



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:37 PM UTC

PDB ID : 1KFY / pdb_00001kfy
Title : QUINOL-FUMARATE REDUCTASE WITH QUINOL INHIBITOR 2-[1-(4-CHLORO-PHENYL)-ETHYL]-4,6-DINITRO-PHENOL
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Deposited on : 2001-11-24
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

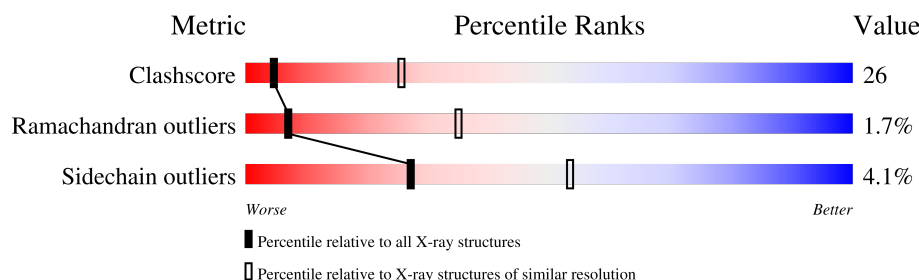
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	602	
1	M	602	
2	B	243	
2	N	243	
3	C	130	
3	O	130	
4	D	119	
4	P	119	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	BRS	B	700	-	-	X	-
5	OAA	A	702	-	X	-	-
8	F3S	N	245	-	-	X	-
9	SF4	N	246	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 16957 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 FUMARATE REDUCTASE FLAVOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4448	2775	802	840	31			
1	M	577	Total	C	N	O	S	0	0	0
			4448	2775	802	840	31			

- Molecule 2 is a protein called Fumarate reductase iron-sulfur protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	19			
2	N	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	19			

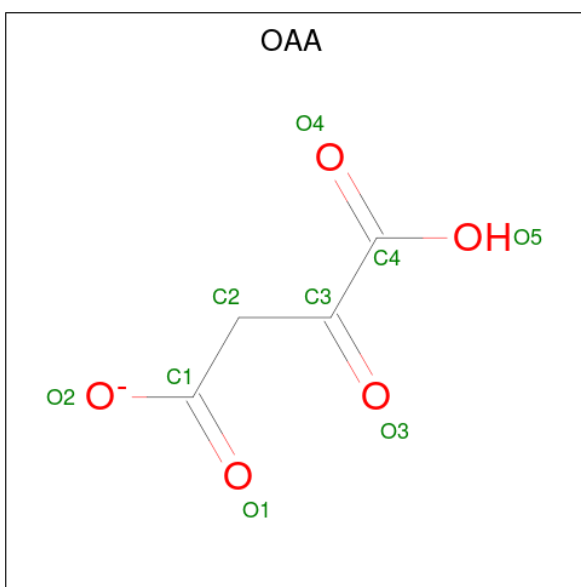
- Molecule 3 is a protein called FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			
3	O	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			

- Molecule 4 is a protein called FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN.

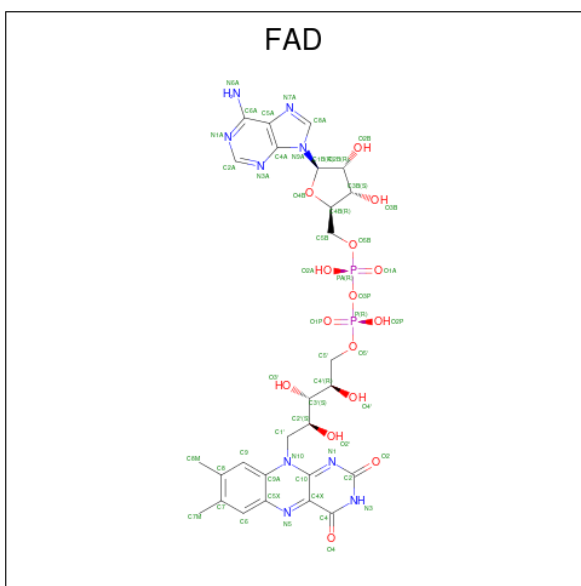
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			
4	P	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

- Molecule 5 is OXALOACETATE ION (CCD ID: OAA) (formula: $C_4H_3O_5$).



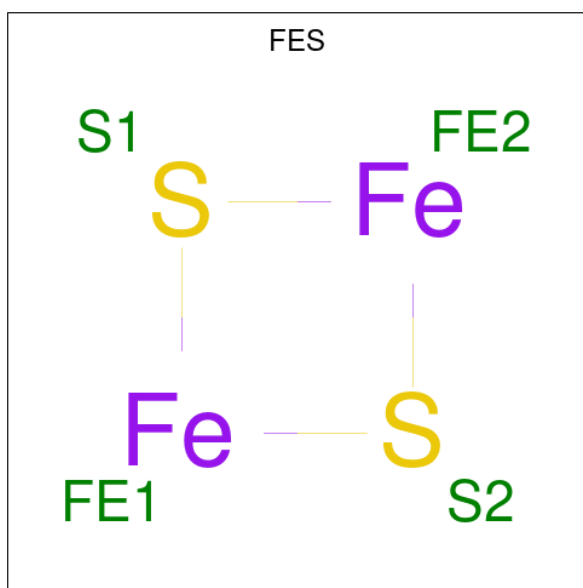
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 9 4 5	0	0
5	M	1	Total C O 9 4 5	0	0

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



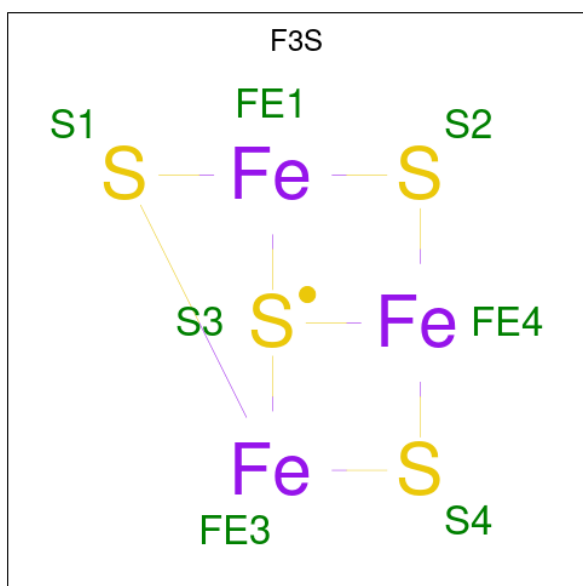
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
6	M	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



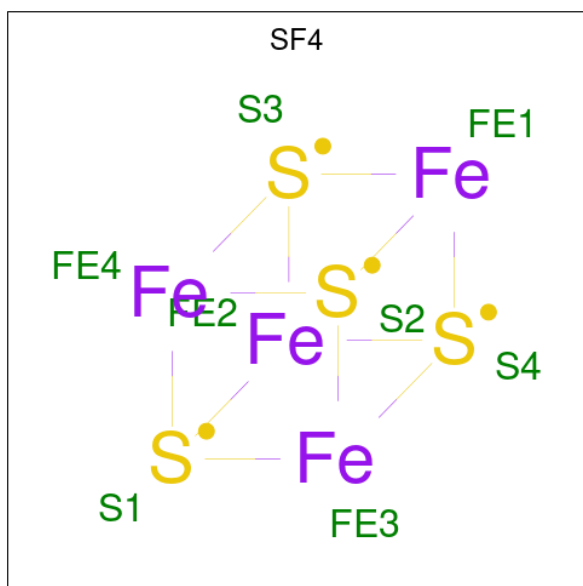
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		

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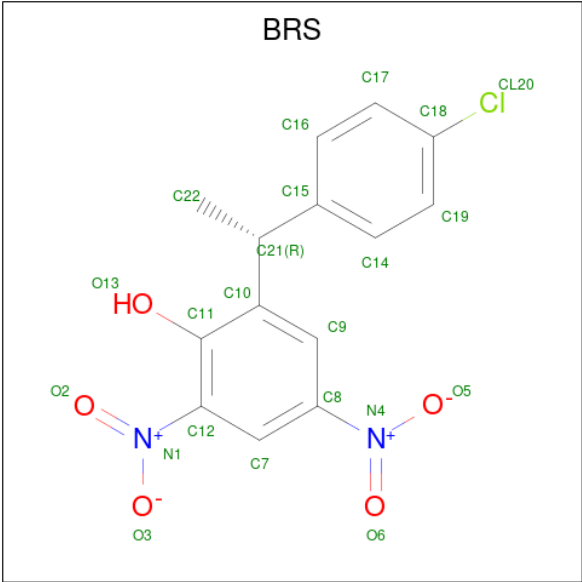
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	N	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



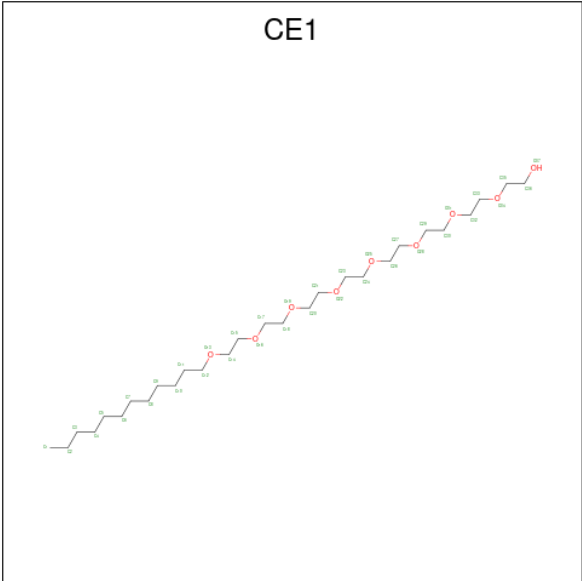
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		
9	N	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 10 is 2-[1-(4-CHLORO-PHENYL)-ETHYL]-4,6-DINITRO-PHENOL (CCD ID: BRS) (formula: C₁₄H₁₁ClN₂O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	Cl	N	O	0	0
			22	14	1	2	5		
10	N	1	Total	C	Cl	N	O	0	0
			22	14	1	2	5		

- Molecule 11 is O-DODECANYL OCTAETHYLENE GLYCOL (CCD ID: CE1) (formula: C₂₈H₅₈O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	D	1	Total	C	O	0	0
			37	28	9		

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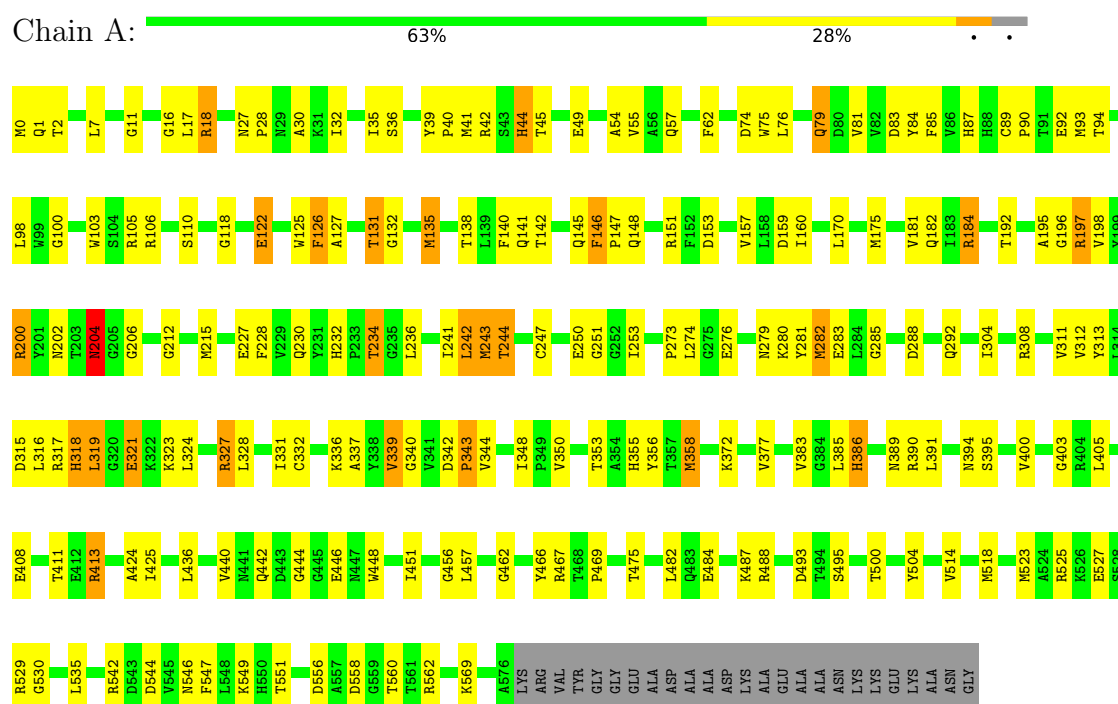
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	O	1	Total	C	O	0	0
			37	28	9		
11	P	1	Total	C	O	0	0
			37	28	9		

3 Residue-property plots

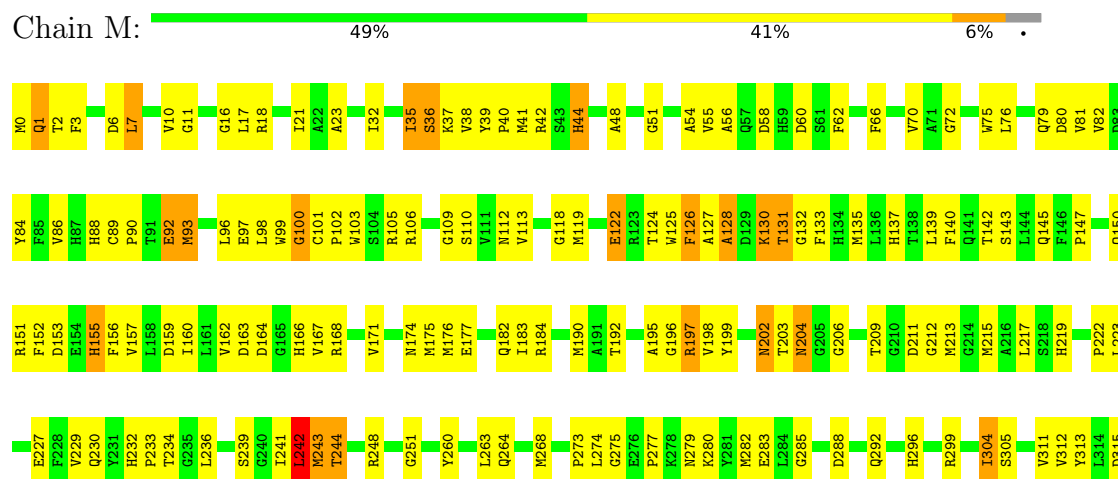
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

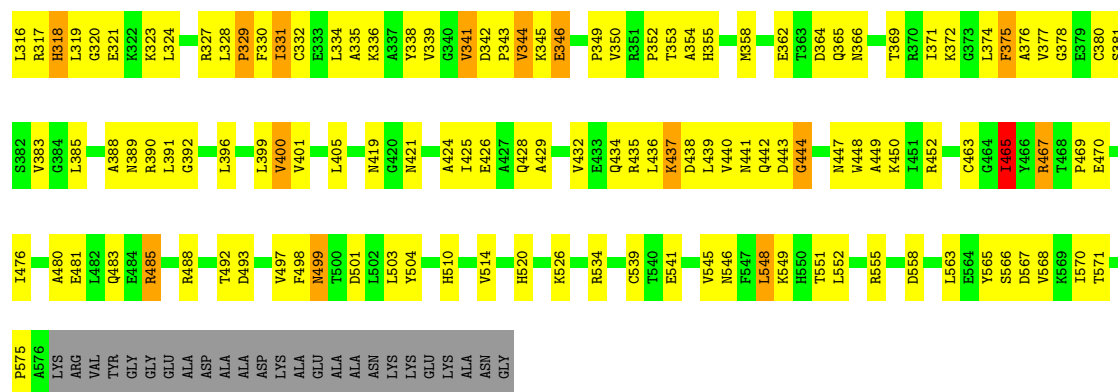
Note EDS was not executed.

• Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN



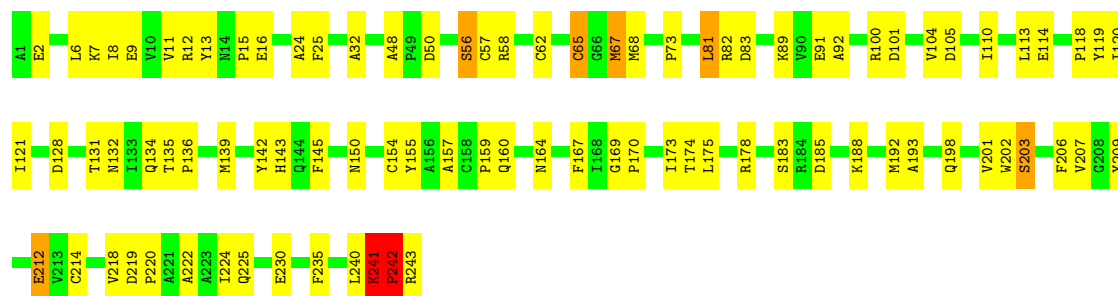
• Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN





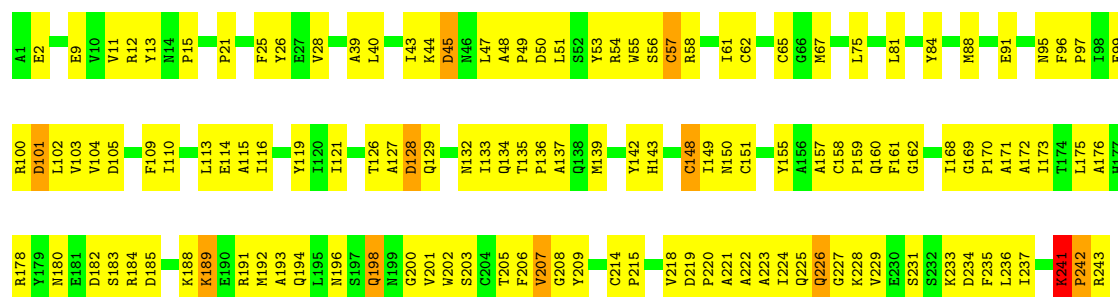
• Molecule 2: Fumarate reductase iron-sulfur protein

Chain B: 63% 34% ..



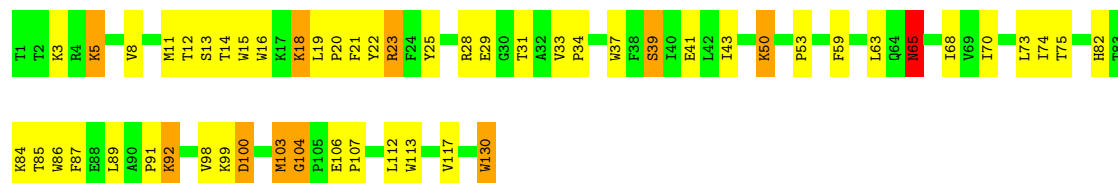
• Molecule 2: Fumarate reductase iron-sulfur protein

Chain N: 46% 49% .



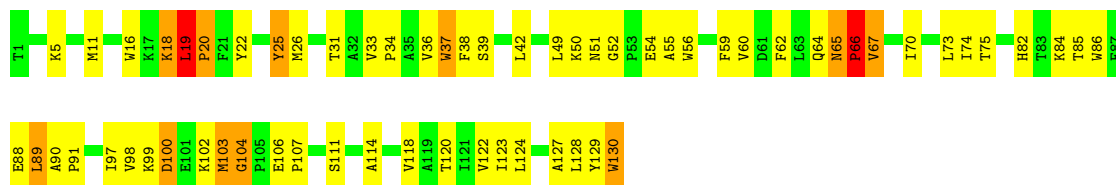
• Molecule 3: FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN

Chain C: 58% 33% 8% .



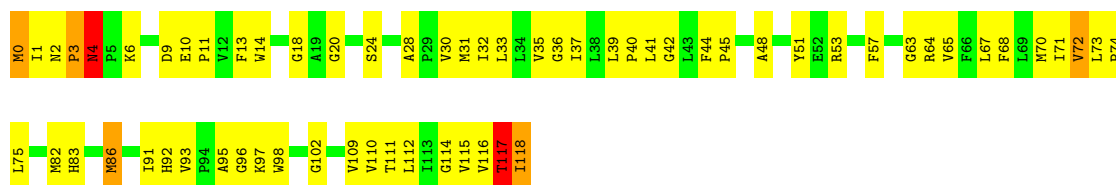
• Molecule 3: FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN

Chain O:  52% 38% 8% .

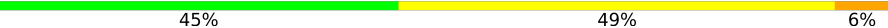


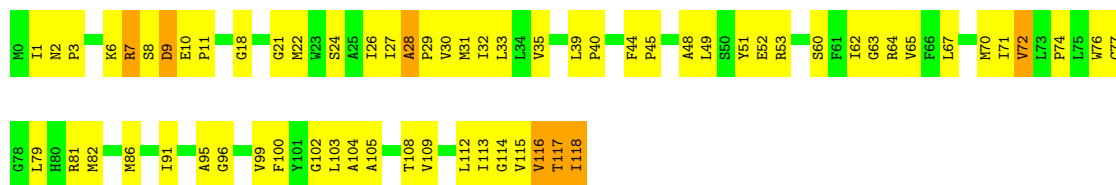
• Molecule 4: FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN

Chain D:  47% 47% . .



• Molecule 4: FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN

Chain P:  45% 49% 6%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.15Å 137.81Å 270.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.264 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	16957	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F3S, SF4, CE1, FAD, FES, BRS, OAA

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	0.87	3/4540 (0.1%)	1.15	26/6139 (0.4%)
1	M	0.72	2/4540 (0.0%)	1.11	24/6139 (0.4%)
2	B	0.80	1/1931 (0.1%)	1.16	9/2617 (0.3%)
2	N	0.74	2/1931 (0.1%)	1.19	10/2617 (0.4%)
3	C	0.96	3/1094 (0.3%)	1.19	9/1496 (0.6%)
3	O	0.88	2/1094 (0.2%)	1.20	10/1496 (0.7%)
4	D	1.00	3/956 (0.3%)	1.29	11/1303 (0.8%)
4	P	0.91	3/956 (0.3%)	1.19	6/1303 (0.5%)
All	All	0.83	19/17042 (0.1%)	1.16	105/23110 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	O	0	1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	117	THR	CA-C	-12.36	1.36	1.52
4	P	117	THR	CA-C	-10.53	1.38	1.52
4	D	3	PRO	C-O	-8.86	1.13	1.24
1	A	135	MET	SD-CE	8.80	2.01	1.79
3	C	65	ASN	C-O	-8.29	1.13	1.24
3	C	104	GLY	C-O	-7.85	1.13	1.24
3	O	104	GLY	C-O	-7.69	1.13	1.24
4	P	3	PRO	C-O	-7.61	1.15	1.23
2	N	242	PRO	CA-C	-7.24	1.42	1.52
1	A	241	ILE	CA-CB	-7.22	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	117	THR	CA-CB	6.68	1.64	1.53
3	O	65	ASN	C-O	-6.41	1.16	1.24
4	P	31	MET	SD-CE	6.39	1.95	1.79
1	M	268	MET	SD-CE	5.84	1.94	1.79
1	M	465	ILE	CA-CB	5.33	1.61	1.54
1	A	243	MET	SD-CE	-5.14	1.66	1.79
3	C	130	TRP	CB-CG	-5.12	1.34	1.50
2	N	172	ALA	CA-CB	-5.10	1.45	1.53
2	B	67	MET	SD-CE	-5.07	1.66	1.79

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	241	LYS	CA-C-N	-12.81	103.83	119.84
2	N	241	LYS	C-N-CA	-12.81	103.83	119.84
4	D	117	THR	N-CA-C	10.96	134.14	110.80
3	C	65	ASN	N-CA-C	10.04	132.01	109.81
2	N	65	CYS	N-CA-C	9.10	123.98	113.15
2	B	65	CYS	N-CA-C	8.68	123.62	112.34
4	D	72	VAL	N-CA-C	7.79	117.75	110.42
4	D	117	THR	CA-C-N	-7.70	107.83	121.70
4	D	117	THR	C-N-CA	-7.70	107.83	121.70
4	P	116	VAL	N-CA-C	-7.67	102.12	113.39
4	D	117	THR	CB-CA-C	-7.66	95.18	110.42
1	A	547	PHE	N-CA-C	7.39	122.02	112.41
4	D	35	VAL	N-CA-C	7.38	117.47	110.53
1	A	106	ARG	N-CA-C	-7.37	100.49	110.36
1	M	75	TRP	N-CA-C	7.35	121.58	112.47
1	M	467	ARG	N-CA-C	7.27	120.78	109.07
1	A	242	LEU	N-CA-C	7.22	120.79	109.96
2	B	48	ALA	CA-C-N	7.21	126.91	119.56
2	B	48	ALA	C-N-CA	7.21	126.91	119.56
3	O	66	PRO	N-CA-C	7.17	127.25	112.47
3	O	25	TYR	N-CA-C	-7.09	103.16	111.03
1	M	100	GLY	N-CA-C	6.95	121.93	113.79
1	A	337	ALA	N-CA-C	6.87	118.84	111.36
2	N	48	ALA	CA-C-N	6.81	126.51	119.56
2	N	48	ALA	C-N-CA	6.81	126.51	119.56
1	M	242	LEU	N-CA-C	6.57	120.21	109.76
1	M	106	ARG	N-CA-C	-6.57	100.54	110.39
3	C	104	GLY	CA-C-O	-6.47	112.27	121.52
4	P	72	VAL	N-CA-C	6.42	116.56	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	400	VAL	CB-CA-C	-6.38	103.70	112.24
2	B	198	GLN	N-CA-C	-6.34	104.80	112.54
4	P	117	THR	CB-CA-C	-6.34	97.79	110.42
1	A	105	ARG	N-CA-C	6.33	119.85	109.85
1	A	204	ASN	N-CA-C	6.29	119.83	110.52
3	O	104	GLY	CA-C-O	-6.26	112.57	121.52
1	M	44	HIS	N-CA-C	6.25	120.00	112.38
1	A	175	MET	N-CA-C	6.12	117.95	111.28
4	P	100	PHE	N-CA-C	6.10	117.62	110.97
4	D	2	ASN	CA-C-N	6.06	126.58	120.04
4	D	2	ASN	C-N-CA	6.06	126.58	120.04
1	A	100	GLY	N-CA-C	6.05	121.99	114.37
1	A	339	VAL	N-CA-C	-6.03	107.42	113.20
1	A	285	GLY	CA-C-N	6.02	126.37	119.93
1	A	285	GLY	C-N-CA	6.02	126.37	119.93
3	O	65	ASN	CA-C-N	-5.93	112.43	119.84
3	O	65	ASN	C-N-CA	-5.93	112.43	119.84
3	C	65	ASN	CA-C-N	5.92	141.22	127.00
3	C	65	ASN	C-N-CA	5.92	141.22	127.00
1	A	312	VAL	N-CA-C	-5.91	99.20	108.95
3	O	130	TRP	CA-CB-CG	5.90	124.82	113.60
1	A	467	ARG	N-CA-C	5.90	119.09	109.59
3	O	19	LEU	N-CA-C	5.88	117.48	110.07
1	A	355	HIS	N-CA-C	5.84	123.25	110.80
2	B	241	LYS	CA-C-N	5.71	126.98	119.84
2	B	241	LYS	C-N-CA	5.71	126.98	119.84
2	N	207	VAL	N-CA-C	-5.70	104.80	110.62
1	A	313	TYR	N-CA-C	5.69	118.51	109.24
1	M	341	VAL	N-CA-C	5.68	116.29	108.12
1	M	346	GLU	N-CA-C	5.68	114.67	108.14
1	M	567	ASP	N-CA-C	5.67	118.67	110.28
1	A	146	PHE	CA-C-N	5.66	125.34	119.56
1	A	146	PHE	C-N-CA	5.66	125.34	119.56
1	M	437	LYS	N-CA-C	-5.63	105.22	111.36
2	N	45	ASP	N-CA-C	5.61	117.20	111.14
1	M	338	TYR	N-CA-C	5.61	120.25	112.45
1	M	285	GLY	CA-C-N	5.60	126.84	119.84
1	M	285	GLY	C-N-CA	5.60	126.84	119.84
3	C	73	LEU	N-CA-C	-5.60	105.26	111.36
1	M	355	HIS	N-CA-C	5.53	122.58	110.80
1	M	381	SER	N-CA-C	5.53	117.16	109.31
1	A	75	TRP	N-CA-C	5.53	119.32	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	198	GLN	N-CA-C	-5.49	105.84	112.54
3	C	65	ASN	C-N-CD	-5.49	108.53	120.60
1	A	110	SER	N-CA-C	-5.48	103.15	110.55
1	M	110	SER	N-CA-C	-5.47	103.16	110.55
4	D	4	ASN	N-CA-C	-5.47	100.89	108.76
1	M	234	THR	N-CA-C	5.45	118.64	107.69
3	O	67	VAL	N-CA-C	5.42	116.05	110.36
2	N	57	CYS	N-CA-C	5.42	117.89	111.33
1	A	386	HIS	N-CA-C	5.36	119.87	113.23
1	M	419	ASN	N-CA-C	5.32	117.96	110.14
1	M	0	MET	CA-C-N	5.29	131.64	121.54
1	M	0	MET	C-N-CA	5.29	131.64	121.54
4	P	28	ALA	N-CA-C	5.26	119.90	112.75
1	A	234	THR	N-CA-C	5.25	118.83	107.49
4	P	117	THR	N-CA-CB	5.25	119.36	110.49
1	A	138	THR	N-CA-C	-5.25	105.46	111.07
1	M	130	LYS	N-CA-C	-5.24	105.97	114.09
1	A	131	THR	N-CA-C	5.22	117.64	111.33
3	O	52	GLY	CA-C-N	5.21	126.35	119.84
3	O	52	GLY	C-N-CA	5.21	126.35	119.84
1	A	126	PHE	N-CA-C	5.21	116.99	109.07
1	M	92	GLU	N-CA-C	5.20	116.95	111.28
2	B	135	THR	CA-C-N	-5.16	113.33	119.05
2	B	135	THR	C-N-CA	-5.16	113.33	119.05
3	C	5	LYS	CA-C-N	5.14	126.27	119.84
3	C	5	LYS	C-N-CA	5.14	126.27	119.84
3	C	65	ASN	CB-CA-C	-5.12	100.08	110.17
2	B	24	ALA	N-CA-C	-5.11	101.31	109.23
4	D	45	PRO	N-CA-C	5.11	119.20	111.19
1	A	1	GLN	N-CA-C	-5.09	103.81	110.53
4	D	65	VAL	CB-CA-C	-5.09	105.46	111.97
2	N	242	PRO	O-C-N	5.07	129.49	122.64
1	A	44	HIS	N-CA-C	5.04	118.69	112.54
1	M	202	ASN	N-CA-C	5.02	115.67	108.74

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	O	129	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	4448	0	4335	161	0
1	M	4448	0	4335	283	0
2	B	1888	0	1837	86	0
2	N	1888	0	1837	130	0
3	C	1058	0	1108	65	0
3	O	1058	0	1108	69	0
4	D	926	0	971	83	0
4	P	926	0	971	78	0
5	A	9	0	2	1	0
5	M	9	0	2	2	0
6	A	53	0	31	6	0
6	M	53	0	31	10	0
7	B	4	0	0	0	0
7	N	4	0	0	0	0
8	B	7	0	0	0	0
8	N	7	0	0	2	0
9	B	8	0	0	0	0
9	N	8	0	0	7	0
10	B	22	0	11	13	0
10	N	22	0	11	5	0
11	D	37	0	58	5	0
11	O	37	0	58	1	0
11	P	37	0	58	2	0
All	All	16957	0	16764	870	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 26.

All (870) 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:135:MET:SD	1:A:135:MET:CE	2.01	1.48
1:M:44:HIS:NE2	6:M:803:FAD:HM82	0.88	1.21
1:A:44:HIS:NE2	6:A:703:FAD:HM82	0.85	1.17
4:D:6:LYS:HG3	4:P:6:LYS:HB3	1.27	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:GLN:NE2	10:B:700:BRS:H222	1.66	1.09
1:M:190:MET:HE1	1:M:215:MET:HE3	1.26	1.08
1:M:421:ASN:HD22	1:M:424:ALA:HB2	1.15	1.08
2:B:225:GLN:HE21	10:B:700:BRS:C22	1.68	1.06
1:A:44:HIS:CE1	6:A:703:FAD:HM82	1.92	1.05
1:M:44:HIS:CD2	6:M:803:FAD:HM82	1.90	1.05
1:M:44:HIS:CE1	6:M:803:FAD:HM82	1.92	1.04
1:M:251:GLY:HA2	1:M:277:PRO:HG2	1.41	1.03
1:A:358:MET:HE3	1:A:389:ASN:HA	1.38	1.02
2:B:225:GLN:HE21	10:B:700:BRS:H222	0.88	1.01
3:C:50:LYS:HD2	4:D:118:ILE:O	1.59	1.01
1:A:44:HIS:CD2	6:A:703:FAD:HM82	1.95	1.01
2:N:148:CYS:SG	9:N:246:SF4:S2	2.59	0.99
9:N:246:SF4:S2	9:N:246:SF4:S4	2.60	0.99
3:C:12:THR:HG22	3:C:14:THR:H	1.22	0.99
1:M:469:PRO:HG3	1:M:534:ARG:HH21	1.28	0.99
3:O:50:LYS:HG3	4:P:118:ILE:HA	1.39	0.98
2:N:116:ILE:HG21	2:N:176:ALA:HB2	1.42	0.98
3:C:50:LYS:HD2	4:D:118:ILE:C	1.87	0.98
3:O:19:LEU:H	3:O:19:LEU:HD23	1.27	0.97
1:M:421:ASN:HD22	1:M:424:ALA:CB	1.77	0.97
2:N:54:ARG:HE	2:N:103:VAL:HG13	1.31	0.96
1:M:316:LEU:HB3	1:M:319:LEU:HD12	1.48	0.93
3:C:50:LYS:HD3	4:D:118:ILE:HG22	1.49	0.91
1:M:447:ASN:HD21	1:M:449:ALA:HB3	1.34	0.90
1:M:42:ARG:HH21	2:N:150:ASN:HB2	1.35	0.90
4:P:117:THR:O	4:P:118:ILE:C	2.13	0.90
4:P:117:THR:HG22	4:P:118:ILE:N	1.88	0.89
3:O:50:LYS:CG	4:P:118:ILE:HA	2.02	0.89
1:A:413:ARG:HH11	1:A:413:ARG:HB2	1.34	0.89
2:N:189:LYS:H	2:N:189:LYS:HD3	1.37	0.88
3:C:99:LYS:O	3:C:100:ASP:HB2	1.74	0.87
4:D:92:HIS:HB3	2:N:243:ARG:HB2	1.55	0.87
2:N:225:GLN:NE2	10:N:800:BRS:H222	1.90	0.87
2:B:241:LYS:O	2:B:243:ARG:N	2.08	0.86
1:M:155:HIS:CD2	1:M:174:ASN:HA	2.10	0.85
4:D:64:ARG:NH1	4:D:117:THR:HG23	1.92	0.85
3:O:86:TRP:HE1	4:P:22:MET:HE2	1.42	0.84
4:D:0:MET:HG2	4:D:1:ILE:H	1.39	0.84
1:M:437:LYS:HG2	1:M:441:ASN:HD21	1.42	0.84
2:N:214:CYS:SG	2:N:218:VAL:HG23	2.16	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:31:THR:HG21	3:O:82:HIS:HB2	1.58	0.84
1:M:304:ILE:HD12	1:M:304:ILE:H	1.39	0.84
1:M:197:ARG:HD2	1:M:206:GLY:HA2	1.58	0.83
1:M:98:LEU:HD11	2:N:127:ALA:HA	1.60	0.83
2:B:15:PRO:HB2	3:C:5:LYS:H	1.43	0.81
1:A:356:TYR:CE2	1:A:390:ARG:HD3	2.14	0.81
3:O:50:LYS:CD	4:P:118:ILE:HA	2.11	0.81
1:A:7:LEU:HD21	1:A:32:ILE:HG12	1.61	0.81
1:A:514:VAL:HG12	1:A:518:MET:HE3	1.62	0.81
1:A:484:GLU:HG3	1:A:488:ARG:NH1	1.96	0.80
2:N:11:VAL:HG21	2:N:91:GLU:HG2	1.63	0.80
1:M:465:ILE:HD13	1:M:465:ILE:H	1.45	0.80
3:O:33:VAL:HB	3:O:34:PRO:HD3	1.63	0.80
1:M:425:ILE:O	1:M:428:GLN:HB2	1.83	0.79
3:C:33:VAL:HB	3:C:34:PRO:HD3	1.63	0.79
2:N:157:ALA:HB1	2:N:209:TYR:CD2	2.18	0.79
1:A:413:ARG:HB2	1:A:413:ARG:NH1	1.96	0.78
1:M:41:MET:HE2	2:N:150:ASN:ND2	1.97	0.78
1:M:152:PHE:HB3	1:M:155:HIS:ND1	1.98	0.78
3:O:128:LEU:HD22	4:P:44:PHE:HB2	1.66	0.77
1:A:184:ARG:HG2	1:A:184:ARG:HH11	1.48	0.77
3:C:50:LYS:CD	4:D:118:ILE:HG22	2.12	0.77
1:A:413:ARG:HH11	1:A:413:ARG:CB	1.97	0.77
2:B:134:GLN:HE21	2:B:139:MET:HE3	1.49	0.77
2:B:13:TYR:OH	3:C:5:LYS:O	2.01	0.77
1:M:421:ASN:ND2	1:M:424:ALA:HB2	1.95	0.77
1:M:549:LYS:HD2	1:M:565:TYR:HB3	1.67	0.76
2:B:241:LYS:C	2:B:243:ARG:H	1.94	0.76
4:D:92:HIS:HB3	2:N:243:ARG:CB	2.14	0.76
1:M:316:LEU:HD22	1:M:319:LEU:HD11	1.68	0.76
2:N:225:GLN:HE21	10:N:800:BRG:H222	1.51	0.75
4:D:63:GLY:O	4:D:67:LEU:HD23	1.87	0.75
1:M:102:PRO:HB2	2:N:139:MET:HE3	1.67	0.75
2:N:159:PRO:HG2	2:N:207:VAL:HG21	1.68	0.75
3:O:104:GLY:O	3:O:107:PRO:HD2	1.86	0.75
3:O:50:LYS:HD2	4:P:117:THR:HG22	1.68	0.74
2:N:116:ILE:HG21	2:N:176:ALA:CB	2.18	0.74
1:M:488:ARG:NH1	1:M:488:ARG:HB3	2.03	0.74
4:D:48:ALA:O	4:D:53:ARG:HD3	1.87	0.74
1:A:279:ASN:O	1:A:280:LYS:HB2	1.88	0.74
4:D:64:ARG:HH22	4:D:117:THR:HG21	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:THR:OG1	1:A:212:GLY:HA3	1.88	0.73
1:M:311:VAL:HG11	1:M:349:PRO:HB2	1.71	0.73
10:B:700:BRS:HC19	4:D:18:GLY:HA2	1.71	0.72
1:M:447:ASN:ND2	1:M:449:ALA:HB3	2.04	0.72
3:C:19:LEU:HD12	3:C:20:PRO:HD2	1.70	0.72
1:M:331:ILE:HD12	1:M:331:ILE:H	1.53	0.72
1:M:96:LEU:HD21	1:M:139:LEU:HD21	1.70	0.72
1:A:0:MET:SD	1:A:182:GLN:HG3	2.29	0.72
1:M:41:MET:HE2	2:N:150:ASN:HD22	1.52	0.72
1:M:311:VAL:HG12	1:M:312:VAL:O	1.89	0.72
4:D:64:ARG:NH2	4:D:117:THR:HG21	2.04	0.72
4:D:0:MET:CG	4:D:1:ILE:H	2.00	0.71
1:M:11:GLY:O	1:M:16:GLY:HA3	1.89	0.71
1:M:469:PRO:HG3	1:M:534:ARG:NH2	2.05	0.71
1:M:436:LEU:O	1:M:440:VAL:HG23	1.89	0.71
2:N:222:ALA:O	2:N:226:GLN:NE2	2.24	0.71
1:A:323:LYS:HG3	1:A:327:ARG:HH11	1.56	0.71
1:A:103:TRP:O	2:B:139:MET:HE1	1.91	0.70
1:M:48:ALA:HB3	1:M:132:GLY:HA3	1.73	0.70
1:M:549:LYS:HA	1:M:568:VAL:HG23	1.73	0.70
4:P:105:ALA:O	4:P:109:VAL:HG23	1.90	0.70
3:O:97:ILE:HD13	3:O:102:LYS:HA	1.73	0.70
1:M:497:VAL:HG21	2:N:15:PRO:HG2	1.73	0.70
1:M:437:LYS:HG2	1:M:441:ASN:ND2	2.07	0.70
1:M:510:HIS:O	1:M:514:VAL:HG23	1.91	0.70
1:A:41:MET:HE2	2:B:150:ASN:HD22	1.57	0.70
1:M:260:TYR:CE1	1:M:264:GLN:NE2	2.60	0.70
3:O:19:LEU:H	3:O:19:LEU:CD2	2.02	0.70
4:D:6:LYS:CG	4:P:6:LYS:HB3	2.14	0.69
1:M:174:ASN:HD22	1:M:177:GLU:H	1.40	0.69
1:M:174:ASN:ND2	1:M:177:GLU:HG2	2.07	0.69
1:M:192:THR:OG1	1:M:212:GLY:HA3	1.91	0.69
4:P:77:CYS:O	4:P:81:ARG:HG3	1.93	0.69
1:M:358:MET:SD	1:M:390:ARG:N	2.65	0.69
1:M:332:CYS:HA	1:M:343:PRO:HG2	1.74	0.69
1:M:444:GLY:HA3	1:M:488:ARG:O	1.93	0.69
3:O:130:TRP:O	4:P:53:ARG:NH2	2.26	0.69
1:M:342:ASP:HB3	1:M:345:LYS:HB3	1.75	0.68
3:O:75:THR:HG22	4:P:32:ILE:HD13	1.73	0.68
3:C:99:LYS:O	3:C:100:ASP:CB	2.35	0.68
1:A:484:GLU:HG3	1:A:488:ARG:HH12	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:10:VAL:HG13	1:M:157:VAL:HG21	1.75	0.68
11:D:710:CE1:H211	11:D:710:CE1:H171	1.76	0.67
1:A:7:LEU:CD2	1:A:32:ILE:HG12	2.23	0.67
1:M:327:ARG:O	1:M:328:LEU:HD23	1.94	0.67
4:D:13:PHE:HE2	4:D:97:LYS:HE2	1.58	0.67
4:P:51:TYR:HD1	4:P:52:GLU:HG3	1.60	0.67
1:M:182:GLN:NE2	1:M:429:ALA:HB1	2.10	0.67
1:M:122:GLU:H	1:M:122:GLU:CD	2.03	0.66
2:N:11:VAL:CG2	2:N:91:GLU:HG2	2.25	0.66
1:A:372:LYS:HE3	1:A:413:ARG:HE	1.60	0.66
1:A:324:LEU:CD1	1:A:344:VAL:HG22	2.26	0.66
3:C:50:LYS:HB3	4:D:118:ILE:HG22	1.78	0.66
1:M:162:VAL:HG13	1:M:166:HIS:O	1.96	0.66
1:M:202:ASN:HA	1:M:353:THR:HG22	1.78	0.66
4:D:0:MET:HG2	4:D:1:ILE:N	2.11	0.65
3:O:50:LYS:HG3	4:P:118:ILE:CA	2.24	0.65
4:P:86:MET:HE3	4:P:91:ILE:HB	1.77	0.65
1:A:390:ARG:HH22	5:A:702:OAA:C4	2.09	0.65
1:A:204:ASN:N	1:A:204:ASN:HD22	1.91	0.65
1:M:444:GLY:HA3	1:M:488:ARG:C	2.22	0.65
2:B:81:LEU:HD23	2:B:81:LEU:N	2.12	0.65
1:M:93:MET:HB3	1:M:125:TRP:CE3	2.31	0.65
1:M:304:ILE:HD12	1:M:304:ILE:N	2.11	0.65
1:M:204:ASN:N	1:M:204:ASN:HD22	1.95	0.64
1:M:217:LEU:HG	1:M:555:ARG:HB3	1.79	0.64
1:A:232:HIS:CE1	1:A:242:LEU:HD11	2.33	0.64
1:A:57:GLN:NE2	1:A:122:GLU:HG2	2.12	0.64
1:M:41:MET:HB2	1:M:137:HIS:CE1	2.32	0.64
2:N:135:THR:HG23	2:N:136:PRO:HD2	1.80	0.64
4:P:24:SER:O	4:P:28:ALA:HB3	1.98	0.64
1:M:168:ARG:HD3	1:M:425:ILE:CD1	2.28	0.63
1:M:435:ARG:HH12	1:M:439:LEU:HD22	1.62	0.63
2:N:81:LEU:N	2:N:81:LEU:HD12	2.12	0.63
4:D:13:PHE:CE2	4:D:97:LYS:HE2	2.33	0.63
10:N:800:BRS:HC19	4:P:18:GLY:HA2	1.80	0.63
3:O:99:LYS:O	3:O:100:ASP:CG	2.41	0.63
4:P:39:LEU:HD13	4:P:49:LEU:HB3	1.81	0.63
1:A:250:GLU:CB	1:A:319:LEU:HD11	2.28	0.63
2:B:15:PRO:CB	3:C:5:LYS:H	2.09	0.63
2:N:40:LEU:HB3	2:N:53:TYR:CE2	2.34	0.63
2:N:54:ARG:NE	2:N:103:VAL:HG13	2.09	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:87:PHE:O	3:C:91:PRO:HD3	1.99	0.62
1:M:242:LEU:HD12	1:M:243:MET:N	2.14	0.62
4:P:51:TYR:CD1	4:P:52:GLU:HG3	2.34	0.62
1:A:27:ASN:ND2	1:A:30:ALA:HB2	2.15	0.62
1:M:435:ARG:HA	1:M:438:ASP:OD2	1.99	0.62
1:A:251:GLY:O	1:A:318:HIS:NE2	2.23	0.62
2:B:6:LEU:HD23	2:B:81:LEU:HD13	1.82	0.62
4:D:112:LEU:O	4:D:116:VAL:HG22	2.00	0.62
2:N:57:CYS:HB3	2:N:62:CYS:HB3	1.79	0.62
1:A:236:LEU:HD11	1:A:243:MET:HE3	1.81	0.62
4:D:64:ARG:NH2	4:D:117:THR:CG2	2.62	0.62
1:M:44:HIS:NE2	6:M:803:FAD:C8	2.61	0.62
2:B:32:ALA:O	2:B:82:ARG:NH1	2.32	0.62
1:M:51:GLY:HA2	1:M:131:THR:HG21	1.82	0.62
4:P:60:SER:O	4:P:64:ARG:HG3	2.00	0.62
1:M:168:ARG:HD3	1:M:425:ILE:HD11	1.80	0.62
3:O:59:PHE:O	3:O:62:PHE:HB3	2.00	0.62
1:M:399:LEU:HD11	6:M:803:FAD:H4'	1.80	0.62
4:D:86:MET:HE3	4:D:86:MET:HA	1.79	0.61
2:N:81:LEU:H	2:N:81:LEU:CD1	2.13	0.61
1:A:253:ILE:HG13	1:A:315:ASP:HB3	1.82	0.61
1:M:230:GLN:HB2	1:M:358:MET:HE2	1.80	0.61
1:A:197:ARG:HD2	1:A:206:GLY:HA2	1.82	0.61
4:D:36:GLY:C	4:D:37:ILE:HG13	2.24	0.61
2:N:196:ASN:ND2	2:N:234:ASP:OD1	2.32	0.61
3:O:106:GLU:H	3:O:106:GLU:CD	2.08	0.61
1:M:156:PHE:CD2	1:M:503:LEU:HD22	2.36	0.61
4:D:64:ARG:HH12	4:D:117:THR:HG23	1.61	0.61
3:O:50:LYS:HD2	4:P:118:ILE:HA	1.81	0.61
4:P:79:LEU:HD23	4:P:82:MET:HE3	1.81	0.61
2:B:155:TYR:CE2	2:B:169:GLY:HA3	2.36	0.61
3:O:86:TRP:HE1	4:P:22:MET:CE	2.11	0.61
1:A:436:LEU:O	1:A:440:VAL:HG23	2.01	0.61
4:D:64:ARG:CZ	4:D:117:THR:HG23	2.30	0.61
1:M:390:ARG:NH1	1:M:392:GLY:HA2	2.15	0.61
3:C:130:TRP:O	4:D:53:ARG:NH2	2.32	0.60
1:M:448:TRP:CH2	1:M:504:TYR:HB3	2.36	0.60
2:N:201:VAL:HG23	2:N:202:TRP:N	2.16	0.60
2:N:39:ALA:O	2:N:43:ILE:HG12	2.02	0.60
2:B:155:TYR:CZ	2:B:169:GLY:HA3	2.37	0.60
2:N:116:ILE:HG22	2:N:191:ARG:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:VAL:HG12	1:A:215:MET:HE1	1.82	0.60
1:M:21:ILE:HG21	1:M:99:TRP:CH2	2.36	0.60
1:M:275:GLY:O	1:M:277:PRO:HD3	2.01	0.60
2:N:169:GLY:O	2:N:173:ILE:HG13	2.02	0.60
2:B:241:LYS:C	2:B:243:ARG:N	2.58	0.60
1:A:321:GLU:OE1	1:A:321:GLU:HA	2.00	0.60
4:P:64:ARG:HB3	4:P:115:VAL:HG22	1.84	0.59
2:B:15:PRO:HB2	3:C:5:LYS:N	2.16	0.59
1:M:447:ASN:HD22	1:M:450:LYS:HG2	1.66	0.59
2:N:135:THR:HG22	2:N:137:ALA:H	1.66	0.59
1:M:545:VAL:C	1:M:546:ASN:HD22	2.09	0.59
2:N:162:GLY:HA3	3:O:11:MET:HE1	1.85	0.59
1:A:42:ARG:HD2	1:A:42:ARG:N	2.18	0.59
2:N:113:LEU:HD11	2:N:175:LEU:HD22	1.85	0.59
1:A:11:GLY:O	1:A:16:GLY:HA3	2.03	0.59
1:M:329:PRO:HG2	1:M:330:PHE:H	1.67	0.59
1:M:396:LEU:HG	6:M:803:FAD:C2	2.32	0.59
3:O:19:LEU:HD21	3:O:22:TYR:CE2	2.38	0.59
1:A:324:LEU:HD12	1:A:344:VAL:HG22	1.84	0.59
10:B:700:BRS:HO13	4:D:14:TRP:HE1	1.50	0.59
4:D:73:LEU:HB2	4:D:74:PRO:HD3	1.85	0.59
2:N:194:GLN:HE22	4:P:1:ILE:HG21	1.68	0.59
4:D:64:ARG:HH22	4:D:117:THR:CG2	2.16	0.58
1:M:236:LEU:HD22	1:M:339:VAL:HG11	1.84	0.58
1:M:311:VAL:HG11	1:M:349:PRO:CB	2.33	0.58
1:M:331:ILE:HD12	1:M:331:ILE:N	2.18	0.58
1:M:331:ILE:H	1:M:331:ILE:CD1	2.15	0.58
3:O:106:GLU:HB2	3:O:107:PRO:HD3	1.83	0.58
1:A:323:LYS:HG3	1:A:327:ARG:NH1	2.18	0.58
10:N:800:BRS:HC19	4:P:18:GLY:CA	2.33	0.58
2:B:8:ILE:HD11	2:B:81:LEU:HD11	1.86	0.58
4:D:67:LEU:O	4:D:71:ILE:HG13	2.04	0.58
1:M:213:MET:HE2	1:M:380:CYS:HA	1.84	0.58
2:N:225:GLN:NE2	2:N:228:LYS:HD2	2.18	0.58
1:A:18:ARG:NH1	1:A:92:GLU:OE1	2.37	0.58
1:M:82:VAL:HG22	1:M:385:LEU:HD12	1.84	0.58
1:M:476:ILE:HG23	1:M:520:HIS:CE1	2.39	0.58
1:M:499:ASN:HD21	1:M:501:ASP:HB3	1.68	0.58
2:N:81:LEU:HD12	2:N:81:LEU:H	1.69	0.58
4:P:10:GLU:N	4:P:11:PRO:CD	2.67	0.58
3:C:113:TRP:O	3:C:117:VAL:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:39:LEU:N	4:P:40:PRO:HD2	2.18	0.58
1:M:171:VAL:HB	1:M:432:VAL:HG11	1.86	0.57
1:M:311:VAL:HG13	1:M:350:VAL:O	2.02	0.57
1:M:296:HIS:ND1	1:M:299:ARG:NH2	2.52	0.57
1:M:332:CYS:O	1:M:336:LYS:HG3	2.04	0.57
2:B:57:CYS:HB3	2:B:62:CYS:HB3	1.86	0.57
1:M:155:HIS:HD2	1:M:174:ASN:HA	1.66	0.57
2:N:119:TYR:CE1	2:N:121:ILE:HD11	2.40	0.57
1:A:527:GLU:OE1	1:A:529:ARG:HD2	2.05	0.57
1:M:358:MET:SD	1:M:389:ASN:HA	2.44	0.57
1:M:183:ILE:HD12	1:M:183:ILE:N	2.20	0.57
3:O:36:VAL:HG23	3:O:37:TRP:N	2.20	0.57
1:A:448:TRP:CH2	1:A:504:TYR:HB3	2.40	0.56
1:M:545:VAL:HG12	1:M:546:ASN:ND2	2.19	0.56
3:O:60:VAL:O	3:O:64:GLN:HG3	2.06	0.56
3:C:130:TRP:N	3:C:130:TRP:CD1	2.69	0.56
1:M:288:ASP:O	1:M:292:GLN:HG3	2.05	0.56
1:M:435:ARG:O	1:M:438:ASP:HB2	2.05	0.56
2:N:206:PHE:CE1	2:N:225:GLN:HG3	2.40	0.56
1:A:28:PRO:HA	1:A:148:GLN:HE21	1.70	0.56
1:A:141:GLN:HB3	2:B:118:PRO:O	2.06	0.56
1:M:48:ALA:HB3	1:M:132:GLY:CA	2.36	0.56
2:N:97:PRO:HG2	2:N:105:ASP:HB3	1.87	0.56
3:C:50:LYS:CD	4:D:118:ILE:C	2.73	0.56
4:D:83:HIS:O	4:D:86:MET:HB2	2.06	0.56
2:N:12:ARG:NH2	2:N:101:ASP:OD1	2.38	0.56
4:P:28:ALA:N	4:P:29:PRO:HD2	2.20	0.56
3:O:33:VAL:O	3:O:36:VAL:HG22	2.06	0.56
1:A:395:SER:OG	6:A:703:FAD:H2'	2.06	0.56
1:M:162:VAL:HG22	1:M:167:VAL:HA	1.86	0.56
1:M:213:MET:CE	1:M:380:CYS:HA	2.36	0.56
3:O:65:ASN:O	3:O:66:PRO:C	2.47	0.56
4:P:35:VAL:O	4:P:40:PRO:HD3	2.06	0.56
2:N:155:TYR:CE2	2:N:169:GLY:HA3	2.41	0.56
1:M:17:LEU:HD13	1:M:140:PHE:N	2.21	0.55
1:M:217:LEU:HG	1:M:555:ARG:CB	2.37	0.55
2:N:188:LYS:HE2	2:N:192:MET:HE2	1.88	0.55
2:N:151:CYS:N	9:N:246:SF4:S4	2.79	0.55
1:A:250:GLU:HB3	1:A:319:LEU:HD11	1.87	0.55
2:B:57:CYS:O	2:B:58:ARG:HB2	2.05	0.55
1:M:174:ASN:ND2	1:M:177:GLU:CG	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:476:ILE:HG23	1:M:520:HIS:HE1	1.71	0.55
2:B:16:GLU:HG2	3:C:3:LYS:HB3	1.89	0.55
3:C:75:THR:HG22	4:D:32:ILE:HD13	1.89	0.55
1:M:113:VAL:HA	1:M:124:THR:O	2.06	0.55
1:A:35:ILE:HG22	1:A:36:SER:N	2.20	0.55
1:A:328:LEU:O	1:A:332:CYS:SG	2.49	0.55
3:C:85:THR:O	3:C:89:LEU:HD12	2.05	0.55
1:M:549:LYS:HD2	1:M:565:TYR:CB	2.37	0.55
2:N:241:LYS:O	2:N:241:LYS:CD	2.55	0.55
2:N:241:LYS:O	2:N:241:LYS:CG	2.55	0.55
2:B:2:GLU:HA	2:B:2:GLU:OE2	2.05	0.55
2:N:233:LYS:O	2:N:237:ILE:HD13	2.06	0.55
3:O:18:LYS:HD2	3:O:19:LEU:HD22	1.87	0.55
1:A:546:ASN:O	1:A:549:LYS:HE2	2.07	0.55
3:O:70:ILE:O	3:O:73:LEU:HB2	2.07	0.55
1:M:499:ASN:HD22	1:M:499:ASN:C	2.15	0.54
2:N:175:LEU:O	2:N:178:ARG:HB3	2.06	0.54
4:D:4:ASN:HD22	4:P:2:ASN:ND2	2.05	0.54
1:M:323:LYS:HG2	1:M:327:ARG:HH21	1.71	0.54
4:P:51:TYR:CD1	4:P:52:GLU:N	2.72	0.54
2:B:81:LEU:HD23	2:B:81:LEU:H	1.72	0.54
3:C:65:ASN:HB3	3:C:68:ILE:H	1.72	0.54
1:M:76:LEU:HD12	1:M:388:ALA:HB2	1.89	0.54
1:M:195:ALA:O	1:M:198:VAL:HG22	2.06	0.54
1:A:170:LEU:C	1:A:170:LEU:HD12	2.31	0.54
3:C:33:VAL:HA	4:D:82:MET:CE	2.37	0.54
1:M:548:LEU:HD21	1:M:575:PRO:HG3	1.89	0.54
1:M:42:ARG:HH21	2:N:150:ASN:CB	2.14	0.54
1:M:239:SER:HB2	1:M:241:ILE:HG13	1.89	0.54
1:M:499:ASN:O	1:M:503:LEU:HG	2.07	0.54
2:N:157:ALA:HB1	2:N:209:TYR:HD2	1.71	0.54
1:M:84:TYR:HE2	1:M:405:LEU:HD22	1.73	0.54
4:D:10:GLU:N	4:D:11:PRO:HD2	2.22	0.54
2:N:13:TYR:HB2	2:N:21:PRO:HB3	1.90	0.54
2:B:56:SER:O	2:B:58:ARG:HG3	2.08	0.54
11:D:710:CE1:H362	4:P:76:TRP:NE1	2.24	0.54
1:M:84:TYR:CE2	1:M:405:LEU:HD22	2.43	0.54
2:B:170:PRO:HA	2:B:224:ILE:HD11	1.90	0.53
1:M:304:ILE:H	1:M:304:ILE:CD1	2.16	0.53
3:O:74:ILE:HA	11:O:811:CE1:H151	1.90	0.53
4:P:64:ARG:O	4:P:115:VAL:HG21	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:CYS:HB2	1:A:90:PRO:HD3	1.90	0.53
1:A:232:HIS:HD2	1:A:234:THR:H	1.56	0.53
2:B:110:ILE:O	2:B:114:GLU:HG3	2.08	0.53
1:M:499:ASN:HA	2:N:100:ARG:HH21	1.73	0.53
1:A:93:MET:HB3	1:A:125:TRP:CZ3	2.44	0.53
1:A:556:ASP:HB2	1:A:558:ASP:OD2	2.08	0.53
4:P:113:ILE:O	4:P:117:THR:N	2.41	0.53
1:M:204:ASN:N	1:M:204:ASN:ND2	2.52	0.53
1:A:469:PRO:HB3	1:A:523:MET:HE1	1.91	0.53
1:M:44:HIS:CE1	1:M:204:ASN:HA	2.44	0.53
1:A:18:ARG:HG2	1:A:400:VAL:HA	1.91	0.53
1:A:395:SER:HB3	6:A:703:FAD:N1	2.24	0.53
1:A:442:GLN:OE1	1:A:487:LYS:HA	2.08	0.53
2:B:225:GLN:HE21	10:B:700:BRS:C21	2.20	0.53
3:C:59:PHE:CE1	3:C:63:LEU:HD11	2.44	0.53
2:N:220:PRO:O	2:N:223:ALA:N	2.41	0.53
4:P:62:ILE:HG23	4:P:63:GLY:N	2.24	0.53
1:A:159:ASP:OD2	1:A:160:ILE:N	2.42	0.53
2:N:139:MET:HA	2:N:142:TYR:CE2	2.44	0.53
3:C:50:LYS:CG	4:D:118:ILE:HG22	2.39	0.53
1:M:190:MET:HE1	1:M:215:MET:CE	2.18	0.53
1:M:279:ASN:O	1:M:280:LYS:HB2	2.09	0.53
2:B:169:GLY:O	2:B:173:ILE:HG13	2.09	0.53
1:M:36:SER:HA	6:M:803:FAD:N3A	2.24	0.53
4:P:62:ILE:O	4:P:65:VAL:HG22	2.09	0.53
1:A:157:VAL:CG1	1:A:215:MET:HE1	2.39	0.52
1:A:204:ASN:N	1:A:204:ASN:ND2	2.52	0.52
2:N:12:ARG:NH1	2:N:50:ASP:OD1	2.23	0.52
2:N:225:GLN:O	2:N:229:VAL:HG23	2.09	0.52
3:O:19:LEU:HD23	3:O:19:LEU:N	2.06	0.52
1:M:209:THR:O	1:M:209:THR:HG22	2.09	0.52
1:M:497:VAL:HG21	2:N:15:PRO:CG	2.38	0.52
1:M:54:ALA:O	1:M:55:VAL:C	2.51	0.52
2:N:81:LEU:N	2:N:81:LEU:CD1	2.71	0.52
2:N:135:THR:CG2	2:N:136:PRO:HD2	2.40	0.52
3:O:130:TRP:C	4:P:53:ARG:NH2	2.67	0.52
2:B:207:VAL:HG22	3:C:25:TYR:CE1	2.45	0.52
3:C:50:LYS:HE2	3:C:50:LYS:HA	1.91	0.52
1:M:97:GLU:OE2	2:N:132:ASN:ND2	2.42	0.52
4:P:117:THR:O	4:P:118:ILE:OXT	2.27	0.52
2:B:134:GLN:HE21	2:B:139:MET:CE	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:66:PHE:HD1	1:M:82:VAL:HG12	1.74	0.52
2:N:241:LYS:O	2:N:241:LYS:HD2	2.09	0.52
1:A:142:THR:O	1:A:145:GLN:HG2	2.08	0.52
2:B:157:ALA:HB1	2:B:209:TYR:CD2	2.45	0.52
1:M:199:TYR:CE1	1:M:229:VAL:HG11	2.44	0.52
1:A:342:ASP:C	1:A:344:VAL:H	2.18	0.52
3:C:98:VAL:HG23	3:C:98:VAL:O	2.10	0.52
1:M:58:ASP:C	1:M:60:ASP:H	2.18	0.52
1:A:253:ILE:CG1	1:A:315:ASP:HB3	2.39	0.52
1:M:390:ARG:HD2	1:M:391:LEU:O	2.10	0.52
3:C:50:LYS:HB3	4:D:118:ILE:CG2	2.39	0.52
1:M:10:VAL:CG1	1:M:157:VAL:HG21	2.40	0.52
1:M:41:MET:CE	2:N:150:ASN:HD22	2.23	0.52
2:B:120:ILE:HD13	2:B:185:ASP:HB2	1.92	0.51
2:B:212:GLU:HG3	3:C:21:PHE:CE2	2.44	0.51
4:D:24:SER:O	4:D:28:ALA:HB3	2.10	0.51
1:M:105:ARG:HG3	2:N:134:GLN:O	2.10	0.51
1:M:195:ALA:O	1:M:198:VAL:HG13	2.11	0.51
3:O:120:THR:HG23	4:P:30:VAL:HB	1.92	0.51
1:A:54:ALA:HB3	1:A:125:TRP:NE1	2.25	0.51
1:A:184:ARG:HG2	1:A:184:ARG:NH1	2.21	0.51
1:M:435:ARG:NH1	1:M:439:LEU:HB2	2.25	0.51
1:M:103:TRP:HH2	1:M:135:MET:SD	2.33	0.51
1:A:446:GLU:HB2	1:A:488:ARG:O	2.11	0.51
1:A:462:GLY:HA3	1:A:475:THR:OG1	2.09	0.51
3:C:87:PHE:CD2	3:C:112:LEU:HD13	2.46	0.51
3:O:127:ALA:O	3:O:128:LEU:HD23	2.10	0.51
1:A:200:ARG:HG3	1:A:457:LEU:HD23	1.93	0.51
4:D:4:ASN:ND2	4:P:2:ASN:ND2	2.58	0.51
4:D:114:GLY:O	4:D:117:THR:HA	2.11	0.51
1:M:99:TRP:CD2	1:M:142:THR:HG21	2.45	0.51
1:M:232:HIS:O	1:M:352:PRO:HA	2.10	0.51
1:M:6:ASP:HB3	1:M:7:LEU:HD23	1.91	0.51
2:N:225:GLN:HE21	10:N:800:BRS:C22	2.21	0.51
3:O:97:ILE:CD1	3:O:102:LYS:HA	2.41	0.51
1:M:199:TYR:OH	1:M:229:VAL:HG21	2.11	0.51
2:N:2:GLU:OE1	2:N:2:GLU:HA	2.10	0.51
2:B:113:LEU:HD23	2:B:113:LEU:O	2.09	0.51
1:M:96:LEU:HD21	1:M:139:LEU:CD2	2.40	0.51
1:M:488:ARG:HB3	1:M:488:ARG:CZ	2.41	0.51
2:N:155:TYR:CZ	2:N:169:GLY:HA3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:HIS:NE2	6:A:703:FAD:C8	2.68	0.51
1:A:316:LEU:O	1:A:319:LEU:HB2	2.09	0.51
2:B:145:PHE:HA	2:B:218:VAL:HG13	1.93	0.51
1:M:130:LYS:O	1:M:133:PHE:HB3	2.11	0.51
1:M:176:MET:O	1:M:497:VAL:HA	2.10	0.51
1:M:222:PRO:CG	1:M:362:GLU:OE1	2.59	0.51
1:M:162:VAL:HG13	1:M:166:HIS:C	2.36	0.51
1:A:253:ILE:HA	1:A:283:GLU:HG2	1.92	0.50
1:A:317:ARG:C	1:A:319:LEU:H	2.19	0.50
2:B:192:MET:O	2:B:193:ALA:C	2.52	0.50
1:M:213:MET:HB3	1:M:223:LEU:HD21	1.92	0.50
1:A:184:ARG:HH11	1:A:184:ARG:CG	2.18	0.50
3:C:104:GLY:HA2	3:C:107:PRO:HD2	1.92	0.50
4:D:28:ALA:O	4:D:32:ILE:HG13	2.11	0.50
1:M:233:PRO:HG2	1:M:248:ARG:HH22	1.76	0.50
1:A:525:ARG:NH1	1:A:527:GLU:OE1	2.42	0.50
1:M:400:VAL:HG23	1:M:401:VAL:N	2.26	0.50
1:A:148:GLN:OE1	1:A:148:GLN:N	2.40	0.50
3:C:11:MET:HE2	3:C:15:TRP:CD1	2.47	0.50
1:M:435:ARG:O	1:M:435:ARG:HD2	2.11	0.50
3:O:84:LYS:HE2	3:O:88:GLU:CD	2.36	0.50
1:A:94:THR:HA	2:B:131:THR:HG22	1.92	0.50
1:A:500:THR:HB	1:A:504:TYR:CZ	2.46	0.50
3:C:82:HIS:HE1	3:C:86:TRP:CE3	2.30	0.50
2:N:235:PHE:HE1	4:P:8:SER:O	1.95	0.50
1:A:228:PHE:O	1:A:358:MET:HB2	2.12	0.50
1:A:236:LEU:HD21	1:A:243:MET:HE3	1.92	0.50
2:N:236:LEU:HD23	2:N:236:LEU:C	2.37	0.50
4:P:117:THR:HG22	4:P:118:ILE:CA	2.41	0.50
1:M:23:ALA:HB3	1:M:32:ILE:HD13	1.93	0.50
1:M:98:LEU:HD11	2:N:127:ALA:CA	2.38	0.50
1:M:488:ARG:NH1	1:M:488:ARG:CB	2.74	0.50
2:N:9:GLU:HG3	2:N:25:PHE:CZ	2.47	0.50
2:B:240:LEU:C	2:B:242:PRO:HD3	2.37	0.50
2:B:241:LYS:O	2:B:241:LYS:HG3	2.11	0.50
2:N:110:ILE:O	2:N:114:GLU:HG3	2.11	0.50
1:M:452:ARG:NH2	2:N:45:ASP:OD2	2.45	0.49
1:M:493:ASP:OD2	1:M:499:ASN:CG	2.55	0.49
3:O:50:LYS:HD2	4:P:118:ILE:CA	2.41	0.49
1:A:336:LYS:O	1:A:340:GLY:HA2	2.11	0.49
3:C:50:LYS:CB	4:D:118:ILE:HG22	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:251:GLY:CA	1:M:277:PRO:HG2	2.29	0.49
3:C:28:ARG:HD2	3:C:29:GLU:OE2	2.13	0.49
3:O:84:LYS:HG3	3:O:85:THR:N	2.27	0.49
1:A:244:THR:HG22	1:A:331:ILE:HG13	1.92	0.49
2:N:96:PHE:HB3	2:N:104:VAL:HB	1.93	0.49
1:A:390:ARG:HD2	1:A:395:SER:HB2	1.94	0.49
4:D:0:MET:CG	4:D:1:ILE:N	2.72	0.49
4:D:102:GLY:HA2	11:D:710:CE1:H62	1.93	0.49
1:M:488:ARG:CB	1:M:488:ARG:HH11	2.25	0.49
2:N:225:GLN:HE22	2:N:228:LYS:HD2	1.76	0.49
4:P:30:VAL:O	4:P:33:LEU:HB3	2.12	0.49
4:P:95:ALA:O	4:P:96:GLY:C	2.55	0.49
1:M:1:GLN:HG2	1:M:2:THR:N	2.27	0.49
1:M:324:LEU:O	1:M:328:LEU:N	2.42	0.49
2:N:208:GLY:N	8:N:245:F3S:S1	2.81	0.49
3:O:36:VAL:HG11	4:P:82:MET:CE	2.43	0.49
1:A:288:ASP:O	1:A:292:GLN:HG3	2.13	0.49
2:B:119:TYR:O	2:B:121:ILE:HG13	2.13	0.49
1:M:222:PRO:HG3	1:M:362:GLU:OE1	2.12	0.49
4:P:7:ARG:HG2	4:P:8:SER:N	2.28	0.49
1:M:321:GLU:HA	1:M:324:LEU:HB3	1.95	0.49
1:M:375:PHE:CD1	1:M:375:PHE:N	2.81	0.49
1:M:421:ASN:ND2	1:M:424:ALA:CB	2.61	0.49
1:A:391:LEU:O	1:A:394:ASN:HB2	2.13	0.49
2:B:175:LEU:O	2:B:178:ARG:HB3	2.13	0.49
3:C:106:GLU:HB2	3:C:107:PRO:HD3	1.95	0.49
2:N:221:ALA:O	2:N:225:GLN:HG2	2.13	0.49
3:O:31:THR:O	3:O:34:PRO:HD2	2.13	0.49
3:O:103:MET:CG	3:O:104:GLY:N	2.76	0.49
1:A:232:HIS:NE2	1:A:242:LEU:HD11	2.28	0.49
2:B:222:ALA:HB2	3:C:92:LYS:HE3	1.95	0.49
4:D:30:VAL:HG13	4:D:31:MET:N	2.27	0.49
2:B:225:GLN:CG	10:B:700:BRS:H222	2.43	0.48
3:C:31:THR:O	3:C:34:PRO:HD2	2.13	0.48
1:M:40:PRO:HB2	1:M:140:PHE:CD1	2.48	0.48
1:M:311:VAL:HG12	1:M:312:VAL:N	2.28	0.48
3:C:106:GLU:CD	3:C:106:GLU:H	2.22	0.48
1:A:85:PHE:CD2	1:A:385:LEU:HD11	2.49	0.48
1:M:66:PHE:CD1	1:M:82:VAL:HG12	2.48	0.48
4:P:72:VAL:HG11	4:P:108:THR:HG23	1.94	0.48
4:D:93:VAL:N	2:N:243:ARG:O	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:103:MET:HG2	3:O:104:GLY:N	2.28	0.48
1:M:7:LEU:CD1	1:M:23:ALA:HB1	2.43	0.48
3:O:85:THR:O	3:O:89:LEU:HD12	2.14	0.48
1:A:184:ARG:NH1	1:A:184:ARG:CG	2.76	0.48
1:A:469:PRO:CB	1:A:523:MET:HE1	2.43	0.48
4:P:9:ASP:C	4:P:11:PRO:HD2	2.39	0.48
3:C:12:THR:CG2	3:C:13:SER:N	2.77	0.48
1:M:465:ILE:HD13	1:M:465:ILE:N	2.21	0.48
1:A:127:ALA:HB3	1:A:131:THR:HA	1.96	0.48
4:D:4:ASN:CG	4:D:4:ASN:O	2.56	0.48
1:M:233:PRO:HG2	1:M:248:ARG:NH2	2.29	0.48
1:M:448:TRP:CG	1:M:449:ALA:N	2.81	0.48
1:A:308:ARG:HH12	1:A:339:VAL:HA	1.79	0.48
4:D:86:MET:CE	4:D:91:ILE:HD12	2.43	0.48
2:N:84:TYR:CD1	2:N:88:MET:HE3	2.49	0.48
2:N:182:ASP:OD2	2:N:184:ARG:HD3	2.14	0.48
1:M:175:MET:HE3	1:M:503:LEU:HD13	1.96	0.47
1:M:463:CYS:HA	1:M:467:ARG:HE	1.78	0.47
1:M:546:ASN:HD22	1:M:546:ASN:N	2.10	0.47
1:M:548:LEU:CD2	1:M:575:PRO:HG3	2.44	0.47
2:N:44:LYS:HD3	2:N:51:LEU:O	2.14	0.47
3:O:65:ASN:O	3:O:65:ASN:OD1	2.32	0.47
2:B:159:PRO:CG	2:B:207:VAL:HG21	2.44	0.47
3:O:50:LYS:HD2	4:P:117:THR:CG2	2.41	0.47
1:M:304:ILE:HG12	1:M:313:TYR:HE2	1.79	0.47
2:N:241:LYS:O	2:N:241:LYS:HG3	2.14	0.47
3:C:28:ARG:NH1	3:C:29:GLU:OE2	2.38	0.47
4:D:92:HIS:HA	2:N:243:ARG:OXT	2.15	0.47
4:D:95:ALA:O	4:D:96:GLY:C	2.57	0.47
1:M:2:THR:HG22	1:M:3:PHE:N	2.29	0.47
4:P:6:LYS:H	4:P:6:LYS:HG3	1.36	0.47
2:N:201:VAL:CG2	2:N:202:TRP:N	2.77	0.47
3:O:98:VAL:HG23	3:O:103:MET:HB2	1.96	0.47
1:A:126:PHE:N	1:A:126:PHE:CD2	2.82	0.47
2:B:81:LEU:N	2:B:81:LEU:CD2	2.77	0.47
1:M:7:LEU:HD11	1:M:23:ALA:HB1	1.97	0.47
1:M:358:MET:HE1	1:M:389:ASN:HA	1.96	0.47
1:M:546:ASN:O	1:M:549:LYS:HE3	2.15	0.47
1:A:250:GLU:HB2	1:A:319:LEU:HD11	1.95	0.47
2:B:7:LYS:HE2	2:B:25:PHE:CD2	2.50	0.47
1:M:17:LEU:O	1:M:21:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:421:ASN:ND2	1:M:424:ALA:H	2.13	0.47
1:A:49:GLU:HG3	1:A:244:THR:HB	1.96	0.47
1:A:408:GLU:O	1:A:411:THR:HB	2.15	0.47
1:M:89:CYS:N	1:M:90:PRO:HD2	2.30	0.47
1:M:159:ASP:OD2	1:M:160:ILE:N	2.48	0.47
2:B:100:ARG:NE	2:B:101:ASP:OD2	2.43	0.46
1:M:88:HIS:O	1:M:401:VAL:HG22	2.15	0.46
1:M:100:GLY:C	2:N:184:ARG:HH22	2.24	0.46
2:N:12:ARG:NE	2:N:101:ASP:OD1	2.48	0.46
1:A:247:CYS:SG	1:A:331:ILE:HG21	2.56	0.46
2:B:11:VAL:HG21	2:B:91:GLU:HG2	1.97	0.46
10:B:700:BRS:HC21	4:D:14:TRP:HZ2	1.80	0.46
1:M:184:ARG:NH2	1:M:426:GLU:HG2	2.30	0.46
1:M:251:GLY:HA2	1:M:277:PRO:CG	2.29	0.46
3:O:22:TYR:O	3:O:25:TYR:HB3	2.15	0.46
3:O:51:ASN:HB2	3:O:55:ALA:CB	2.45	0.46
4:P:48:ALA:HA	4:P:53:ARG:HD3	1.97	0.46
1:A:39:TYR:O	1:A:40:PRO:C	2.58	0.46
1:A:182:GLN:OE1	1:A:184:ARG:NH1	2.46	0.46
1:A:451:ILE:HG23	1:A:482:LEU:HD22	1.96	0.46
1:A:466:TYR:CD2	1:A:535:LEU:HD21	2.51	0.46
2:B:68:MET:HE1	2:B:73:PRO:HD3	1.96	0.46
1:M:242:LEU:HD12	1:M:242:LEU:C	2.40	0.46
2:N:28:VAL:HG22	2:N:43:ILE:HD11	1.97	0.46
1:A:145:GLN:HB3	2:B:119:TYR:CZ	2.50	0.46
4:D:53:ARG:HH11	4:D:53:ARG:HG2	1.81	0.46
4:D:57:PHE:CZ	4:D:63:GLY:HA2	2.51	0.46
1:M:316:LEU:O	1:M:317:ARG:C	2.58	0.46
4:P:114:GLY:O	4:P:118:ILE:HG22	2.14	0.46
1:M:219:HIS:O	1:M:371:ILE:HD11	2.15	0.46
1:M:481:GLU:O	1:M:485:ARG:HG2	2.15	0.46
1:A:55:VAL:HG21	1:A:62:PHE:CD2	2.51	0.46
1:A:94:THR:HG23	2:B:131:THR:HG22	1.97	0.46
1:A:556:ASP:OD2	1:A:562:ARG:NE	2.49	0.46
1:M:342:ASP:OD1	1:M:344:VAL:HG22	2.16	0.46
2:N:220:PRO:O	2:N:221:ALA:C	2.59	0.46
2:B:188:LYS:NZ	2:B:230:GLU:HG3	2.30	0.46
10:B:700:BRS:HC19	4:D:18:GLY:CA	2.43	0.46
1:M:428:GLN:O	1:M:432:VAL:HG23	2.15	0.46
1:M:551:THR:HG23	1:M:563:LEU:HD22	1.98	0.46
4:P:1:ILE:N	4:P:1:ILE:HD12	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:26:ILE:HG22	4:P:27:ILE:HG13	1.96	0.46
1:A:542:ARG:NH2	1:A:544:ASP:OD2	2.46	0.46
3:C:33:VAL:HG22	4:D:82:MET:HE2	1.96	0.46
1:M:100:GLY:O	1:M:101:CYS:C	2.58	0.46
1:M:206:GLY:HA3	2:N:55:TRP:CZ3	2.51	0.46
2:N:12:ARG:HH22	2:N:50:ASP:C	2.24	0.46
1:A:304:ILE:HD12	1:A:304:ILE:H	1.80	0.46
4:D:9:ASP:HB2	11:P:810:CE1:H242	1.98	0.46
1:M:18:ARG:HG2	1:M:400:VAL:HA	1.98	0.46
1:M:330:PHE:HB3	1:M:331:ILE:HD12	1.97	0.46
1:M:421:ASN:O	1:M:425:ILE:HG13	2.17	0.46
1:M:174:ASN:ND2	1:M:177:GLU:H	2.11	0.45
3:O:18:LYS:HD2	3:O:19:LEU:CD2	2.46	0.45
3:O:38:PHE:CE2	3:O:42:LEU:HD11	2.52	0.45
3:C:8:VAL:O	3:C:8:VAL:HG12	2.14	0.45
1:M:339:VAL:O	1:M:341:VAL:HG23	2.16	0.45
2:N:109:PHE:CE2	2:N:113:LEU:HD22	2.51	0.45
2:N:158:CYS:HA	8:N:245:F3S:S4	2.56	0.45
3:O:128:LEU:O	4:P:45:PRO:HG2	2.17	0.45
2:B:214:CYS:SG	2:B:218:VAL:HB	2.56	0.45
3:C:98:VAL:HG22	3:C:103:MET:HB3	1.98	0.45
4:D:117:THR:O	4:D:118:ILE:C	2.54	0.45
2:N:28:VAL:CG2	2:N:43:ILE:HD11	2.46	0.45
2:N:192:MET:O	2:N:193:ALA:C	2.58	0.45
2:B:57:CYS:O	2:B:58:ARG:CB	2.63	0.45
1:M:35:ILE:CD1	1:M:155:HIS:HB3	2.46	0.45
1:A:250:GLU:O	1:A:319:LEU:HD11	2.17	0.45
4:D:42:GLY:O	4:D:44:PHE:N	2.48	0.45
1:M:151:ARG:NH1	1:M:153:ASP:OD2	2.49	0.45
2:N:202:TRP:NE1	2:N:231:SER:OG	2.48	0.45
4:P:51:TYR:HD1	4:P:52:GLU:H	1.55	0.45
3:C:12:THR:HG22	3:C:13:SER:N	2.30	0.45
1:M:92:GLU:HB3	1:M:400:VAL:HB	1.99	0.45
1:M:184:ARG:HG3	1:M:184:ARG:HH11	1.82	0.45
4:P:53:ARG:NH1	4:P:53:ARG:HG2	2.32	0.45
3:C:70:ILE:O	3:C:74:ILE:HG13	2.16	0.45
1:M:145:GLN:O	1:M:147:PRO:HD3	2.16	0.45
1:M:299:ARG:HE	1:M:299:ARG:HB2	1.54	0.45
2:N:168:ILE:HD11	2:N:173:ILE:HG12	1.99	0.45
1:M:492:THR:HG22	1:M:492:THR:O	2.16	0.45
4:P:67:LEU:O	4:P:71:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:102:GLY:O	4:P:103:LEU:C	2.60	0.45
1:M:570:ILE:HG22	1:M:571:THR:N	2.31	0.45
1:M:150:GLN:HG3	1:M:152:PHE:CE1	2.51	0.44
1:M:341:VAL:HG13	1:M:346:GLU:HB2	1.99	0.44
1:M:480:ALA:O	1:M:483:GLN:HB2	2.17	0.44
1:M:1:GLN:HG2	1:M:2:THR:H	1.83	0.44
1:M:105:ARG:NH1	2:N:134:GLN:H	2.15	0.44
1:M:273:PRO:O	1:M:274:LEU:C	2.58	0.44
1:M:443:ASP:CG	1:M:444:GLY:N	2.74	0.44
2:N:198:GLN:O	2:N:203:SER:HB2	2.17	0.44
2:N:214:CYS:SG	9:N:246:SF4:S1	3.15	0.44
3:O:33:VAL:HB	3:O:34:PRO:CD	2.42	0.44
1:A:282:MET:HB3	1:A:283:GLU:OE1	2.17	0.44
3:C:39:SER:O	3:C:43:ILE:HG13	2.18	0.44
4:D:39:LEU:HB3	4:D:40:PRO:CD	2.47	0.44
4:D:117:THR:HB	4:D:118:ILE:O	2.17	0.44
1:M:38:VAL:O	1:M:39:TYR:C	2.61	0.44
1:M:377:VAL:HG22	1:M:378:GLY:N	2.33	0.44
1:A:17:LEU:HD22	1:A:140:PHE:HA	1.99	0.44
4:D:20:GLY:HA2	4:D:73:LEU:HB3	2.00	0.44
4:D:30:VAL:CG1	4:D:31:MET:N	2.81	0.44
4:D:72:VAL:O	4:D:75:LEU:HB2	2.18	0.44
2:N:126:THR:OG1	2:N:129:GLN:HG3	2.18	0.44
2:N:218:VAL:O	2:N:219:ASP:HB3	2.18	0.44
4:P:112:LEU:O	4:P:116:VAL:HG22	2.18	0.44
3:C:15:TRP:CD2	3:C:16:TRP:N	2.85	0.44
2:N:170:PRO:HG2	2:N:171:ALA:H	1.82	0.44
4:P:79:LEU:HD12	4:P:104:ALA:HB2	1.98	0.44
1:A:2:THR:HA	1:A:182:GLN:O	2.18	0.44
1:A:244:THR:HG22	1:A:331:ILE:CG1	2.47	0.44
1:A:356:TYR:CZ	1:A:390:ARG:HD3	2.51	0.44
2:B:206:PHE:CE1	2:B:225:GLN:HG3	2.53	0.44
4:P:109:VAL:O	4:P:112:LEU:HB3	2.17	0.44
2:B:142:TYR:O	2:B:143:HIS:C	2.57	0.44
2:B:201:VAL:HG23	2:B:202:TRP:N	2.32	0.44
1:M:127:ALA:C	1:M:128:ALA:O	2.60	0.44
1:M:399:LEU:HD11	6:M:803:FAD:C4'	2.46	0.44
1:A:151:ARG:NH1	1:A:153:ASP:OD2	2.49	0.44
2:B:81:LEU:O	2:B:83:ASP:N	2.51	0.44
2:B:113:LEU:HD23	2:B:113:LEU:C	2.43	0.44
2:B:160:GLN:OE1	2:B:160:GLN:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:40:PRO:O	4:D:41:LEU:HD23	2.18	0.44
1:M:196:GLY:C	1:M:198:VAL:H	2.26	0.44
1:A:386:HIS:ND1	1:A:390:ARG:HG3	2.33	0.44
2:B:81:LEU:O	2:B:82:ARG:C	2.60	0.44
4:D:64:ARG:NH1	4:D:115:VAL:O	2.51	0.44
1:M:328:LEU:N	1:M:329:PRO:CD	2.81	0.44
1:M:364:ASP:CG	1:M:366:ASN:H	2.26	0.44
1:M:434:GLN:HA	1:M:434:GLN:NE2	2.33	0.44
1:M:190:MET:O	1:M:376:ALA:HA	2.18	0.43
1:M:203:THR:C	1:M:204:ASN:HD22	2.25	0.43
1:M:435:ARG:HD2	1:M:435:ARG:C	2.43	0.43
2:N:75:LEU:HD11	2:N:215:PRO:HG3	2.00	0.43
3:O:49:LEU:HD13	3:O:56:TRP:CE3	2.53	0.43
3:C:37:TRP:CZ2	3:C:41:GLU:OE1	2.71	0.43
1:M:2:THR:CG2	1:M:3:PHE:N	2.81	0.43
1:M:526:LYS:HA	1:M:534:ARG:NH1	2.33	0.43
2:N:133:ILE:O	2:N:133:ILE:HG22	2.17	0.43
3:O:111:SER:O	3:O:114:ALA:HB3	2.18	0.43
3:O:124:LEU:HD23	3:O:124:LEU:HA	1.79	0.43
1:A:304:ILE:HD12	1:A:304:ILE:N	2.33	0.43
1:A:324:LEU:O	1:A:328:LEU:N	2.46	0.43
4:D:70:MET:HE3	4:D:70:MET:O	2.17	0.43
2:N:142:TYR:O	2:N:143:HIS:C	2.60	0.43
2:N:159:PRO:CG	2:N:207:VAL:HG21	2.44	0.43
1:A:40:PRO:HB2	1:A:140:PHE:CD1	2.53	0.43
2:B:240:LEU:O	2:B:242:PRO:CD	2.66	0.43
1:M:316:LEU:HD22	1:M:319:LEU:CD1	2.43	0.43
1:A:273:PRO:O	1:A:274:LEU:C	2.59	0.43
2:B:164:ASN:OD1	2:B:164:ASN:C	2.59	0.43
3:O:65:ASN:O	3:O:67:VAL:N	2.51	0.43
2:B:225:GLN:CD	10:B:700:BRS:H222	2.38	0.43
1:M:35:ILE:CG1	1:M:36:SER:N	2.81	0.43
1:M:274:LEU:HD22	1:M:318:HIS:CD2	2.53	0.43
1:M:304:ILE:HG22	1:M:305:SER:N	2.34	0.43
1:M:435:ARG:HH12	1:M:439:LEU:CD2	2.27	0.43
3:O:86:TRP:CH2	4:P:21:GLY:HA3	2.54	0.43
1:A:493:ASP:OD1	1:A:495:SER:OG	2.28	0.43
2:B:136:PRO:HB2	3:C:100:ASP:OD1	2.18	0.43
3:C:87:PHE:O	3:C:91:PRO:CD	2.67	0.43
4:D:86:MET:HA	4:D:86:MET:CE	2.44	0.43
1:M:2:THR:HA	1:M:182:GLN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:44:LYS:NZ	2:N:49:PRO:O	2.42	0.43
1:A:358:MET:HE3	1:A:389:ASN:CA	2.27	0.43
2:B:167:PHE:CD1	2:B:203:SER:HB3	2.54	0.43
4:D:109:VAL:O	4:D:110:VAL:C	2.62	0.43
1:M:331:ILE:HA	1:M:334:LEU:HD12	2.01	0.43
1:M:439:LEU:O	1:M:442:GLN:HB3	2.19	0.43
2:N:149:ILE:HG12	9:N:246:SF4:S3	2.59	0.43
1:A:83:ASP:O	1:A:87:HIS:HD2	2.02	0.43
4:D:64:ARG:CZ	4:D:117:THR:CG2	2.96	0.43
1:M:320:GLY:O	1:M:324:LEU:HB2	2.19	0.43
1:A:311:VAL:HB	1:A:350:VAL:O	2.19	0.43
1:M:449:ALA:HB1	2:N:45:ASP:OD2	2.18	0.43
1:A:343:PRO:HG3	1:A:348:ILE:HD11	2.00	0.42
1:A:377:VAL:HG21	1:A:403:GLY:HA2	2.01	0.42
2:B:225:GLN:HG3	10:B:700:BRG:H222	2.00	0.42
4:D:13:PHE:HZ	11:D:710:CE1:H102	1.83	0.42
1:M:118:GLY:O	1:M:119:MET:C	2.62	0.42
1:M:315:ASP:OD1	1:M:317:ARG:HG3	2.19	0.42
3:O:73:LEU:HD23	3:O:73:LEU:HA	1.79	0.42
3:O:90:ALA:N	3:O:91:PRO:HD2	2.33	0.42
1:A:118:GLY:HA2	1:A:279:ASN:HD21	1.84	0.42
1:M:112:ASN:C	1:M:126:PHE:HE2	2.27	0.42
1:M:184:ARG:HG3	1:M:184:ARG:NH1	2.33	0.42
4:D:98:TRP:NE1	11:D:710:CE1:H141	2.34	0.42
1:M:66:PHE:O	1:M:70:VAL:HG23	2.18	0.42
1:M:493:ASP:OD2	1:M:499:ASN:ND2	2.53	0.42
3:O:118:VAL:O	3:O:122:VAL:HG23	2.19	0.42
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.73	0.42
2:B:6:LEU:CD2	2:B:81:LEU:HD13	2.48	0.42
2:N:26:TYR:HB3	2:N:47:LEU:HD13	2.00	0.42
1:A:84:TYR:OH	1:A:405:LEU:HD13	2.19	0.42
1:A:135:MET:CE	1:A:135:MET:CG	2.94	0.42
1:A:202:ASN:HA	1:A:353:THR:HG22	2.00	0.42
4:D:48:ALA:HA	4:D:53:ARG:HD3	2.01	0.42
1:A:281:TYR:O	1:A:282:MET:C	2.63	0.42
1:M:105:ARG:HH12	2:N:134:GLN:H	1.68	0.42
3:O:19:LEU:HA	3:O:20:PRO:HD3	1.90	0.42
3:O:123:ILE:HD12	4:P:30:VAL:HG11	2.00	0.42
2:B:188:LYS:HZ1	2:B:230:GLU:HG3	1.83	0.42
3:C:82:HIS:CE1	3:C:86:TRP:CE3	3.08	0.42
2:N:58:ARG:HH11	2:N:58:ARG:HD2	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:61:ILE:O	2:N:61:ILE:HG13	2.19	0.42
2:N:67:MET:SD	2:N:102:LEU:HD13	2.60	0.42
2:N:150:ASN:HA	9:N:246:SF4:S4	2.60	0.42
1:A:196:GLY:HA3	1:A:204:ASN:OD1	2.20	0.42
1:M:369:THR:HG23	1:M:374:LEU:O	2.19	0.42
3:O:19:LEU:CD2	3:O:19:LEU:N	2.72	0.42
3:O:36:VAL:HG11	4:P:82:MET:HE1	2.00	0.42
2:B:154:CYS:SG	2:B:170:PRO:HG2	2.60	0.42
10:B:700:BRS:O5	3:C:89:LEU:HB2	2.19	0.42
3:C:15:TRP:CE3	3:C:16:TRP:N	2.88	0.42
1:M:72:GLY:O	1:M:389:ASN:HB3	2.20	0.42
1:M:127:ALA:O	1:M:128:ALA:C	2.63	0.42
1:M:434:GLN:HA	1:M:434:GLN:HE21	1.84	0.42
1:M:552:LEU:HD11	1:M:566:SER:OG	2.20	0.42
3:O:16:TRP:CD1	3:O:26:MET:HE2	2.55	0.42
4:P:22:MET:O	4:P:26:ILE:HD13	2.19	0.42
1:A:181:VAL:HG12	1:A:182:GLN:N	2.34	0.42
2:B:9:GLU:CD	2:B:89:LYS:HG3	2.45	0.42
3:C:15:TRP:O	3:C:18:LYS:HG2	2.20	0.42
1:M:498:PHE:CD2	2:N:103:VAL:HG21	2.55	0.42
2:N:95:ASN:O	2:N:161:PHE:HE2	2.02	0.42
3:O:36:VAL:CG2	3:O:37:TRP:N	2.82	0.42
3:O:98:VAL:HG21	3:O:103:MET:HE3	2.02	0.42
11:P:810:CE1:H171	11:P:810:CE1:H211	2.02	0.42
3:C:33:VAL:HB	3:C:34:PRO:CD	2.43	0.41
1:M:152:PHE:O	1:M:155:HIS:HB2	2.20	0.41
1:A:200:ARG:NH1	1:A:457:LEU:HD21	2.35	0.41
1:A:558:ASP:OD2	1:A:558:ASP:N	2.54	0.41
2:B:105:ASP:OD1	2:B:105:ASP:C	2.63	0.41
3:C:53:PRO:HD3	4:D:51:TYR:CZ	2.54	0.41
4:D:67:LEU:N	4:D:67:LEU:HD22	2.34	0.41
1:M:2:THR:HG23	1:M:184:ARG:HG2	2.01	0.41
1:M:155:HIS:O	6:M:803:FAD:H2A	2.19	0.41
1:M:222:PRO:HG2	1:M:362:GLU:OE1	2.20	0.41
2:N:201:VAL:HG23	2:N:202:TRP:CD2	2.55	0.41
4:P:24:SER:O	4:P:28:ALA:CB	2.67	0.41
1:M:329:PRO:HG2	1:M:330:PHE:N	2.34	0.41
1:A:62:PHE:CE2	1:A:90:PRO:HG2	2.55	0.41
1:A:81:VAL:HG21	1:A:383:VAL:O	2.21	0.41
1:A:413:ARG:HA	1:A:413:ARG:HD3	1.73	0.41
2:B:67:MET:HE2	2:B:67:MET:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:ARG:O	2:B:101:ASP:C	2.61	0.41
2:B:174:THR:OG1	2:B:220:PRO:HA	2.19	0.41
4:D:67:LEU:HD13	4:D:67:LEU:HA	1.88	0.41
1:M:316:LEU:HB3	1:M:319:LEU:CD1	2.33	0.41
4:P:70:MET:O	4:P:74:PRO:HG2	2.20	0.41
1:A:198:VAL:O	1:A:456:GLY:HA2	2.21	0.41
1:A:529:ARG:O	1:A:530:GLY:C	2.63	0.41
1:M:119:MET:HE2	1:M:391:LEU:HG	2.02	0.41
1:M:150:GLN:HG3	1:M:152:PHE:HE1	1.86	0.41
1:M:263:LEU:CD1	1:M:283:GLU:HA	2.50	0.41
1:M:390:ARG:HH22	5:M:802:OAA:C4	2.34	0.41
2:N:116:ILE:HD11	2:N:168:ILE:HD12	2.01	0.41
1:A:146:PHE:HA	1:A:147:PRO:HD2	1.88	0.41
2:B:9:GLU:HG3	2:B:25:PHE:CZ	2.55	0.41
10:B:700:BRS:O13	4:D:14:TRP:NE1	2.42	0.41
3:C:23:ARG:HB3	3:C:23:ARG:HH11	1.86	0.41
4:D:93:VAL:H	2:N:243:ARG:C	2.26	0.41
1:M:375:PHE:N	1:M:375:PHE:HD1	2.19	0.41
2:N:214:CYS:HB2	9:N:246:SF4:S1	2.60	0.41
2:N:224:ILE:O	2:N:227:GLY:N	2.54	0.41
4:P:79:LEU:HD23	4:P:82:MET:CE	2.49	0.41
1:A:41:MET:HG2	1:A:42:ARG:HD2	2.02	0.41
1:A:98:LEU:HD23	2:B:132:ASN:ND2	2.36	0.41
1:A:195:ALA:O	1:A:198:VAL:HG22	2.20	0.41
1:A:247:CYS:HB3	1:A:316:LEU:HD21	2.03	0.41
4:D:42:GLY:HA2	4:D:44:PHE:CE2	2.56	0.41
1:M:335:ALA:HA	1:M:339:VAL:HG22	2.03	0.41
1:A:54:ALA:O	1:A:55:VAL:C	2.64	0.41
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.79	0.41
1:A:227:GLU:OE1	1:A:551:THR:OG1	2.26	0.41
1:A:232:HIS:CD2	1:A:242:LEU:CD1	3.04	0.41
2:B:235:PHE:CD2	2:B:235:PHE:C	2.99	0.41
3:C:59:PHE:CZ	3:C:63:LEU:HD11	2.55	0.41
4:D:68:PHE:HD1	4:D:111:THR:HG22	1.85	0.41
1:M:80:ASP:OD2	1:M:365:GLN:HG2	2.21	0.41
1:M:100:GLY:O	2:N:184:ARG:NH2	2.52	0.41
1:M:329:PRO:CG	1:M:330:PHE:H	2.32	0.41
1:M:534:ARG:HD3	1:M:539:CYS:HB3	2.03	0.41
2:B:174:THR:O	2:B:175:LEU:C	2.62	0.41
2:B:212:GLU:HG3	3:C:21:PHE:HE2	1.85	0.41
1:M:37:LYS:NZ	1:M:211:ASP:OD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:100:GLY:C	2:N:184:ARG:NH2	2.79	0.41
1:M:176:MET:SD	2:N:99:GLU:HG3	2.61	0.41
1:M:279:ASN:O	1:M:280:LYS:CB	2.69	0.41
1:A:232:HIS:CD2	1:A:234:THR:H	2.35	0.41
1:A:236:LEU:CD1	1:A:243:MET:HE3	2.51	0.41
3:C:65:ASN:O	3:C:65:ASN:CG	2.62	0.41
1:M:81:VAL:HG21	1:M:383:VAL:O	2.20	0.41
1:M:122:GLU:CD	1:M:122:GLU:N	2.77	0.41
1:M:242:LEU:HD11	1:M:244:THR:HA	2.03	0.41
1:A:157:VAL:HG12	1:A:215:MET:CE	2.49	0.40
4:D:30:VAL:O	4:D:33:LEU:HB3	2.22	0.40
1:M:105:ARG:NH1	1:M:109:GLY:O	2.53	0.40
1:M:122:GLU:N	1:M:122:GLU:OE2	2.49	0.40
1:M:353:THR:HG22	1:M:354:ALA:N	2.36	0.40
2:N:155:TYR:HE1	2:N:171:ALA:CB	2.33	0.40
2:N:226:GLN:HE21	2:N:226:GLN:HB2	1.60	0.40
3:O:130:TRP:C	4:P:53:ARG:HH21	2.29	0.40
1:A:230:GLN:HB2	1:A:358:MET:HE1	2.03	0.40
1:A:321:GLU:OE1	1:A:321:GLU:CA	2.68	0.40
2:B:92:ALA:HB1	2:B:104:VAL:CG1	2.51	0.40
2:B:219:ASP:OD2	3:C:92:LYS:HE2	2.22	0.40
1:M:62:PHE:HB3	1:M:86:VAL:HG23	2.02	0.40
1:M:311:VAL:CG1	1:M:312:VAL:N	2.84	0.40
2:N:180:ASN:OD1	2:N:188:LYS:HA	2.21	0.40
4:P:72:VAL:HG12	4:P:76:TRP:CD1	2.56	0.40
1:A:89:CYS:N	1:A:90:PRO:CD	2.84	0.40
2:B:12:ARG:HH22	2:B:50:ASP:CG	2.29	0.40
2:B:240:LEU:C	2:B:242:PRO:CD	2.94	0.40
3:C:22:TYR:O	3:C:25:TYR:HB3	2.21	0.40
1:M:126:PHE:CD2	1:M:126:PHE:N	2.89	0.40
2:N:160:GLN:NE2	2:N:205:THR:CG2	2.84	0.40
2:N:200:GLY:O	2:N:201:VAL:C	2.64	0.40
4:P:62:ILE:HG23	4:P:63:GLY:H	1.85	0.40
4:P:104:ALA:O	4:P:108:THR:OG1	2.31	0.40
1:A:283:GLU:OE1	1:A:283:GLU:N	2.44	0.40
1:M:56:ALA:HB2	1:M:125:TRP:HE1	1.86	0.40
1:M:242:LEU:HD21	5:M:802:OAA:O1	2.22	0.40
3:O:99:LYS:O	3:O:100:ASP:OD1	2.38	0.40
4:P:53:ARG:HG2	4:P:53:ARG:HH11	1.87	0.40
1:A:45:THR:O	1:A:132:GLY:HA3	2.21	0.40
1:A:79:GLN:HB2	1:A:569:LYS:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:MET:HB3	1:A:125:TRP:CE3	2.57	0.40
1:A:413:ARG:HH11	1:A:413:ARG:CA	2.34	0.40
1:A:424:ALA:O	1:A:425:ILE:C	2.64	0.40
4:D:75:LEU:HA	4:D:75:LEU:HD23	1.84	0.40
1:M:44:HIS:CD2	6:M:803:FAD:C8M	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	575/602 (96%)	525 (91%)	43 (8%)	7 (1%)	10	41
1	M	575/602 (96%)	506 (88%)	59 (10%)	10 (2%)	7	35
2	B	241/243 (99%)	218 (90%)	19 (8%)	4 (2%)	7	35
2	N	241/243 (99%)	212 (88%)	23 (10%)	6 (2%)	4	28
3	C	128/130 (98%)	116 (91%)	9 (7%)	3 (2%)	5	30
3	O	128/130 (98%)	114 (89%)	10 (8%)	4 (3%)	3	25
4	D	117/119 (98%)	103 (88%)	13 (11%)	1 (1%)	14	46
4	P	117/119 (98%)	106 (91%)	10 (8%)	1 (1%)	14	46
All	All	2122/2188 (97%)	1900 (90%)	186 (9%)	36 (2%)	7	35

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	242	PRO
1	M	1	GLN
1	M	244	THR
3	O	18	LYS
1	A	79	GLN

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Mol	Chain	Res	Type
1	A	244	THR
1	A	321	GLU
2	B	56	SER
3	C	18	LYS
1	M	79	GLN
2	N	56	SER
1	A	318	HIS
1	M	128	ALA
1	M	318	HIS
2	N	128	ASP
3	O	66	PRO
3	O	100	ASP
2	B	183	SER
2	N	101	ASP
2	N	115	ALA
2	N	183	SER
1	A	282	MET
3	C	100	ASP
1	M	131	THR
1	M	329	PRO
1	M	344	VAL
3	O	103	MET
1	A	343	PRO
2	B	241	LYS
4	D	117	THR
1	M	282	MET
3	C	65	ASN
1	M	444	GLY
2	N	242	PRO
4	P	99	VAL
1	A	444	GLY

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	460/475 (97%)	447 (97%)	13 (3%)	38	60
1	M	460/475 (97%)	434 (94%)	26 (6%)	18	46
2	B	205/205 (100%)	199 (97%)	6 (3%)	37	60
2	N	205/205 (100%)	199 (97%)	6 (3%)	37	60
3	C	111/111 (100%)	105 (95%)	6 (5%)	20	47
3	O	111/111 (100%)	104 (94%)	7 (6%)	16	44
4	D	97/97 (100%)	92 (95%)	5 (5%)	21	48
4	P	97/97 (100%)	94 (97%)	3 (3%)	35	59
All	All	1746/1776 (98%)	1674 (96%)	72 (4%)	27	53

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	74	ASP
1	A	122	GLU
1	A	184	ARG
1	A	197	ARG
1	A	200	ARG
1	A	204	ASN
1	A	276	GLU
1	A	319	LEU
1	A	327	ARG
1	A	358	MET
1	A	413	ARG
1	A	560	THR
2	B	65	CYS
2	B	81	LEU
2	B	128	ASP
2	B	203	SER
2	B	212	GLU
2	B	242	PRO
3	C	23	ARG
3	C	39	SER
3	C	50	LYS
3	C	84	LYS
3	C	92	LYS

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Mol	Chain	Res	Type
3	C	103	MET
4	D	0	MET
4	D	3	PRO
4	D	4	ASN
4	D	86	MET
4	D	118	ILE
1	M	7	LEU
1	M	35	ILE
1	M	36	SER
1	M	93	MET
1	M	122	GLU
1	M	126	PHE
1	M	143	SER
1	M	155	HIS
1	M	163	ASP
1	M	164	ASP
1	M	197	ARG
1	M	204	ASN
1	M	227	GLU
1	M	242	LEU
1	M	243	MET
1	M	304	ILE
1	M	331	ILE
1	M	372	LYS
1	M	375	PHE
1	M	465	ILE
1	M	470	GLU
1	M	485	ARG
1	M	499	ASN
1	M	541	GLU
1	M	548	LEU
1	M	558	ASP
2	N	128	ASP
2	N	148	CYS
2	N	185	ASP
2	N	189	LYS
2	N	226	GLN
2	N	241	LYS
3	O	5	LYS
3	O	19	LEU
3	O	20	PRO
3	O	37	TRP

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Mol	Chain	Res	Type
3	O	39	SER
3	O	54	GLU
3	O	89	LEU
4	P	7	ARG
4	P	9	ASP
4	P	118	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	67	HIS
1	A	87	HIS
1	A	95	GLN
1	A	141	GLN
1	A	155	HIS
1	A	204	ASN
1	A	232	HIS
1	A	279	ASN
1	A	428	GLN
1	A	434	GLN
2	B	134	GLN
2	B	150	ASN
2	B	194	GLN
2	B	196	ASN
2	B	225	GLN
3	C	51	ASN
3	C	64	GLN
3	C	72	ASN
3	C	82	HIS
4	D	4	ASN
4	D	59	GLN
4	D	92	HIS
1	M	1	GLN
1	M	27	ASN
1	M	57	GLN
1	M	137	HIS
1	M	174	ASN
1	M	182	GLN
1	M	186	ASN
1	M	204	ASN
1	M	230	GLN

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Mol	Chain	Res	Type
1	M	264	GLN
1	M	292	GLN
1	M	366	ASN
1	M	409	GLN
1	M	421	ASN
1	M	434	GLN
1	M	441	ASN
1	M	447	ASN
1	M	499	ASN
1	M	520	HIS
1	M	546	ASN
1	M	550	HIS
2	N	95	ASN
2	N	150	ASN
2	N	160	GLN
2	N	225	GLN
2	N	226	GLN
3	O	65	ASN
3	O	72	ASN
3	O	95	ASN
4	P	2	ASN
4	P	4	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 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	$\# Z > 2$
10	BRS	N	800	-	23,23,23	2.34	6 (26%)	26,33,33	1.57	6 (23%)
7	FES	N	244	2	0,4,4	-	-	-	-	-
5	OAA	M	802	-	8,8,8	1.28	0	8,10,10	1.09	1 (12%)
7	FES	B	244	2	0,4,4	-	-	-	-	-
10	BRS	B	700	-	23,23,23	2.54	10 (43%)	26,33,33	1.87	7 (26%)
9	SF4	N	246	2	0,12,12	-	-	-	-	-
11	CE1	D	710	-	36,36,36	1.17	2 (5%)	35,35,35	1.56	8 (22%)
6	FAD	M	803	1	58,58,58	1.73	14 (24%)	85,89,89	1.54	14 (16%)
8	F3S	B	245	2	0,9,9	-	-	-	-	-
8	F3S	N	245	2	0,9,9	-	-	-	-	-
9	SF4	B	246	2	0,12,12	-	-	-	-	-
11	CE1	P	810	-	36,36,36	1.10	3 (8%)	35,35,35	1.67	9 (25%)
6	FAD	A	703	1	58,58,58	2.24	12 (20%)	85,89,89	1.64	21 (24%)
5	OAA	A	702	-	8,8,8	2.22	4 (50%)	8,10,10	2.21	3 (37%)
11	CE1	O	811	-	36,36,36	1.10	0	35,35,35	1.60	10 (28%)

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
10	BRS	N	800	-	-	5/12/16/16	0/2/2/2
7	FES	N	244	2	-	-	0/1/1/1
5	OAA	M	802	-	-	4/8/8/8	-
7	FES	B	244	2	-	-	0/1/1/1
10	BRS	B	700	-	-	6/12/16/16	0/2/2/2
11	CE1	D	710	-	-	17/34/34/34	-
9	SF4	N	246	2	-	-	0/6/5/5
6	FAD	M	803	1	-	5/34/50/50	0/6/6/6
11	CE1	P	810	-	-	14/34/34/34	-
8	F3S	B	245	2	-	-	0/3/3/3
8	F3S	N	245	2	-	-	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SF4	B	246	2	-	-	0/6/5/5
6	FAD	A	703	1	-	7/34/50/50	0/6/6/6
5	OAA	A	702	-	-	4/8/8/8	-
11	CE1	O	811	-	-	17/34/34/34	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	703	FAD	PA-O3P	-9.33	1.49	1.59
6	A	703	FAD	P-O3P	-9.07	1.49	1.59
10	N	800	BRS	C12-N1	6.60	1.57	1.45
6	M	803	FAD	PA-O3P	-5.79	1.53	1.59
10	B	700	BRS	C17-C16	5.37	1.47	1.38
6	M	803	FAD	P-O3P	-4.79	1.54	1.59
10	B	700	BRS	C12-N1	4.67	1.54	1.45
10	B	700	BRS	C8-N4	3.98	1.54	1.45
10	N	800	BRS	C12-C11	3.98	1.46	1.40
5	A	702	OAA	C3-C4	3.94	1.59	1.53
10	B	700	BRS	C17-C18	3.76	1.45	1.38
6	A	703	FAD	C10-N10	3.76	1.45	1.37
10	B	700	BRS	C15-C21	3.65	1.58	1.52
5	A	702	OAA	O3-C3	3.52	1.30	1.23
10	B	700	BRS	C12-C11	3.35	1.45	1.40
6	A	703	FAD	P-O5'	-3.34	1.46	1.59
10	N	800	BRS	C15-C21	3.23	1.58	1.52
10	B	700	BRS	C18-CL20	3.15	1.81	1.74
6	M	803	FAD	C4A-N3A	2.99	1.40	1.34
10	N	800	BRS	C8-N4	2.99	1.52	1.45
10	N	800	BRS	C11-C10	2.83	1.43	1.39
10	B	700	BRS	C19-C14	2.78	1.43	1.38
6	A	703	FAD	C9-C9A	2.69	1.44	1.39
6	M	803	FAD	O4B-C1B	2.69	1.48	1.42
6	M	803	FAD	C10-N10	2.68	1.43	1.37
6	M	803	FAD	P-O5'	-2.66	1.49	1.59
6	A	703	FAD	C4A-N9A	-2.63	1.32	1.37
10	N	800	BRS	C16-C15	2.61	1.43	1.39
11	P	810	CE1	C30-C29	2.53	1.61	1.49
11	D	710	CE1	C27-C26	2.53	1.61	1.49
11	D	710	CE1	O25-C26	2.51	1.52	1.42
10	B	700	BRS	C16-C15	2.50	1.43	1.39
6	M	803	FAD	C5A-C4A	2.50	1.43	1.39
6	M	803	FAD	C5A-N7A	-2.49	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	703	FAD	C5A-N7A	-2.45	1.34	1.39
6	A	703	FAD	C4A-N3A	2.34	1.38	1.34
6	M	803	FAD	C9A-N10	2.29	1.45	1.41
5	A	702	OAA	O2-C1	2.28	1.38	1.30
6	A	703	FAD	O4B-C1B	2.28	1.47	1.42
6	A	703	FAD	C4X-N5	2.27	1.35	1.30
11	P	810	CE1	O28-C29	2.17	1.51	1.42
6	M	803	FAD	C1'-C2'	2.16	1.55	1.52
6	A	703	FAD	C5A-C4A	2.14	1.42	1.39
6	M	803	FAD	C8A-N7A	2.14	1.35	1.31
6	A	703	FAD	O2'-C2'	-2.13	1.38	1.43
6	M	803	FAD	C5X-N5	-2.12	1.35	1.39
5	A	702	OAA	O5-C4	2.11	1.36	1.30
10	B	700	BRS	C14-C15	2.06	1.42	1.39
11	P	810	CE1	C35-C36	2.05	1.60	1.49
6	M	803	FAD	C1B-N9A	2.03	1.51	1.46
6	M	803	FAD	C9-C9A	2.01	1.42	1.39

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	703	FAD	N3A-C2A-N1A	-5.36	120.47	128.58
6	M	803	FAD	N3A-C2A-N1A	-5.34	120.50	128.58
6	A	703	FAD	N3A-C4A-N9A	4.00	133.98	127.17
6	M	803	FAD	C4'-C3'-C2'	-3.81	107.22	113.57
6	M	803	FAD	N3A-C4A-N9A	3.71	133.48	127.17
6	M	803	FAD	C5A-C4A-N3A	-3.70	121.62	126.72
6	A	703	FAD	C4A-N9A-C8A	3.68	109.60	105.74
5	A	702	OAA	O4-C4-C3	3.65	126.35	121.81
5	A	702	OAA	O3-C3-C2	3.62	125.97	120.41
6	A	703	FAD	C5A-C4A-N3A	-3.58	121.79	126.72
6	M	803	FAD	C4-N3-C2	-3.56	119.33	125.64
10	N	800	BRS	C9-C10-C21	-3.41	117.89	122.20
10	B	700	BRS	C9-C10-C11	3.39	120.96	117.49
6	A	703	FAD	C2A-N3A-C4A	3.38	120.08	111.83
6	A	703	FAD	C5X-N5-C4X	3.29	123.42	118.09
6	M	803	FAD	C2A-N3A-C4A	3.28	119.84	111.83
10	B	700	BRS	C17-C18-CL20	3.27	124.19	119.36
6	M	803	FAD	C5X-N5-C4X	3.02	122.98	118.09
11	O	811	CE1	O16-C17-C18	2.99	124.00	110.35
10	B	700	BRS	O2-N1-C12	2.99	124.14	119.03
10	N	800	BRS	C7-C12-C11	-2.98	118.51	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	703	FAD	O4B-C1B-N9A	2.95	113.75	108.09
10	B	700	BRS	C19-C18-C17	-2.95	117.59	121.24
11	P	810	CE1	O25-C26-C27	2.90	123.56	110.35
6	M	803	FAD	C4X-C4-N3	2.86	120.52	113.25
6	A	703	FAD	C4-N3-C2	-2.85	120.58	125.64
5	A	702	OAA	O3-C3-C4	2.75	123.60	119.67
10	B	700	BRS	C14-C19-C18	2.73	121.99	119.24
6	A	703	FAD	C4'-C3'-C2'	-2.73	109.03	113.57
11	P	810	CE1	O22-C23-C24	2.69	122.60	110.35
10	N	800	BRS	O2-N1-C12	2.69	123.63	119.03
10	N	800	BRS	C7-C8-N4	2.68	121.05	118.74
6	M	803	FAD	C4A-N9A-C8A	2.67	108.54	105.74
6	M	803	FAD	O4-C4-C4X	-2.65	119.53	126.53
10	B	700	BRS	C22-C21-C10	-2.52	107.86	112.21
11	P	810	CE1	O22-C21-C20	2.51	121.77	110.35
11	D	710	CE1	O16-C17-C18	2.49	121.71	110.35
11	O	811	CE1	O19-C18-C17	2.49	121.69	110.35
10	N	800	BRS	C9-C10-C11	2.45	119.99	117.49
6	A	703	FAD	N9A-C8A-N7A	-2.44	110.48	113.94
6	M	803	FAD	C10-N1-C2	2.43	122.12	116.85
11	P	810	CE1	O28-C29-C30	2.43	121.44	110.35
6	A	703	FAD	C4X-C4-N3	2.40	119.35	113.25
11	D	710	CE1	O13-C14-C15	2.37	121.17	110.35
6	M	803	FAD	C2A-N1A-C6A	2.36	122.61	118.73
6	A	703	FAD	C7M-C7-C6	-2.34	115.45	119.57
6	A	703	FAD	C5'-C4'-C3'	2.34	116.63	112.22
6	A	703	FAD	C10-C4X-N5	-2.33	120.05	124.81
11	O	811	CE1	O28-C27-C26	2.33	120.95	110.35
6	A	703	FAD	C4X-C10-N1	-2.32	118.89	124.59
6	A	703	FAD	C10-N1-C2	2.30	121.83	116.85
11	D	710	CE1	O22-C21-C20	2.28	120.73	110.35
11	O	811	CE1	O22-C23-C24	2.25	120.61	110.35
11	O	811	CE1	O25-C26-C27	2.25	120.59	110.35
11	D	710	CE1	O13-C12-C11	2.24	122.07	110.32
6	M	803	FAD	O4B-C1B-N9A	2.23	112.38	108.09
11	O	811	CE1	O16-C15-C14	2.23	120.54	110.35
6	A	703	FAD	O4-C4-C4X	-2.23	120.65	126.53
11	O	811	CE1	O34-C35-C36	2.22	119.91	110.11
11	D	710	CE1	O28-C29-C30	2.21	120.43	110.35
11	P	810	CE1	O31-C32-C33	2.21	120.41	110.35
11	D	710	CE1	O22-C23-C24	2.20	120.40	110.35
11	P	810	CE1	O13-C12-C11	2.19	121.84	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	N	800	BRS	C22-C21-C10	-2.18	108.45	112.21
11	O	811	CE1	O25-C24-C23	2.17	120.26	110.35
6	A	703	FAD	O3P-P-O1P	-2.17	104.18	110.70
11	D	710	CE1	O31-C32-C33	2.14	120.09	110.35
11	P	810	CE1	O16-C17-C18	2.14	120.09	110.35
6	A	703	FAD	C4-C4X-N5	2.13	121.14	118.21
10	B	700	BRS	C7-C8-N4	2.12	120.56	118.74
11	P	810	CE1	O25-C24-C23	2.09	119.87	110.35
11	O	811	CE1	O31-C30-C29	2.08	119.84	110.35
5	M	802	OAA	O4-C4-C3	2.08	124.39	121.81
6	M	803	FAD	C5'-C4'-C3'	2.07	116.12	112.22
6	A	703	FAD	O2P-P-O3P	2.06	112.84	107.27
11	D	710	CE1	O19-C18-C17	2.06	119.72	110.35
11	O	811	CE1	O13-C14-C15	2.06	119.72	110.35
6	A	703	FAD	C7M-C7-C8	2.02	124.88	120.76
11	P	810	CE1	O37-C36-C35	2.01	123.67	111.82

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	702	OAA	O3-C3-C4-O4
5	A	702	OAA	O3-C3-C4-O5
5	A	702	OAA	C2-C3-C4-O5
5	M	802	OAA	O3-C3-C4-O4
5	M	802	OAA	O3-C3-C4-O5
5	M	802	OAA	C2-C3-C4-O5
6	A	703	FAD	N10-C1'-C2'-O2'
6	A	703	FAD	N10-C1'-C2'-C3'
6	A	703	FAD	PA-O3P-P-O5'
6	M	803	FAD	N10-C1'-C2'-O2'
6	M	803	FAD	N10-C1'-C2'-C3'
6	M	803	FAD	PA-O3P-P-O5'
11	P	810	CE1	O13-C14-C15-O16
11	P	810	CE1	O28-C29-C30-O31
11	O	811	CE1	C17-C18-O19-C20
11	D	710	CE1	O28-C29-C30-O31
11	D	710	CE1	O34-C35-C36-O37
11	D	710	CE1	O25-C26-C27-O28
11	D	710	CE1	O13-C14-C15-O16
11	P	810	CE1	O22-C23-C24-O25
11	P	810	CE1	O34-C35-C36-O37

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Mol	Chain	Res	Type	Atoms
11	P	810	CE1	C11-C10-C9-C8
11	O	811	CE1	O25-C26-C27-O28
11	P	810	CE1	O25-C26-C27-O28
11	O	811	CE1	C7-C8-C9-C10
11	D	710	CE1	C2-C3-C4-C5
11	D	710	CE1	C6-C7-C8-C9
11	O	811	CE1	C6-C7-C8-C9
11	O	811	CE1	O34-C35-C36-O37
11	O	811	CE1	C36-C35-O34-C33
11	P	810	CE1	C36-C35-O34-C33
5	A	702	OAA	C2-C3-C4-O4
5	M	802	OAA	C2-C3-C4-O4
11	D	710	CE1	C36-C35-O34-C33
11	P	810	CE1	C33-C32-O31-C30
11	O	811	CE1	C3-C4-C5-C6
11	O	811	CE1	C32-C33-O34-C35
11	D	710	CE1	C11-C12-O13-C14
10	B	700	BRS	C11-C10-C21-C15
6	A	703	FAD	C5B-O5B-PA-O1A
6	M	803	FAD	C5B-O5B-PA-O1A
11	D	710	CE1	C24-C23-O22-C21
11	O	811	CE1	C20-C21-O22-C23
11	O	811	CE1	O28-C29-C30-O31
11	D	710	CE1	C11-C10-C9-C8
10	N	800	BRS	C11-C10-C21-C15
11	D	710	CE1	C14-C15-O16-C17
11	P	810	CE1	C24-C23-O22-C21
11	P	810	CE1	C4-C5-C6-C7
11	D	710	CE1	C18-C17-O16-C15
10	B	700	BRS	C11-C10-C21-C22
11	P	810	CE1	C6-C7-C8-C9
11	D	710	CE1	O22-C23-C24-O25
11	D	710	CE1	O16-C17-C18-O19
11	P	810	CE1	O16-C17-C18-O19
10	N	800	BRS	C11-C10-C21-C22
6	M	803	FAD	O4B-C4B-C5B-O5B
11	O	811	CE1	C11-C12-O13-C14
11	O	811	CE1	C24-C23-O22-C21
6	A	703	FAD	O4B-C4B-C5B-O5B
10	N	800	BRS	C16-C15-C21-C22
10	N	800	BRS	C9-C10-C21-C15
10	B	700	BRS	C9-C10-C21-C15

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Mol	Chain	Res	Type	Atoms
11	D	710	CE1	C30-C29-O28-C27
10	B	700	BRS	C9-C10-C21-C22
11	O	811	CE1	O16-C17-C18-O19
10	B	700	BRS	C14-C15-C21-C22
10	B	700	BRS	C16-C15-C21-C22
10	N	800	BRS	C14-C15-C21-C22
11	P	810	CE1	C11-C12-O13-C14
11	O	811	CE1	O22-C23-C24-O25
11	D	710	CE1	O19-C20-C21-O22
11	O	811	CE1	O19-C20-C21-O22
11	O	811	CE1	O31-C32-C33-O34
11	P	810	CE1	O19-C20-C21-O22
11	D	710	CE1	C23-C24-O25-C26
11	O	811	CE1	O13-C14-C15-O16
6	A	703	FAD	PA-O3P-P-O1P
6	A	703	FAD	PA-O3P-P-O2P

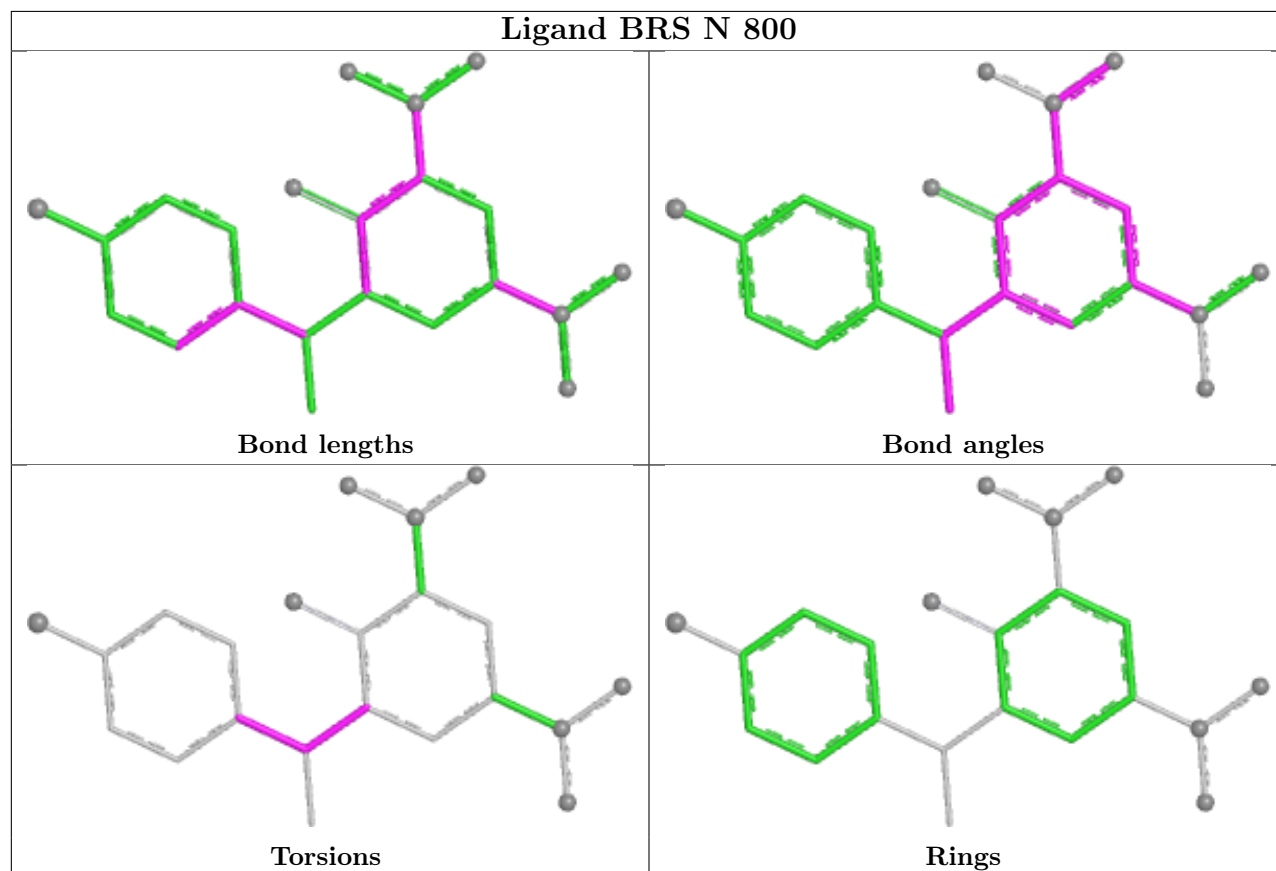
There are no ring outliers.

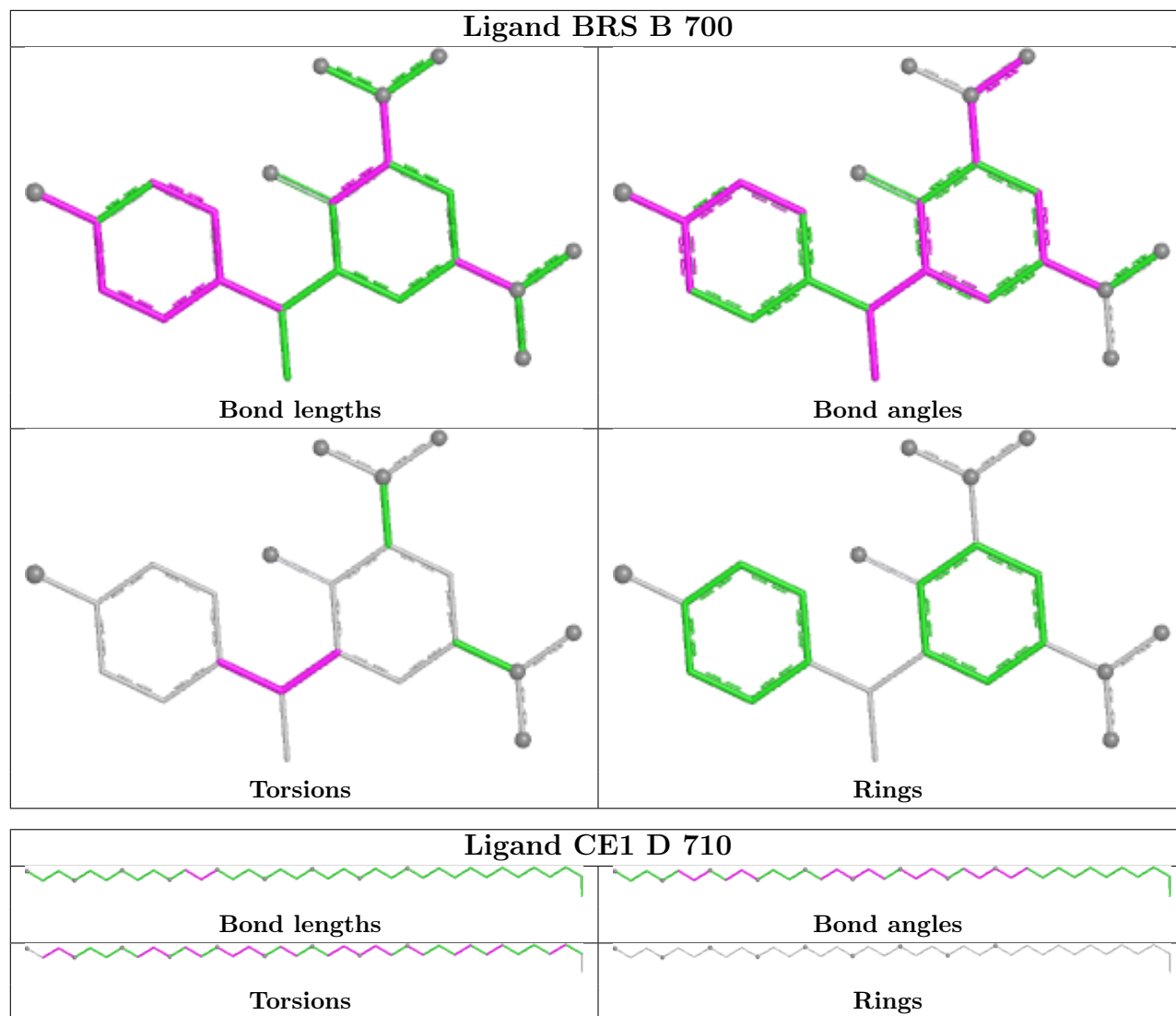
11 monomers are involved in 54 short contacts:

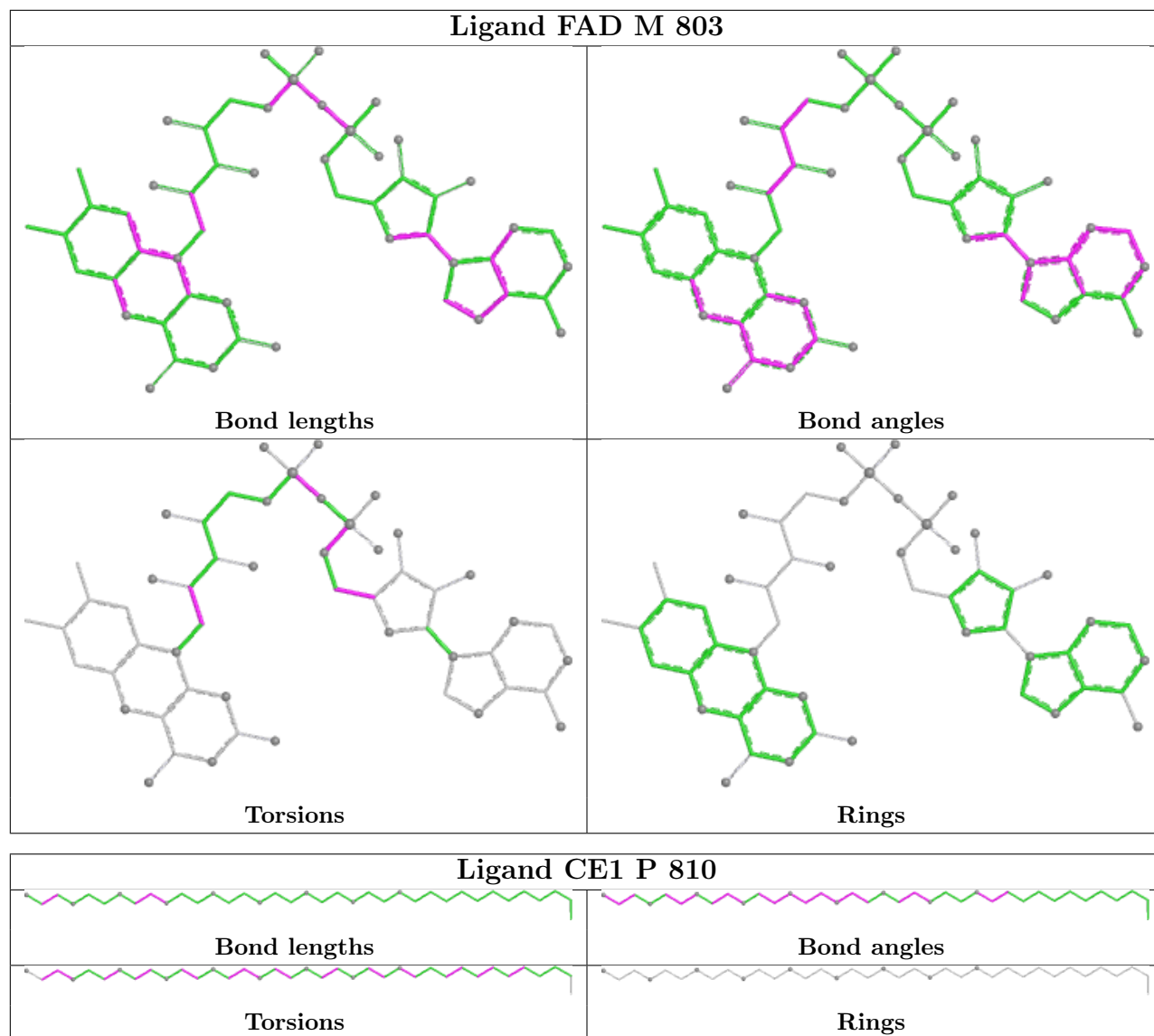
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	N	800	BRS	5	0
5	M	802	OAA	2	0
10	B	700	BRS	13	0
9	N	246	SF4	7	0
11	D	710	CE1	5	0
6	M	803	FAD	10	0
8	N	245	F3S	2	0
11	P	810	CE1	2	0
6	A	703	FAD	6	0
5	A	702	OAA	1	0
11	O	811	CE1	1	0

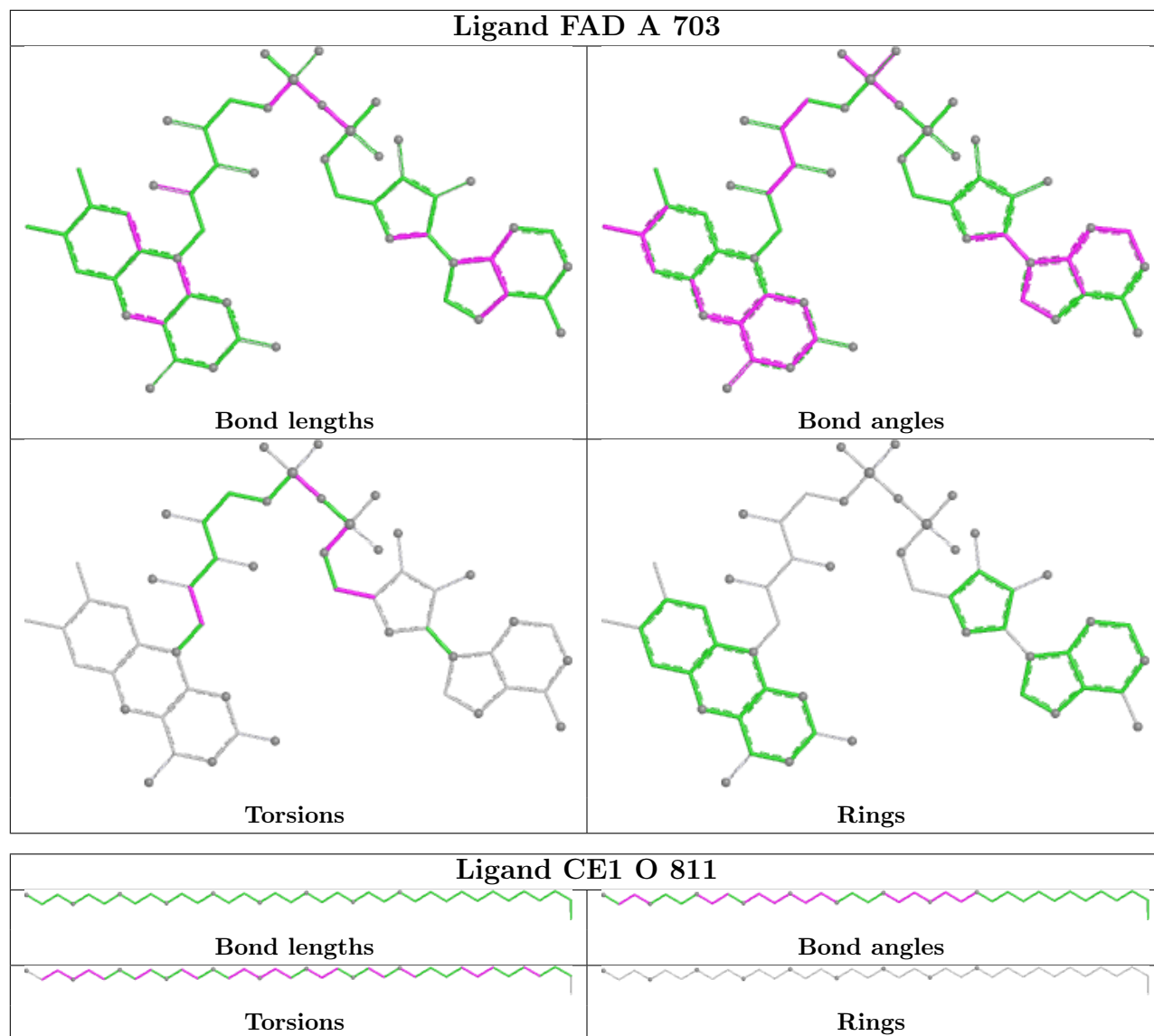
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.