



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 01:26 PM EDT

PDB ID : 1KF6 / pdb_00001kf6
Title : E. coli Quinol-Fumarate Reductase with Bound Inhibitor HQNO
Authors : Iverson, T.M.; Luna-Chavez, C.; Croal, L.R.; Cecchini, G.; Rees, D.C.
Deposited on : 2001-11-19
Resolution : 2.70 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) : 2.50

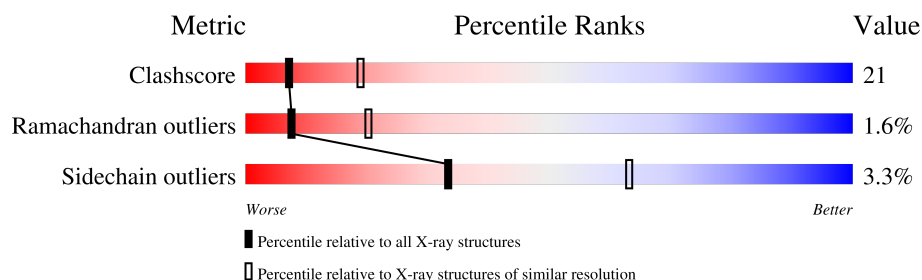
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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
12	SF4	N	246	-	-	X	-
7	ACT	N	803	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 17071 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			

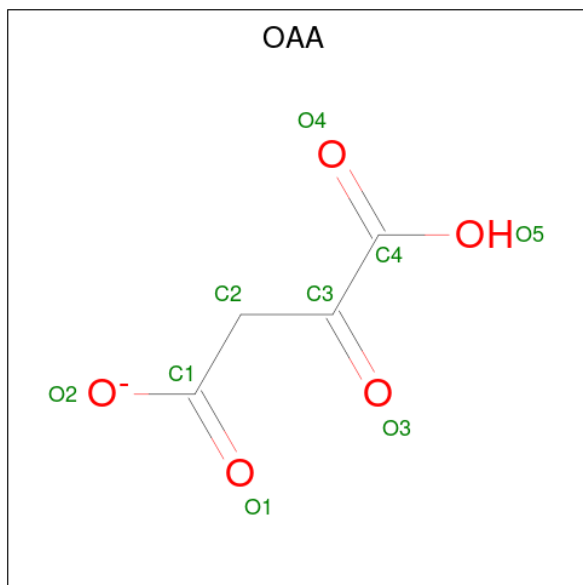
- Molecule 4 is a protein called FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN.

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 POTASSIUM ION (CCD ID: K) (formula: K).

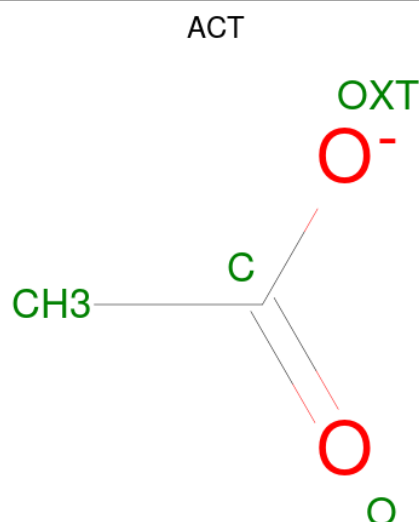
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	M	1	Total K 1 1	0	0

- Molecule 6 is OXALOACETATE ION (CCD ID: OAA) (formula: $C_4H_3O_5$).



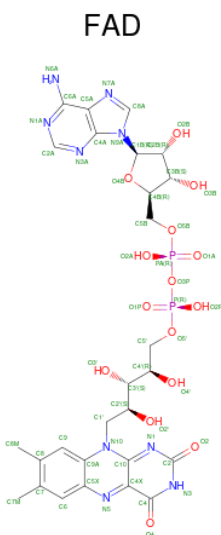
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 9 4 5	0	0
6	M	1	Total C O 9 4 5	0	0

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	N	1	Total 4	C 2	O 2	0	0

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



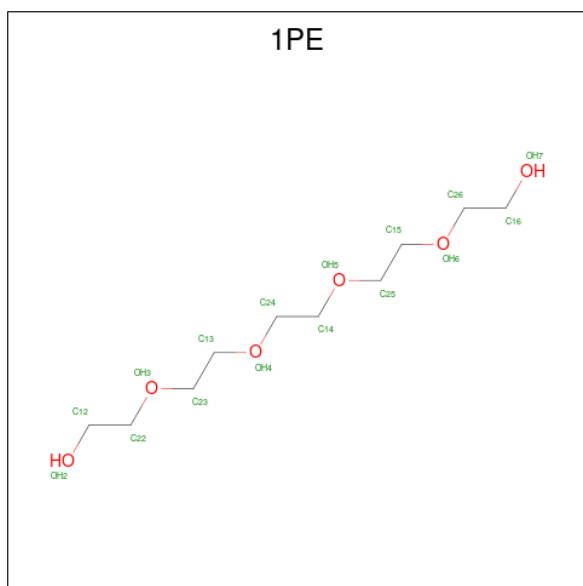
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total 53	C 27	N 9	O 15	P 2	0	0

Continued on next page...

Continued from previous page...

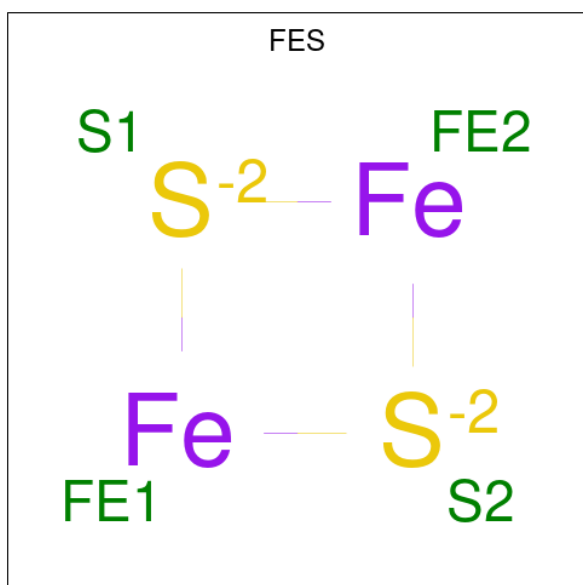
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 9 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



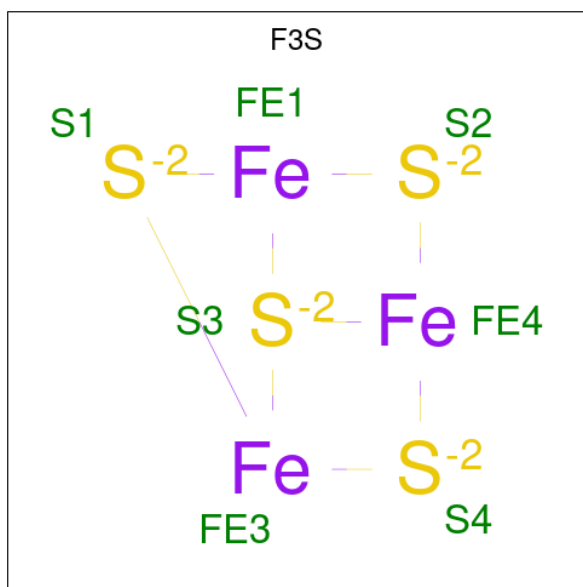
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	C	O	0
			16	10	6	

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



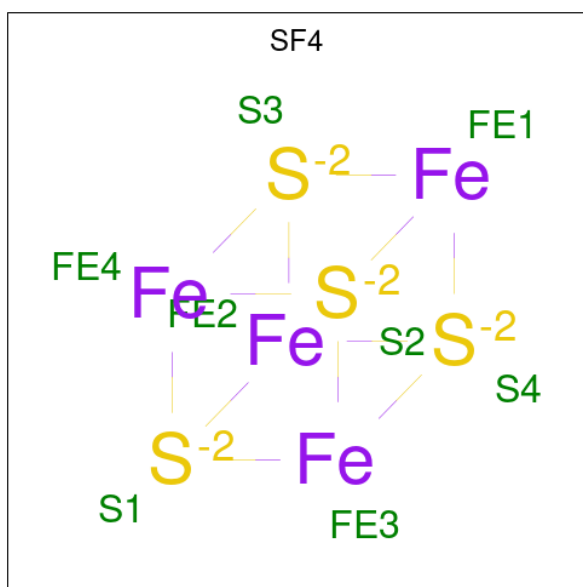
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			4	2	2		
10	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 11 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



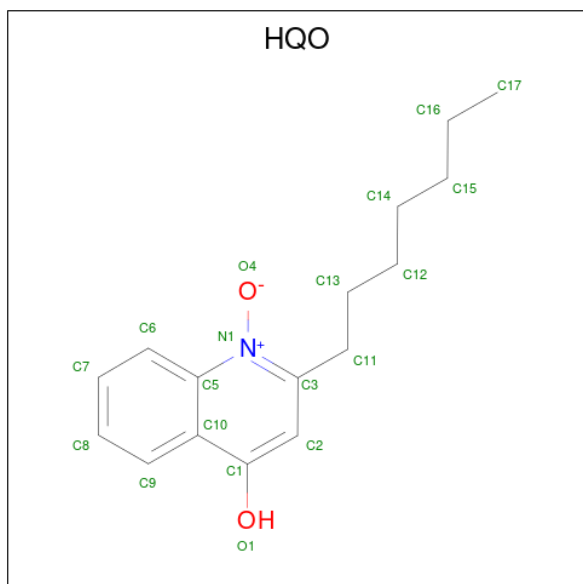
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	0
			7	3	4		
11	N	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 12 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 13 is 2-HEPTYL-4-HYDROXY QUINOLINE N-OXIDE (CCD ID: HQO) (formula: $C_{16}H_{21}NO_2$).



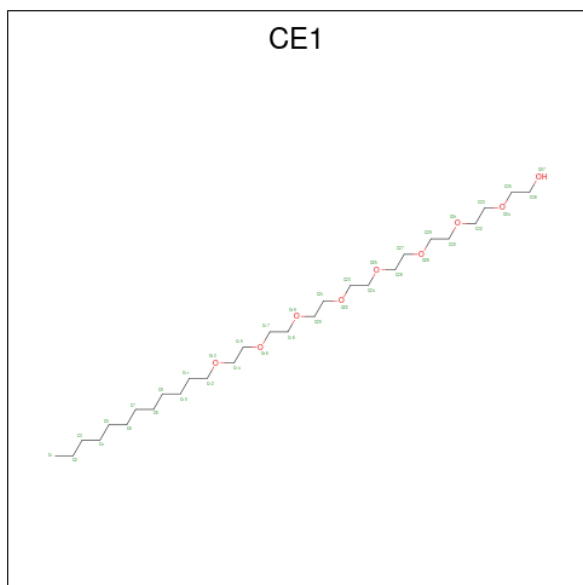
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	N	O	0	0
			19	16	1	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	N	1	Total	C	N	O	0	0
			19	16	1	2		

- Molecule 14 is O-DODECANYL OCTAETHYLENE GLYCOL (CCD ID: CE1) (formula: $C_{28}H_{58}O_9$).



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

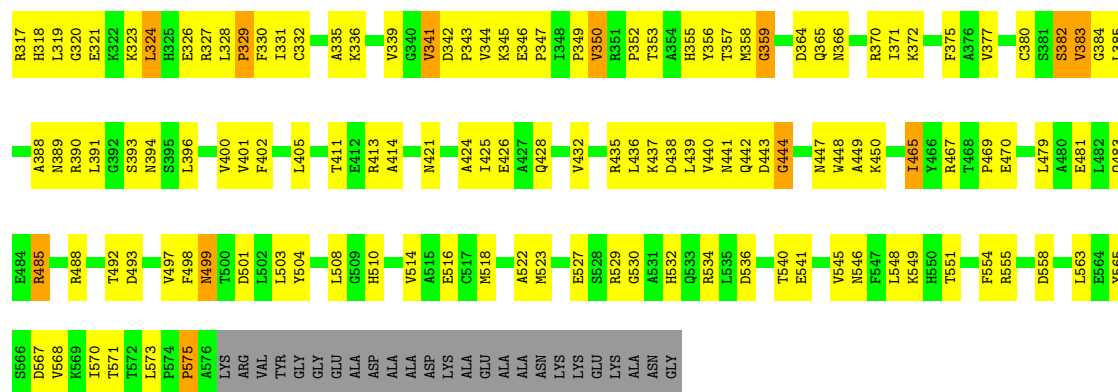
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	10	Total	O	0	0
			10	10		
15	B	1	Total	O	0	0
			1	1		
15	M	4	Total	O	0	0
			4	4		

Continued on next page...

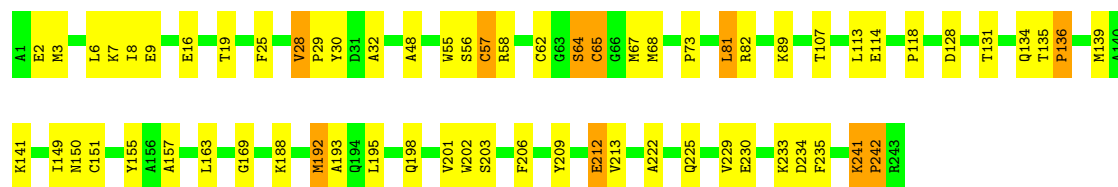
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	N	1	Total	O	0	0
			1	1		



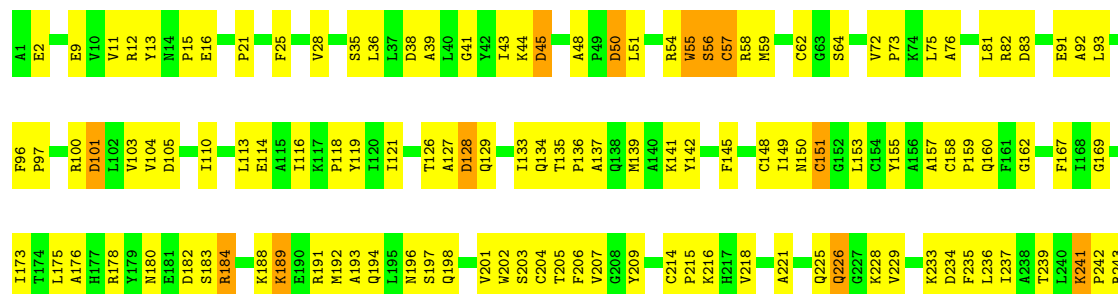
• Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN

Chain B: 73% 23% .



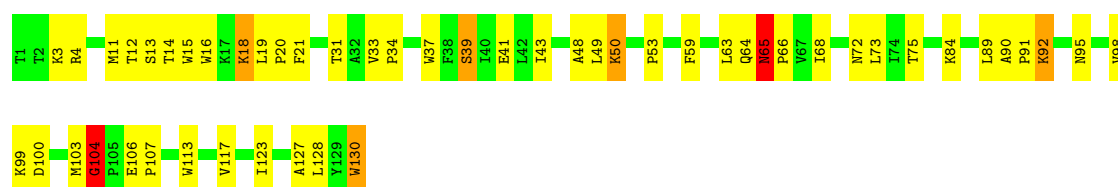
• Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN

Chain N: 50% 45% 5%



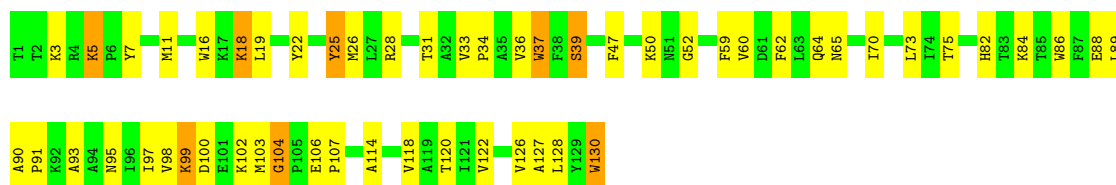
• Molecule 3: FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN

Chain C: 61% 34% . .



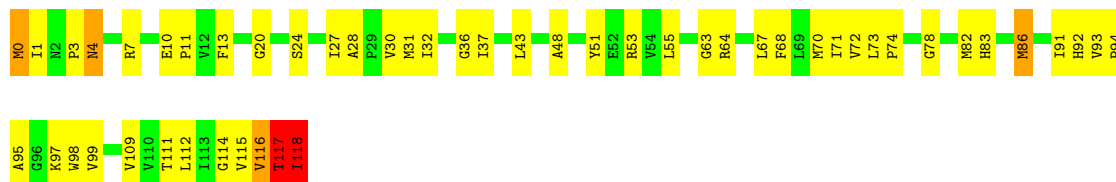
• Molecule 3: FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN

Chain O: 58% 35% 6%



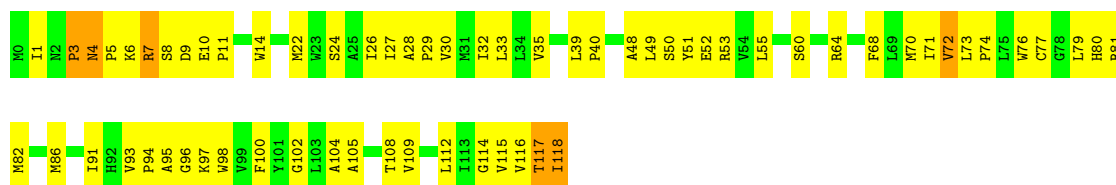
• Molecule 4: FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN

Chain D: 57% 38% . .



• Molecule 4: FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN

Chain P: 46% 49% 5%



4 Data and refinement statistics

Xtriage (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	96.50Å 137.84Å 273.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.231 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17071	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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: FES, CE1, K, ACT, FAD, 1PE, HQO, F3S, OAA, SF4

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	1.04	1/4540 (0.0%)	1.23	23/6139 (0.4%)
1	M	0.68	3/4540 (0.1%)	1.11	10/6139 (0.2%)
2	B	0.99	2/1931 (0.1%)	1.22	14/2617 (0.5%)
2	N	0.74	3/1931 (0.2%)	1.13	6/2617 (0.2%)
3	C	0.99	6/1094 (0.5%)	1.21	6/1496 (0.4%)
3	O	0.87	5/1094 (0.5%)	1.14	4/1496 (0.3%)
4	D	1.01	4/956 (0.4%)	1.24	4/1303 (0.3%)
4	P	0.91	4/956 (0.4%)	1.12	4/1303 (0.3%)
All	All	0.90	28/17042 (0.2%)	1.17	71/23110 (0.3%)

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	C	0	2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	117	THR	CA-C	-12.17	1.40	1.53
3	C	65	ASN	C-O	-11.70	1.09	1.24
4	D	118	ILE	C-OXT	10.96	1.45	1.23
3	O	65	ASN	C-O	-8.75	1.12	1.24
4	D	117	THR	CA-C	-8.45	1.41	1.52
1	A	575	PRO	C-O	-8.34	1.13	1.23
3	O	104	GLY	C-O	-7.99	1.13	1.24
4	D	3	PRO	C-O	-7.73	1.14	1.24
2	B	241	LYS	C-O	-7.54	1.14	1.24
4	P	118	ILE	C-OXT	7.51	1.38	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	241	LYS	C-O	-7.38	1.14	1.24
4	P	3	PRO	C-O	-7.18	1.14	1.23
3	O	130	TRP	CA-CB	7.03	1.67	1.53
1	M	575	PRO	C-O	-6.95	1.15	1.24
3	O	99	LYS	C-O	-6.84	1.15	1.24
1	M	357	THR	C-O	6.14	1.31	1.24
3	C	104	GLY	C-O	-6.12	1.15	1.24
3	C	65	ASN	CA-CB	-6.11	1.43	1.53
2	N	242	PRO	CA-C	-5.86	1.43	1.52
3	C	130	TRP	C-OXT	5.84	1.35	1.23
3	C	104	GLY	CA-C	-5.74	1.43	1.51
2	N	151	CYS	CA-CB	5.67	1.62	1.53
1	M	359	GLY	C-O	5.63	1.32	1.23
4	P	118	ILE	CA-CB	5.53	1.69	1.54
3	O	104	GLY	CA-C	-5.51	1.44	1.51
3	C	99	LYS	C-O	-5.46	1.15	1.23
2	B	242	PRO	CA-CB	5.14	1.62	1.53
4	D	4	ASN	CA-CB	5.10	1.59	1.53

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	116	VAL	N-CA-C	-11.52	101.43	112.83
2	B	65	CYS	N-CA-C	11.16	126.00	112.38
2	B	64	SER	CA-C-N	9.68	136.09	120.60
2	B	64	SER	C-N-CA	9.68	136.09	120.60
4	D	72	VAL	N-CA-C	7.78	118.36	110.82
3	C	48	ALA	N-CA-C	-7.27	103.38	112.90
1	A	53	ALA	N-CA-C	7.16	120.88	110.28
2	N	48	ALA	CA-C-N	7.08	126.78	119.56
2	N	48	ALA	C-N-CA	7.08	126.78	119.56
3	O	104	GLY	CA-C-O	-7.01	111.49	121.52
1	A	249	GLY	N-CA-C	-6.98	106.99	114.67
1	A	381	SER	N-CA-C	6.95	119.96	109.95
2	B	65	CYS	N-CA-CB	-6.78	98.79	110.32
1	A	337	ALA	N-CA-C	6.76	118.45	111.14
4	P	72	VAL	N-CA-C	6.70	117.32	110.82
2	B	57	CYS	N-CA-C	6.53	118.39	111.28
4	P	14	TRP	N-CA-C	-6.47	104.31	111.36
3	C	65	ASN	CA-C-O	-6.21	111.65	120.16
1	A	225	ASP	N-CA-C	6.20	119.98	111.54
1	A	175	MET	N-CA-C	6.17	118.01	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	350	VAL	N-CA-C	6.17	116.05	108.53
2	B	192	MET	N-CA-C	6.11	118.72	111.33
1	A	419	ASN	N-CA-C	6.05	118.51	110.53
1	M	573	LEU	CA-C-N	6.02	124.00	119.66
1	M	573	LEU	C-N-CA	6.02	124.00	119.66
3	C	104	GLY	CA-C-O	-5.99	112.95	121.52
1	A	422	GLU	N-CA-C	5.93	118.50	111.33
4	P	117	THR	O-C-N	5.90	129.07	122.11
1	M	106	ARG	N-CA-C	-5.88	101.58	110.39
3	C	64	GLN	N-CA-C	5.85	120.14	112.89
1	A	110	SER	N-CA-C	-5.79	102.89	110.53
1	M	232	HIS	N-CA-C	-5.74	101.65	110.32
1	A	386	HIS	N-CA-C	5.73	120.33	113.23
2	B	198	GLN	N-CA-C	-5.72	105.19	111.82
1	A	204	ASN	N-CA-C	5.70	118.95	110.52
1	M	341	VAL	O-C-N	5.70	129.20	123.10
1	A	65	HIS	N-CA-C	-5.68	105.23	111.82
3	C	89	LEU	N-CA-C	5.68	117.55	111.36
3	O	52	GLY	CA-C-N	5.66	126.92	119.84
3	O	52	GLY	C-N-CA	5.66	126.92	119.84
1	A	276	GLU	N-CA-C	5.65	122.29	109.81
2	N	242	PRO	O-C-N	5.64	128.73	122.24
3	O	25	TYR	N-CA-C	-5.63	104.53	111.40
1	A	27	ASN	CA-C-N	5.57	125.25	119.56
1	A	27	ASN	C-N-CA	5.57	125.25	119.56
4	D	27	ILE	N-CA-C	5.57	119.94	113.42
1	A	312	VAL	N-CA-C	-5.56	100.69	108.80
1	A	106	ARG	N-CA-C	-5.53	102.95	110.36
2	B	48	ALA	CA-C-N	5.52	125.23	119.82
2	B	48	ALA	C-N-CA	5.52	125.23	119.82
1	M	355	HIS	N-CA-C	5.52	119.57	111.34
1	A	467	ARG	N-CA-C	5.45	118.28	109.40
2	N	184	ARG	N-CA-C	-5.41	106.54	114.39
2	N	57	CYS	N-CA-C	5.41	118.67	111.75
2	B	28	VAL	N-CA-C	5.40	114.04	107.61
1	A	105	ARG	N-CA-C	5.36	118.01	109.81
1	M	115	ARG	N-CA-C	5.29	118.43	109.76
4	P	100	PHE	N-CA-C	5.26	116.82	111.14
2	B	19	THR	N-CA-C	-5.25	106.02	112.90
1	M	567	ASP	N-CA-C	5.25	117.90	110.50
2	B	203	SER	N-CA-C	-5.22	106.68	113.16
2	N	45	ASP	N-CA-C	5.22	116.65	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	THR	N-CA-C	-5.22	102.12	110.10
2	B	65	CYS	CB-CA-C	-5.21	99.32	110.32
3	C	73	LEU	N-CA-C	-5.13	105.77	111.36
1	M	75	TRP	N-CA-C	5.11	118.81	112.47
1	A	174	ASN	N-CA-C	-5.11	101.80	109.15
1	A	451	ILE	N-CA-C	-5.09	105.58	110.72
1	A	234	THR	N-CA-C	5.08	118.31	107.70
4	D	117	THR	O-C-N	5.04	129.29	122.59
2	B	107	THR	N-CA-C	5.01	117.39	111.33

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	65	ASN	Mainchain,Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4448	0	4335	128	0
1	M	4448	0	4335	270	0
2	B	1888	0	1837	54	0
2	N	1888	0	1837	112	0
3	C	1058	0	1108	49	0
3	O	1058	0	1108	52	0
4	D	926	0	971	48	0
4	P	926	0	971	68	0
5	A	1	0	0	0	0
5	M	1	0	0	0	0
6	A	9	0	2	2	0
6	M	9	0	2	0	0
7	A	4	0	3	0	0
7	B	4	0	3	0	0
7	N	4	0	3	2	0
8	A	53	0	31	7	0
8	M	53	0	31	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	16	0	20	5	0
10	B	4	0	0	0	0
10	N	4	0	0	0	0
11	B	7	0	0	0	0
11	N	7	0	0	1	0
12	B	8	0	0	0	0
12	N	8	0	0	4	0
13	C	19	0	20	3	0
13	N	19	0	20	2	0
14	O	111	0	174	0	0
14	P	74	0	116	5	0
15	A	10	0	0	1	0
15	B	1	0	0	0	0
15	M	4	0	0	0	0
15	N	1	0	0	0	0
All	All	17071	0	16927	706	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 21.

All (706) 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:44:HIS:NE2	8:A:721:FAD:C8M	1.89	1.33
1:M:44:HIS:NE2	8:M:821:FAD:HM82	1.02	1.33
1:M:44:HIS:NE2	8:M:821:FAD:C8M	1.98	1.27
1:A:44:HIS:NE2	8:A:721:FAD:HM82	0.93	1.24
1:M:421:ASN:HD22	1:M:424:ALA:HB2	1.17	1.04
1:A:44:HIS:CE1	8:A:721:FAD:HM82	1.91	1.04
3:C:12:THR:HG22	3:C:14:THR:H	1.18	1.03
1:A:358:MET:HE3	1:A:389:ASN:HA	1.40	1.00
1:M:465:ILE:HD13	1:M:465:ILE:H	1.29	0.97
2:N:116:ILE:HG21	2:N:176:ALA:HB2	1.47	0.96
3:O:86:TRP:HE1	4:P:22:MET:HE2	1.28	0.96
1:M:197:ARG:HD2	1:M:206:GLY:HA2	1.48	0.95
3:O:33:VAL:HB	3:O:34:PRO:HD3	1.52	0.92
2:N:189:LYS:H	2:N:189:LYS:HD3	1.34	0.91
1:M:102:PRO:HB2	2:N:139:MET:HE3	1.52	0.91
1:M:190:MET:HE1	1:M:215:MET:HE3	1.51	0.90
1:M:469:PRO:HG3	1:M:534:ARG:HH21	1.36	0.90
3:C:33:VAL:HG22	4:D:82:MET:HE2	1.52	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:44:HIS:CE1	8:M:821:FAD:HM82	2.08	0.88
3:O:75:THR:HG22	4:P:32:ILE:HD13	1.56	0.87
2:N:54:ARG:HE	2:N:103:VAL:HG13	1.39	0.87
1:M:304:ILE:HD12	1:M:304:ILE:H	1.40	0.86
2:N:15:PRO:HB2	3:O:5:LYS:H	1.41	0.85
1:M:316:LEU:HB3	1:M:319:LEU:HD12	1.59	0.85
1:M:447:ASN:HD21	1:M:449:ALA:HB3	1.42	0.84
1:M:7:LEU:HD21	1:M:411:THR:HA	1.60	0.84
1:M:421:ASN:HD22	1:M:424:ALA:CB	1.91	0.83
12:N:246:SF4:FE3	12:N:246:SF4:S2	1.69	0.83
3:O:19:LEU:H	3:O:19:LEU:HD23	1.44	0.83
1:A:413:ARG:HH11	1:A:413:ARG:HB2	1.43	0.82
3:C:104:GLY:HA2	3:C:107:PRO:HD2	1.62	0.82
3:O:31:THR:HG21	3:O:82:HIS:HB2	1.62	0.81
1:M:44:HIS:CD2	8:M:821:FAD:HM82	2.12	0.81
1:M:155:HIS:CD2	1:M:174:ASN:HA	2.15	0.81
1:M:549:LYS:HD2	1:M:565:TYR:HB3	1.62	0.81
3:O:126:VAL:HA	3:O:130:TRP:HB3	1.65	0.79
1:M:174:ASN:HD22	1:M:177:GLU:H	1.27	0.79
1:M:41:MET:HE2	2:N:150:ASN:ND2	1.98	0.79
2:N:113:LEU:HD11	2:N:175:LEU:HD22	1.65	0.78
1:M:41:MET:HE2	2:N:150:ASN:HD22	1.51	0.76
1:A:292:GLN:HE22	9:A:705:1PE:H261	1.51	0.75
1:M:236:LEU:HD22	1:M:339:VAL:HG11	1.67	0.75
2:N:116:ILE:HG21	2:N:176:ALA:CB	2.16	0.75
2:N:141:LYS:NZ	3:O:95:ASN:HB3	2.01	0.75
12:N:246:SF4:FE4	12:N:246:SF4:S1	1.77	0.75
4:P:51:TYR:HD1	4:P:52:GLU:HG3	1.49	0.75
2:N:206:PHE:HD1	13:N:800:HQO:H112	1.52	0.74
2:B:134:GLN:HE21	2:B:139:MET:HE3	1.52	0.74
4:D:67:LEU:O	4:D:71:ILE:HG13	1.86	0.74
1:M:42:ARG:HH21	2:N:150:ASN:HB2	1.51	0.74
1:M:311:VAL:HG12	1:M:312:VAL:O	1.88	0.74
1:M:437:LYS:HG2	1:M:441:ASN:HD21	1.51	0.74
4:P:105:ALA:O	4:P:109:VAL:HG23	1.88	0.74
2:N:141:LYS:HZ1	3:O:95:ASN:HB3	1.53	0.73
1:M:465:ILE:HD13	1:M:465:ILE:N	2.03	0.73
1:M:152:PHE:HB3	1:M:155:HIS:ND1	2.02	0.73
2:B:225:GLN:HE22	13:C:700:HQO:H111	1.53	0.73
1:M:437:LYS:HG2	1:M:441:ASN:ND2	2.04	0.73
3:O:106:GLU:HB2	3:O:107:PRO:HD3	1.69	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:97:ILE:HD13	3:O:102:LYS:HA	1.70	0.72
1:M:488:ARG:NH1	1:M:488:ARG:HB3	2.04	0.72
1:M:251:GLY:HA2	1:M:277:PRO:HG2	1.70	0.72
1:M:88:HIS:O	1:M:401:VAL:HG22	1.89	0.72
2:N:11:VAL:HG21	2:N:91:GLU:HG2	1.70	0.72
14:P:810:CE1:H171	14:P:810:CE1:H211	1.72	0.72
4:P:104:ALA:O	4:P:108:THR:OG1	2.08	0.72
1:A:42:ARG:HG2	2:B:64:SER:HB3	1.71	0.71
1:A:184:ARG:HG2	1:A:184:ARG:HH11	1.54	0.71
3:C:19:LEU:HD12	3:C:20:PRO:HD2	1.72	0.71
3:C:12:THR:HG22	3:C:14:THR:N	2.02	0.71
3:O:50:LYS:HD2	4:P:117:THR:HG22	1.72	0.71
3:O:130:TRP:O	4:P:53:ARG:NH2	2.24	0.70
3:O:50:LYS:HD2	4:P:117:THR:CG2	2.21	0.70
4:P:60:SER:O	4:P:64:ARG:HG3	1.91	0.70
1:M:316:LEU:HD22	1:M:319:LEU:HD11	1.73	0.70
1:M:545:VAL:HG12	1:M:546:ASN:ND2	2.06	0.70
1:M:447:ASN:HD22	1:M:450:LYS:HG2	1.57	0.69
1:M:497:VAL:HG21	2:N:15:PRO:HG2	1.73	0.69
1:A:514:VAL:HG12	1:A:518:MET:HE3	1.72	0.69
3:C:50:LYS:HB3	4:D:118:ILE:HG22	1.74	0.69
4:P:51:TYR:CD1	4:P:52:GLU:HG3	2.27	0.69
1:M:89:CYS:N	1:M:90:PRO:HD2	2.07	0.69
1:M:465:ILE:H	1:M:465:ILE:CD1	1.95	0.69
4:P:79:LEU:HD23	4:P:82:MET:HE3	1.75	0.69
2:B:225:GLN:NE2	13:C:700:HQO:H111	2.07	0.69
1:A:413:ARG:HH11	1:A:413:ARG:CB	2.05	0.69
1:M:187:ALA:HB2	1:M:414:ALA:HB2	1.74	0.69
1:A:323:LYS:HG3	1:A:327:ARG:HH11	1.58	0.69
3:C:15:TRP:O	3:C:18:LYS:HG2	1.92	0.69
1:M:99:TRP:CD2	1:M:142:THR:HG21	2.27	0.69
1:A:484:GLU:HG3	1:A:488:ARG:NH1	2.08	0.69
3:O:120:THR:HG23	4:P:30:VAL:HB	1.76	0.68
1:A:390:ARG:HH22	6:A:702:OAA:C4	2.07	0.68
1:M:1:GLN:HG2	1:M:2:THR:H	1.57	0.68
1:M:447:ASN:ND2	1:M:449:ALA:HB3	2.08	0.68
1:M:549:LYS:HA	1:M:568:VAL:HG23	1.76	0.68
1:A:413:ARG:HB2	1:A:413:ARG:NH1	2.08	0.68
1:M:435:ARG:HA	1:M:438:ASP:OD2	1.94	0.68
1:M:421:ASN:ND2	1:M:424:ALA:HB2	2.01	0.67
1:M:342:ASP:HB3	1:M:345:LYS:HB3	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:GLU:HG3	1:A:488:ARG:HH12	1.60	0.67
2:B:222:ALA:HB2	3:C:92:LYS:HE3	1.77	0.67
3:C:33:VAL:HA	4:D:82:MET:CE	2.25	0.66
4:D:20:GLY:HA2	4:D:73:LEU:HB3	1.77	0.66
1:M:174:ASN:ND2	1:M:177:GLU:HG2	2.09	0.66
1:M:332:CYS:HA	1:M:343:PRO:HG2	1.78	0.66
3:C:50:LYS:HE2	3:C:50:LYS:HA	1.77	0.66
1:M:444:GLY:HA3	1:M:488:ARG:C	2.21	0.66
4:P:48:ALA:HA	4:P:53:ARG:HD3	1.78	0.66
4:P:72:VAL:HG11	4:P:108:THR:HG23	1.77	0.66
3:O:75:THR:HG22	4:P:32:ILE:CD1	2.25	0.66
1:M:230:GLN:HB2	1:M:358:MET:HE2	1.78	0.65
1:M:84:TYR:HE2	1:M:405:LEU:HD22	1.61	0.65
2:N:196:ASN:ND2	2:N:234:ASP:OD1	2.30	0.65
2:N:236:LEU:HD23	2:N:236:LEU:C	2.22	0.65
3:C:33:VAL:HB	3:C:34:PRO:HD3	1.78	0.65
1:A:469:PRO:HB3	1:A:523:MET:HE1	1.77	0.65
1:A:103:TRP:O	2:B:139:MET:HE1	1.96	0.65
1:A:197:ARG:HD2	1:A:206:GLY:HA2	1.79	0.65
4:P:7:ARG:HG2	4:P:8:SER:N	2.10	0.65
2:N:225:GLN:O	2:N:229:VAL:HG23	1.97	0.64
1:M:89:CYS:H	1:M:90:PRO:HD2	1.60	0.64
1:M:444:GLY:HA3	1:M:488:ARG:O	1.98	0.64
2:N:13:TYR:HB2	2:N:21:PRO:HB3	1.79	0.64
1:A:27:ASN:ND2	1:A:30:ALA:HB2	2.12	0.64
4:D:0:MET:HG2	4:D:1:ILE:H	1.63	0.64
4:P:77:CYS:O	4:P:81:ARG:HG3	1.97	0.64
1:A:324:LEU:CD1	1:A:344:VAL:HG22	2.28	0.64
1:M:217:LEU:HG	1:M:555:ARG:HB3	1.78	0.63
1:M:391:LEU:O	1:M:394:ASN:HB2	1.98	0.63
1:M:275:GLY:O	1:M:277:PRO:HD3	1.99	0.63
4:P:9:ASP:C	4:P:11:PRO:HD2	2.24	0.63
3:O:60:VAL:O	3:O:64:GLN:HG3	1.99	0.63
2:B:16:GLU:OE2	3:C:3:LYS:HD2	1.98	0.63
1:M:251:GLY:HA2	1:M:277:PRO:CG	2.28	0.63
1:M:327:ARG:O	1:M:328:LEU:HD23	1.98	0.63
1:M:435:ARG:HH12	1:M:439:LEU:HD22	1.64	0.63
2:N:57:CYS:HB3	2:N:62:CYS:HB3	1.79	0.63
3:O:36:VAL:HG11	4:P:82:MET:HE1	1.79	0.63
1:A:279:ASN:O	1:A:280:LYS:HB2	1.99	0.62
4:P:24:SER:O	4:P:28:ALA:HB3	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:469:PRO:HA	1:M:523:MET:HE1	1.82	0.62
3:O:106:GLU:H	3:O:106:GLU:CD	2.08	0.62
1:M:436:LEU:O	1:M:440:VAL:HG23	1.99	0.62
1:M:499:ASN:HD22	1:M:499:ASN:C	2.06	0.62
2:N:135:THR:HG23	2:N:136:PRO:HD2	1.82	0.62
3:C:33:VAL:HA	4:D:82:MET:HE3	1.80	0.62
1:M:202:ASN:HA	1:M:353:THR:HG22	1.82	0.62
2:N:206:PHE:CE1	2:N:225:GLN:HG3	2.35	0.62
1:M:175:MET:HE3	1:M:503:LEU:HD13	1.82	0.62
1:M:41:MET:HB2	1:M:137:HIS:CE1	2.34	0.62
1:M:199:TYR:CE1	1:M:229:VAL:HG11	2.35	0.61
1:M:51:GLY:HA2	1:M:131:THR:HG21	1.82	0.61
1:M:332:CYS:O	1:M:336:LYS:HG3	2.00	0.61
3:C:130:TRP:N	3:C:130:TRP:CD1	2.69	0.61
4:D:48:ALA:O	4:D:53:ARG:HD3	2.00	0.61
4:D:13:PHE:HE2	4:D:97:LYS:HE2	1.65	0.61
3:O:18:LYS:HD2	3:O:19:LEU:HD22	1.81	0.61
1:A:336:LYS:O	1:A:340:GLY:HA2	2.00	0.60
2:N:188:LYS:HE2	2:N:192:MET:HE2	1.82	0.60
4:D:86:MET:HE3	4:D:86:MET:HA	1.82	0.60
1:M:545:VAL:C	1:M:546:ASN:HD22	2.08	0.60
4:P:22:MET:O	4:P:26:ILE:HD13	2.01	0.60
1:M:11:GLY:O	1:M:16:GLY:HA3	2.01	0.60
1:M:82:VAL:HG22	1:M:385:LEU:HD12	1.82	0.60
1:M:192:THR:OG1	1:M:212:GLY:HA3	2.02	0.60
2:N:206:PHE:CD1	13:N:800:HQO:H112	2.33	0.60
4:D:63:GLY:O	4:D:67:LEU:HD23	2.02	0.59
1:A:94:THR:HG23	2:B:131:THR:HG22	1.83	0.59
3:C:106:GLU:CD	3:C:106:GLU:H	2.10	0.59
1:M:92:GLU:HB3	1:M:400:VAL:HB	1.83	0.59
1:M:195:ALA:O	1:M:198:VAL:HG22	2.02	0.59
1:A:28:PRO:HA	1:A:148:GLN:HE21	1.65	0.59
1:M:156:PHE:CD2	1:M:503:LEU:HD22	2.37	0.59
3:O:86:TRP:HE1	4:P:22:MET:CE	2.09	0.59
1:A:148:GLN:OE1	1:A:148:GLN:N	2.30	0.59
1:M:96:LEU:HD21	1:M:139:LEU:HD21	1.85	0.59
1:A:343:PRO:HG3	1:A:348:ILE:HD11	1.85	0.59
3:O:50:LYS:HG3	4:P:118:ILE:HA	1.84	0.59
1:A:372:LYS:HE3	1:A:413:ARG:HE	1.67	0.59
2:B:57:CYS:O	2:B:58:ARG:HB2	2.02	0.59
4:D:78:GLY:O	4:D:82:MET:HG3	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:84:TYR:CE2	1:M:405:LEU:HD22	2.38	0.59
1:A:289:LYS:NZ	9:A:705:1PE:H262	2.18	0.59
2:N:44:LYS:HD3	2:N:51:LEU:O	2.03	0.58
1:A:232:HIS:HD2	1:A:234:THR:H	1.50	0.58
1:M:44:HIS:CE1	1:M:204:ASN:HA	2.38	0.58
2:N:116:ILE:HG22	2:N:191:ARG:HD3	1.86	0.58
4:P:3:PRO:O	4:P:4:ASN:C	2.46	0.58
1:A:200:ARG:NH1	1:A:201:TYR:OH	2.37	0.58
2:B:241:LYS:HG3	2:B:241:LYS:O	2.02	0.58
1:M:181:VAL:HG12	1:M:182:GLN:H	1.67	0.58
1:M:331:ILE:HD12	1:M:331:ILE:H	1.69	0.58
2:N:157:ALA:HB1	2:N:209:TYR:CD2	2.38	0.58
1:A:390:ARG:HD2	1:A:395:SER:HB2	1.86	0.58
2:N:54:ARG:NE	2:N:103:VAL:HG13	2.13	0.58
4:P:117:THR:O	4:P:118:ILE:C	2.46	0.58
3:O:36:VAL:HG11	4:P:82:MET:CE	2.33	0.57
3:O:98:VAL:HG23	3:O:103:MET:HB2	1.85	0.57
1:A:556:ASP:HB2	1:A:558:ASP:OD2	2.04	0.57
1:M:448:TRP:CH2	1:M:504:TYR:HB3	2.38	0.57
1:M:341:VAL:HG13	1:M:346:GLU:HB2	1.86	0.57
1:A:366:ASN:HB3	1:A:409:GLN:HG3	1.84	0.57
1:M:58:ASP:C	1:M:60:ASP:H	2.11	0.57
4:P:64:ARG:HB3	4:P:115:VAL:HG22	1.87	0.57
1:M:181:VAL:HG12	1:M:182:GLN:N	2.19	0.57
1:A:324:LEU:HD12	1:A:344:VAL:HG22	1.86	0.57
2:B:157:ALA:HB1	2:B:209:TYR:CD2	2.39	0.57
2:N:11:VAL:CG2	2:N:91:GLU:HG2	2.34	0.57
1:M:209:THR:O	1:M:209:THR:HG22	2.04	0.57
2:B:206:PHE:HD1	13:C:700:HQO:H112	1.69	0.56
1:A:462:GLY:HA3	1:A:475:THR:OG1	2.05	0.56
1:M:122:GLU:H	1:M:122:GLU:CD	2.13	0.56
3:O:16:TRP:CD1	3:O:26:MET:HE2	2.41	0.56
4:D:68:PHE:HD1	4:D:111:THR:HG22	1.70	0.56
2:N:2:GLU:OE1	2:N:2:GLU:HA	2.04	0.56
1:A:18:ARG:HG2	1:A:400:VAL:HA	1.88	0.56
1:M:304:ILE:HG12	1:M:313:TYR:HE2	1.71	0.56
4:P:76:TRP:NE1	14:P:810:CE1:H362	2.21	0.56
1:M:510:HIS:O	1:M:514:VAL:HG23	2.06	0.56
2:B:188:LYS:NZ	2:B:230:GLU:HG3	2.20	0.56
4:D:83:HIS:O	4:D:86:MET:HB2	2.06	0.56
1:M:358:MET:SD	1:M:390:ARG:N	2.79	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:104:GLY:O	3:O:107:PRO:HD2	2.06	0.55
2:N:135:THR:HG22	2:N:137:ALA:H	1.71	0.55
1:A:321:GLU:OE1	1:A:321:GLU:HA	2.06	0.55
1:M:152:PHE:O	1:M:155:HIS:HB2	2.06	0.55
1:M:260:TYR:CE1	1:M:264:GLN:NE2	2.75	0.55
4:P:112:LEU:O	4:P:116:VAL:HG22	2.07	0.55
1:A:41:MET:HE2	2:B:150:ASN:HD22	1.70	0.55
3:C:50:LYS:HD3	4:D:118:ILE:HG22	1.88	0.55
1:M:435:ARG:O	1:M:438:ASP:HB2	2.07	0.55
3:O:19:LEU:HD21	3:O:22:TYR:CE2	2.41	0.55
1:A:250:GLU:HB3	1:A:319:LEU:HD11	1.89	0.55
4:D:112:LEU:O	4:D:116:VAL:HG22	2.06	0.55
1:M:311:VAL:HG11	1:M:349:PRO:HB2	1.89	0.55
1:M:323:LYS:HG2	1:M:327:ARG:HH21	1.71	0.55
2:N:201:VAL:HG23	2:N:202:TRP:N	2.21	0.55
3:O:19:LEU:H	3:O:19:LEU:CD2	2.19	0.55
2:N:21:PRO:HD2	3:O:7:TYR:CE2	2.42	0.55
2:B:2:GLU:HA	2:B:2:GLU:OE2	2.06	0.55
2:B:8:ILE:HD11	2:B:81:LEU:HD11	1.89	0.55
1:M:62:PHE:HB3	1:M:86:VAL:HG23	1.89	0.55
2:N:202:TRP:CZ2	4:P:11:PRO:HG3	2.42	0.54
1:A:182:GLN:OE1	1:A:184:ARG:NH1	2.33	0.54
1:A:323:LYS:HG3	1:A:327:ARG:NH1	2.22	0.54
1:A:527:GLU:OE1	1:A:529:ARG:HD2	2.07	0.54
2:B:155:TYR:CE2	2:B:169:GLY:HA3	2.43	0.54
1:M:162:VAL:HG22	1:M:167:VAL:HA	1.89	0.54
1:M:358:MET:HE1	1:M:389:ASN:HA	1.89	0.54
1:M:219:HIS:O	1:M:371:ILE:HD11	2.07	0.54
3:O:70:ILE:O	3:O:73:LEU:HB2	2.07	0.54
1:M:168:ARG:HD3	1:M:425:ILE:CD1	2.37	0.54
2:B:32:ALA:O	2:B:82:ARG:NH1	2.40	0.54
3:C:50:LYS:HB3	4:D:118:ILE:CG2	2.36	0.54
2:N:162:GLY:HA3	3:O:11:MET:HE1	1.90	0.54
4:P:72:VAL:CG1	4:P:108:THR:HG23	2.38	0.54
1:A:341:VAL:HG13	1:A:346:GLU:HB2	1.88	0.54
1:M:242:LEU:HD12	1:M:243:MET:N	2.22	0.54
1:M:253:ILE:HA	1:M:283:GLU:HG2	1.90	0.54
2:N:81:LEU:N	2:N:81:LEU:HD12	2.22	0.54
2:B:57:CYS:HB3	2:B:62:CYS:HB3	1.90	0.54
1:M:551:THR:HG23	1:M:563:LEU:HD22	1.90	0.54
1:A:7:LEU:HD21	1:A:32:ILE:HG12	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:95:GLN:OE1	1:M:98:LEU:HD12	2.07	0.54
1:M:308:ARG:NH1	1:M:339:VAL:HG12	2.23	0.54
1:M:100:GLY:O	1:M:101:CYS:C	2.52	0.53
1:A:317:ARG:C	1:A:319:LEU:H	2.17	0.53
1:M:217:LEU:HG	1:M:555:ARG:CB	2.39	0.53
1:A:11:GLY:O	1:A:16:GLY:HA3	2.08	0.53
1:A:184:ARG:HG2	1:A:184:ARG:NH1	2.22	0.53
1:M:331:ILE:HD12	1:M:331:ILE:N	2.23	0.53
1:M:76:LEU:HD12	1:M:388:ALA:HB2	1.90	0.53
2:N:134:GLN:NE2	2:N:184:ARG:HD3	2.23	0.53
4:P:73:LEU:HB2	4:P:74:PRO:HD3	1.90	0.53
3:C:98:VAL:HG23	3:C:98:VAL:O	2.08	0.53
4:D:98:TRP:NE1	14:P:810:CE1:H141	2.24	0.53
1:M:147:PRO:HD2	1:M:148:GLN:OE1	2.09	0.53
1:M:311:VAL:HG11	1:M:349:PRO:CB	2.39	0.53
1:A:192:THR:OG1	1:A:212:GLY:HA3	2.08	0.53
1:A:200:ARG:HG3	1:A:457:LEU:HD23	1.91	0.53
4:P:86:MET:HE3	4:P:91:ILE:HB	1.91	0.53
1:M:7:LEU:HD12	1:M:23:ALA:HB1	1.91	0.53
4:P:102:GLY:HA2	14:P:710:CE1:H42	1.91	0.53
1:M:425:ILE:O	1:M:428:GLN:HB2	2.09	0.52
3:O:91:PRO:C	3:O:93:ALA:H	2.16	0.52
1:M:81:VAL:HG21	1:M:383:VAL:O	2.09	0.52
1:M:168:ARG:HD3	1:M:425:ILE:HD11	1.91	0.52
1:M:545:VAL:HG12	1:M:546:ASN:HD22	1.74	0.52
1:M:213:MET:HE2	1:M:380:CYS:HA	1.90	0.52
1:A:90:PRO:HB2	15:A:758:HOH:O	2.09	0.52
1:M:151:ARG:NH1	1:M:153:ASP:OD2	2.43	0.52
1:M:331:ILE:H	1:M:331:ILE:CD1	2.23	0.52
1:M:382:SER:C	1:M:384:GLY:H	2.17	0.52
2:N:9:GLU:HG3	2:N:25:PHE:CZ	2.44	0.52
4:P:39:LEU:HD13	4:P:49:LEU:HB3	1.90	0.52
1:A:436:LEU:O	1:A:440:VAL:HG23	2.10	0.52
2:B:242:PRO:HG3	4:P:94:PRO:HD3	1.89	0.52
4:P:10:GLU:N	4:P:11:PRO:CD	2.73	0.52
1:A:118:GLY:HA2	1:A:279:ASN:HD21	1.73	0.52
4:D:13:PHE:CE2	4:D:97:LYS:HE2	2.45	0.52
2:N:139:MET:HA	2:N:142:TYR:CE2	2.45	0.52
1:A:292:GLN:NE2	9:A:705:1PE:H261	2.21	0.52
1:A:469:PRO:CB	1:A:523:MET:HE1	2.37	0.52
2:B:229:VAL:HG12	2:B:233:LYS:HE3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:LYS:CB	4:D:118:ILE:HG22	2.40	0.52
2:N:169:GLY:O	2:N:173:ILE:HG13	2.10	0.52
1:A:232:HIS:CE1	1:A:242:LEU:HD11	2.45	0.52
1:M:10:VAL:HG13	1:M:157:VAL:HG21	1.91	0.52
2:N:97:PRO:HG2	2:N:105:ASP:HB3	1.92	0.52
2:N:233:LYS:O	2:N:237:ILE:HD13	2.10	0.52
3:C:113:TRP:O	3:C:117:VAL:HG23	2.09	0.52
3:O:98:VAL:HG21	3:O:103:MET:HE3	1.92	0.52
1:M:7:LEU:HD11	1:M:411:THR:OG1	2.10	0.51
1:M:328:LEU:N	1:M:329:PRO:HD3	2.24	0.51
1:A:356:TYR:CE2	1:A:390:ARG:HD3	2.45	0.51
2:N:28:VAL:HG22	2:N:43:ILE:HD11	1.92	0.51
1:M:467:ARG:NH1	1:M:532:HIS:ND1	2.58	0.51
1:A:236:LEU:HD11	1:A:243:MET:HE3	1.93	0.51
2:B:212:GLU:HG3	3:C:21:PHE:CE2	2.45	0.51
1:M:227:GLU:HB2	1:M:522:ALA:HB2	1.93	0.51
1:M:546:ASN:HD22	1:M:546:ASN:N	2.06	0.51
3:C:59:PHE:CE1	3:C:63:LEU:HD11	2.46	0.51
1:M:98:LEU:HD11	2:N:127:ALA:HA	1.92	0.51
1:M:328:LEU:N	1:M:329:PRO:CD	2.74	0.51
2:N:113:LEU:CD1	2:N:175:LEU:HD22	2.39	0.51
4:D:93:VAL:N	2:N:243:ARG:O	2.42	0.51
1:M:171:VAL:HG11	1:M:432:VAL:HG11	1.93	0.51
2:N:28:VAL:CG2	2:N:43:ILE:HD11	2.41	0.51
2:N:198:GLN:O	2:N:203:SER:HB2	2.10	0.51
3:C:50:LYS:CG	4:D:118:ILE:HG22	2.41	0.50
4:D:73:LEU:HB2	4:D:74:PRO:HD3	1.93	0.50
1:M:364:ASP:CG	1:M:366:ASN:H	2.19	0.50
1:M:145:GLN:O	1:M:147:PRO:HD3	2.12	0.50
1:M:296:HIS:ND1	1:M:299:ARG:NH2	2.59	0.50
1:M:308:ARG:HH12	1:M:339:VAL:HG12	1.76	0.50
3:O:33:VAL:O	3:O:36:VAL:HG22	2.11	0.50
1:M:0:MET:SD	1:M:182:GLN:HB2	2.51	0.50
1:M:21:ILE:HG21	1:M:99:TRP:CH2	2.47	0.50
1:M:158:LEU:HD11	1:M:436:LEU:HD22	1.93	0.50
1:M:413:ARG:NH1	1:M:413:ARG:HB2	2.26	0.50
1:M:311:VAL:HG13	1:M:350:VAL:O	2.11	0.50
2:N:241:LYS:O	2:N:243:ARG:HG3	2.12	0.50
1:A:42:ARG:CG	2:B:64:SER:HB3	2.42	0.50
1:M:39:TYR:HE2	2:N:54:ARG:HH12	1.59	0.50
1:M:174:ASN:ND2	1:M:177:GLU:H	2.03	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:ASP:OD1	4:D:7:ARG:NH2	2.44	0.50
3:C:50:LYS:HD2	4:D:118:ILE:O	2.11	0.50
1:M:171:VAL:HB	1:M:432:VAL:HG11	1.94	0.50
1:M:435:ARG:NH1	1:M:439:LEU:HB2	2.27	0.50
1:A:342:ASP:C	1:A:344:VAL:H	2.20	0.49
1:M:75:TRP:O	1:M:568:VAL:HG11	2.12	0.49
1:A:316:LEU:O	1:A:319:LEU:HB2	2.10	0.49
1:M:162:VAL:HG13	1:M:166:HIS:C	2.37	0.49
1:M:162:VAL:HG13	1:M:166:HIS:O	2.12	0.49
1:M:330:PHE:HB3	1:M:331:ILE:HD12	1.94	0.49
3:O:118:VAL:O	3:O:122:VAL:HG23	2.12	0.49
4:P:118:ILE:HG23	4:P:118:ILE:OXT	2.11	0.49
3:C:127:ALA:O	3:C:128:LEU:HD23	2.12	0.49
1:A:159:ASP:OD2	1:A:160:ILE:N	2.46	0.49
1:M:42:ARG:HD2	2:N:64:SER:OG	2.13	0.49
1:M:66:PHE:HD1	1:M:82:VAL:HG12	1.78	0.49
1:M:114:ARG:C	1:M:122:GLU:HB2	2.36	0.49
1:M:196:GLY:HA3	1:M:204:ASN:OD1	2.13	0.49
1:M:316:LEU:HB3	1:M:319:LEU:CD1	2.35	0.49
2:N:92:ALA:HB1	2:N:104:VAL:CG1	2.42	0.49
2:N:96:PHE:HB3	2:N:104:VAL:HB	1.94	0.49
2:N:189:LYS:H	2:N:189:LYS:CD	2.12	0.49
3:O:33:VAL:HB	3:O:34:PRO:CD	2.34	0.49
4:D:10:GLU:N	4:D:11:PRO:HD2	2.27	0.49
1:M:187:ALA:CB	1:M:414:ALA:HB2	2.41	0.49
1:M:304:ILE:HD12	1:M:304:ILE:N	2.18	0.49
2:N:180:ASN:OD1	2:N:188:LYS:HA	2.12	0.49
4:P:28:ALA:N	4:P:29:PRO:HD2	2.28	0.49
1:M:141:GLN:HB3	2:N:118:PRO:O	2.13	0.49
1:M:488:ARG:HB3	1:M:488:ARG:HH11	1.75	0.49
1:A:549:LYS:HD2	1:A:565:TYR:HB3	1.95	0.49
2:B:135:THR:O	2:B:136:PRO:C	2.52	0.49
1:M:38:VAL:O	1:M:39:TYR:C	2.56	0.49
1:M:104:SER:O	1:M:105:ARG:HD3	2.12	0.49
1:M:155:HIS:HD2	1:M:174:ASN:HA	1.74	0.49
3:C:11:MET:HE3	3:C:15:TRP:CG	2.48	0.49
1:M:171:VAL:CG1	1:M:432:VAL:HG11	2.42	0.49
2:N:159:PRO:HG2	2:N:207:VAL:HG21	1.94	0.49
3:O:90:ALA:N	3:O:91:PRO:HD2	2.28	0.49
3:O:127:ALA:O	3:O:128:LEU:HD23	2.13	0.49
4:P:55:LEU:CD1	4:P:118:ILE:HD11	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:435:ARG:HH12	1:M:439:LEU:CD2	2.25	0.48
1:M:549:LYS:HD2	1:M:565:TYR:CB	2.39	0.48
2:N:201:VAL:CG2	2:N:202:TRP:N	2.76	0.48
1:A:115:ARG:HD3	1:A:279:ASN:ND2	2.28	0.48
1:M:213:MET:CE	1:M:380:CYS:HA	2.43	0.48
1:M:236:LEU:HD22	1:M:339:VAL:CG1	2.41	0.48
1:A:109:GLY:HA2	2:B:134:GLN:O	2.13	0.48
1:M:304:ILE:HG22	1:M:305:SER:N	2.28	0.48
1:A:44:HIS:NE2	8:A:721:FAD:C8	2.73	0.48
2:B:201:VAL:HG23	2:B:202:TRP:N	2.28	0.48
1:A:196:GLY:HA3	1:A:204:ASN:OD1	2.14	0.48
1:A:448:TRP:CH2	1:A:504:TYR:HB3	2.49	0.48
1:M:62:PHE:CD2	1:M:87:HIS:HA	2.49	0.48
2:N:175:LEU:O	2:N:178:ARG:HB3	2.13	0.48
1:A:556:ASP:OD2	1:A:562:ARG:NE	2.43	0.48
4:D:93:VAL:HA	4:D:94:PRO:HD2	1.73	0.48
1:A:85:PHE:CD2	1:A:385:LEU:HD11	2.49	0.48
1:M:1:GLN:HG2	1:M:2:THR:N	2.27	0.48
4:P:39:LEU:HB2	4:P:49:LEU:HD13	1.96	0.48
4:P:70:MET:O	4:P:74:PRO:HG2	2.13	0.48
3:C:75:THR:HG22	4:D:32:ILE:HD13	1.96	0.48
1:M:159:ASP:OD2	1:M:160:ILE:N	2.47	0.48
1:M:469:PRO:HG3	1:M:534:ARG:NH2	2.16	0.48
1:A:273:PRO:O	1:A:274:LEU:C	2.57	0.48
1:M:35:ILE:CD1	1:M:155:HIS:HB3	2.44	0.48
1:M:63:GLU:O	1:M:66:PHE:HB3	2.14	0.47
1:M:130:LYS:O	1:M:133:PHE:HB3	2.14	0.47
2:N:54:ARG:O	2:N:55:TRP:HB3	2.15	0.47
1:M:165:GLY:O	1:M:372:LYS:HB2	2.13	0.47
1:A:224:ARG:NH2	1:A:382:SER:O	2.41	0.47
1:A:439:LEU:HD12	1:A:442:GLN:NE2	2.29	0.47
2:N:81:LEU:H	2:N:81:LEU:CD1	2.27	0.47
2:B:149:ILE:HG13	2:B:151:CYS:HB3	1.96	0.47
1:M:184:ARG:NH2	1:M:426:GLU:HG2	2.29	0.47
1:M:66:PHE:CD1	1:M:82:VAL:HG12	2.50	0.47
1:M:286:PRO:O	1:M:290:VAL:HG23	2.15	0.47
1:M:311:VAL:HG12	1:M:312:VAL:N	2.30	0.47
1:M:499:ASN:HD21	1:M:501:ASP:HB3	1.79	0.47
2:N:194:GLN:HE22	4:P:1:ILE:HG21	1.79	0.47
2:B:28:VAL:HG12	2:B:29:PRO:O	2.14	0.47
2:B:113:LEU:HD23	2:B:113:LEU:O	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:VAL:HG21	1:A:403:GLY:HA2	1.97	0.47
1:M:493:ASP:OD1	2:N:50:ASP:HB3	2.15	0.47
2:N:135:THR:CG2	2:N:136:PRO:HD2	2.45	0.47
2:B:195:LEU:O	2:B:201:VAL:HG22	2.15	0.47
1:M:382:SER:C	1:M:384:GLY:N	2.73	0.47
1:M:479:LEU:HB3	1:M:516:GLU:HG2	1.97	0.47
1:A:89:CYS:HB2	1:A:90:PRO:HD3	1.96	0.47
3:C:31:THR:O	3:C:34:PRO:HD2	2.15	0.47
3:C:53:PRO:HD3	4:D:51:TYR:CZ	2.50	0.47
3:O:39:SER:OG	4:P:71:ILE:O	2.33	0.47
1:A:151:ARG:NH2	2:B:114:GLU:OE2	2.48	0.46
2:B:134:GLN:NE2	2:B:139:MET:HE3	2.27	0.46
3:C:50:LYS:CD	4:D:118:ILE:HG22	2.46	0.46
1:A:244:THR:H	1:A:331:ILE:HD11	1.79	0.46
1:M:232:HIS:O	1:M:352:PRO:HA	2.15	0.46
2:N:160:GLN:NE2	2:N:205:THR:OG1	2.47	0.46
4:P:10:GLU:N	4:P:11:PRO:HD2	2.30	0.46
1:A:232:HIS:NE2	1:A:242:LEU:HD11	2.30	0.46
1:A:287:ARG:H	9:A:705:1PE:H122	1.81	0.46
1:M:247:CYS:CB	1:M:314:LEU:HD21	2.46	0.46
1:M:393:SER:HA	8:M:821:FAD:O2	2.15	0.46
1:A:184:ARG:NH1	1:A:184:ARG:CG	2.78	0.46
2:B:188:LYS:HZ1	2:B:230:GLU:HG3	1.81	0.46
4:D:64:ARG:NH1	4:D:117:THR:HG23	2.30	0.46
1:M:479:LEU:O	1:M:483:GLN:HG2	2.16	0.46
1:A:142:THR:O	1:A:145:GLN:HG2	2.15	0.46
1:A:244:THR:HG22	1:A:331:ILE:HG13	1.97	0.46
4:D:36:GLY:C	4:D:37:ILE:HG13	2.40	0.46
1:M:229:VAL:HG22	1:M:518:MET:HE2	1.97	0.46
4:P:39:LEU:N	4:P:40:PRO:HD2	2.30	0.46
2:N:133:ILE:O	2:N:133:ILE:HG22	2.14	0.46
2:N:145:PHE:HA	2:N:218:VAL:HG13	1.97	0.46
4:P:96:GLY:O	4:P:97:LYS:C	2.57	0.46
2:N:214:CYS:SG	12:N:246:SF4:S1	3.14	0.46
4:P:109:VAL:O	4:P:112:LEU:HB3	2.16	0.46
1:M:40:PRO:HB2	1:M:140:PHE:CD1	2.51	0.46
2:N:15:PRO:CB	3:O:5:LYS:H	2.18	0.46
4:D:70:MET:HE3	4:D:70:MET:O	2.15	0.46
1:M:174:ASN:ND2	1:M:177:GLU:CG	2.77	0.46
2:N:158:CYS:HA	2:N:159:PRO:HD3	1.85	0.46
1:M:263:LEU:CD1	1:M:283:GLU:HA	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:304:ILE:H	1:M:304:ILE:CD1	2.16	0.45
2:N:81:LEU:HD12	2:N:81:LEU:H	1.81	0.45
2:N:167:PHE:CD1	2:N:203:SER:HB3	2.51	0.45
1:A:40:PRO:HB2	1:A:140:PHE:CD1	2.51	0.45
1:A:206:GLY:HA3	2:B:55:TRP:CH2	2.51	0.45
1:M:315:ASP:OD1	1:M:317:ARG:HG3	2.15	0.45
1:M:448:TRP:CG	1:M:449:ALA:N	2.84	0.45
2:N:41:GLY:CA	7:N:803:ACT:H2	2.46	0.45
1:A:536:ASP:O	1:A:539:CYS:HB2	2.16	0.45
1:A:546:ASN:O	1:A:549:LYS:HE2	2.16	0.45
3:C:49:LEU:HG	4:D:55:LEU:HD12	1.98	0.45
4:D:24:SER:O	4:D:28:ALA:HB3	2.15	0.45
3:O:89:LEU:C	3:O:91:PRO:HD2	2.41	0.45
4:P:93:VAL:HA	4:P:94:PRO:HD2	1.78	0.45
1:A:176:MET:HG3	3:C:4:ARG:HD3	1.98	0.45
1:A:202:ASN:HA	1:A:353:THR:HG22	1.99	0.45
4:D:48:ALA:HA	4:D:53:ARG:HD3	1.98	0.45
1:M:396:LEU:HG	8:M:821:FAD:C2	2.46	0.45
2:N:39:ALA:O	2:N:43:ILE:HG12	2.16	0.45
4:P:95:ALA:HB1	4:P:98:TRP:HB2	1.98	0.45
1:M:279:ASN:O	1:M:280:LYS:HB2	2.17	0.45
2:B:3:MET:HE2	2:B:30:TYR:C	2.41	0.45
1:M:158:LEU:O	1:M:159:ASP:HB2	2.17	0.45
1:M:546:ASN:O	1:M:549:LYS:HE3	2.17	0.45
1:M:93:MET:HB3	1:M:125:TRP:CE3	2.50	0.45
1:A:317:ARG:O	1:A:319:LEU:N	2.50	0.45
1:A:366:ASN:O	1:A:367:CYS:HB2	2.16	0.45
1:A:385:LEU:HD23	1:A:386:HIS:CE1	2.52	0.45
3:C:33:VAL:HG22	4:D:82:MET:CE	2.36	0.45
3:O:36:VAL:HG23	3:O:37:TRP:N	2.32	0.45
4:P:9:ASP:OD2	4:P:9:ASP:N	2.49	0.45
1:A:332:CYS:O	1:A:336:LYS:HG3	2.17	0.45
3:C:90:ALA:N	3:C:91:PRO:CD	2.80	0.45
1:M:320:GLY:O	1:M:324:LEU:HB2	2.17	0.45
1:M:498:PHE:CD2	2:N:103:VAL:HG21	2.51	0.45
2:N:12:ARG:NH2	2:N:101:ASP:OD1	2.49	0.45
1:A:141:GLN:HB3	2:B:118:PRO:O	2.17	0.45
1:A:448:TRP:CG	1:A:449:ALA:N	2.85	0.45
4:D:86:MET:CE	4:D:91:ILE:HD12	2.47	0.45
4:P:51:TYR:CD1	4:P:52:GLU:N	2.82	0.44
1:A:45:THR:O	1:A:132:GLY:HA3	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:64:ARG:HH12	4:D:117:THR:HG23	1.82	0.44
1:M:239:SER:OG	1:M:241:ILE:HG13	2.17	0.44
1:M:488:ARG:HB3	1:M:488:ARG:CZ	2.46	0.44
2:N:119:TYR:CE1	2:N:121:ILE:HD11	2.52	0.44
2:N:162:GLY:HA3	3:O:11:MET:CE	2.47	0.44
2:N:235:PHE:CE1	4:P:9:ASP:HA	2.51	0.44
4:P:30:VAL:O	4:P:33:LEU:HB3	2.17	0.44
1:A:93:MET:HB3	1:A:125:TRP:CZ3	2.52	0.44
2:B:7:LYS:HE2	2:B:25:PHE:CD2	2.52	0.44
1:M:61:SER:C	1:M:63:GLU:N	2.74	0.44
1:M:226:MET:SD	1:M:359:GLY:C	3.00	0.44
2:N:155:TYR:CZ	2:N:169:GLY:HA3	2.53	0.44
1:M:17:LEU:O	1:M:21:ILE:HG13	2.18	0.44
1:M:9:ILE:HD13	1:M:19:ALA:HB3	2.00	0.44
2:N:192:MET:O	2:N:193:ALA:C	2.59	0.44
1:M:96:LEU:HD23	1:M:96:LEU:HA	1.86	0.44
1:A:0:MET:SD	1:A:182:GLN:HG3	2.58	0.44
3:C:123:ILE:HD12	4:D:30:VAL:HG11	2.00	0.44
2:B:192:MET:O	2:B:193:ALA:C	2.60	0.44
4:D:92:HIS:HB3	2:N:243:ARG:CB	2.48	0.44
3:O:114:ALA:O	3:O:118:VAL:HG23	2.18	0.44
1:A:324:LEU:HD23	1:A:328:LEU:HD12	2.00	0.44
4:P:64:ARG:O	4:P:115:VAL:HG21	2.17	0.44
1:A:356:TYR:HE1	8:A:721:FAD:O3'	2.01	0.43
2:B:209:TYR:CZ	3:C:19:LEU:HD21	2.53	0.43
1:M:89:CYS:N	1:M:90:PRO:CD	2.78	0.43
1:M:171:VAL:CB	1:M:432:VAL:HG11	2.48	0.43
1:M:316:LEU:O	1:M:317:ARG:C	2.61	0.43
1:M:488:ARG:HH11	1:M:488:ARG:CB	2.29	0.43
4:P:55:LEU:HD12	4:P:118:ILE:HD11	1.99	0.43
1:A:100:GLY:O	1:A:101:CYS:C	2.61	0.43
3:O:84:LYS:HE2	3:O:88:GLU:OE2	2.17	0.43
1:A:244:THR:HG22	1:A:331:ILE:CG1	2.49	0.43
4:D:114:GLY:O	4:D:117:THR:HA	2.18	0.43
1:M:46:VAL:HG23	1:M:133:PHE:HA	2.00	0.43
1:M:335:ALA:HA	1:M:339:VAL:HG22	2.00	0.43
1:M:435:ARG:O	1:M:435:ARG:HD2	2.18	0.43
1:M:546:ASN:ND2	1:M:546:ASN:N	2.66	0.43
4:P:50:SER:O	4:P:51:TYR:C	2.61	0.43
1:M:118:GLY:O	1:M:119:MET:C	2.62	0.43
1:M:203:THR:O	8:M:821:FAD:HM83	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:382:SER:O	1:M:384:GLY:N	2.51	0.43
1:M:548:LEU:HD12	1:M:568:VAL:HG21	1.99	0.43
1:A:232:HIS:CD2	1:A:234:THR:H	2.33	0.43
2:B:136:PRO:HB2	3:C:100:ASP:OD1	2.17	0.43
3:C:37:TRP:CZ2	3:C:41:GLU:OE1	2.72	0.43
1:M:21:ILE:O	1:M:25:GLN:HG3	2.19	0.43
1:M:329:PRO:HG2	1:M:330:PHE:H	1.83	0.43
2:N:75:LEU:HD11	2:N:215:PRO:HG3	2.00	0.43
2:N:155:TYR:CE2	2:N:169:GLY:HA3	2.54	0.43
2:N:197:SER:HB2	4:P:5:PRO:HG2	2.00	0.43
1:A:328:LEU:N	1:A:329:PRO:CD	2.81	0.43
1:A:253:ILE:HG13	1:A:315:ASP:HB3	1.99	0.43
1:A:289:LYS:HZ3	9:A:705:1PE:H262	1.84	0.43
1:M:311:VAL:CG1	1:M:312:VAL:N	2.81	0.43
2:N:35:SER:O	2:N:38:ASP:HB2	2.19	0.43
2:N:149:ILE:HG23	2:N:216:LYS:HG3	1.99	0.43
1:M:239:SER:CB	1:M:241:ILE:HG13	2.49	0.43
1:M:326:GLU:HG2	1:M:326:GLU:O	2.18	0.43
2:N:82:ARG:HG3	2:N:83:ASP:OD1	2.19	0.43
2:N:221:ALA:O	2:N:225:GLN:HG2	2.19	0.43
1:A:204:ASN:N	1:A:204:ASN:HD22	2.17	0.43
2:B:73:PRO:HG2	2:B:213:VAL:HG11	2.01	0.43
3:C:49:LEU:HG	4:D:55:LEU:CD1	2.49	0.43
4:D:53:ARG:HH11	4:D:53:ARG:HG2	1.84	0.43
1:M:156:PHE:C	1:M:156:PHE:CD1	2.97	0.43
2:N:57:CYS:O	2:N:59:MET:HG2	2.19	0.43
1:A:78:GLU:OE2	1:A:568:VAL:HA	2.19	0.42
1:M:499:ASN:C	1:M:499:ASN:ND2	2.72	0.42
2:N:36:LEU:HD23	2:N:76:ALA:CB	2.49	0.42
2:N:135:THR:HG22	2:N:137:ALA:N	2.33	0.42
1:A:346:GLU:HB3	1:A:347:PRO:CD	2.49	0.42
4:D:4:ASN:HD21	4:P:6:LYS:HE3	1.84	0.42
2:N:81:LEU:N	2:N:81:LEU:CD1	2.82	0.42
2:N:110:ILE:O	2:N:114:GLU:HG3	2.19	0.42
4:P:95:ALA:O	4:P:96:GLY:C	2.62	0.42
1:A:89:CYS:N	1:A:90:PRO:CD	2.81	0.42
4:D:64:ARG:NH1	4:D:115:VAL:O	2.51	0.42
1:A:120:LYS:HG2	1:A:121:ILE:HD13	2.01	0.42
1:A:198:VAL:HA	1:A:455:MET:HE3	2.02	0.42
2:B:188:LYS:NZ	2:B:230:GLU:CG	2.81	0.42
1:M:44:HIS:NE2	8:M:821:FAD:C8	2.78	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:273:PRO:C	1:M:275:GLY:N	2.77	0.42
1:M:497:VAL:O	1:M:498:PHE:C	2.62	0.42
4:P:35:VAL:O	4:P:40:PRO:HD3	2.19	0.42
1:A:243:MET:HA	1:A:331:ILE:HD12	2.01	0.42
4:D:30:VAL:HG13	4:D:31:MET:N	2.34	0.42
1:M:58:ASP:C	1:M:60:ASP:N	2.78	0.42
1:M:365:GLN:O	1:M:366:ASN:ND2	2.48	0.42
1:M:481:GLU:O	1:M:485:ARG:HG2	2.18	0.42
1:M:548:LEU:HD21	1:M:575:PRO:HG3	2.02	0.42
4:P:10:GLU:OE2	4:P:80:HIS:HE1	2.02	0.42
4:P:68:PHE:CE1	4:P:72:VAL:HG21	2.55	0.42
1:A:42:ARG:HD2	1:A:42:ARG:N	2.35	0.42
1:A:379:GLU:HB2	8:A:721:FAD:H5'2	2.02	0.42
2:B:6:LEU:HD23	2:B:81:LEU:HD13	2.02	0.42
1:M:469:PRO:CD	1:M:536:ASP:HB3	2.50	0.42
2:N:137:ALA:HB2	3:O:100:ASP:OD1	2.20	0.42
3:O:59:PHE:O	3:O:62:PHE:HB3	2.20	0.42
4:P:79:LEU:HD23	4:P:82:MET:CE	2.45	0.42
1:M:92:GLU:HG3	1:M:400:VAL:O	2.20	0.42
1:M:100:GLY:O	2:N:184:ARG:NH2	2.51	0.42
1:M:435:ARG:HD2	1:M:435:ARG:C	2.45	0.42
2:N:54:ARG:HH21	2:N:103:VAL:CG1	2.33	0.42
1:M:85:PHE:CD2	1:M:385:LEU:HD11	2.55	0.42
2:N:45:ASP:OD1	7:N:803:ACT:H1	2.20	0.42
1:A:542:ARG:NH2	1:A:544:ASP:OD2	2.41	0.42
1:M:51:GLY:O	1:M:396:LEU:HD12	2.19	0.42
1:M:184:ARG:HH11	1:M:184:ARG:HG3	1.85	0.42
1:M:321:GLU:HA	1:M:324:LEU:HB3	2.02	0.42
1:M:370:ARG:HH12	1:M:554:PHE:HZ	1.67	0.42
2:N:206:PHE:HA	11:N:245:F3S:S1	2.60	0.42
2:B:28:VAL:HA	2:B:29:PRO:HD3	1.92	0.41
1:M:18:ARG:HG2	1:M:400:VAL:HA	2.01	0.41
2:N:72:VAL:HA	2:N:73:PRO:HD3	1.77	0.41
1:M:248:ARG:C	1:M:250:GLU:N	2.77	0.41
1:M:377:VAL:HG21	1:M:402:PHE:O	2.19	0.41
1:A:68:ASP:HB3	1:A:391:LEU:HD21	2.01	0.41
2:B:8:ILE:HD11	2:B:81:LEU:CD1	2.50	0.41
2:B:163:LEU:HD21	3:C:11:MET:HE2	2.02	0.41
3:C:39:SER:O	3:C:43:ILE:HG13	2.21	0.41
1:M:0:MET:O	1:M:1:GLN:HB2	2.19	0.41
2:N:16:GLU:HG2	3:O:3:LYS:HG2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:28:ARG:HD2	4:P:81:ARG:HH22	1.85	0.41
1:A:242:LEU:HD21	6:A:702:OAA:O1	2.20	0.41
3:C:59:PHE:CZ	3:C:63:LEU:HD11	2.55	0.41
1:M:9:ILE:HD12	1:M:20:ALA:HB2	2.03	0.41
1:M:106:ARG:NH1	1:M:111:VAL:O	2.53	0.41
1:M:180:LEU:HD21	1:M:436:LEU:CD2	2.51	0.41
2:N:126:THR:OG1	2:N:129:GLN:HG3	2.21	0.41
3:C:50:LYS:HE2	3:C:50:LYS:CA	2.49	0.41
1:M:48:ALA:HB3	1:M:132:GLY:HA3	2.02	0.41
2:N:151:CYS:HB2	2:N:153:LEU:HG	2.03	0.41
1:A:209:THR:OG1	1:A:507:GLU:HG2	2.20	0.41
1:A:443:ASP:HA	1:A:490:ARG:HG3	2.03	0.41
2:B:113:LEU:HD23	2:B:113:LEU:C	2.45	0.41
3:C:12:THR:CG2	3:C:13:SER:N	2.83	0.41
3:C:15:TRP:CD2	3:C:16:TRP:N	2.88	0.41
1:M:527:GLU:OE2	1:M:529:ARG:NH1	2.54	0.41
2:N:182:ASP:C	2:N:184:ARG:H	2.28	0.41
4:P:72:VAL:HG12	4:P:76:TRP:CD1	2.56	0.41
2:B:68:MET:HE1	2:B:73:PRO:HD3	2.02	0.41
1:M:199:TYR:OH	1:M:229:VAL:HG21	2.21	0.41
1:M:342:ASP:HA	1:M:343:PRO:HD3	1.84	0.41
1:M:439:LEU:O	1:M:442:GLN:HB3	2.20	0.41
3:O:89:LEU:O	3:O:90:ALA:C	2.62	0.41
1:A:96:LEU:CD1	1:A:135:MET:HE3	2.50	0.41
3:C:72:ASN:HD22	3:C:72:ASN:HA	1.61	0.41
1:M:570:ILE:HG22	1:M:571:THR:N	2.35	0.41
2:N:150:ASN:HA	12:N:246:SF4:S4	2.61	0.41
14:P:710:CE1:H211	14:P:710:CE1:H171	2.02	0.41
1:A:59:HIS:CD2	1:A:59:HIS:H	2.39	0.41
1:A:127:ALA:O	1:A:128:ALA:C	2.61	0.41
2:B:188:LYS:HZ2	2:B:230:GLU:CG	2.34	0.41
2:B:235:PHE:CD2	2:B:235:PHE:C	2.99	0.41
1:M:26:ALA:O	1:M:28:PRO:HD3	2.21	0.41
1:M:233:PRO:HG2	1:M:248:ARG:HH22	1.84	0.41
1:M:233:PRO:HG2	1:M:248:ARG:NH2	2.36	0.41
1:M:316:LEU:O	1:M:319:LEU:HG	2.21	0.41
2:N:214:CYS:SG	2:N:218:VAL:HG23	2.60	0.41
3:O:47:PHE:HE2	4:P:114:GLY:HA3	1.86	0.41
1:A:57:GLN:NE2	1:A:122:GLU:HG2	2.36	0.41
1:A:93:MET:HE1	1:A:397:ALA:HA	2.03	0.41
1:A:204:ASN:N	1:A:204:ASN:ND2	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:7:LEU:CD2	1:M:411:THR:HA	2.39	0.41
1:M:62:PHE:HB3	1:M:86:VAL:CG2	2.50	0.41
1:M:102:PRO:HB2	2:N:139:MET:CE	2.36	0.41
1:M:443:ASP:CG	1:M:444:GLY:N	2.78	0.41
2:B:9:GLU:CD	2:B:89:LYS:HG3	2.45	0.40
2:B:67:MET:HE2	2:B:67:MET:HB3	1.93	0.40
1:M:485:ARG:HH11	1:M:485:ARG:HB3	1.85	0.40
2:N:56:SER:O	2:N:58:ARG:HG3	2.21	0.40
1:A:529:ARG:NH1	1:A:542:ARG:HG2	2.36	0.40
3:C:18:LYS:HB2	3:C:19:LEU:H	1.61	0.40
1:M:208:VAL:O	1:M:208:VAL:HG12	2.19	0.40
1:M:356:TYR:HD1	1:M:358:MET:HG2	1.86	0.40
4:P:26:ILE:HG22	4:P:27:ILE:N	2.35	0.40
1:A:48:ALA:HA	8:A:721:FAD:C6	2.51	0.40
1:A:256:ASN:OD1	1:A:256:ASN:C	2.64	0.40
2:B:141:LYS:HE3	3:C:95:ASN:OD1	2.21	0.40
3:C:65:ASN:HB3	3:C:68:ILE:H	1.86	0.40
4:D:95:ALA:HB2	2:N:239:THR:HG22	2.03	0.40
1:M:156:PHE:C	1:M:156:PHE:HD1	2.30	0.40
1:M:213:MET:HB3	1:M:223:LEU:HD21	2.04	0.40
1:M:311:VAL:HG13	1:M:350:VAL:N	2.36	0.40
1:M:324:LEU:O	1:M:328:LEU:N	2.47	0.40
1:M:508:LEU:O	1:M:508:LEU:HD12	2.21	0.40
1:A:152:PHE:HB3	1:A:155:HIS:CG	2.56	0.40
1:M:76:LEU:HD23	1:M:76:LEU:HA	1.98	0.40
1:M:313:TYR:CD1	1:M:347:PRO:HB2	2.57	0.40
1:M:529:ARG:O	1:M:530:GLY:C	2.65	0.40
2:N:116:ILE:HG22	2:N:116:ILE:O	2.21	0.40
2:N:226:GLN:HE21	2:N:226:GLN:HB2	1.62	0.40
1:M:6:ASP:O	1:M:185:ALA:HB1	2.21	0.40
2:N:204:CYS:O	2:N:228:LYS:NZ	2.42	0.40
3:O:25:TYR:HD1	3:O:28:ARG:HH21	1.69	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	575/602 (96%)	541 (94%)	30 (5%)	4 (1%)	18	41
1	M	575/602 (96%)	487 (85%)	75 (13%)	13 (2%)	5	13
2	B	241/243 (99%)	224 (93%)	16 (7%)	1 (0%)	30	54
2	N	241/243 (99%)	215 (89%)	20 (8%)	6 (2%)	4	11
3	C	128/130 (98%)	120 (94%)	4 (3%)	4 (3%)	3	8
3	O	128/130 (98%)	114 (89%)	12 (9%)	2 (2%)	7	20
4	D	117/119 (98%)	111 (95%)	3 (3%)	3 (3%)	4	11
4	P	117/119 (98%)	102 (87%)	14 (12%)	1 (1%)	14	35
All	All	2122/2188 (97%)	1914 (90%)	174 (8%)	34 (2%)	7	20

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	18	LYS
3	C	65	ASN
1	M	244	THR
1	M	382	SER
1	A	318	HIS
1	M	79	GLN
1	M	540	THR
2	N	183	SER
3	O	18	LYS
2	B	56	SER
4	D	43	LEU
1	A	389	ASN
3	C	66	PRO
1	M	329	PRO
1	M	492	THR
2	N	55	TRP
2	N	93	LEU
2	N	101	ASP
3	O	99	LYS
1	A	244	THR
1	M	119	MET
1	M	257	LYS
1	M	344	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	56	SER
1	A	343	PRO
4	D	117	THR
1	M	318	HIS
1	M	324	LEU
2	N	128	ASP
1	M	444	GLY
4	P	4	ASN
1	M	383	VAL
3	C	104	GLY
4	D	99	VAL

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	460/475 (97%)	445 (97%)	15 (3%)	33	63
1	M	460/475 (97%)	441 (96%)	19 (4%)	27	56
2	B	205/205 (100%)	200 (98%)	5 (2%)	43	72
2	N	205/205 (100%)	199 (97%)	6 (3%)	37	67
3	C	111/111 (100%)	106 (96%)	5 (4%)	24	52
3	O	111/111 (100%)	108 (97%)	3 (3%)	39	69
4	D	97/97 (100%)	93 (96%)	4 (4%)	27	56
4	P	97/97 (100%)	96 (99%)	1 (1%)	68	86
All	All	1746/1776 (98%)	1688 (97%)	58 (3%)	33	63

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	74	ASP
1	A	96	LEU
1	A	122	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	197	ARG
1	A	200	ARG
1	A	276	GLU
1	A	319	LEU
1	A	327	ARG
1	A	358	MET
1	A	411	THR
1	A	413	ARG
1	A	489	VAL
1	A	528	SER
1	A	560	THR
2	B	65	CYS
2	B	81	LEU
2	B	128	ASP
2	B	136	PRO
2	B	212	GLU
3	C	39	SER
3	C	50	LYS
3	C	84	LYS
3	C	92	LYS
3	C	103	MET
4	D	0	MET
4	D	86	MET
4	D	109	VAL
4	D	118	ILE
1	M	35	ILE
1	M	93	MET
1	M	122	GLU
1	M	143	SER
1	M	155	HIS
1	M	163	ASP
1	M	164	ASP
1	M	197	ARG
1	M	227	GLU
1	M	242	LEU
1	M	243	MET
1	M	304	ILE
1	M	375	PHE
1	M	465	ILE
1	M	470	GLU
1	M	485	ARG
1	M	499	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	541	GLU
1	M	558	ASP
2	N	50	ASP
2	N	100	ARG
2	N	128	ASP
2	N	148	CYS
2	N	189	LYS
2	N	226	GLN
3	O	5	LYS
3	O	37	TRP
3	O	39	SER
4	P	7	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	57	GLN
1	A	87	HIS
1	A	95	GLN
1	A	141	GLN
1	A	155	HIS
1	A	232	HIS
1	A	258	ASN
1	A	279	ASN
1	A	292	GLN
1	A	296	HIS
1	A	428	GLN
1	A	434	GLN
1	A	442	GLN
2	B	134	GLN
2	B	144	GLN
2	B	150	ASN
2	B	194	GLN
2	B	196	ASN
3	C	51	ASN
3	C	72	ASN
4	D	4	ASN
4	D	59	GLN
1	M	1	GLN
1	M	27	ASN
1	M	57	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	137	HIS
1	M	174	ASN
1	M	186	ASN
1	M	204	ASN
1	M	232	HIS
1	M	292	GLN
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
2	N	71	ASN
2	N	95	ASN
2	N	123	ASN
2	N	129	GLN
2	N	150	ASN
2	N	160	GLN
2	N	186	HIS
2	N	217	HIS
2	N	226	GLN
3	O	72	ASN
4	P	80	HIS
4	P	83	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ACT	N	803	-	3,3,3	1.21	0	3,3,3	1.05	0
6	OAA	A	702	-	8,8,8	1.30	1 (12%)	8,10,10	1.59	1 (12%)
14	CE1	P	710	-	36,36,36	1.14	0	35,35,35	1.89	15 (42%)
7	ACT	B	704	-	3,3,3	0.81	0	3,3,3	0.98	0
12	SF4	N	246	2	0,12,12	-	-	-	-	-
7	ACT	A	703	-	3,3,3	0.97	0	3,3,3	1.32	0
14	CE1	P	810	-	36,36,36	1.14	0	35,35,35	1.98	15 (42%)
14	CE1	O	811	-	36,36,36	1.14	0	35,35,35	1.95	16 (45%)
14	CE1	O	813	-	36,36,36	1.21	0	35,35,35	1.94	15 (42%)
8	FAD	A	721	-	58,58,58	1.81	14 (24%)	85,89,89	1.59	18 (21%)
13	HQO	N	800	-	19,20,20	3.55	8 (42%)	20,26,26	1.09	2 (10%)
10	FES	B	244	2	0,4,4	-	-	-	-	-
14	CE1	O	812	-	36,36,36	1.14	0	35,35,35	1.88	15 (42%)
11	F3S	B	245	2	0,9,9	-	-	-	-	-
8	FAD	M	821	-	58,58,58	1.56	7 (12%)	85,89,89	1.58	15 (17%)
12	SF4	B	246	2	0,12,12	-	-	-	-	-
11	F3S	N	245	2	0,9,9	-	-	-	-	-
6	OAA	M	802	-	8,8,8	1.29	1 (12%)	8,10,10	1.60	1 (12%)
10	FES	N	244	2	0,4,4	-	-	-	-	-
13	HQO	C	700	-	19,20,20	3.55	8 (42%)	20,26,26	1.09	2 (10%)
9	1PE	A	705	-	15,15,15	1.65	0	14,14,14	2.27	9 (64%)

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
11	F3S	N	245	2	-	-	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OAA	A	702	-	-	4/8/8/8	-
6	OAA	M	802	-	-	4/8/8/8	-
14	CE1	O	811	-	-	16/34/34/34	-
14	CE1	O	813	-	-	13/34/34/34	-
14	CE1	P	710	-	-	16/34/34/34	-
12	SF4	B	246	2	-	-	0/6/5/5
10	FES	B	244	2	-	-	0/1/1/1
10	FES	N	244	2	-	-	0/1/1/1
8	FAD	A	721	-	-	6/34/50/50	0/6/6/6
12	SF4	N	246	2	-	-	0/6/5/5
8	FAD	M	821	-	-	6/34/50/50	0/6/6/6
13	HQO	N	800	-	-	3/7/7/7	0/2/2/2
13	HQO	C	700	-	-	3/7/7/7	0/2/2/2
9	1PE	A	705	-	-	6/13/13/13	-
14	CE1	P	810	-	-	15/34/34/34	-
14	CE1	O	812	-	-	17/34/34/34	-
11	F3S	B	245	2	-	-	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	800	HQO	O4-N1	-13.29	1.23	1.38
13	C	700	HQO	O4-N1	-13.29	1.23	1.38
8	A	721	FAD	P-O3P	-5.22	1.53	1.59
8	A	721	FAD	PA-O3P	-4.84	1.54	1.59
8	M	821	FAD	P-O3P	-4.46	1.54	1.59
8	A	721	FAD	C5A-N7A	-3.71	1.32	1.39
8	M	821	FAD	C5'-C4'	3.61	1.56	1.51
8	A	721	FAD	C10-N10	3.57	1.45	1.37
8	M	821	FAD	PA-O3P	-3.57	1.55	1.59
8	A	721	FAD	C8A-N9A	-3.56	1.31	1.37
8	M	821	FAD	C4A-N3A	3.44	1.40	1.34
13	C	700	HQO	O1-C1	-3.31	1.26	1.36
13	N	800	HQO	O1-C1	-3.31	1.26	1.36
13	N	800	HQO	C11-C3	-3.23	1.42	1.50
13	C	700	HQO	C11-C3	-3.22	1.42	1.50
8	A	721	FAD	C4A-N9A	-2.98	1.31	1.37
8	A	721	FAD	C10-N1	2.94	1.39	1.33
8	M	821	FAD	C5A-N7A	-2.79	1.34	1.39
8	M	821	FAD	C10-N10	2.77	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	800	HQO	C2-C3	2.73	1.43	1.38
8	A	721	FAD	C9-C9A	2.73	1.44	1.39
13	C	700	HQO	C2-C3	2.71	1.43	1.38
13	N	800	HQO	C7-C6	2.71	1.42	1.36
13	C	700	HQO	C7-C6	2.69	1.42	1.36
13	N	800	HQO	C8-C9	2.58	1.42	1.36
13	C	700	HQO	C8-C9	2.53	1.42	1.36
13	N	800	HQO	C8-C7	2.52	1.43	1.38
8	A	721	FAD	C4-N3	2.52	1.43	1.38
13	C	700	HQO	C8-C7	2.51	1.43	1.38
8	M	821	FAD	C9-C8	2.45	1.43	1.39
8	A	721	FAD	C4X-N5	2.39	1.35	1.30
6	M	802	OAA	O2-C1	2.38	1.38	1.30
6	A	702	OAA	O2-C1	2.38	1.38	1.30
13	N	800	HQO	C10-C5	2.27	1.46	1.42
13	C	700	HQO	C10-C5	2.25	1.46	1.42
8	A	721	FAD	P-O5'	-2.22	1.50	1.59
8	A	721	FAD	C9A-C5X	2.09	1.44	1.41
8	A	721	FAD	C2'-C3'	-2.04	1.49	1.53
8	A	721	FAD	PA-O5B	-2.01	1.51	1.59

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	821	FAD	N3A-C2A-N1A	-5.84	119.73	128.58
14	P	810	CE1	O28-C27-C26	4.60	131.30	110.35
8	A	721	FAD	C5A-C4A-N3A	-4.10	121.06	126.72
8	A	721	FAD	N3A-C4A-N9A	4.10	134.14	127.17
8	M	821	FAD	C4-N3-C2	-4.07	118.42	125.64
8	M	821	FAD	N3A-C4A-N9A	3.86	133.73	127.17
8	M	821	FAD	C5A-C4A-N3A	-3.76	121.54	126.72
8	A	721	FAD	C4-N3-C2	-3.67	119.13	125.64
8	A	721	FAD	N3A-C2A-N1A	-3.57	123.17	128.58
6	M	802	OAA	O3-C3-C2	3.56	125.88	120.41
6	A	702	OAA	O3-C3-C2	3.55	125.86	120.41
8	M	821	FAD	C2A-N3A-C4A	3.27	119.81	111.83
8	A	721	FAD	C5'-C4'-C3'	3.24	118.34	112.22
8	A	721	FAD	O3'-C3'-C2'	-3.23	101.58	108.93
14	O	813	CE1	O22-C23-C24	3.20	124.96	110.35
14	O	811	CE1	O19-C18-C17	3.20	124.92	110.35
14	P	710	CE1	O28-C27-C26	3.16	124.76	110.35
14	O	813	CE1	O22-C21-C20	3.16	124.76	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	812	CE1	O22-C21-C20	3.15	124.73	110.35
14	O	812	CE1	O22-C23-C24	3.13	124.61	110.35
14	O	812	CE1	O13-C14-C15	3.12	124.59	110.35
14	P	810	CE1	O28-C29-C30	3.10	124.49	110.35
14	P	810	CE1	O13-C14-C15	3.10	124.48	110.35
8	A	721	FAD	C5X-N5-C4X	3.09	123.09	118.09
14	P	710	CE1	O25-C24-C23	3.08	124.41	110.35
14	O	811	CE1	O16-C17-C18	3.08	124.38	110.35
14	O	811	CE1	O22-C23-C24	3.08	124.37	110.35
8	M	821	FAD	C5X-N5-C4X	3.05	123.02	118.09
14	O	813	CE1	O34-C35-C36	3.04	123.52	110.11
14	O	811	CE1	O16-C15-C14	3.04	124.19	110.35
14	O	812	CE1	O16-C15-C14	3.01	124.07	110.35
14	P	710	CE1	O13-C14-C15	2.99	123.97	110.35
14	P	810	CE1	O22-C23-C24	2.98	123.96	110.35
8	M	821	FAD	C4X-C4-N3	2.98	120.85	113.25
14	O	813	CE1	O19-C18-C17	2.98	123.92	110.35
14	P	710	CE1	O22-C23-C24	2.96	123.85	110.35
9	A	705	1PE	OH5-C25-C15	2.92	123.65	110.35
14	P	710	CE1	O34-C33-C32	2.91	123.60	110.35
14	O	812	CE1	O34-C35-C36	2.89	122.85	110.11
14	O	813	CE1	O25-C24-C23	2.88	123.49	110.35
14	P	810	CE1	O25-C24-C23	2.88	123.46	110.35
9	A	705	1PE	OH3-C22-C12	2.87	122.76	110.11
14	O	813	CE1	O16-C15-C14	2.87	123.43	110.35
8	A	721	FAD	C10-N1-C2	2.87	123.06	116.85
14	O	812	CE1	O19-C18-C17	2.86	123.40	110.35
14	O	813	CE1	O25-C26-C27	2.84	123.31	110.35
8	A	721	FAD	C2A-N3A-C4A	2.83	118.75	111.83
14	O	813	CE1	O31-C32-C33	2.83	123.25	110.35
14	O	812	CE1	O34-C33-C32	2.81	123.15	110.35
14	O	811	CE1	O31-C32-C33	2.80	123.11	110.35
8	A	721	FAD	C4A-N9A-C8A	2.78	108.66	105.74
9	A	705	1PE	OH4-C24-C14	2.78	123.03	110.35
14	O	813	CE1	O28-C29-C30	2.78	123.01	110.35
14	O	811	CE1	O19-C20-C21	2.77	122.99	110.35
9	A	705	1PE	OH4-C13-C23	2.76	122.95	110.35
14	P	710	CE1	O16-C15-C14	2.74	122.84	110.35
14	O	811	CE1	O22-C21-C20	2.73	122.77	110.35
14	O	811	CE1	O34-C35-C36	2.72	122.12	110.11
14	O	811	CE1	O25-C24-C23	2.72	122.75	110.35
14	P	710	CE1	O19-C20-C21	2.70	122.68	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	P	710	CE1	O34-C35-C36	2.70	122.03	110.11
14	O	811	CE1	O34-C33-C32	2.70	122.68	110.35
8	A	721	FAD	C9A-C5X-N5	-2.69	119.60	122.45
8	M	821	FAD	C9A-C5X-N5	-2.69	119.60	122.45
14	O	812	CE1	O16-C17-C18	2.68	122.57	110.35
14	P	810	CE1	O34-C33-C32	2.68	122.57	110.35
14	O	812	CE1	O31-C32-C33	2.68	122.57	110.35
14	P	810	CE1	O31-C30-C29	2.66	122.50	110.35
14	O	813	CE1	O13-C14-C15	2.65	122.41	110.35
14	P	810	CE1	O22-C21-C20	2.63	122.32	110.35
14	P	810	CE1	O16-C17-C18	2.62	122.28	110.35
14	P	810	CE1	O34-C35-C36	2.61	121.61	110.11
14	O	813	CE1	O34-C33-C32	2.61	122.25	110.35
8	A	721	FAD	C4X-C4-N3	2.59	119.84	113.25
14	O	812	CE1	O31-C30-C29	2.59	122.14	110.35
9	A	705	1PE	OH3-C23-C13	2.59	122.14	110.35
8	A	721	FAD	O4-C4-C4X	-2.58	119.71	126.53
14	O	812	CE1	O25-C24-C23	2.58	122.11	110.35
14	O	811	CE1	O28-C27-C26	2.58	122.10	110.35
13	C	700	HQO	O1-C1-C10	2.58	120.83	116.42
13	N	800	HQO	O1-C1-C10	2.57	120.82	116.42
9	A	705	1PE	OH6-C15-C25	2.56	122.04	110.35
14	P	810	CE1	O19-C20-C21	2.56	122.03	110.35
14	O	811	CE1	O13-C14-C15	2.55	121.98	110.35
14	O	811	CE1	O31-C30-C29	2.54	121.95	110.35
8	M	821	FAD	C4A-N9A-C8A	2.54	108.41	105.74
9	A	705	1PE	OH6-C26-C16	2.54	121.29	110.11
14	O	811	CE1	O28-C29-C30	2.53	121.88	110.35
14	O	813	CE1	O28-C27-C26	2.52	121.82	110.35
8	M	821	FAD	O4B-C1B-N9A	2.51	112.92	108.09
14	P	710	CE1	O31-C30-C29	2.51	121.80	110.35
14	O	813	CE1	O31-C30-C29	2.51	121.77	110.35
14	P	710	CE1	O22-C21-C20	2.48	121.67	110.35
14	P	710	CE1	O28-C29-C30	2.47	121.62	110.35
14	P	810	CE1	O16-C15-C14	2.47	121.62	110.35
8	A	721	FAD	O4B-C1B-N9A	2.46	112.82	108.09
14	P	710	CE1	O31-C32-C33	2.45	121.54	110.35
14	O	811	CE1	O25-C26-C27	2.44	121.48	110.35
14	P	710	CE1	O19-C18-C17	2.42	121.39	110.35
8	M	821	FAD	C4'-C3'-C2'	-2.39	109.59	113.57
14	P	710	CE1	O25-C26-C27	2.39	121.24	110.35
14	P	810	CE1	O31-C32-C33	2.39	121.24	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	813	CE1	C10-C11-C12	-2.38	103.11	113.47
9	A	705	1PE	OH5-C14-C24	2.36	121.09	110.35
8	A	721	FAD	O3P-P-O1P	-2.32	103.72	110.70
8	A	721	FAD	C4X-C10-N1	-2.32	118.89	124.59
8	M	821	FAD	C10-N1-C2	2.32	121.87	116.85
8	M	821	FAD	O4-C4-C4X	-2.31	120.43	126.53
14	O	812	CE1	O28-C27-C26	2.31	120.86	110.35
14	O	812	CE1	O28-C29-C30	2.29	120.80	110.35
14	O	813	CE1	O16-C17-C18	2.29	120.79	110.35
13	N	800	HQO	C1-C2-C3	2.29	120.17	118.45
13	C	700	HQO	C1-C2-C3	2.26	120.16	118.45
14	O	812	CE1	O25-C26-C27	2.26	120.64	110.35
14	P	710	CE1	O16-C17-C18	2.25	120.59	110.35
14	O	812	CE1	O19-C20-C21	2.24	120.57	110.35
14	P	810	CE1	O19-C18-C17	2.23	120.53	110.35
14	P	810	CE1	O25-C26-C27	2.20	120.38	110.35
8	M	821	FAD	C5'-C4'-C3'	2.16	116.30	112.22
8	A	721	FAD	C10-C4X-N5	-2.11	120.50	124.81
9	A	705	1PE	OH2-C12-C22	2.10	124.19	111.82
8	A	721	FAD	C4-C4X-N5	2.07	121.07	118.21
8	M	821	FAD	C2A-N1A-C6A	2.06	122.11	118.73
14	O	811	CE1	C10-C11-C12	-2.01	104.75	113.47

There are no chirality outliers.

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	702	OAA	O3-C3-C4-O4
6	A	702	OAA	O3-C3-C4-O5
6	A	702	OAA	C2-C3-C4-O5
6	M	802	OAA	O3-C3-C4-O4
6	M	802	OAA	O3-C3-C4-O5
6	M	802	OAA	C2-C3-C4-O5
8	A	721	FAD	N10-C1'-C2'-O2'
8	A	721	FAD	N10-C1'-C2'-C3'
8	A	721	FAD	PA-O3P-P-O5'
8	M	821	FAD	N10-C1'-C2'-O2'
8	M	821	FAD	N10-C1'-C2'-C3'
8	M	821	FAD	PA-O3P-P-O5'
14	O	811	CE1	C17-C18-O19-C20
14	O	812	CE1	O28-C29-C30-O31
14	O	813	CE1	O25-C26-C27-O28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	P	710	CE1	O28-C29-C30-O31
14	P	710	CE1	O13-C14-C15-O16
14	P	710	CE1	O22-C23-C24-O25
9	A	705	1PE	OH5-C14-C24-OH4
9	A	705	1PE	OH7-C16-C26-OH6
14	P	810	CE1	O25-C26-C27-O28
13	C	700	HQO	C3-C11-C13-C12
13	N	800	HQO	C3-C11-C13-C12
14	O	811	CE1	O28-C29-C30-O31
14	O	812	CE1	O13-C14-C15-O16
14	P	810	CE1	O34-C35-C36-O37
14	P	810	CE1	O28-C29-C30-O31
13	C	700	HQO	C14-C12-C13-C11
13	N	800	HQO	C14-C12-C13-C11
14	O	813	CE1	C6-C7-C8-C9
14	O	813	CE1	C7-C8-C9-C10
14	P	710	CE1	O34-C35-C36-O37
14	O	813	CE1	O13-C14-C15-O16
14	O	812	CE1	O25-C26-C27-O28
14	P	810	CE1	O22-C23-C24-O25
14	O	811	CE1	C7-C8-C9-C10
14	P	710	CE1	C11-C10-C9-C8
14	O	813	CE1	C3-C4-C5-C6
14	P	810	CE1	O13-C14-C15-O16
14	O	812	CE1	C6-C7-C8-C9
14	P	710	CE1	O25-C26-C27-O28
14	O	812	CE1	C3-C4-C5-C6
14	O	811	CE1	C3-C4-C5-C6
14	P	810	CE1	C2-C3-C4-C5
14	O	811	CE1	C6-C7-C8-C9
14	O	812	CE1	C7-C8-C9-C10
14	O	812	CE1	C2-C3-C4-C5
14	P	810	CE1	C6-C7-C8-C9
14	O	811	CE1	O34-C35-C36-O37
9	A	705	1PE	C13-C23-OH3-C22
14	O	813	CE1	C23-C24-O25-C26
6	A	702	OAA	C2-C3-C4-O4
6	M	802	OAA	C2-C3-C4-O4
14	P	710	CE1	C33-C32-O31-C30
9	A	705	1PE	C15-C25-OH5-C14
14	P	810	CE1	C11-C12-O13-C14
14	O	811	CE1	C36-C35-O34-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	O	813	CE1	C33-C32-O31-C30
14	O	813	CE1	C4-C5-C6-C7
14	O	813	CE1	C20-C21-O22-C23
14	P	810	CE1	C11-C10-C9-C8
14	P	710	CE1	C36-C35-O34-C33
14	O	812	CE1	C24-C23-O22-C21
14	O	811	CE1	O25-C26-C27-O28
9	A	705	1PE	C14-C24-OH4-C13
14	O	813	CE1	C18-C17-O16-C15
14	P	710	CE1	C4-C5-C6-C7
14	O	811	CE1	O22-C23-C24-O25
13	C	700	HQO	C12-C14-C15-C16
13	N	800	HQO	C12-C14-C15-C16
14	O	812	CE1	O34-C35-C36-O37
9	A	705	1PE	OH2-C12-C22-OH3
14	P	810	CE1	C30-C29-O28-C27
14	O	812	CE1	C11-C12-O13-C14
14	P	710	CE1	C32-C33-O34-C35
14	P	810	CE1	C36-C35-O34-C33
14	O	812	CE1	C32-C33-O34-C35
14	O	812	CE1	C4-C5-C6-C7
14	P	710	CE1	C11-C12-O13-C14
14	P	810	CE1	C18-C17-O16-C15
14	O	812	CE1	C33-C32-O31-C30
14	P	810	CE1	O19-C20-C21-O22
14	O	812	CE1	C30-C29-O28-C27
14	O	811	CE1	C32-C33-O34-C35
14	O	811	CE1	C20-C21-O22-C23
14	O	811	CE1	C24-C23-O22-C21
14	P	810	CE1	C24-C23-O22-C21
14	O	813	CE1	O28-C29-C30-O31
14	O	811	CE1	C11-C12-O13-C14
14	P	710	CE1	C24-C23-O22-C21
8	A	721	FAD	PA-O3P-P-O1P
8	A	721	FAD	PA-O3P-P-O2P
8	M	821	FAD	PA-O3P-P-O1P
14	O	813	CE1	O31-C32-C33-O34
8	A	721	FAD	O4B-C4B-C5B-O5B
8	M	821	FAD	O4B-C4B-C5B-O5B
14	P	710	CE1	C1-C2-C3-C4
14	P	710	CE1	O19-C20-C21-O22
14	O	811	CE1	O19-C20-C21-O22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	P	710	CE1	C6-C7-C8-C9
14	O	811	CE1	O13-C14-C15-O16
14	O	812	CE1	O22-C23-C24-O25
14	O	812	CE1	O19-C20-C21-O22
14	O	811	CE1	C1-C2-C3-C4
14	O	812	CE1	O31-C32-C33-O34
14	O	813	CE1	C21-C20-O19-C18
14	P	810	CE1	O16-C17-C18-O19
14	P	710	CE1	O16-C17-C18-O19
8	M	821	FAD	PA-O3P-P-O2P

There are no ring outliers.

11 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	N	803	ACT	2	0
6	A	702	OAA	2	0
14	P	710	CE1	2	0
12	N	246	SF4	4	0
14	P	810	CE1	3	0
8	A	721	FAD	7	0
13	N	800	HQO	2	0
8	M	821	FAD	8	0
11	N	245	F3S	1	0
13	C	700	HQO	3	0
9	A	705	1PE	5	0

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

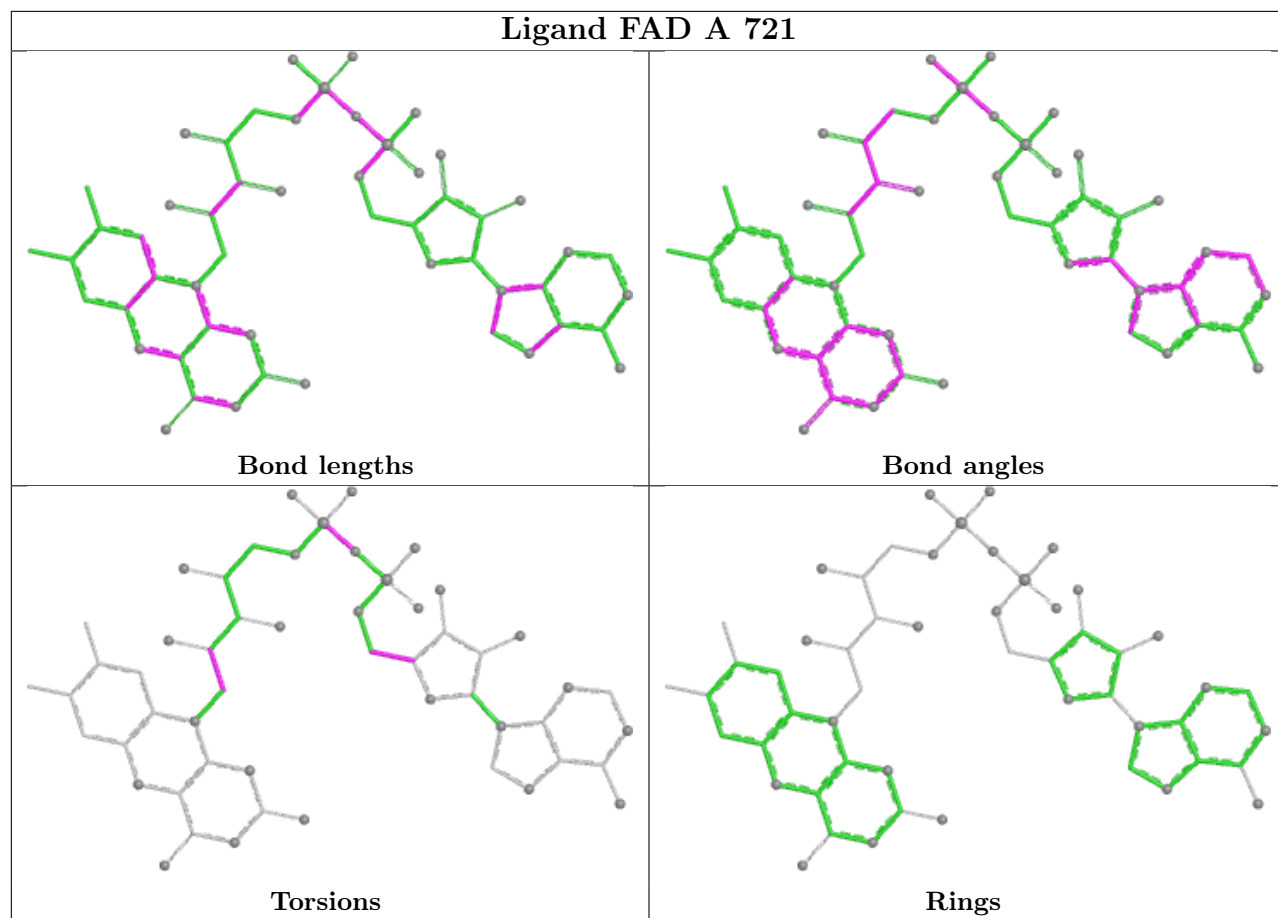
Ligand CE1 P 710	
 Bond lengths	 Bond angles
 Torsions	 Rings

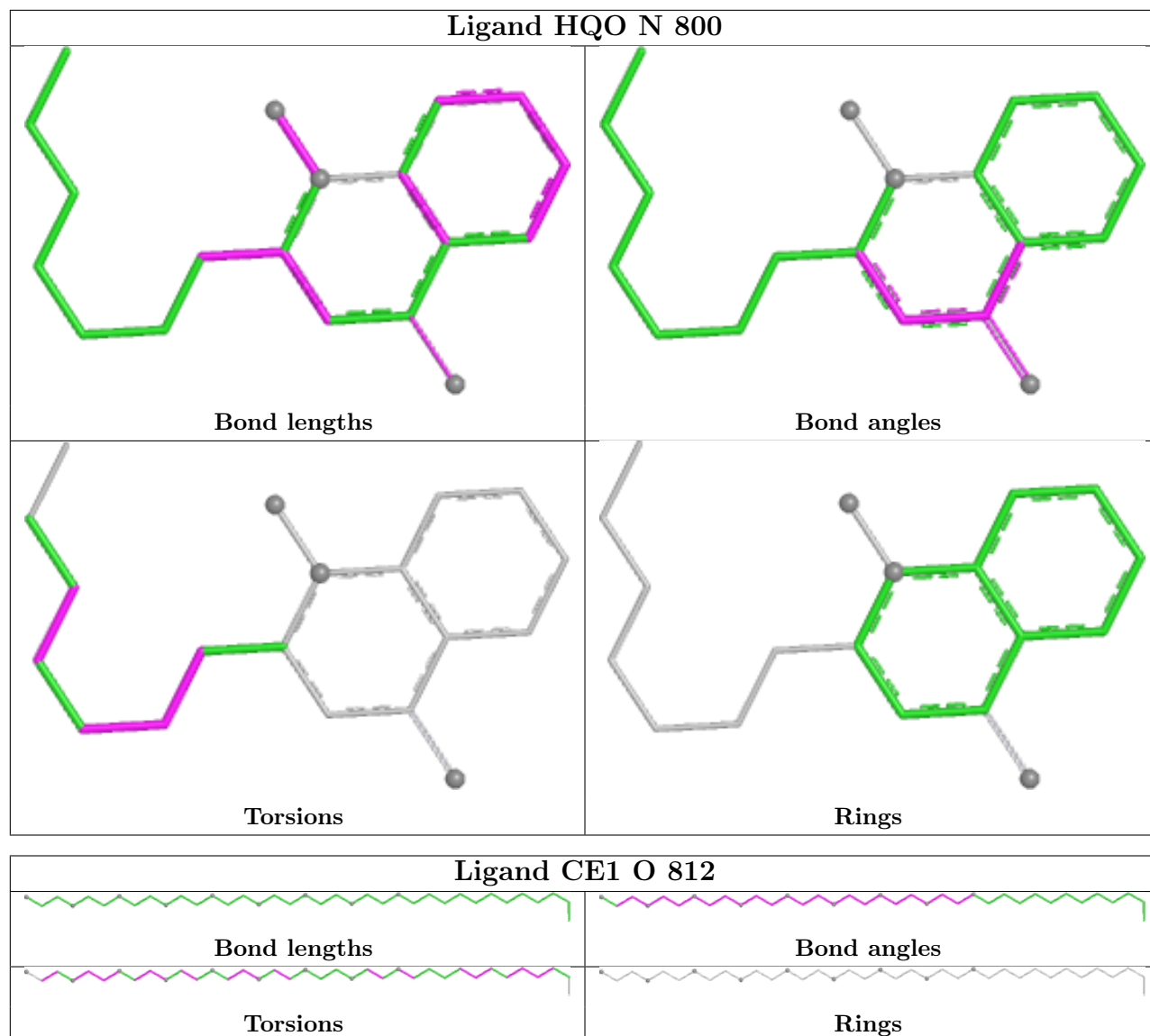
Ligand CE1 P 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

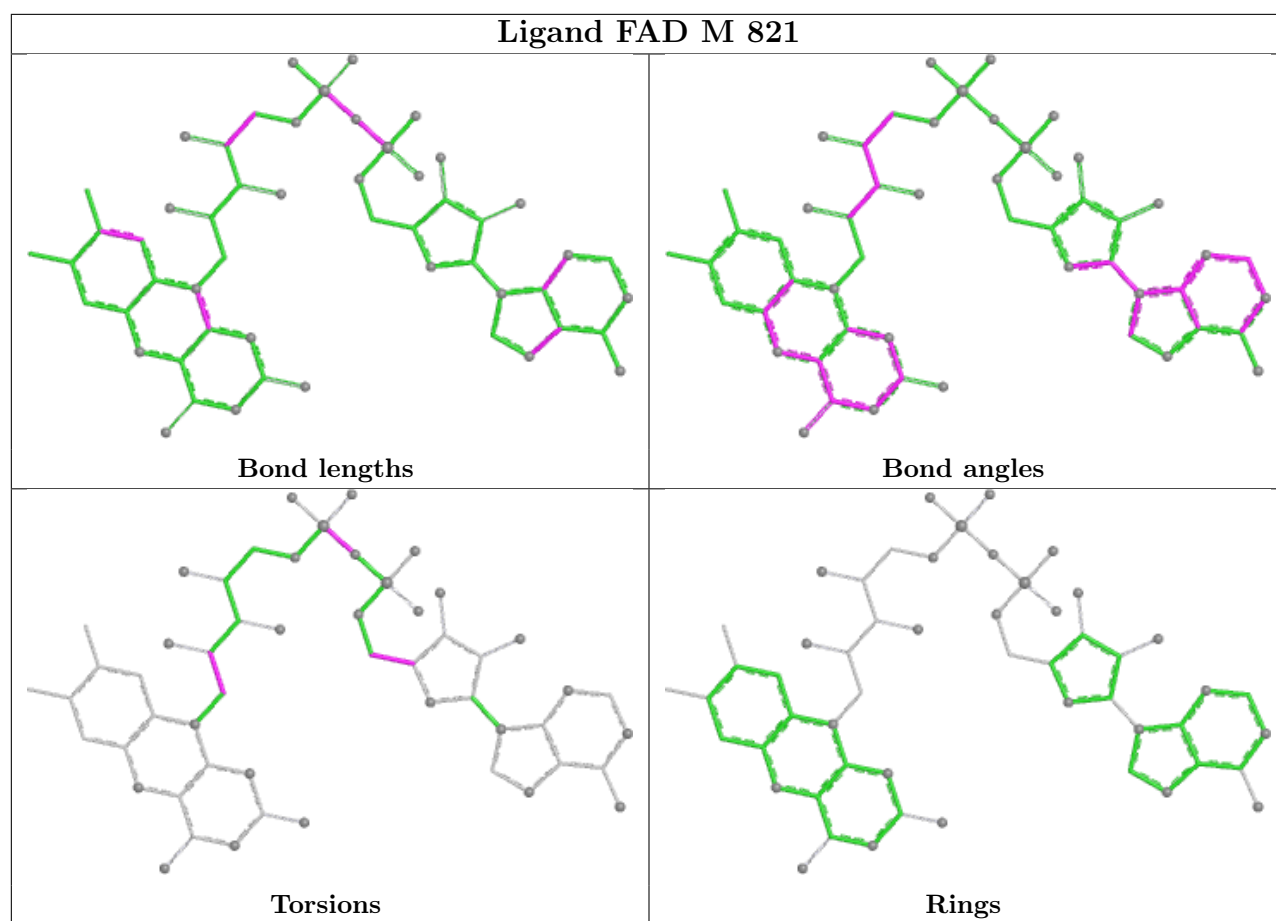
Ligand CE1 O 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

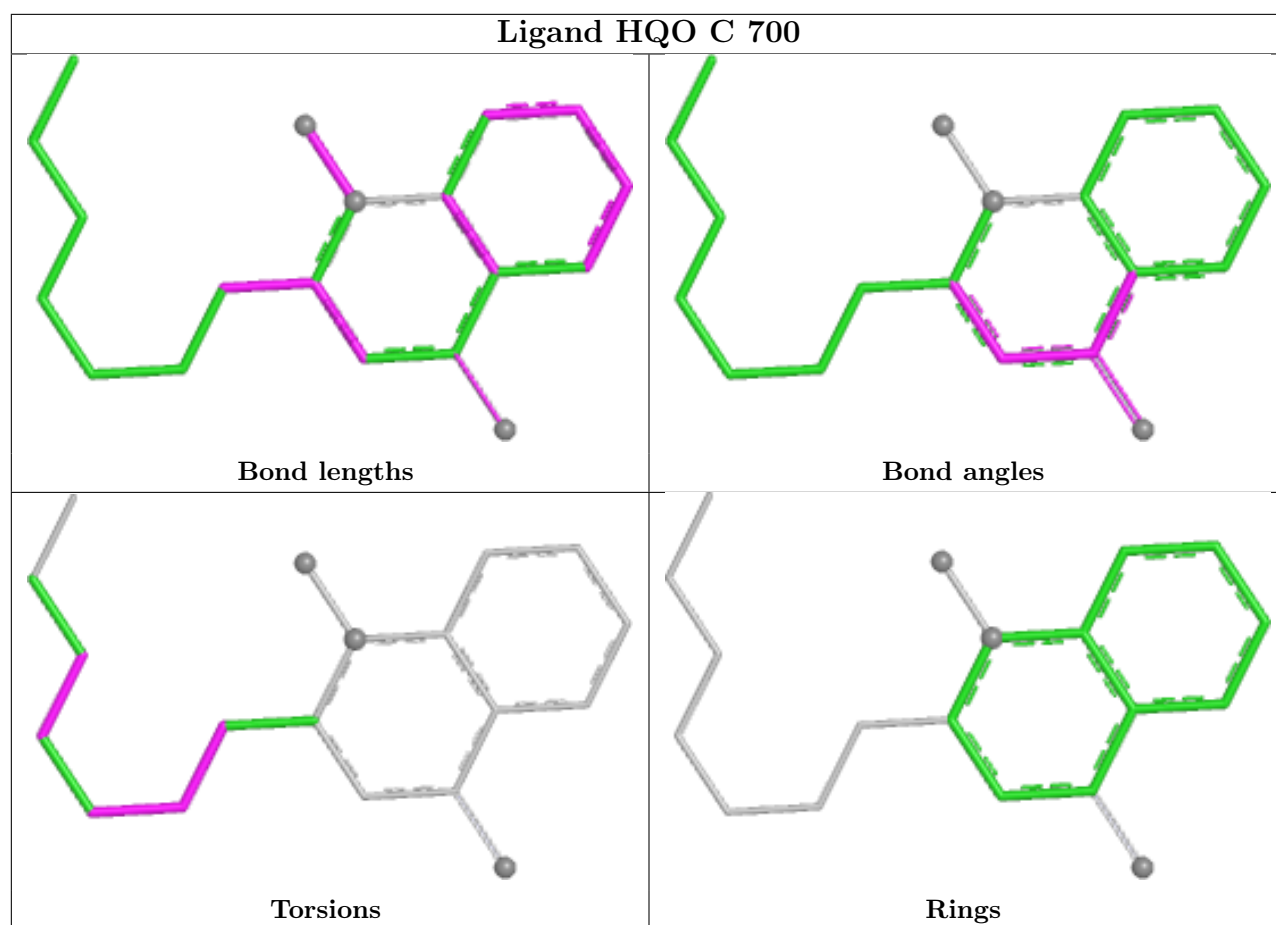
Ligand CE1 O 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FAD A 721









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.