.40
1:B:58:THR:O	1:B:63:GLY:N	2.54	0.40
1:B:460:LEU:HA	1:B:464:GLN:OE1	2.22	0.40
1:C:249:ARG:HA	1:C:249:ARG:HD2	1.80	0.40
1:C:318:VAL:HG23	1:C:319:THR:O	2.22	0.40
1:D:221:ARG:NH1	1:D:252:VAL:HG21	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	489/513 (95%)	442 (90%)	40 (8%)	7 (1%)	9	30
1	B	485/513 (94%)	441 (91%)	40 (8%)	4 (1%)	16	44
1	C	485/513 (94%)	435 (90%)	43 (9%)	7 (1%)	9	30
1	D	482/513 (94%)	437 (91%)	41 (8%)	4 (1%)	16	44
All	All	1941/2052 (95%)	1755 (90%)	164 (8%)	22 (1%)	11	36

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	495	ALA
1	C	9	LYS
1	C	138	HIS
1	A	138	HIS
1	B	476	ALA
1	C	260	GLU
1	D	476	ALA
1	A	260	GLU
1	A	498	CYS
1	C	8	PRO
1	D	138	HIS
1	B	22	SER
1	D	260	GLU
1	A	245	ILE
1	A	493	LEU
1	C	476	ALA
1	C	327	PRO
1	A	327	PRO
1	B	245	ILE
1	C	245	ILE
1	D	245	ILE
1	B	473	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	402/422 (95%)	352 (88%)	50 (12%)	4	16
1	B	401/422 (95%)	353 (88%)	48 (12%)	5	17
1	C	401/422 (95%)	360 (90%)	41 (10%)	7	23
1	D	398/422 (94%)	353 (89%)	45 (11%)	5	19
All	All	1602/1688 (95%)	1418 (88%)	184 (12%)	5	18

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	18	ILE
1	A	39	MET
1	A	40	VAL
1	A	46	PRO
1	A	48	PRO
1	A	51	THR
1	A	52	ARG
1	A	58	THR
1	A	64	CYS
1	A	67	LYS
1	A	81	GLN
1	A	84	ARG
1	A	93	THR
1	A	109	ILE
1	A	111	SER
1	A	121	ARG
1	A	137	PRO
1	A	141	LYS
1	A	143	THR
1	A	149	GLU
1	A	166	ARG
1	A	170	ILE
1	A	175	GLU

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Mol	Chain	Res	Type
1	A	179	SER
1	A	185	SER
1	A	212	ILE
1	A	236	ILE
1	A	238	GLU
1	A	255	LYS
1	A	272	GLN
1	A	280	ILE
1	A	291	ILE
1	A	303	GLU
1	A	304	THR
1	A	309	ILE
1	A	318	VAL
1	A	320	ASP
1	A	327	PRO
1	A	341	GLU
1	A	362	THR
1	A	368	GLU
1	A	373	THR
1	A	376	THR
1	A	397	GLU
1	A	413	ILE
1	A	473	PRO
1	A	474	VAL
1	A	491	SER
1	A	497	CYS
1	B	45	THR
1	B	46	PRO
1	B	48	PRO
1	B	52	ARG
1	B	64	CYS
1	B	70	MET
1	B	84	ARG
1	B	92	GLU
1	B	93	THR
1	B	94	VAL
1	B	100	ARG
1	B	109	ILE
1	B	114	TRP
1	B	133	GLN
1	B	137	PRO
1	B	140	ILE

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Mol	Chain	Res	Type
1	B	143	THR
1	B	145	ASN
1	B	161	THR
1	B	170	ILE
1	B	171	PRO
1	B	180	SER
1	B	194	LEU
1	B	195	VAL
1	B	240	MET
1	B	270	VAL
1	B	274	THR
1	B	299	LYS
1	B	303	GLU
1	B	305	VAL
1	B	332	ILE
1	B	347	ILE
1	B	367	TYR
1	B	376	THR
1	B	377	PRO
1	B	396	GLU
1	B	397	GLU
1	B	399	ILE
1	B	400	GLU
1	B	413	ILE
1	B	432	ASN
1	B	433	GLU
1	B	435	VAL
1	B	456	LEU
1	B	457	LYS
1	B	474	VAL
1	B	488	SER
1	B	492	ILE
1	C	7	LEU
1	C	9	LYS
1	C	15	LEU
1	C	48	PRO
1	C	52	ARG
1	C	64	CYS
1	C	93	THR
1	C	107	ASN
1	C	109	ILE
1	C	126	VAL

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Mol	Chain	Res	Type
1	C	133	GLN
1	C	137	PRO
1	C	140	ILE
1	C	143	THR
1	C	144	ASN
1	C	149	GLU
1	C	150	LYS
1	C	153	SER
1	C	180	SER
1	C	185	SER
1	C	193	THR
1	C	194	LEU
1	C	200	TYR
1	C	223	ILE
1	C	247	PHE
1	C	248	ILE
1	C	250	GLN
1	C	272	GLN
1	C	275	ASN
1	C	277	GLU
1	C	279	ILE
1	C	289	LEU
1	C	303	GLU
1	C	305	VAL
1	C	309	ILE
1	C	318	VAL
1	C	327	PRO
1	C	336	LEU
1	C	376	THR
1	C	424	LYS
1	C	474	VAL
1	D	18	ILE
1	D	64	CYS
1	D	80	LEU
1	D	91	GLU
1	D	92	GLU
1	D	93	THR
1	D	107	ASN
1	D	111	SER
1	D	117	ARG
1	D	141	LYS
1	D	144	ASN

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Mol	Chain	Res	Type
1	D	146	LYS
1	D	149	GLU
1	D	159	ILE
1	D	175	GLU
1	D	187	PRO
1	D	194	LEU
1	D	219	MET
1	D	230	GLN
1	D	254	ILE
1	D	259	ILE
1	D	277	GLU
1	D	280	ILE
1	D	297	THR
1	D	303	GLU
1	D	309	ILE
1	D	318	VAL
1	D	332	ILE
1	D	340	VAL
1	D	361	SER
1	D	368	GLU
1	D	370	VAL
1	D	376	THR
1	D	377	PRO
1	D	386	SER
1	D	398	ASN
1	D	399	ILE
1	D	429	THR
1	D	433	GLU
1	D	457	LYS
1	D	461	THR
1	D	482	LEU
1	D	487	ARG
1	D	488	SER
1	D	492	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	96	HIS
1	A	113	ASN
1	A	129	ASN

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Mol	Chain	Res	Type
1	A	133	GLN
1	A	230	GLN
1	A	285	ASN
1	A	323	GLN
1	A	369	ASN
1	A	418	ASN
1	A	444	ASN
1	A	464	GLN
1	B	234	ASN
1	B	250	GLN
1	B	285	ASN
1	B	355	GLN
1	C	78	GLN
1	C	107	ASN
1	C	113	ASN
1	C	144	ASN
1	C	145	ASN
1	C	234	ASN
1	C	243	HIS
1	C	258	GLN
1	C	272	GLN
1	C	275	ASN
1	C	285	ASN
1	C	323	GLN
1	C	369	ASN
1	C	419	ASN
1	C	444	ASN
1	C	464	GLN
1	D	33	GLN
1	D	129	ASN
1	D	144	ASN
1	D	145	ASN
1	D	258	GLN
1	D	275	ASN
1	D	419	ASN
1	D	464	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
2	FAD	D	900	-	58,58,58	1.34	7 (12%)	85,89,89	1.63	20 (23%)
3	SO4	B	901	-	4,4,4	0.48	0	6,6,6	0.45	0
2	FAD	B	900	-	58,58,58	1.39	8 (13%)	85,89,89	1.61	19 (22%)
3	SO4	C	901	-	4,4,4	0.56	0	6,6,6	0.32	0
2	FAD	C	900	-	58,58,58	1.56	13 (22%)	85,89,89	1.72	18 (21%)
2	FAD	A	900	-	58,58,58	1.45	8 (13%)	85,89,89	1.63	20 (23%)
3	SO4	A	901	-	4,4,4	0.55	0	6,6,6	0.50	0
3	SO4	D	901	-	4,4,4	0.47	0	6,6,6	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	D	900	-	-	2/34/50/50	0/6/6/6
2	FAD	A	900	-	-	2/34/50/50	0/6/6/6
2	FAD	B	900	-	-	2/34/50/50	0/6/6/6
2	FAD	C	900	-	-	2/34/50/50	0/6/6/6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	FAD	P-O3P	5.67	1.65	1.59
2	B	900	FAD	C5A-C4A	3.89	1.46	1.39
2	A	900	FAD	P-O3P	3.85	1.63	1.59
2	D	900	FAD	P-O3P	3.78	1.63	1.59
2	A	900	FAD	C5A-C4A	3.39	1.45	1.39
2	D	900	FAD	C5A-C4A	3.34	1.45	1.39
2	B	900	FAD	C6-C5X	3.25	1.44	1.40
2	D	900	FAD	PA-O3P	3.24	1.63	1.59
2	C	900	FAD	C5X-N5	-2.87	1.34	1.39
2	B	900	FAD	P-O3P	2.83	1.62	1.59
2	C	900	FAD	O2-C2	-2.76	1.18	1.24
2	A	900	FAD	C9A-C5X	2.73	1.45	1.41
2	D	900	FAD	C6-C5X	2.70	1.44	1.40
2	C	900	FAD	PA-O3P	2.64	1.62	1.59
2	C	900	FAD	C2-N1	-2.61	1.30	1.36
2	A	900	FAD	C2-N1	-2.59	1.30	1.36
2	D	900	FAD	C9-C9A	2.52	1.43	1.39
2	A	900	FAD	C6A-N6A	2.50	1.40	1.34
2	A	900	FAD	O4B-C1B	2.46	1.47	1.42
2	C	900	FAD	C9-C9A	2.45	1.43	1.39
2	D	900	FAD	C6A-N6A	2.43	1.40	1.34
2	B	900	FAD	C9A-C5X	2.40	1.45	1.41
2	A	900	FAD	PA-O3P	2.39	1.62	1.59
2	C	900	FAD	O4B-C1B	2.36	1.47	1.42
2	C	900	FAD	C9A-C5X	2.35	1.45	1.41
2	C	900	FAD	O4B-C4B	-2.29	1.39	1.45
2	B	900	FAD	C5X-N5	-2.27	1.35	1.39
2	C	900	FAD	C4X-C4	2.18	1.52	1.44
2	C	900	FAD	P-O2P	2.14	1.65	1.55
2	A	900	FAD	C4X-C10	2.13	1.50	1.44
2	D	900	FAD	C4X-C10	2.13	1.50	1.44
2	B	900	FAD	C4X-C10	2.11	1.50	1.44
2	C	900	FAD	C1'-C2'	2.10	1.55	1.52
2	C	900	FAD	C4X-N5	2.10	1.35	1.30
2	B	900	FAD	C2A-N1A	2.09	1.37	1.33
2	B	900	FAD	C4X-C4	2.03	1.52	1.44

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	FAD	C5A-C4A-N3A	-5.12	119.66	126.72
2	C	900	FAD	N3A-C4A-N9A	4.73	135.21	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	FAD	C5A-C4A-N3A	-4.71	120.23	126.72
2	C	900	FAD	N3A-C2A-N1A	-4.67	121.52	128.58
2	B	900	FAD	C5A-C4A-N3A	-4.66	120.30	126.72
2	A	900	FAD	N3A-C2A-N1A	-4.57	121.66	128.58
2	C	900	FAD	C4-C4X-N5	4.48	124.40	118.21
2	D	900	FAD	N3A-C4A-N9A	4.34	134.55	127.17
2	D	900	FAD	N3A-C2A-N1A	-4.28	122.11	128.58
2	A	900	FAD	N3A-C4A-N9A	4.28	134.44	127.17
2	A	900	FAD	C5A-C4A-N3A	-4.07	121.11	126.72
2	B	900	FAD	N3A-C2A-N1A	-4.00	122.53	128.58
2	B	900	FAD	N3A-C4A-N9A	3.98	133.94	127.17
2	D	900	FAD	C4-C4X-N5	3.95	123.66	118.21
2	C	900	FAD	C5A-N7A-C8A	3.79	109.40	103.45
2	C	900	FAD	C2A-N3A-C4A	3.65	120.74	111.83
2	C	900	FAD	O2-C2-N1	-3.63	115.77	121.80
2	A	900	FAD	C4-C4X-N5	3.44	122.96	118.21
2	D	900	FAD	C5A-N7A-C8A	3.43	108.83	103.45
2	A	900	FAD	C5A-N7A-C8A	3.37	108.75	103.45
2	B	900	FAD	C5A-N7A-C8A	3.37	108.74	103.45
2	B	900	FAD	C4-C4X-N5	3.37	122.86	118.21
2	A	900	FAD	O2-C2-N1	-3.33	116.26	121.80
2	D	900	FAD	C2A-N3A-C4A	3.32	119.93	111.83
2	D	900	FAD	O2-C2-N1	-3.19	116.50	121.80
2	A	900	FAD	C2A-N3A-C4A	3.16	119.56	111.83
2	B	900	FAD	C10-N1-C2	3.12	123.59	116.85
2	B	900	FAD	C2A-N3A-C4A	2.92	118.97	111.83
2	C	900	FAD	C4A-C5A-N7A	-2.85	107.32	110.58
2	B	900	FAD	C4-N3-C2	-2.73	120.79	125.64
2	C	900	FAD	C10-N1-C2	2.73	122.76	116.85
2	B	900	FAD	O2-C2-N1	-2.66	117.37	121.80
2	D	900	FAD	C4A-C5A-N7A	-2.61	107.60	110.58
2	B	900	FAD	C4A-C5A-N7A	-2.60	107.61	110.58
2	A	900	FAD	O4B-C1B-C2B	-2.58	101.09	106.62
2	C	900	FAD	N9A-C8A-N7A	-2.58	110.28	113.94
2	B	900	FAD	O4B-C1B-C2B	-2.52	101.23	106.62
2	D	900	FAD	C10-C4X-N5	-2.52	119.67	124.81
2	D	900	FAD	N9A-C8A-N7A	-2.50	110.39	113.94
2	A	900	FAD	C10-N1-C2	2.48	122.22	116.85
2	C	900	FAD	C4-N3-C2	-2.46	121.27	125.64
2	B	900	FAD	O4-C4-C4X	-2.46	120.04	126.53
2	B	900	FAD	C4X-C10-N1	-2.43	118.62	124.59
2	C	900	FAD	C5X-N5-C4X	2.41	121.99	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	FAD	C10-C4X-N5	-2.39	119.92	124.81
2	D	900	FAD	C10-N1-C2	2.38	122.00	116.85
2	A	900	FAD	C2A-N1A-C6A	2.38	122.64	118.73
2	D	900	FAD	C2A-N1A-C6A	2.32	122.54	118.73
2	A	900	FAD	O4-C4-C4X	-2.31	120.44	126.53
2	C	900	FAD	C4X-C10-N1	-2.31	118.93	124.59
2	A	900	FAD	C4A-N9A-C8A	2.30	108.15	105.74
2	A	900	FAD	C4A-C5A-N7A	-2.29	107.96	110.58
2	A	900	FAD	N9A-C8A-N7A	-2.29	110.69	113.94
2	D	900	FAD	C4X-C10-N1	-2.27	119.02	124.59
2	C	900	FAD	N3-C2-N1	2.27	124.32	119.50
2	D	900	FAD	C4-N3-C2	-2.26	121.63	125.64
2	D	900	FAD	N3-C2-N1	2.23	124.25	119.50
2	D	900	FAD	C4X-C10-N10	2.23	119.67	116.48
2	A	900	FAD	C4-N3-C2	-2.20	121.73	125.64
2	A	900	FAD	P-O5'-C5'	-2.18	108.84	121.35
2	D	900	FAD	O4B-C1B-C2B	-2.18	101.95	106.62
2	B	900	FAD	P-O5'-C5'	-2.14	109.09	121.35
2	B	900	FAD	C5X-N5-C4X	2.14	121.55	118.09
2	B	900	FAD	C5X-C9A-N10	2.12	119.89	117.97
2	D	900	FAD	C4A-N9A-C8A	2.11	107.96	105.74
2	B	900	FAD	C10-C4X-N5	-2.10	120.52	124.81
2	A	900	FAD	C5X-N5-C4X	2.09	121.46	118.09
2	C	900	FAD	C2A-N1A-C6A	2.08	122.14	118.73
2	C	900	FAD	C4'-C3'-C2'	-2.06	110.14	113.57
2	A	900	FAD	C10-C4X-N5	-2.06	120.60	124.81
2	A	900	FAD	C4X-C10-N1	-2.04	119.58	124.59
2	B	900	FAD	N9A-C8A-N7A	-2.03	111.05	113.94
2	C	900	FAD	C4A-N9A-C8A	2.03	107.87	105.74
2	A	900	FAD	C4X-C10-N10	2.02	119.37	116.48
2	B	900	FAD	C2A-N1A-C6A	2.01	122.04	118.73
2	D	900	FAD	C5B-C4B-C3B	-2.01	107.99	115.21
2	D	900	FAD	P-O5'-C5'	-2.00	109.89	121.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	FAD	O4B-C4B-C5B-O5B
2	A	900	FAD	C3B-C4B-C5B-O5B
2	B	900	FAD	O4B-C4B-C5B-O5B
2	B	900	FAD	C3B-C4B-C5B-O5B

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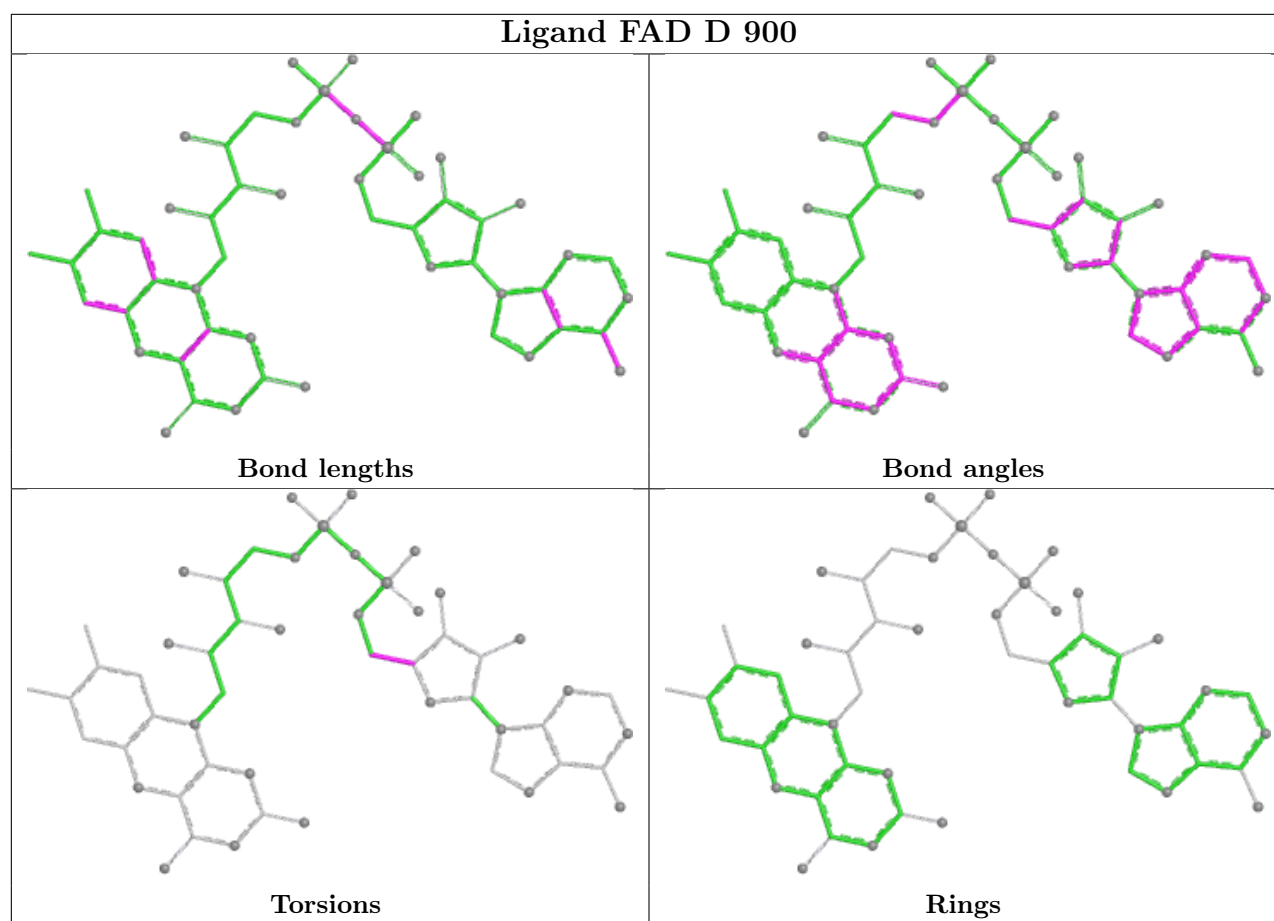
Mol	Chain	Res	Type	Atoms
2	C	900	FAD	O4B-C4B-C5B-O5B
2	D	900	FAD	O4B-C4B-C5B-O5B
2	D	900	FAD	C3B-C4B-C5B-O5B
2	C	900	FAD	C3B-C4B-C5B-O5B

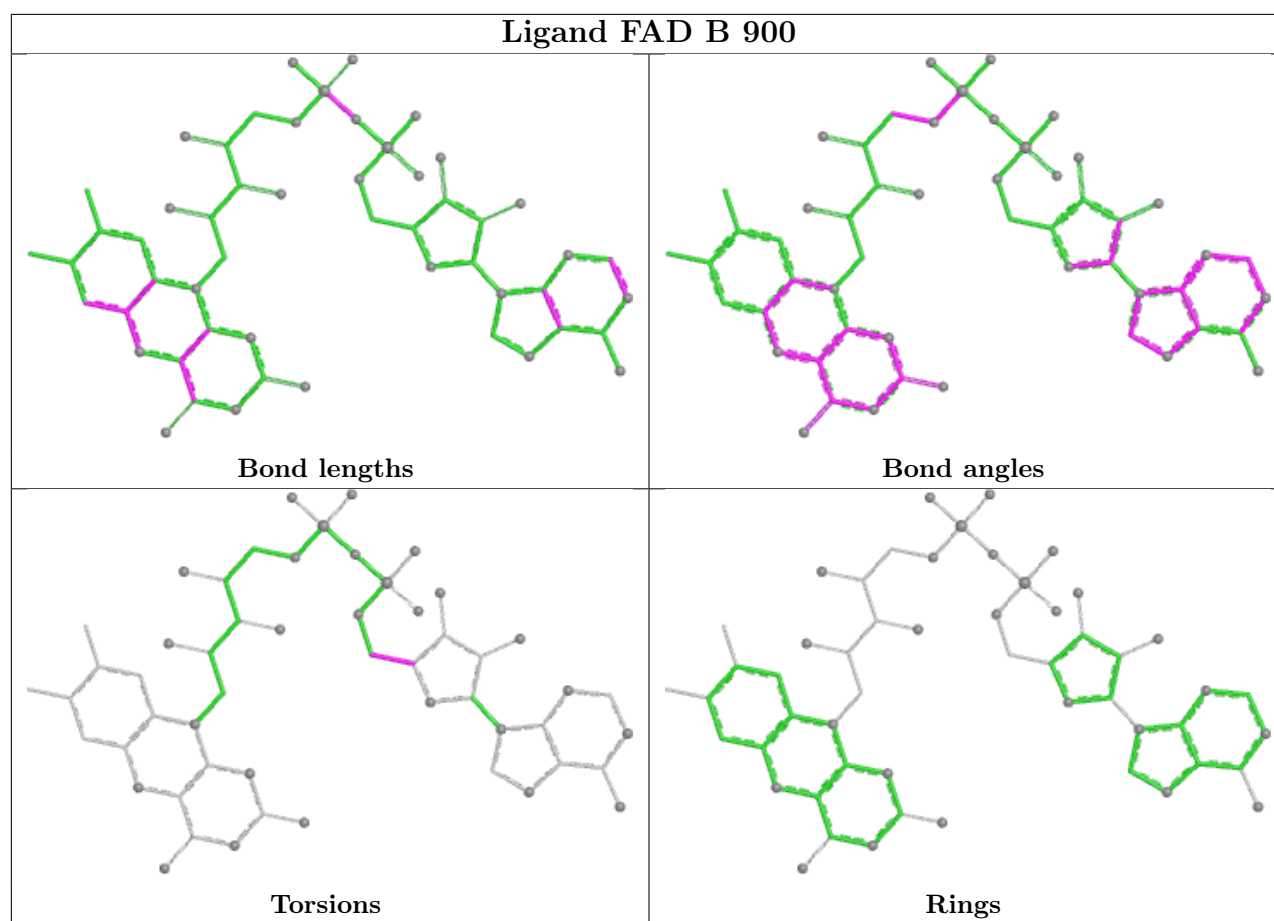
There are no ring outliers.

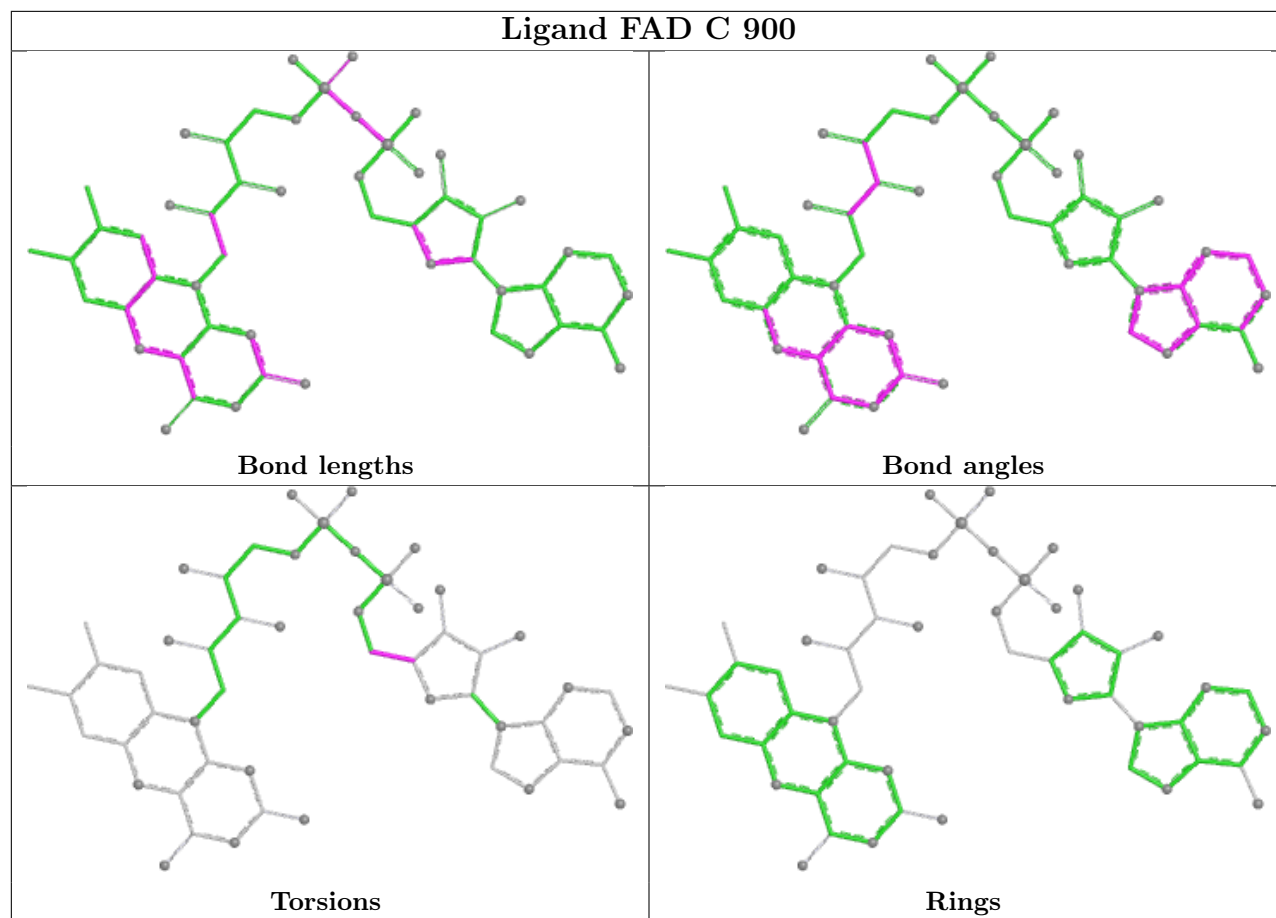
3 monomers are involved in 3 short contacts:

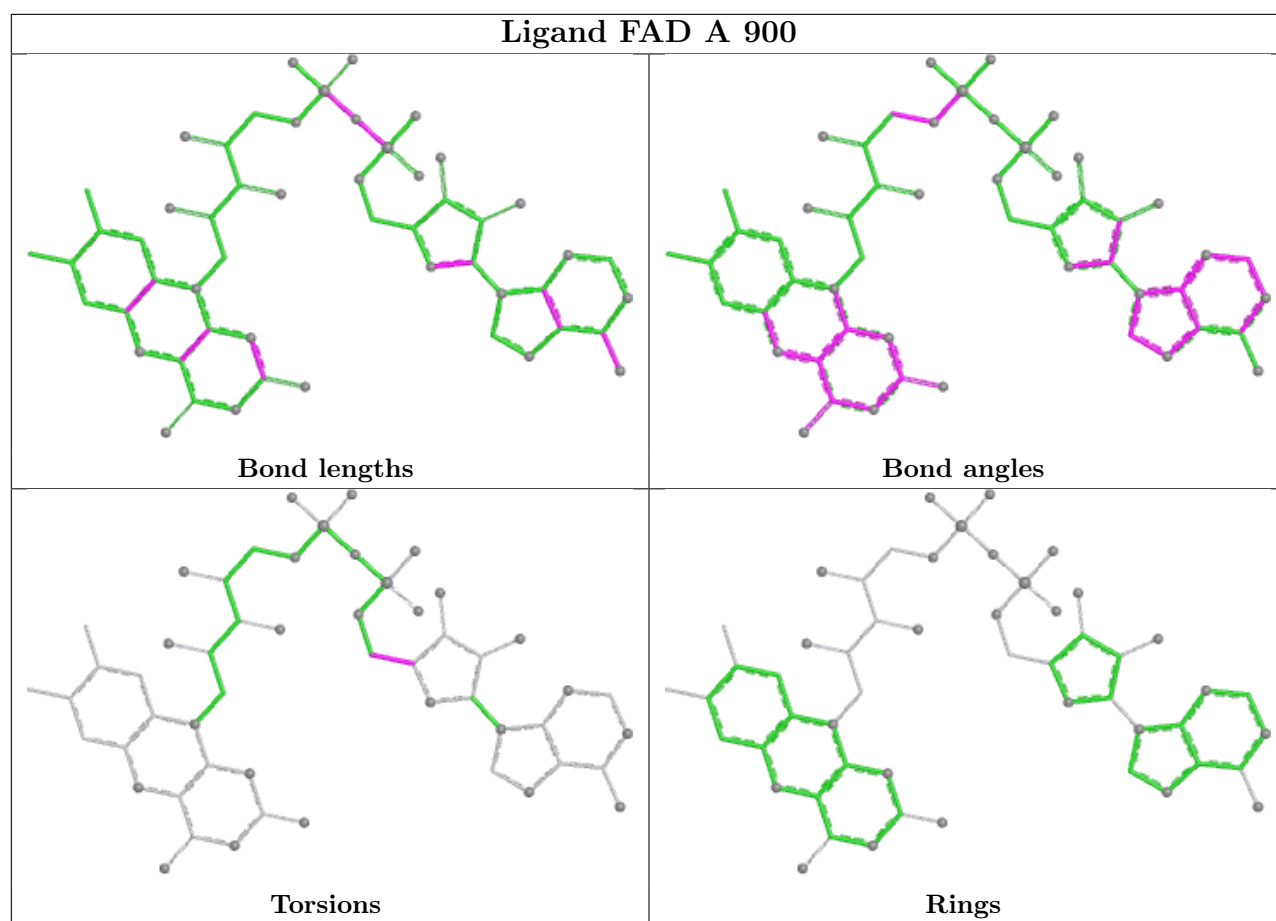
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	SO4	1	0
2	C	900	FAD	1	0
2	A	900	FAD	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	491/513 (95%)	-0.37	4 (0%) 82 75	21, 45, 65, 112	0
1	B	487/513 (94%)	-0.41	3 (0%) 85 80	21, 41, 65, 95	0
1	C	487/513 (94%)	-0.21	3 (0%) 85 80	27, 49, 69, 104	0
1	D	484/513 (94%)	-0.30	1 (0%) 91 88	25, 48, 73, 96	0
All	All	1949/2052 (94%)	-0.32	11 (0%) 85 80	21, 46, 69, 112	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	493	LEU	3.1
1	C	7	LEU	3.0
1	C	8	PRO	2.9
1	A	495	ALA	2.8
1	A	499	GLY	2.7
1	B	200	TYR	2.6
1	A	498	CYS	2.5
1	C	493	LEU	2.4
1	D	493	LEU	2.4
1	B	7	LEU	2.2
1	A	494	GLN	2.1

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

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

6.3 Carbohydrates [i](#)

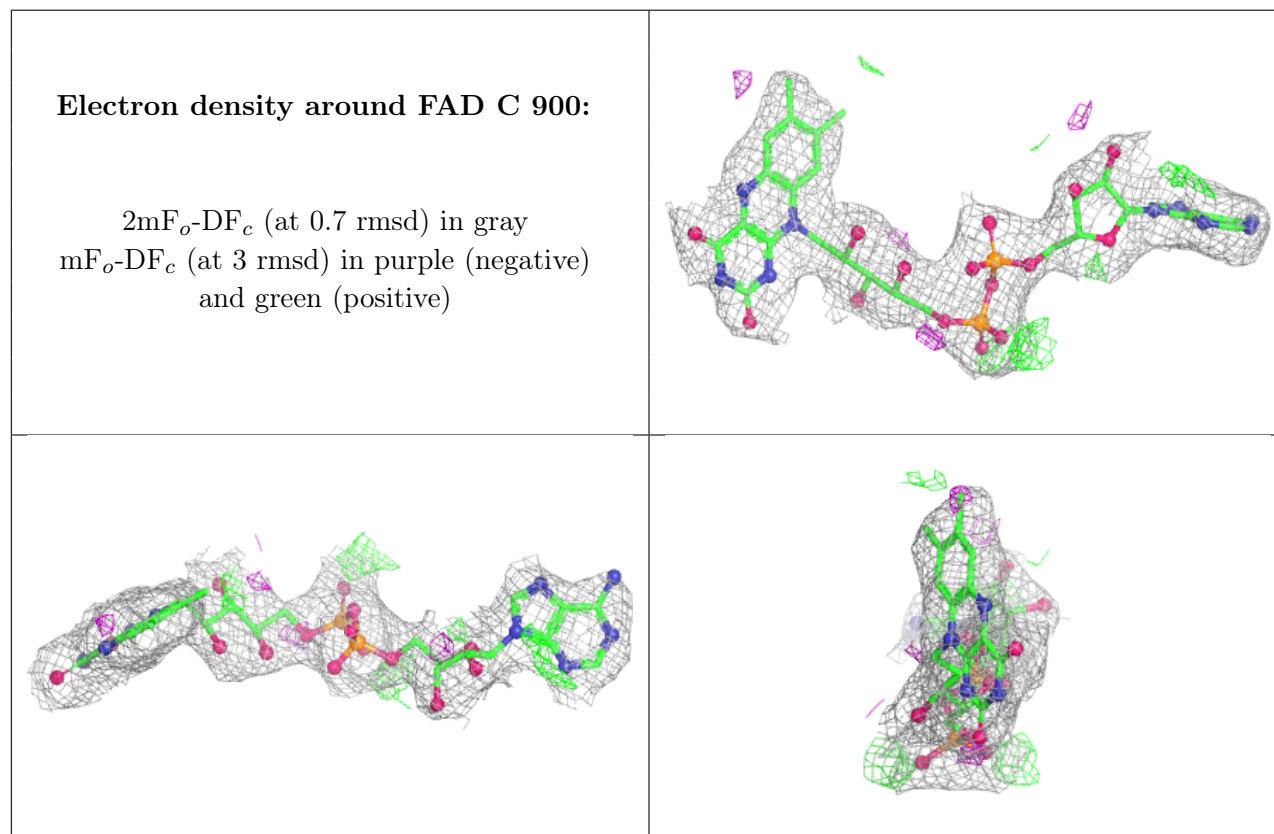
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

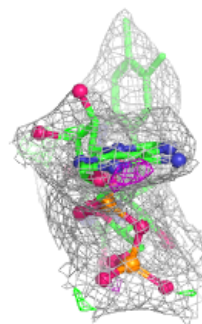
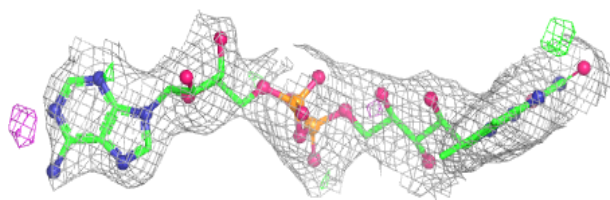
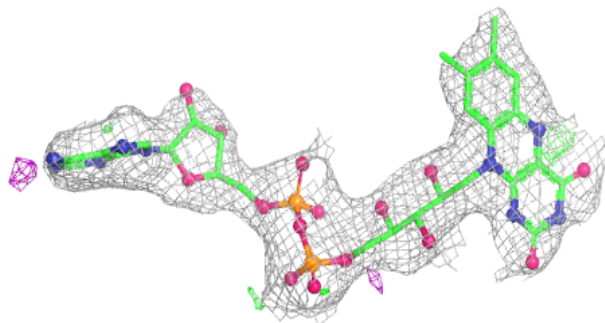
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	D	901	5/5	0.85	0.11	71,73,74,75	0
3	SO4	C	901	5/5	0.87	0.08	67,67,68,68	0
3	SO4	A	901	5/5	0.89	0.09	68,69,71,71	0
3	SO4	B	901	5/5	0.90	0.08	63,65,66,66	0
2	FAD	C	900	53/53	0.94	0.09	39,45,53,53	0
2	FAD	A	900	53/53	0.95	0.08	37,49,55,56	0
2	FAD	B	900	53/53	0.97	0.07	23,28,39,40	0
2	FAD	D	900	53/53	0.97	0.07	27,33,48,49	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.

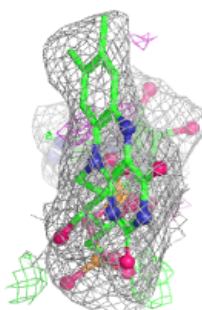
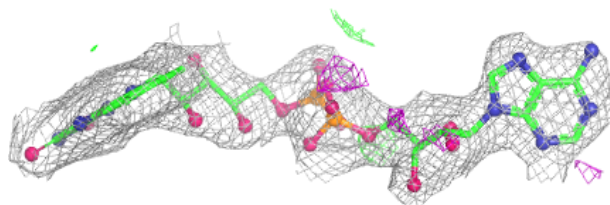
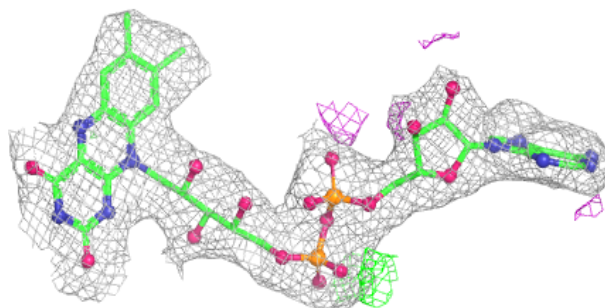


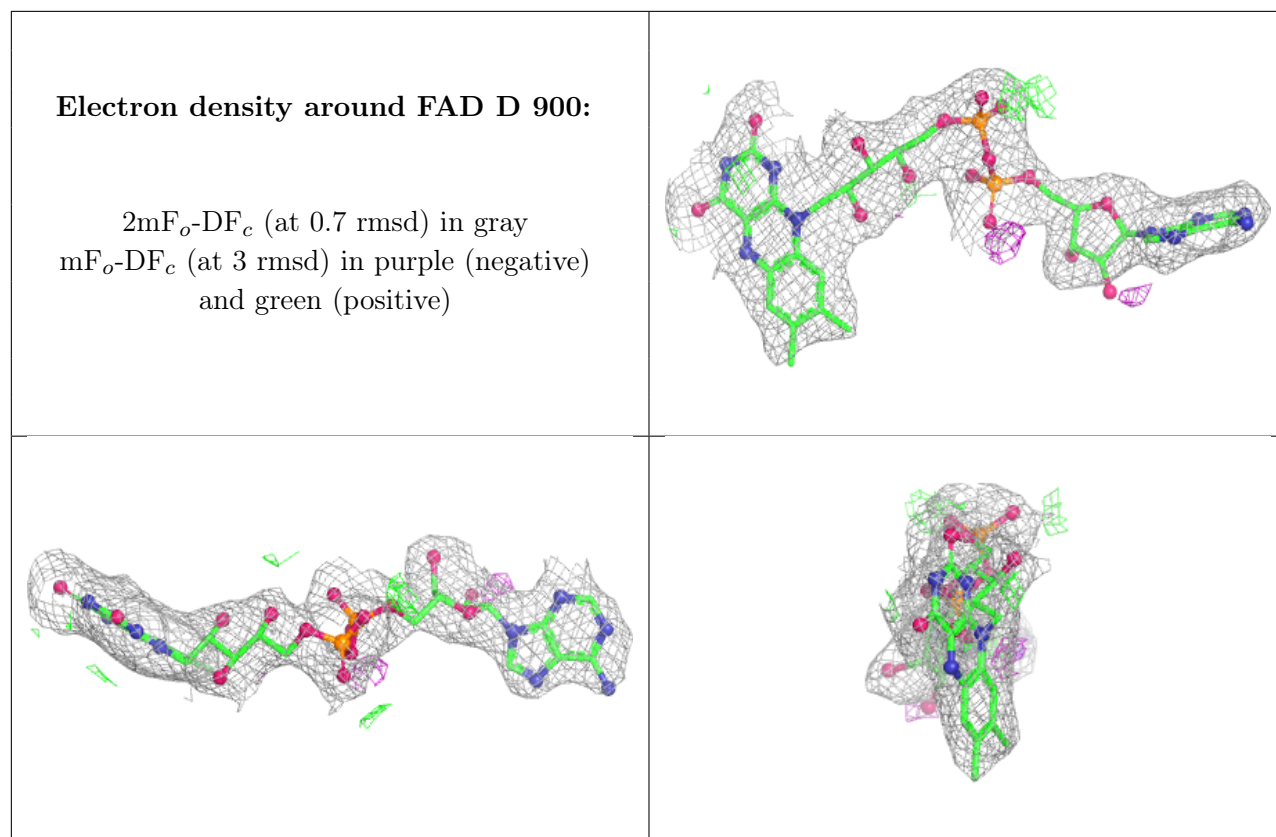
Electron density around FAD A 900:

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

**Electron density around FAD B 900:**

$2mF_o-DF_c$ (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.