



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:35 am BST

PDB ID : 1HBO
Title : METHYL-COENZYME M REDUCTASE MCR-RED1-SILENT
Authors : Grabarse, W.
Deposited on : 2001-04-20
Resolution : 1.78 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

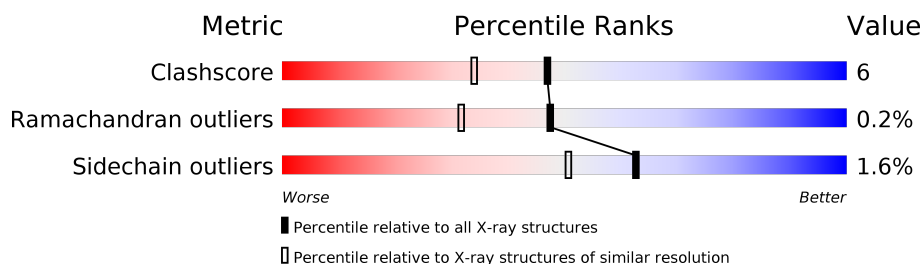
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	549	
1	D	549	
2	B	442	
2	E	442	
3	C	248	
3	F	248	

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
6	COM	A	1552	-	X	X	-
7	GOL	D	1554	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 21713 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 METHYL-COENZYME M REDUCTASE I ALPHA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	23	13	0
			4291	2712	723	836	20			
1	D	548	Total	C	N	O	S	23	14	0
			4294	2715	721	838	20			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	MHS	HIS	modified residue	UNP P11558
A	271	AGM	ARG	modified residue	UNP P11558
A	400	MGN	GLN	modified residue	UNP P11558
A	445	GL3	GLY	modified residue	UNP P11558
A	452	SMC	CYS	modified residue	UNP P11558
D	257	MHS	HIS	modified residue	UNP P11558
D	271	AGM	ARG	modified residue	UNP P11558
D	400	MGN	GLN	modified residue	UNP P11558
D	445	GL3	GLY	modified residue	UNP P11558
D	452	SMC	CYS	modified residue	UNP P11558

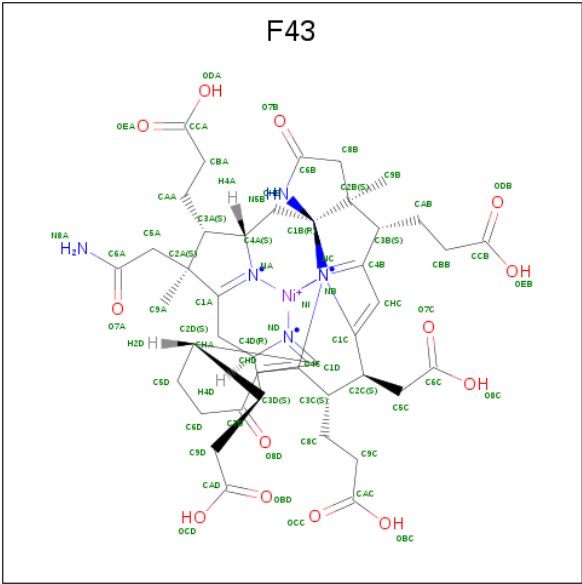
- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE I BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	25	22	0
			3388	2142	564	661	21			
2	E	442	Total	C	N	O	S	41	19	0
			3382	2143	558	660	21			

- Molecule 3 is a protein called METHYL-COENZYME M REDUCTASE I GAMMA SUB-UNIT.

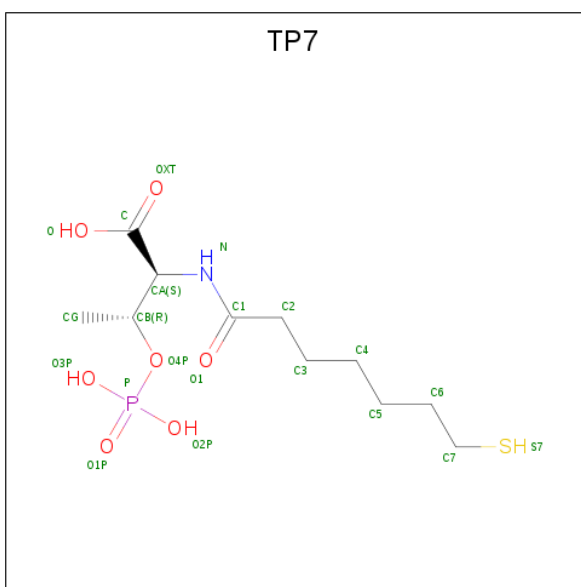
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total	C	N	O	S	39	5	0
			2007	1242	355	398	12			
3	F	247	Total	C	N	O	S	44	5	0
			2006	1242	354	398	12			

- Molecule 4 is FACTOR 430 (three-letter code: F43) (formula: C₄₂H₅₁N₆NiO₁₃).



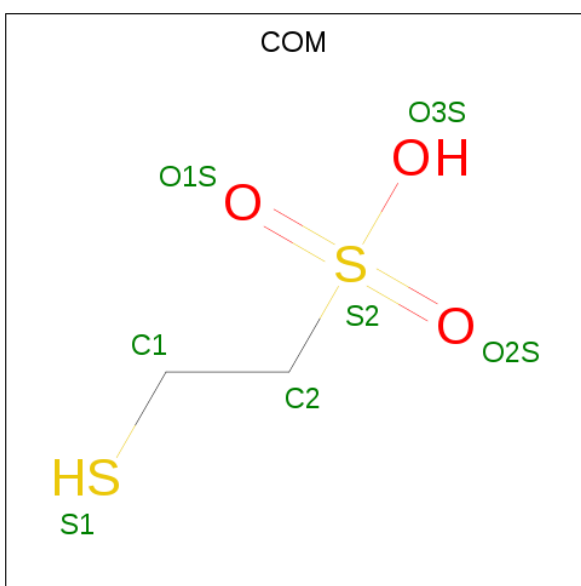
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
4	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 5 is Coenzyme B (three-letter code: TP7) (formula: C₁₁H₂₂NO₇PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
5	D	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		

- Molecule 6 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: $C_2H_6O_3S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			7	2	3	2		
6	D	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Zn	0	1
			1	1		

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	2	Total Na 2 2	0	0
9	A	4	Total Na 4 4	0	0
9	D	2	Total Na 2 2	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	2	Total Mg 2 2	0	0
10	C	1	Total Mg 1 1	0	0
10	F	1	Total Mg 1 1	0	0

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total Cl 1 1	0	0
11	E	1	Total Cl 1 1	0	0

- Molecule 12 is water.

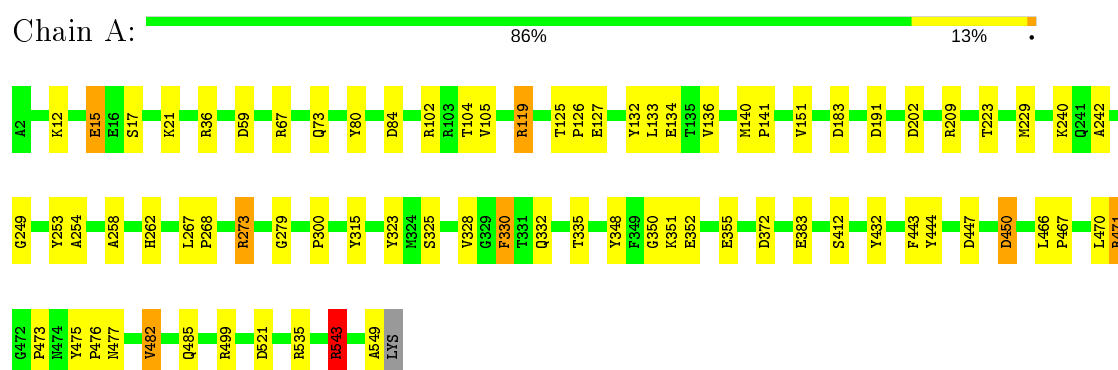
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	436	Total O 436 436	0	28
12	B	380	Total O 380 380	0	33
12	C	256	Total O 256 256	0	25
12	D	430	Total O 430 430	0	35
12	E	352	Total O 352 352	0	33
12	F	242	Total O 242 242	0	15

3 Residue-property plots

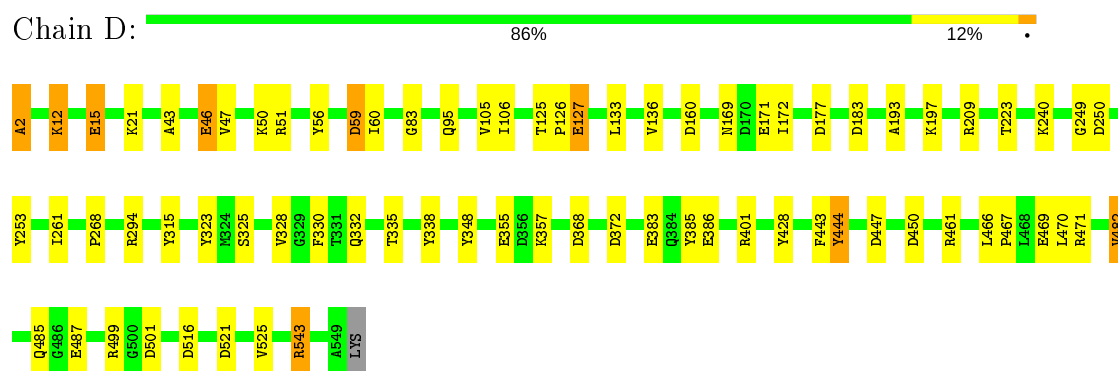
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

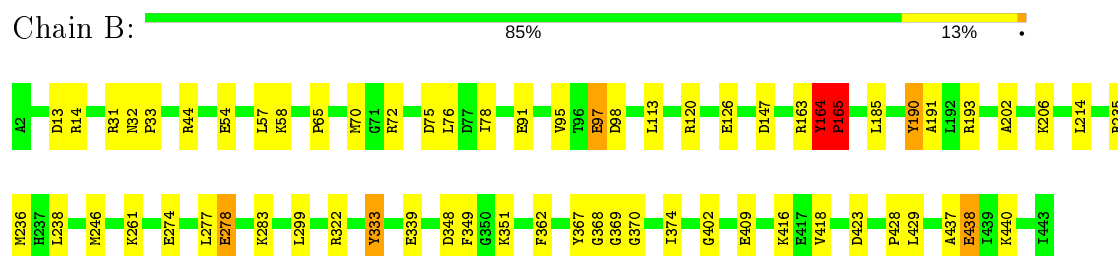
• Molecule 1: METHYL-COENZYME M REDUCTASE I ALPHA SUBUNIT




• Molecule 1: METHYL-COENZYME M REDUCTASE I ALPHA SUBUNIT

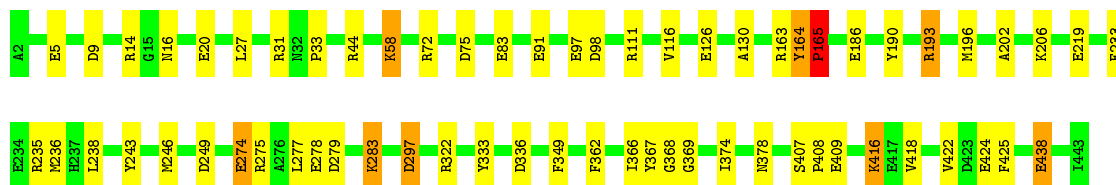


• Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT




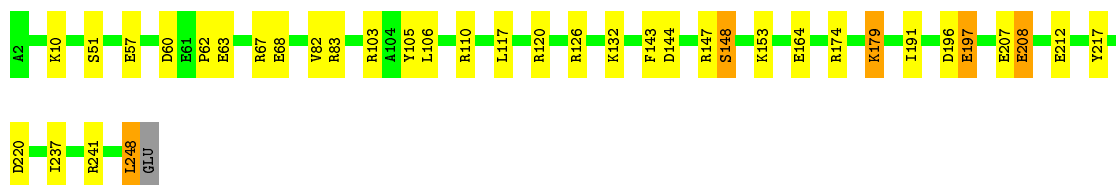
• Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT

Chain E:  86% 12% .




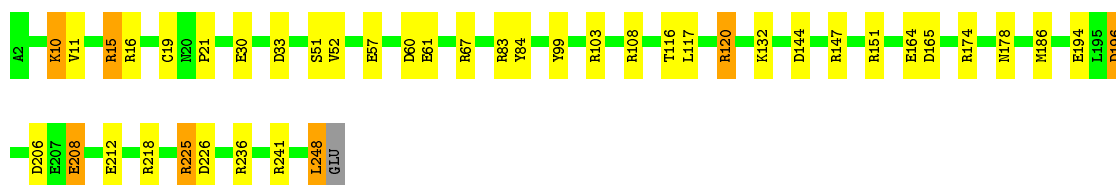
• Molecule 3: METHYL-COENZYME M REDUCTASE I GAMMA SUBUNIT

Chain C:  85% 13% .



• Molecule 3: METHYL-COENZYME M REDUCTASE I GAMMA SUBUNIT

Chain F:  83% 14% .



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.70 Å 117.30 Å 122.40 Å 90.00° 92.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.78	Depositor
% Data completeness (in resolution range)	96.5 (10.00-1.78)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.177 , 0.213	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21713	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: GOL, MG, CL, ZN, NA, AGM, F43, MGN, TP7, SMC, GL3, COM, MHS

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	0.72	3/4411 (0.1%)	1.33	26/5986 (0.4%)
1	D	1.05	6/4416 (0.1%)	1.42	37/5994 (0.6%)
2	B	0.66	3/3529 (0.1%)	1.31	33/4775 (0.7%)
2	E	1.19	8/3503 (0.2%)	1.52	43/4743 (0.9%)
3	C	1.15	10/2072 (0.5%)	1.36	22/2790 (0.8%)
3	F	1.02	11/2070 (0.5%)	1.41	30/2789 (1.1%)
All	All	0.96	41/20001 (0.2%)	1.39	191/27077 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
2	B	0	2
2	E	0	2
3	C	0	1
All	All	0	7

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	127	GLU	CG-CD	-46.53	0.82	1.51
2	E	91[A]	GLU	CG-CD	36.20	2.06	1.51
2	E	91[B]	GLU	CG-CD	36.20	2.06	1.51
2	E	83	GLU	CG-CD	30.40	1.97	1.51
3	C	179	LYS	CD-CE	25.79	2.15	1.51
3	C	164	GLU	CG-CD	24.29	1.88	1.51
3	F	57	GLU	CG-CD	18.79	1.80	1.51
1	D	240	LYS	CE-NZ	-17.02	1.06	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	61	GLU	CB-CG	15.87	1.82	1.52
3	C	60	ASP	CG-OD2	-15.64	0.89	1.25
3	F	196	ASP	CB-CG	-15.46	1.19	1.51
1	D	15	GLU	CB-CG	-15.06	1.23	1.52
3	C	197	GLU	CG-CD	-13.69	1.31	1.51
3	F	248	LEU	CA-C	12.59	1.85	1.52
1	A	21	LYS	CD-CE	11.66	1.80	1.51
2	E	58	LYS	CG-CD	11.02	1.90	1.52
1	D	50	LYS	CD-CE	10.30	1.76	1.51
2	B	91	GLU	CG-CD	10.00	1.67	1.51
3	F	164	GLU	CG-CD	9.95	1.66	1.51
3	F	164	GLU	CB-CG	9.53	1.70	1.52
1	A	127	GLU	CG-CD	9.08	1.65	1.51
2	E	438	GLU	CG-CD	9.08	1.65	1.51
3	F	208	GLU	CB-CG	-8.86	1.35	1.52
3	F	10	LYS	CG-CD	-8.20	1.24	1.52
3	C	63	GLU	CB-CG	-8.07	1.36	1.52
1	D	355	GLU	CG-CD	8.02	1.64	1.51
3	F	132	LYS	CG-CD	7.85	1.79	1.52
1	D	2	ALA	CA-C	7.42	1.72	1.52
3	C	207	GLU	CB-CG	7.35	1.66	1.52
3	C	60	ASP	CG-OD1	7.30	1.42	1.25
2	B	283	LYS	CG-CD	7.12	1.76	1.52
3	C	208	GLU	CB-CG	-7.04	1.38	1.52
1	A	15	GLU	CB-CG	6.89	1.65	1.52
2	B	261	LYS	CG-CD	-6.77	1.29	1.52
3	F	194	GLU	CB-CG	6.77	1.65	1.52
3	C	10	LYS	CG-CD	6.77	1.75	1.52
2	E	97	GLU	CG-CD	-6.45	1.42	1.51
2	E	416	LYS	CD-CE	6.12	1.66	1.51
3	C	132	LYS	CG-CD	-6.07	1.31	1.52
2	E	297	ASP	CB-CG	5.73	1.63	1.51
3	F	60	ASP	CB-CG	5.44	1.63	1.51

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	91[A]	GLU	CG-CD-OE2	-23.78	70.73	118.30
2	E	91[B]	GLU	CG-CD-OE2	-23.78	70.73	118.30
2	E	297	ASP	CB-CG-OD1	-23.75	96.93	118.30
3	C	60	ASP	CB-CG-OD1	-22.86	97.73	118.30
2	E	297	ASP	CB-CG-OD2	21.90	138.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2	ALA	CA-C-O	-17.19	84.01	120.10
1	D	2	ALA	CA-C-N	15.84	152.04	117.20
2	B	98	ASP	CA-CB-CG	-14.99	80.42	113.40
1	D	127	GLU	CB-CG-CD	14.32	152.85	114.20
1	D	2	ALA	CB-CA-C	-14.24	88.74	110.10
2	E	91[A]	GLU	CG-CD-OE1	13.22	144.74	118.30
2	E	91[B]	GLU	CG-CD-OE1	13.22	144.74	118.30
1	D	12	LYS	CD-CE-NZ	-12.90	82.03	111.70
1	D	12	LYS	CG-CD-CE	12.04	148.01	111.90
1	D	127	GLU	CG-CD-OE2	-11.59	95.12	118.30
1	D	294	ARG	NE-CZ-NH2	-11.41	114.60	120.30
3	F	208	GLU	CA-CB-CG	10.91	137.40	113.40
2	B	163	ARG	NE-CZ-NH1	-10.78	114.91	120.30
1	D	543	ARG	NE-CZ-NH2	10.72	125.66	120.30
2	E	438	GLU	CB-CG-CD	-10.51	85.82	114.20
3	F	196	ASP	CA-CB-CG	10.22	135.87	113.40
2	E	91[A]	GLU	CB-CG-CD	-10.07	87.02	114.20
2	E	91[B]	GLU	CB-CG-CD	-10.07	87.02	114.20
1	A	127	GLU	CG-CD-OE2	9.94	138.17	118.30
1	A	499	ARG	NE-CZ-NH2	9.71	125.15	120.30
3	C	60	ASP	OD1-CG-OD2	9.69	141.72	123.30
1	A	183	ASP	CB-CG-OD1	9.62	126.95	118.30
1	D	127	GLU	CG-CD-OE1	9.56	137.42	118.30
3	F	16	ARG	NE-CZ-NH2	9.49	125.04	120.30
2	B	165	PRO	CA-N-CD	-9.39	98.35	111.50
2	B	165	PRO	N-CA-CB	9.31	114.47	103.30
1	D	51	ARG	NE-CZ-NH1	-9.25	115.67	120.30
2	E	72	ARG	NE-CZ-NH1	-9.14	115.73	120.30
2	E	333	TYR	CB-CG-CD2	-9.09	115.55	121.00
1	D	15	GLU	CA-CB-CG	9.08	133.38	113.40
2	B	31[A]	ARG	NE-CZ-NH2	8.95	124.78	120.30
2	B	31[B]	ARG	NE-CZ-NH2	8.95	124.78	120.30
3	C	57	GLU	CA-CB-CG	8.90	132.99	113.40
3	F	218	ARG	NE-CZ-NH1	-8.83	115.89	120.30
3	F	147	ARG	NE-CZ-NH2	8.75	124.67	120.30
3	C	174	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	A	521	ASP	CB-CG-OD1	8.58	126.02	118.30
2	E	165	PRO	N-CA-CB	8.52	113.52	103.30
2	E	163	ARG	NE-CZ-NH1	-8.51	116.05	120.30
1	A	127	GLU	CG-CD-OE1	-8.34	101.62	118.30
2	E	9	ASP	CB-CG-OD1	8.31	125.78	118.30
1	A	543	ARG	NE-CZ-NH1	-8.30	116.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	31[A]	ARG	NE-CZ-NH1	-8.28	116.16	120.30
2	B	31[B]	ARG	NE-CZ-NH1	-8.28	116.16	120.30
2	E	44	ARG	NE-CZ-NH2	8.26	124.43	120.30
2	E	111	ARG	NE-CZ-NH2	8.25	124.43	120.30
2	E	165	PRO	CA-N-CD	-8.14	100.10	111.50
1	D	469	GLU	OE1-CD-OE2	-8.08	113.61	123.30
1	A	84	ASP	CB-CG-OD1	-8.07	111.04	118.30
3	F	196	ASP	CB-CG-OD2	8.00	125.50	118.30
3	F	174	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	D	368	ASP	CB-CG-OD1	7.83	125.35	118.30
2	B	97	GLU	CB-CG-CD	-7.74	93.30	114.20
1	D	355	GLU	CB-CG-CD	-7.68	93.46	114.20
3	F	15	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	D	543	ARG	NE-CZ-NH1	-7.61	116.50	120.30
2	E	438	GLU	CG-CD-OE1	-7.48	103.33	118.30
2	B	322	ARG	NE-CZ-NH2	7.45	124.03	120.30
3	C	147	ARG	NE-CZ-NH2	7.37	123.99	120.30
1	A	543	ARG	CA-CB-CG	7.36	129.59	113.40
3	F	120	ARG	NE-CZ-NH2	-7.28	116.66	120.30
3	C	103	ARG	NE-CZ-NH2	7.28	123.94	120.30
3	F	212	GLU	CA-CB-CG	7.27	129.40	113.40
1	A	482	VAL	CB-CA-C	-7.25	97.63	111.40
1	D	428	TYR	CB-CG-CD1	-7.17	116.70	121.00
1	A	102	ARG	NE-CZ-NH1	-7.17	116.71	120.30
1	D	51	ARG	NE-CZ-NH2	7.14	123.87	120.30
2	E	438	GLU	CG-CD-OE2	7.02	132.34	118.30
2	E	97	GLU	CG-CD-OE2	-6.99	104.32	118.30
1	D	160	ASP	CB-CG-OD1	6.99	124.59	118.30
1	D	447	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	191	ASP	CB-CG-OD1	6.97	124.57	118.30
1	D	209[A]	ARG	CD-NE-CZ	6.89	133.25	123.60
1	D	209[B]	ARG	CD-NE-CZ	6.89	133.25	123.60
3	F	196	ASP	CB-CG-OD1	-6.82	112.16	118.30
3	C	126	ARG	NE-CZ-NH1	-6.81	116.89	120.30
2	B	278	GLU	CG-CD-OE2	-6.79	104.72	118.30
3	F	236	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	D	401	ARG	NE-CZ-NH2	6.78	123.69	120.30
2	E	83	GLU	CB-CG-CD	-6.78	95.90	114.20
2	B	120	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	A	549	ALA	CA-C-O	-6.72	105.99	120.10
1	A	59	ASP	CB-CG-OD1	6.71	124.34	118.30
2	B	278	GLU	CG-CD-OE1	6.70	131.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	322	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	A	273	ARG	NE-CZ-NH1	-6.65	116.98	120.30
3	F	57	GLU	CB-CG-CD	6.64	132.13	114.20
1	A	36	ARG	CD-NE-CZ	6.64	132.89	123.60
3	F	61	GLU	CB-CG-CD	6.62	132.06	114.20
1	D	444	TYR	CB-CG-CD1	-6.61	117.03	121.00
3	F	67	ARG	NE-CZ-NH1	-6.61	117.00	120.30
1	A	202	ASP	CB-CG-OD1	6.61	124.25	118.30
3	C	208	GLU	CA-CB-CG	6.60	127.91	113.40
2	B	193	ARG	NE-CZ-NH1	-6.59	117.00	120.30
2	E	322	ARG	NE-CZ-NH2	6.59	123.60	120.30
2	E	193	ARG	NE-CZ-NH1	-6.57	117.02	120.30
2	B	164	TYR	CA-C-O	-6.53	106.40	120.10
3	C	126	ARG	NE-CZ-NH2	6.48	123.54	120.30
2	E	249	ASP	CB-CG-OD2	6.45	124.10	118.30
3	F	33	ASP	CB-CG-OD2	6.45	124.10	118.30
2	B	44	ARG	NE-CZ-NH1	6.42	123.51	120.30
2	E	126	GLU	OE1-CD-OE2	-6.42	115.60	123.30
2	E	275	ARG	NE-CZ-NH1	-6.39	117.11	120.30
2	E	5	GLU	CB-CG-CD	6.37	131.39	114.20
1	D	59	ASP	CB-CG-OD1	6.36	124.02	118.30
1	D	386	GLU	OE1-CD-OE2	-6.34	115.69	123.30
1	D	46	GLU	CB-CG-CD	6.29	131.20	114.20
2	B	438	GLU	CB-CG-CD	-6.22	97.41	114.20
3	F	147	ARG	NE-CZ-NH1	-6.22	117.19	120.30
3	C	57	GLU	CB-CG-CD	-6.21	97.45	114.20
3	F	206	ASP	CB-CG-OD2	6.20	123.88	118.30
2	E	20	GLU	CA-CB-CG	6.19	127.03	113.40
2	E	58	LYS	CB-CG-CD	-6.18	95.52	111.60
1	D	482	VAL	CB-CA-C	-6.13	99.75	111.40
2	B	14	ARG	CD-NE-CZ	6.08	132.11	123.60
3	F	61	GLU	CA-CB-CG	6.04	126.70	113.40
1	A	119	ARG	NE-CZ-NH2	-6.04	117.28	120.30
2	B	164	TYR	CB-CG-CD2	-6.03	117.38	121.00
3	F	225	ARG	NE-CZ-NH1	-6.00	117.30	120.30
3	F	30	GLU	OE1-CD-OE2	-5.97	116.14	123.30
3	F	10	LYS	CB-CG-CD	5.96	127.11	111.60
1	D	487	GLU	OE1-CD-OE2	-5.95	116.16	123.30
2	B	14	ARG	NE-CZ-NH1	-5.94	117.33	120.30
2	E	190	TYR	CB-CG-CD2	-5.93	117.44	121.00
3	C	217	TYR	CA-CB-CG	5.92	124.66	113.40
2	E	274	GLU	CA-CB-CG	5.92	126.42	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	190	TYR	CB-CG-CD2	-5.87	117.48	121.00
2	B	14	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	A	471	ARG	NE-CZ-NH1	-5.84	117.38	120.30
3	F	151	ARG	NE-CZ-NH1	-5.79	117.41	120.30
1	D	521	ASP	CB-CG-OD1	5.77	123.50	118.30
3	C	174	ARG	NH1-CZ-NH2	5.72	125.69	119.40
2	B	13	ASP	CB-CG-OD2	5.70	123.43	118.30
2	E	283	LYS	CG-CD-CE	5.69	128.97	111.90
3	F	60	ASP	CB-CG-OD1	-5.68	113.19	118.30
2	B	147	ASP	CB-CG-OD1	5.67	123.41	118.30
3	F	60	ASP	CB-CG-OD2	5.65	123.38	118.30
1	D	499	ARG	NE-CZ-NH2	5.64	123.12	120.30
3	C	220	ASP	CB-CG-OD2	5.64	123.38	118.30
2	E	20	GLU	CB-CG-CD	5.63	129.39	114.20
2	B	423	ASP	CB-CG-OD1	5.62	123.36	118.30
3	F	108	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	323	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	A	132	TYR	CB-CG-CD2	-5.61	117.64	121.00
2	B	98	ASP	CB-CG-OD2	5.59	123.33	118.30
2	E	164	TYR	CA-C-O	-5.57	108.41	120.10
3	C	197	GLU	CB-CG-CD	5.57	129.23	114.20
2	B	283	LYS	CB-CG-CD	-5.55	97.16	111.60
3	C	197	GLU	CG-CD-OE2	-5.55	107.20	118.30
1	D	338	TYR	CB-CG-CD1	5.53	124.32	121.00
2	E	235	ARG	NE-CZ-NH2	5.51	123.06	120.30
3	C	212	GLU	CG-CD-OE1	5.50	129.30	118.30
3	C	105	TYR	CB-CG-CD2	5.50	124.30	121.00
1	D	372	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	432	TYR	CB-CG-CD1	-5.46	117.72	121.00
2	E	279	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	372	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	330	PHE	CB-CG-CD1	5.40	124.58	120.80
2	E	75	ASP	CB-CG-OD1	5.38	123.14	118.30
3	C	110	ARG	CD-NE-CZ	5.38	131.13	123.60
2	E	243	TYR	CB-CG-CD2	-5.37	117.78	121.00
2	B	333	TYR	CB-CG-CD2	-5.37	117.78	121.00
3	C	144	ASP	CB-CG-OD2	5.37	123.13	118.30
1	D	56	TYR	CB-CG-CD2	5.36	124.22	121.00
3	F	165	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	535	ARG	NE-CZ-NH1	-5.35	117.62	120.30
2	B	333	TYR	CA-CB-CG	-5.35	103.23	113.40
3	F	83	ARG	NE-CZ-NH1	-5.35	117.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	14	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	D	183	ASP	CB-CG-OD1	5.28	123.06	118.30
1	A	36	ARG	NE-CZ-NH2	5.25	122.92	120.30
2	B	235	ARG	NE-CZ-NH2	5.21	122.91	120.30
3	C	68	GLU	OE1-CD-OE2	-5.13	117.14	123.30
2	E	416	LYS	CD-CE-NZ	5.12	123.47	111.70
2	E	31	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	B	72	ARG	NE-CZ-NH2	-5.10	117.75	120.30
3	C	103	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
3	C	241	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	D	323	TYR	CB-CG-CD2	-5.09	117.95	121.00
2	E	322	ARG	CD-NE-CZ	5.08	130.71	123.60
1	D	385	TYR	CB-CG-CD1	-5.06	117.97	121.00
3	F	144	ASP	CB-CG-OD1	-5.06	113.75	118.30
2	B	164	TYR	C-N-CD	-5.04	109.52	120.60
1	A	477	ASN	CB-CG-OD1	-5.03	111.55	121.60
3	F	241	ARG	NE-CZ-NH1	-5.01	117.80	120.30
2	E	243	TYR	CB-CG-CD1	5.01	124.00	121.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	164	TYR	Mainchain,Peptide
3	C	197	GLU	Sidechain
1	D	127	GLU	Sidechain
1	D	2	ALA	Mainchain
2	E	164	TYR	Mainchain,Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4291	0	4093	60	0
1	D	4294	0	4112	50	1
2	B	3388	0	3369	49	0
2	E	3382	0	3363	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2007	0	1937	16	0
3	F	2006	0	1937	13	0
4	A	62	0	43	4	0
4	D	62	0	43	2	0
5	A	21	0	19	1	0
5	D	21	0	19	1	0
6	A	7	0	5	4	0
6	D	7	0	5	2	0
7	A	18	0	24	4	0
7	B	6	0	8	0	0
7	C	6	0	8	0	0
7	D	18	0	24	9	0
7	E	6	0	8	0	0
8	A	1	0	0	0	0
9	A	4	0	0	0	0
9	B	2	0	0	0	0
9	D	2	0	0	0	0
10	A	2	0	0	0	0
10	C	1	0	0	0	0
10	F	1	0	0	0	0
11	B	1	0	0	0	0
11	E	1	0	0	0	0
12	A	436	0	0	9	0
12	B	380	0	0	9	0
12	C	256	0	0	2	0
12	D	430	0	0	12	0
12	E	352	0	0	10	0
12	F	242	0	0	2	0
All	All	21713	0	19017	237	1

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 6.

All (237) 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)
7:D:1554:GOL:O3	12:D:2428[B]:HOH:O	1.56	1.22
2:E:233[B]:PHE:HB2	12:E:2240[B]:HOH:O	1.44	1.15
2:E:233[B]:PHE:HD2	2:E:236[B]:MET:HE2	1.12	1.13
2:E:196[B]:MET:CE	2:E:374:ILE:HG22	1.84	1.06
7:D:1554:GOL:C3	12:D:2429[B]:HOH:O	2.04	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:196[B]:MET:CE	2:E:374:ILE:HA	1.87	1.05
1:D:466[B]:LEU:HD23	1:D:470:LEU:HB2	1.39	1.04
2:E:233[B]:PHE:CD2	2:E:236[B]:MET:HE2	1.94	1.03
2:B:185[B]:LEU:HD21	2:B:191:ALA:N	1.77	0.98
7:D:1554:GOL:O3	12:D:2429[B]:HOH:O	1.80	0.97
2:B:277[B]:LEU:HD13	2:B:278:GLU:H	1.28	0.95
1:D:466[B]:LEU:CD2	1:D:470:LEU:HB2	1.96	0.94
2:E:193:ARG:HG2	12:E:2231[B]:HOH:O	1.66	0.93
1:A:466[B]:LEU:CD2	1:A:470:LEU:HB2	1.98	0.93
2:E:233[B]:PHE:CD2	2:E:236[B]:MET:CE	2.52	0.91
1:A:466[B]:LEU:HD21	1:A:470:LEU:CB	2.00	0.90
2:B:185[B]:LEU:HD22	2:B:190:TYR:HB2	1.54	0.90
2:E:196[B]:MET:HE2	2:E:374:ILE:HA	1.54	0.88
2:E:196[B]:MET:HE1	2:E:374:ILE:HG22	1.54	0.88
2:E:196[B]:MET:HE3	2:E:374:ILE:HA	1.55	0.87
2:E:277[B]:LEU:HD13	2:E:278:GLU:N	1.89	0.86
2:E:233[B]:PHE:HD2	2:E:236[B]:MET:CE	1.89	0.86
1:D:466[B]:LEU:HD21	1:D:470:LEU:C	1.96	0.86
2:E:219:GLU:OE1	12:E:2231[B]:HOH:O	1.94	0.86
1:D:466[B]:LEU:HD21	1:D:470:LEU:CB	2.07	0.85
12:B:2334:HOH:O	1:D:250:ASP:HA	1.76	0.84
1:A:466[B]:LEU:HD23	1:A:470:LEU:HB2	1.59	0.84
2:B:185[B]:LEU:HD22	2:B:190:TYR:CB	2.07	0.84
2:B:349:PHE:HZ	3:C:248:LEU:HD21	1.44	0.83
1:A:466[B]:LEU:CD2	1:A:467:PRO:O	2.26	0.83
1:D:466[B]:LEU:CD2	1:D:470:LEU:CB	2.57	0.82
2:B:58[A]:LYS:HE3	2:B:75:ASP:OD1	1.80	0.81
2:E:196[B]:MET:HE2	2:E:374:ILE:HG22	1.64	0.80
2:B:277[B]:LEU:CD2	12:B:2291:HOH:O	2.28	0.80
2:E:196[B]:MET:CE	2:E:374:ILE:CG2	2.61	0.78
1:A:466[B]:LEU:HD21	1:A:470:LEU:C	2.03	0.77
2:B:185[B]:LEU:CD2	2:B:190:TYR:C	2.54	0.76
1:A:466[B]:LEU:HD21	1:A:470:LEU:HB2	1.65	0.76
1:A:466[A]:LEU:HD22	2:E:165:PRO:HD2	1.67	0.75
2:E:219:GLU:HA	12:E:2231[B]:HOH:O	1.85	0.75
1:A:383[B]:GLU:HG3	12:A:2328:HOH:O	1.85	0.75
7:D:1554:GOL:C2	12:D:2429[B]:HOH:O	2.28	0.75
2:E:196[B]:MET:CE	2:E:374:ILE:CA	2.65	0.74
1:A:466[B]:LEU:HD23	1:A:467:PRO:O	1.89	0.71
2:B:277[B]:LEU:HD21	12:B:2291:HOH:O	1.89	0.71
2:E:196[B]:MET:HE3	2:E:374:ILE:CA	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:THR:HB	1:A:126:PRO:HD2	1.72	0.70
2:E:366[B]:ILE:HG13	2:E:367[B]:TYR:CD1	2.25	0.70
2:E:349:PHE:CZ	3:F:248:LEU:HD21	2.27	0.70
1:A:466[B]:LEU:HD22	1:A:471:ARG:HG3	1.74	0.69
1:A:466[B]:LEU:HD22	1:A:467:PRO:O	1.92	0.69
2:B:277[B]:LEU:HD13	2:B:278:GLU:N	2.07	0.69
2:B:70[B]:MET:HE3	1:D:501:ASP:HB3	1.73	0.69
2:E:58:LYS:HG3	12:E:2094:HOH:O	1.94	0.68
2:B:185[B]:LEU:CD2	2:B:191:ALA:N	2.54	0.68
2:B:236[A]:MET:HB2	3:C:248:LEU:HD12	1.76	0.68
2:B:349:PHE:CZ	3:C:248:LEU:HD21	2.28	0.67
2:E:27:LEU:HD22	2:E:246[B]:MET:SD	2.35	0.67
2:E:202:ALA:HB1	2:E:416:LYS:HB2	1.77	0.67
2:B:236[B]:MET:HB2	3:C:248:LEU:HD12	1.77	0.67
3:F:226:ASP:OD2	12:F:2222:HOH:O	2.13	0.65
2:E:206[B]:LYS:NZ	2:E:409:GLU:OE1	2.19	0.65
7:A:1554:GOL:H12	12:A:2400:HOH:O	1.96	0.65
2:B:370[B]:GLY:HA3	2:B:374:ILE:HG12	1.77	0.65
1:D:328:VAL:HB	4:D:1550:F43:H9A1	1.78	0.65
2:E:196[B]:MET:HE2	2:E:374:ILE:CA	2.26	0.64
2:B:185[B]:LEU:CD2	2:B:190:TYR:CB	2.76	0.64
1:A:328:VAL:HB	4:A:1550:F43:H9A1	1.78	0.64
2:E:366[B]:ILE:CG1	2:E:367[B]:TYR:CE1	2.81	0.64
2:B:185[B]:LEU:HD22	2:B:190:TYR:CA	2.27	0.64
1:A:249:GLY:O	2:E:369[B]:GLY:HA2	1.98	0.63
1:D:43:ALA:HA	1:D:46:GLU:HG2	1.81	0.62
1:D:525[B]:VAL:HG22	12:D:2393:HOH:O	1.98	0.62
2:E:196[B]:MET:HE3	2:E:374:ILE:CB	2.30	0.62
2:B:70[B]:MET:CE	1:D:501:ASP:HB3	2.29	0.62
2:E:366[B]:ILE:HG13	2:E:367[B]:TYR:CE1	2.34	0.62
12:E:2321:HOH:O	3:F:52[B]:VAL:HG21	2.00	0.62
2:E:196[B]:MET:CE	2:E:374:ILE:CB	2.77	0.61
2:E:233[B]:PHE:CE2	2:E:236[B]:MET:HE1	2.34	0.61
1:D:383[A]:GLU:OE2	3:F:225:ARG:NH2	2.32	0.61
1:D:466[B]:LEU:CD2	1:D:471:ARG:N	2.64	0.60
1:A:254:ALA:HA	1:A:258:ALA:HB3	1.82	0.60
1:A:466[B]:LEU:CD2	1:A:470:LEU:CB	2.64	0.60
5:D:1551:TP7:H62C	2:E:367[B]:TYR:CD2	2.36	0.60
1:D:466[B]:LEU:HD21	1:D:470:LEU:HB3	1.84	0.59
1:D:268:PRO:HG3	12:D:2364:HOH:O	2.02	0.59
2:E:362:PHE:O	2:E:368[B]:GLY:HA3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466[B]:LEU:HD22	1:A:471:ARG:CG	2.33	0.58
2:B:185[B]:LEU:HD21	2:B:191:ALA:CA	2.32	0.58
2:B:206[B]:LYS:NZ	2:B:409:GLU:OE1	2.30	0.58
1:D:21:LYS:HE3	12:D:2332[B]:HOH:O	2.03	0.58
1:A:125:THR:HB	1:A:126:PRO:CD	2.34	0.57
2:E:277[B]:LEU:HD13	2:E:278:GLU:CA	2.34	0.57
1:A:466[B]:LEU:HD21	1:A:470:LEU:CA	2.35	0.57
2:E:233[B]:PHE:CD2	2:E:236[B]:MET:HE1	2.40	0.57
1:A:262[B]:HIS:ND1	12:A:2244[B]:HOH:O	2.33	0.57
1:D:466[B]:LEU:HD22	1:D:471:ARG:N	2.20	0.57
1:D:177:ASP:OD2	12:D:2188:HOH:O	2.18	0.57
1:A:268:PRO:HG3	12:A:2364:HOH:O	2.05	0.56
1:A:134[B]:GLU:HG2	1:D:60:ILE:HD11	1.87	0.56
2:E:362:PHE:CE2	2:E:367[B]:TYR:HB3	2.41	0.56
2:E:233[B]:PHE:CE2	2:E:236[B]:MET:CE	2.88	0.55
7:D:1554:GOL:H2	12:D:2429[B]:HOH:O	2.00	0.55
1:A:443:PHE:HB2	6:A:1552:COM:O1S	2.07	0.55
2:B:165:PRO:HD2	1:D:466[A]:LEU:HD22	1.89	0.55
1:D:466[B]:LEU:CD2	1:D:470:LEU:C	2.73	0.55
3:C:153[B]:LYS:NZ	12:C:2163[B]:HOH:O	1.83	0.54
1:A:466[B]:LEU:HD21	1:A:471:ARG:N	2.21	0.54
1:A:315:TYR:HB3	1:A:485:GLN:HE21	1.73	0.54
2:B:54:GLU:HA	2:B:78:ILE:HD12	1.89	0.54
4:D:1550:F43:NB	6:D:1552:COM:H22	2.23	0.54
1:A:330:PHE:CZ	5:A:1551:TP7:H71C	2.43	0.53
1:D:466[B]:LEU:HD22	1:D:471:ARG:HG3	1.90	0.53
2:E:366[B]:ILE:HD11	2:E:367[B]:TYR:CE1	2.43	0.53
1:A:229:MET:CE	2:E:367[A]:TYR:HA	2.39	0.53
1:A:105[B]:VAL:HG12	12:A:2244[B]:HOH:O	2.10	0.52
2:E:236[B]:MET:SD	3:F:248:LEU:HD11	2.49	0.52
2:E:366[B]:ILE:CG1	2:E:367[B]:TYR:CD1	2.93	0.52
2:E:196[B]:MET:HE2	2:E:374:ILE:CG2	2.32	0.52
2:B:185[B]:LEU:CD2	2:B:190:TYR:CA	2.86	0.51
2:B:362:PHE:O	2:B:368[B]:GLY:HA3	2.10	0.51
2:B:214:LEU:HB2	2:B:428:PRO:HG3	1.92	0.51
1:D:106:ILE:HB	1:D:261:ILE:HB	1.93	0.51
1:D:466[B]:LEU:HD22	1:D:471:ARG:CG	2.40	0.51
2:E:349:PHE:HZ	3:F:248:LEU:HD21	1.76	0.51
1:D:516:ASP:HA	7:D:1554:GOL:H32	1.93	0.50
1:D:443:PHE:HB2	6:D:1552:COM:O1S	2.12	0.50
1:D:466[B]:LEU:HD21	1:D:470:LEU:CA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113[A]:LEU:HD13	2:B:418:VAL:HG13	1.94	0.50
1:A:105[B]:VAL:CG1	12:A:2244[B]:HOH:O	2.59	0.50
1:D:466[B]:LEU:CD2	1:D:467:PRO:O	2.60	0.50
1:D:43:ALA:O	1:D:46:GLU:HG3	2.11	0.50
1:A:133:LEU:HA	1:A:136:VAL:HG12	1.93	0.50
2:B:58[A]:LYS:NZ	2:B:76:LEU:O	2.45	0.50
1:D:169:ASN:OD1	1:D:171:GLU:OE1	2.29	0.50
1:A:104:THR:HG21	1:A:209[B]:ARG:HH21	1.76	0.49
2:B:57:LEU:HD12	2:B:78:ILE:HD11	1.93	0.49
12:B:2334:HOH:O	1:D:253:TYR:HB3	2.12	0.49
1:D:315:TYR:HB3	1:D:485:GLN:HE21	1.77	0.49
2:E:16:ASN:HA	12:E:2013:HOH:O	2.13	0.49
4:A:1550:F43:H8B2	6:A:1552:COM:O3S	2.12	0.49
1:D:172[A]:ILE:HD12	12:D:2223:HOH:O	2.13	0.49
2:B:54:GLU:CA	2:B:78:ILE:HD12	2.43	0.48
7:D:1554:GOL:C3	12:D:2428[B]:HOH:O	2.39	0.48
3:F:178:ASN:HB2	12:F:2182:HOH:O	2.14	0.48
2:E:424:GLU:H	2:E:424:GLU:CD	2.17	0.48
1:A:466[B]:LEU:CD2	1:A:471:ARG:N	2.77	0.47
4:A:1550:F43:N5B	6:A:1552:COM:H22	2.30	0.47
2:B:369[B]:GLY:HA3	1:D:249:GLY:O	2.14	0.47
2:E:277[B]:LEU:CD1	2:E:278:GLU:N	2.72	0.47
1:A:73:GLN:HB2	1:A:80:TYR:CE2	2.50	0.46
2:B:202:ALA:HB1	2:B:416:LYS:HB2	1.97	0.46
2:B:339:GLU:HB3	3:C:237[B]:ILE:HD13	1.98	0.46
1:A:242:ALA:HB2	3:F:84:TYR:CE2	2.51	0.46
1:A:267:LEU:HD12	1:A:273:ARG:HB2	1.98	0.46
1:A:105[B]:VAL:HG13	1:A:223:THR:CG2	2.46	0.46
2:B:362:PHE:CE2	2:B:367[B]:TYR:HB3	2.51	0.46
2:E:196[B]:MET:HE3	2:E:374:ILE:HB	1.97	0.46
1:D:461:ARG:HD3	2:E:233[B]:PHE:CD1	2.49	0.46
1:A:249:GLY:HA3	12:E:2312:HOH:O	2.16	0.46
3:C:179:LYS:HG3	12:C:2185:HOH:O	2.15	0.46
2:B:95:VAL:HB	12:B:2139:HOH:O	2.15	0.45
1:A:443:PHE:HB2	6:A:1552:COM:H12	1.98	0.45
1:D:466[B]:LEU:HD23	1:D:467:PRO:O	2.16	0.45
2:E:407:SER:HB2	2:E:408:PRO:HD2	1.97	0.45
1:A:151:VAL:HG11	1:D:83:GLY:HA3	1.99	0.45
2:B:70[B]:MET:HE3	1:D:501:ASP:CB	2.45	0.45
3:F:99:TYR:CD2	3:F:116:THR:HG21	2.52	0.45
2:B:238:LEU:HD11	12:B:2378[B]:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466[B]:LEU:HD21	1:A:470:LEU:HB3	1.90	0.44
2:B:246:MET:CE	2:B:429:LEU:HD12	2.46	0.44
2:B:185[B]:LEU:HD22	2:B:190:TYR:N	2.33	0.44
3:F:117:LEU:HD22	3:F:120:ARG:HD3	1.99	0.44
1:A:253:TYR:HB2	2:E:369[B]:GLY:HA3	1.99	0.44
3:C:117:LEU:HB2	3:C:120:ARG:HG3	2.00	0.44
2:E:238:LEU:HD11	12:E:2351[B]:HOH:O	2.17	0.44
1:D:133:LEU:HA	1:D:136:VAL:HG12	2.00	0.44
1:A:352:GLU:OE2	7:A:1555:GOL:H32	2.18	0.44
2:B:274:GLU:HA	2:B:277[B]:LEU:HD12	1.44	0.44
3:C:143:PHE:CD1	3:C:148[A]:SER:HB2	2.53	0.44
1:A:119:ARG:HG3	12:E:2321:HOH:O	2.17	0.43
1:A:105[B]:VAL:HG13	1:A:223:THR:HG22	2.00	0.43
2:E:274:GLU:O	2:E:277[B]:LEU:HD12	2.17	0.43
1:A:476:PRO:HD3	2:E:165:PRO:HG2	1.99	0.43
1:A:134[B]:GLU:HG2	1:D:60:ILE:CD1	2.49	0.43
2:B:348:ASP:CG	2:B:351[A]:LYS:HE2	2.38	0.43
2:B:277[B]:LEU:HD22	12:B:2291:HOH:O	2.09	0.43
7:A:1555:GOL:H11	12:A:2007:HOH:O	2.18	0.43
1:A:229:MET:HE1	2:E:367[A]:TYR:HA	1.99	0.43
3:C:248:LEU:HD23	3:C:248:LEU:HA	1.66	0.43
1:D:193:ALA:O	1:D:197:LYS:HG3	2.19	0.43
3:C:62:PRO:HG2	3:C:67:ARG:NH2	2.34	0.43
1:A:475:TYR:HA	1:A:476:PRO:HD3	1.89	0.42
1:D:105[B]:VAL:HG13	1:D:223:THR:HG22	2.01	0.42
7:D:1555:GOL:H11	12:D:2001:HOH:O	2.19	0.42
1:D:105[B]:VAL:HG13	1:D:223:THR:CG2	2.49	0.42
1:A:140:MET:HB3	1:A:141:PRO:HD3	2.01	0.42
3:C:117:LEU:HD22	3:C:120:ARG:HD3	2.01	0.42
1:A:351:LYS:O	1:A:355:GLU:HB2	2.18	0.42
1:D:348:TYR:HB3	7:D:1555:GOL:H31	2.01	0.42
2:E:362:PHE:HE2	2:E:367[B]:TYR:HB3	1.81	0.42
2:B:164:TYR:CD1	2:B:165:PRO:HA	2.54	0.42
1:D:125:THR:HB	1:D:126:PRO:HD2	2.02	0.42
1:A:134[A]:GLU:HG2	1:D:60:ILE:HD11	2.02	0.42
1:A:348:TYR:HB3	7:A:1555:GOL:H31	2.01	0.42
1:D:332:GLN:HA	1:D:335:THR:OG1	2.19	0.42
1:D:330:PHE:CD2	1:D:482:VAL:CG1	3.03	0.42
2:B:299:LEU:HB2	3:C:248:LEU:HD22	2.01	0.42
1:D:46:GLU:HG3	1:D:47:VAL:N	2.35	0.41
2:E:422:VAL:HB	2:E:425:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LYS:HA	12:A:2226:HOH:O	2.19	0.41
3:C:82:VAL:O	3:C:83:ARG:HD2	2.21	0.41
2:B:333:TYR:HB2	3:C:106:LEU:HD22	2.03	0.41
2:E:366[B]:ILE:CD1	2:E:367[B]:TYR:CE1	3.03	0.41
1:A:332:GLN:HA	1:A:335:THR:OG1	2.19	0.41
1:A:447:ASP:HA	1:A:450:ASP:OD1	2.20	0.41
1:A:543:ARG:HD2	1:D:95:GLN:OE1	2.21	0.41
2:B:32:ASN:HA	2:B:33:PRO:HD2	1.99	0.41
3:C:191:ILE:HA	3:C:191:ILE:HD12	1.89	0.41
2:E:116:VAL:HG21	2:E:130:ALA:HA	2.03	0.41
4:A:1550:F43:C9A	4:A:1550:F43:CBA	2.99	0.40
2:E:186:GLU:HG3	2:E:378:ASN:O	2.21	0.40
3:F:19:CYS:O	3:F:21:PRO:HD3	2.21	0.40
1:A:300:PRO:HD2	12:A:2280:HOH:O	2.20	0.40
2:B:185[B]:LEU:HD22	2:B:190:TYR:H	1.87	0.40
2:B:437:ALA:O	2:B:440:LYS:HG2	2.21	0.40
3:F:11:VAL:O	3:F:15:ARG:HG3	2.21	0.40
1:A:279:GLY:HA2	1:A:473:PRO:HB2	2.03	0.40
2:B:370[B]:GLY:HA2	12:B:2334:HOH:O	2.21	0.40
1:A:350:GLY:HA3	1:A:412:SER:OG	2.22	0.40
2:E:336[B]:ASP:OD1	3:F:103:ARG:NE	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:ASP:OD2	1:D:357:LYS:NZ[2_644]	2.04	0.16

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	554/549 (101%)	535 (97%)	18 (3%)	1 (0%)	47	32
1	D	555/549 (101%)	535 (96%)	19 (3%)	1 (0%)	47	32
2	B	462/442 (104%)	444 (96%)	16 (4%)	2 (0%)	34	19
2	E	459/442 (104%)	451 (98%)	7 (2%)	1 (0%)	47	32
3	C	250/248 (101%)	243 (97%)	7 (3%)	0	100	100
3	F	250/248 (101%)	242 (97%)	8 (3%)	0	100	100
All	All	2530/2478 (102%)	2450 (97%)	75 (3%)	5 (0%)	47	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	165	PRO
2	E	165	PRO
1	D	325	SER
1	A	325	SER
2	B	402	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/434 (103%)	439 (98%)	7 (2%)	62	51
1	D	447/434 (103%)	442 (99%)	5 (1%)	73	65
2	B	359/341 (105%)	355 (99%)	4 (1%)	73	65
2	E	356/341 (104%)	351 (99%)	5 (1%)	67	56
3	C	220/216 (102%)	213 (97%)	7 (3%)	39	22
3	F	220/216 (102%)	214 (97%)	6 (3%)	44	28
All	All	2048/1982 (103%)	2014 (98%)	34 (2%)	62	48

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	15	GLU
1	A	17	SER
1	A	444	TYR
1	A	450	ASP
1	A	482	VAL
1	A	543	ARG
2	B	65	PRO
2	B	97	GLU
2	B	126	GLU
2	B	438	GLU
3	C	51[A]	SER
3	C	51[B]	SER
3	C	148[A]	SER
3	C	148[B]	SER
3	C	196	ASP
3	C	208	GLU
3	C	248	LEU
1	D	12	LYS
1	D	15	GLU
1	D	444	TYR
1	D	450	ASP
1	D	543	ARG
2	E	33	PRO
2	E	98	ASP
2	E	283	LYS
2	E	297	ASP
2	E	438	GLU
3	F	10	LYS
3	F	51[A]	SER
3	F	51[B]	SER
3	F	186	MET
3	F	196	ASP
3	F	208	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	485	GLN
1	D	42	ASN
1	D	187	GLN
1	D	365	ASN
1	D	485	GLN

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Mol	Chain	Res	Type
2	E	40	GLN
3	F	235	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	AGM	D	271	1	10,11,12	0.50	0	6,13,15	0.82	0
1	GL3	D	445	1	2,3,4	2.73	1 (50%)	1,2,4	0.20	0
1	GL3	A	445	1	2,3,4	2.71	1 (50%)	1,2,4	0.11	0
1	MHS	A	257	1	7,11,12	1.78	1 (14%)	6,14,16	0.96	0
1	SMC	A	452	1	5,6,7	1.47	1 (20%)	2,6,8	1.30	0
1	MGN	A	400	1	6,9,10	0.60	0	5,12,14	2.44	1 (20%)
1	AGM	A	271	1	10,11,12	0.69	0	6,13,15	1.54	1 (16%)
1	MHS	D	257	1	7,11,12	1.76	1 (14%)	6,14,16	0.79	0
1	MGN	D	400	1	6,9,10	0.92	0	5,12,14	2.11	1 (20%)
1	SMC	D	452	1	5,6,7	0.79	0	2,6,8	0.99	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	AGM	D	271	1	-	2/10/11/13	-
1	GL3	D	445	1	-	1/1/1/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GL3	A	445	1	-	1/1/1/2	-
1	MHS	A	257	1	-	0/5/6/8	0/1/1/1
1	SMC	A	452	1	-	1/3/5/7	-
1	MGN	A	400	1	-	0/7/9/12	-
1	AGM	A	271	1	-	2/10/11/13	-
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1
1	MGN	D	400	1	-	0/7/9/12	-
1	SMC	D	452	1	-	1/3/5/7	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	MHS	CM-ND1	4.38	1.57	1.47
1	D	257	MHS	CM-ND1	4.13	1.57	1.47
1	D	445	GL3	C-S	-3.82	1.67	1.80
1	A	445	GL3	C-S	-3.79	1.67	1.80
1	A	452	SMC	CB-SG	-3.01	1.76	1.80

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	400	MGN	CB2-CA-CB1	-5.20	101.85	111.00
1	D	400	MGN	CB2-CA-CB1	-4.27	103.48	111.00
1	A	271	AGM	NH1-CZ-NE1	2.82	125.84	119.55

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	452	SMC	CA-CB-SG-CS
1	D	452	SMC	CA-CB-SG-CS
1	D	445	GL3	S-C-CA-N
1	D	271	AGM	CE2-CD-NE1-CZ
1	A	271	AGM	CE2-CD-NE1-CZ
1	A	445	GL3	S-C-CA-N
1	D	271	AGM	NE1-CD-CG-CB
1	A	271	AGM	NE1-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 15 are monoatomic - leaving 15 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$
6	COM	D	1552	4	6,6,6	1.53	1 (16%)	7,8,8	2.99	3 (42%)
5	TP7	A	1551	-	16,20,20	2.21	7 (43%)	18,26,26	2.14	5 (27%)
7	GOL	D	1554	-	5,5,5	0.58	0	5,5,5	0.93	0
4	F43	A	1550	1,6	46,71,71	3.71	14 (30%)	48,118,118	2.54	24 (50%)
7	GOL	A	1553	-	5,5,5	0.71	0	5,5,5	1.06	0
7	GOL	D	1553	-	5,5,5	0.78	0	5,5,5	0.65	0
4	F43	D	1550	1,6	46,71,71	3.67	14 (30%)	48,118,118	2.26	23 (47%)
7	GOL	C	1249	-	5,5,5	0.59	0	5,5,5	0.62	0
7	GOL	E	1444	-	5,5,5	0.66	0	5,5,5	0.88	0
7	GOL	B	1444	-	5,5,5	0.76	0	5,5,5	1.13	0
7	GOL	A	1554	-	5,5,5	0.74	0	5,5,5	1.09	0
5	TP7	D	1551	-	16,20,20	2.18	6 (37%)	18,26,26	1.93	5 (27%)
7	GOL	D	1555	-	5,5,5	0.63	0	5,5,5	1.07	0
6	COM	A	1552	4	6,6,6	1.68	2 (33%)	7,8,8	2.30	5 (71%)
7	GOL	A	1555	-	5,5,5	0.60	0	5,5,5	1.17	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	COM	D	1552	4	-	3/4/4/4	-
5	TP7	A	1551	-	-	2/20/24/24	-
7	GOL	D	1554	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	F43	A	1550	1,6	-	1/18/185/185	-
7	GOL	A	1553	-	-	2/4/4/4	-
7	GOL	D	1553	-	-	0/4/4/4	-
4	F43	D	1550	1,6	-	1/18/185/185	-
7	GOL	C	1249	-	-	2/4/4/4	-
7	GOL	E	1444	-	-	2/4/4/4	-
7	GOL	B	1444	-	-	4/4/4/4	-
7	GOL	A	1554	-	-	2/4/4/4	-
5	TP7	D	1551	-	-	3/20/24/24	-
7	GOL	D	1555	-	-	2/4/4/4	-
6	COM	A	1552	4	-	4/4/4/4	-
7	GOL	A	1555	-	-	2/4/4/4	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1550	F43	NI-NA	19.36	2.31	1.89
4	D	1550	F43	NI-NA	13.62	2.18	1.89
4	D	1550	F43	NI-NB	11.61	2.14	1.89
4	A	1550	F43	C4A-NA	-7.55	1.37	1.49
4	D	1550	F43	NI-ND	7.40	2.05	1.89
4	D	1550	F43	C4A-NA	-6.30	1.39	1.49
4	D	1550	F43	C6D-C7D	5.83	1.58	1.50
4	A	1550	F43	NI-ND	5.76	2.01	1.89
5	A	1551	TP7	C2-C1	-5.66	1.40	1.51
4	A	1550	F43	C9D-C3D	-5.34	1.47	1.54
4	D	1550	F43	C9D-C3D	-5.10	1.47	1.54
5	D	1551	TP7	C2-C1	-5.09	1.41	1.51
4	D	1550	F43	CHA-C4D	4.98	1.58	1.53
4	A	1550	F43	C6D-C7D	4.90	1.57	1.50
4	D	1550	F43	CAA-C3A	3.98	1.61	1.53
4	D	1550	F43	C1C-NC	3.97	1.46	1.37
4	D	1550	F43	C9B-C2B	-3.91	1.46	1.54
5	D	1551	TP7	P-O4P	3.46	1.65	1.59
4	A	1550	F43	C1C-NC	3.40	1.44	1.37
5	D	1551	TP7	C1-N	3.33	1.41	1.34
6	A	1552	COM	O2S-S2	3.30	1.54	1.45
4	A	1550	F43	CAA-C3A	3.26	1.59	1.53
4	A	1550	F43	C9B-C2B	-3.20	1.47	1.54
4	D	1550	F43	C5D-C2D	-3.19	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1550	F43	C5D-C2D	-3.16	1.47	1.53
5	A	1551	TP7	C1-N	3.09	1.40	1.34
4	D	1550	F43	C2B-C3B	3.02	1.66	1.57
6	D	1552	COM	O3S-S2	3.01	1.58	1.47
5	A	1551	TP7	CB-CA	-2.73	1.47	1.53
5	D	1551	TP7	CA-N	-2.70	1.41	1.46
5	A	1551	TP7	P-O4P	2.66	1.64	1.59
5	A	1551	TP7	CA-N	-2.65	1.41	1.46
4	A	1550	F43	C2A-C3A	2.42	1.59	1.54
4	A	1550	F43	NI-NB	2.37	1.94	1.89
4	D	1550	F43	CHD-C7D	2.34	1.51	1.46
5	D	1551	TP7	CB-CA	-2.31	1.48	1.53
4	A	1550	F43	C2B-C3B	2.13	1.63	1.57
5	A	1551	TP7	O1-C1	2.11	1.27	1.23
5	D	1551	TP7	P-O3P	-2.09	1.46	1.54
6	A	1552	COM	C2-S2	2.07	1.80	1.77
5	A	1551	TP7	P-O2P	-2.07	1.46	1.54
4	A	1550	F43	CHD-C7D	2.03	1.50	1.46
4	D	1550	F43	C2A-C3A	2.02	1.58	1.54
4	A	1550	F43	CHB-C1B	2.01	1.54	1.53

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1550	F43	C4A-NA-C1A	6.82	117.23	108.97
4	D	1550	F43	O8D-C7D-C6D	-6.57	110.10	120.86
6	D	1552	COM	O1S-S2-C2	5.65	113.72	106.92
4	A	1550	F43	C3D-C4D-ND	5.12	110.30	102.34
4	D	1550	F43	O7B-C6B-N5B	-5.04	118.58	125.13
4	A	1550	F43	C2B-C1B-NB	4.50	108.57	101.84
5	D	1551	TP7	O1-C1-N	-4.47	115.40	122.95
5	A	1551	TP7	O1-C1-N	-4.42	115.48	122.95
4	A	1550	F43	O8D-C7D-C6D	-4.35	113.73	120.86
5	A	1551	TP7	C5-C6-C7	-4.26	105.50	113.09
4	D	1550	F43	CAB-C3B-C2B	-4.10	110.42	119.09
4	A	1550	F43	C3B-C4B-CHC	-4.01	114.66	123.32
4	D	1550	F43	C3D-C4D-ND	3.90	108.41	102.34
5	A	1551	TP7	C4-C3-C2	3.85	127.04	113.19
5	D	1551	TP7	C4-C3-C2	3.81	126.88	113.19
5	A	1551	TP7	O1-C1-C2	3.75	128.87	122.02
4	A	1550	F43	C4B-CHC-C1C	3.74	131.96	125.84
6	D	1552	COM	O3S-S2-O2S	-3.62	102.43	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1550	F43	C5D-C2D-C1D	3.53	115.20	110.45
6	A	1552	COM	O3S-S2-O2S	-3.35	103.08	111.27
4	A	1550	F43	O7B-C6B-C8B	-3.35	122.50	126.59
5	D	1551	TP7	C5-C6-C7	-3.30	107.22	113.09
4	A	1550	F43	O7B-C6B-N5B	-3.29	120.86	125.13
4	D	1550	F43	C3B-C4B-CHC	-3.27	116.27	123.32
4	A	1550	F43	C6D-C5D-C2D	3.14	117.81	111.46
4	D	1550	F43	C4A-NA-C1A	3.09	112.71	108.97
4	A	1550	F43	C9A-C2A-C5A	3.05	115.83	110.80
4	D	1550	F43	O7A-C6A-N8A	-3.04	114.20	122.50
4	A	1550	F43	C6D-C7D-CHD	3.03	122.64	116.95
4	A	1550	F43	C9B-C2B-C3B	2.98	120.59	112.96
4	D	1550	F43	C5D-C2D-C1D	2.93	114.40	110.45
6	A	1552	COM	O2S-S2-C2	-2.93	103.39	106.92
4	A	1550	F43	CAB-C3B-C2B	-2.87	113.02	119.09
5	A	1551	TP7	C6-C7-S7	2.85	122.10	112.96
4	A	1550	F43	C2A-C3A-C4A	-2.80	98.08	102.36
4	A	1550	F43	CAB-C3B-C4B	2.79	116.11	111.19
4	A	1550	F43	CAB-CBB-CCB	-2.75	107.67	113.59
6	D	1552	COM	C2-C1-S1	-2.67	106.33	113.10
4	D	1550	F43	CAB-C3B-C4B	2.67	115.90	111.19
4	A	1550	F43	C5C-C2C-C3C	-2.65	108.15	114.94
6	A	1552	COM	O3S-S2-C2	2.64	110.04	105.77
4	D	1550	F43	C3A-C4A-NA	2.64	106.31	102.30
4	D	1550	F43	C2B-C1B-NB	2.60	105.72	101.84
4	A	1550	F43	C8C-C3C-C4C	-2.59	103.66	112.19
4	A	1550	F43	C2B-C3B-C4B	-2.59	98.71	101.63
5	D	1551	TP7	C6-C7-S7	2.56	121.19	112.96
4	A	1550	F43	C3A-C4A-NA	2.55	106.17	102.30
4	D	1550	F43	C6D-C7D-CHD	2.53	121.70	116.95
4	D	1550	F43	C5A-C6A-N8A	2.44	124.26	116.52
4	D	1550	F43	C2A-C3A-C4A	-2.43	98.65	102.36
4	D	1550	F43	CBB-CAB-C3B	-2.39	107.77	114.69
4	A	1550	F43	C4D-ND-C1D	-2.39	105.37	108.51
4	A	1550	F43	C1C-NC-C4C	2.34	112.55	107.42
4	D	1550	F43	C9B-C2B-C3B	2.32	118.89	112.96
4	D	1550	F43	O8D-C7D-CHD	2.31	126.69	122.75
4	D	1550	F43	O7B-C6B-C8B	-2.28	123.81	126.59
5	D	1551	TP7	O3P-P-O2P	2.19	116.02	107.64
4	D	1550	F43	C2B-C3B-C4B	-2.19	99.16	101.63
4	D	1550	F43	C5C-C2C-C3C	-2.16	109.42	114.94
4	A	1550	F43	O7A-C6A-C5A	-2.12	115.29	121.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1550	F43	C6D-C5D-C2D	2.12	115.73	111.46
6	A	1552	COM	O1S-S2-C2	2.09	109.43	106.92
4	D	1550	F43	C4B-CHC-C1C	2.08	129.25	125.84
4	D	1550	F43	C8C-C3C-C4C	-2.05	105.45	112.19
6	A	1552	COM	C2-C1-S1	-2.03	107.95	113.10

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	1554	GOL	C1-C2-C3-O3
7	D	1554	GOL	O2-C2-C3-O3
6	A	1552	COM	C1-C2-S2-O1S
6	A	1552	COM	C1-C2-S2-O2S
7	A	1555	GOL	C1-C2-C3-O3
6	D	1552	COM	C1-C2-S2-O1S
6	D	1552	COM	C1-C2-S2-O2S
6	D	1552	COM	C1-C2-S2-O3S
7	E	1444	GOL	C1-C2-C3-O3
7	A	1554	GOL	O1-C1-C2-C3
7	D	1555	GOL	C1-C2-C3-O3
7	A	1553	GOL	O1-C1-C2-O2
7	A	1553	GOL	O1-C1-C2-C3
5	D	1551	TP7	C5-C6-C7-S7
7	B	1444	GOL	C1-C2-C3-O3
4	A	1550	F43	C3A-CAA-CBA-CCA
5	D	1551	TP7	C2-C3-C4-C5
7	E	1444	GOL	O2-C2-C3-O3
4	D	1550	F43	C3A-CAA-CBA-CCA
7	B	1444	GOL	O1-C1-C2-C3
5	A	1551	TP7	C2-C3-C4-C5
7	A	1555	GOL	O2-C2-C3-O3
7	A	1554	GOL	O1-C1-C2-O2
7	D	1555	GOL	O2-C2-C3-O3
7	B	1444	GOL	O2-C2-C3-O3
5	D	1551	TP7	C4-C5-C6-C7
6	A	1552	COM	S1-C1-C2-S2
6	A	1552	COM	C1-C2-S2-O3S
7	C	1249	GOL	O1-C1-C2-O2
7	C	1249	GOL	O1-C1-C2-C3
7	D	1554	GOL	O1-C1-C2-O2
7	B	1444	GOL	O1-C1-C2-O2

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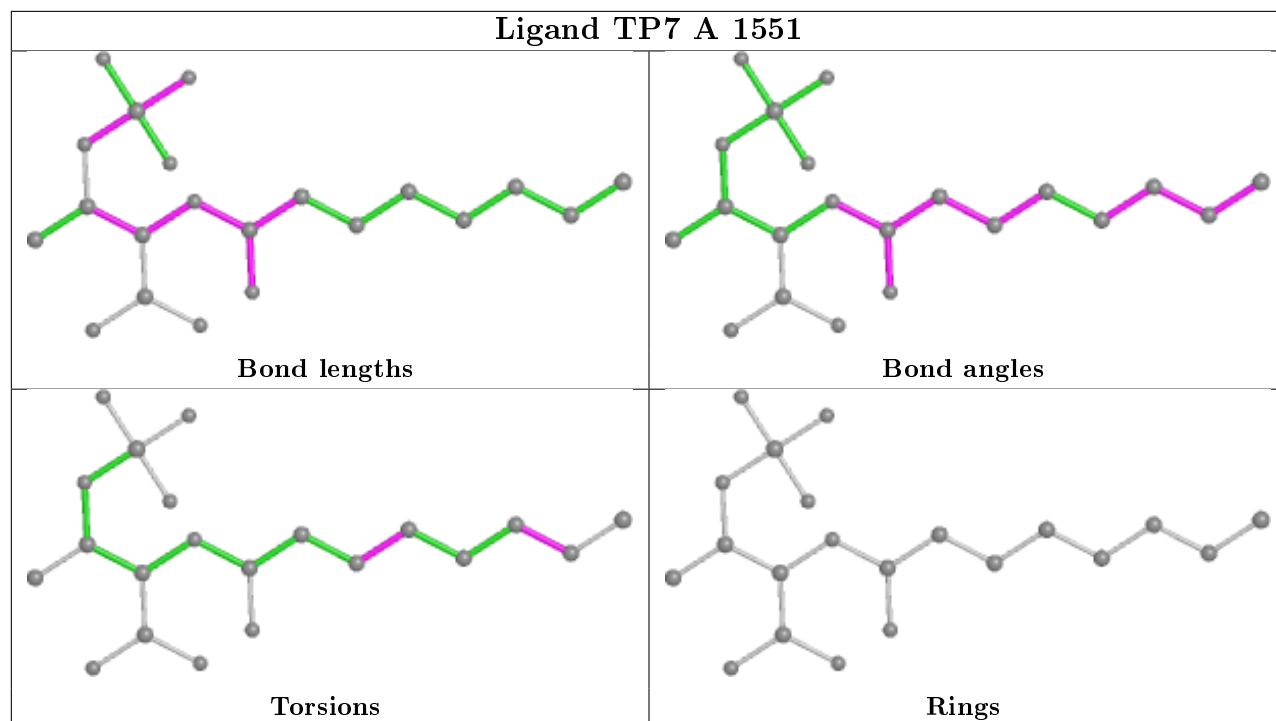
Mol	Chain	Res	Type	Atoms
5	A	1551	TP7	C5-C6-C7-S7

There are no ring outliers.

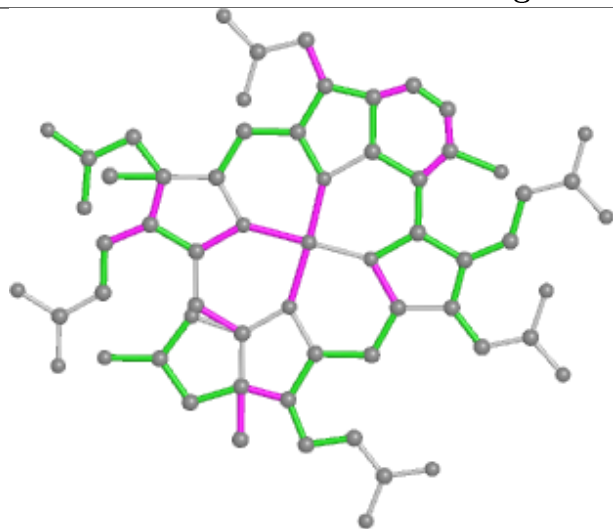
10 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1552	COM	2	0
5	A	1551	TP7	1	0
7	D	1554	GOL	7	0
4	A	1550	F43	4	0
4	D	1550	F43	2	0
7	A	1554	GOL	1	0
5	D	1551	TP7	1	0
7	D	1555	GOL	2	0
6	A	1552	COM	4	0
7	A	1555	GOL	3	0

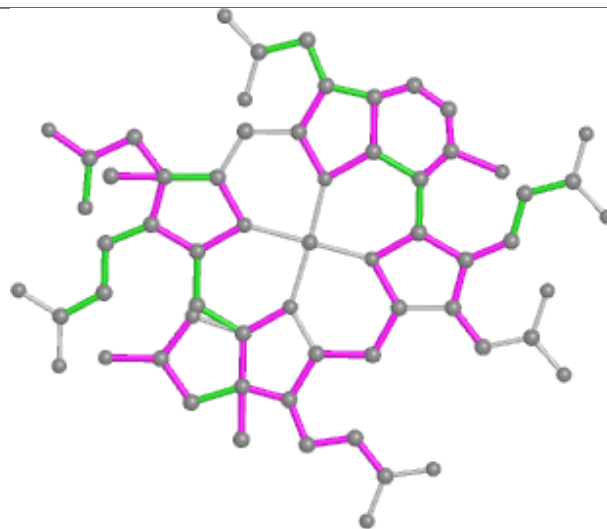
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



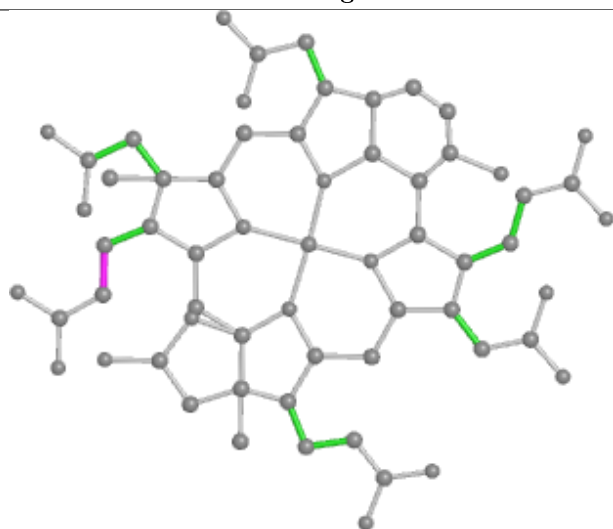
Ligand F43 A 1550



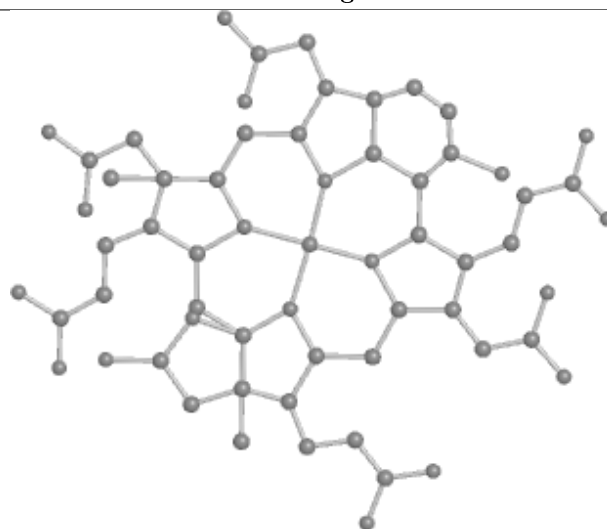
Bond lengths



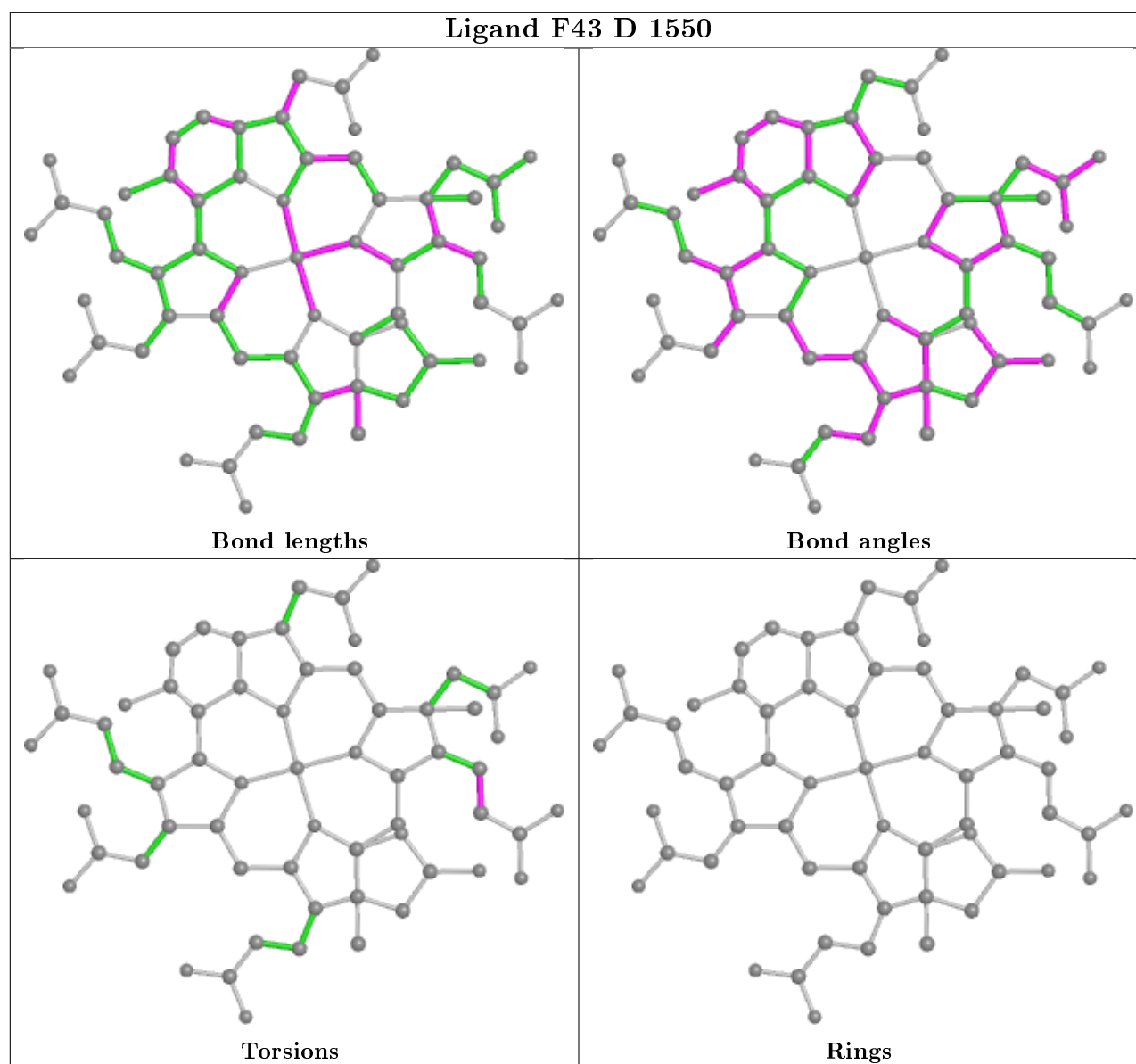
Bond angles

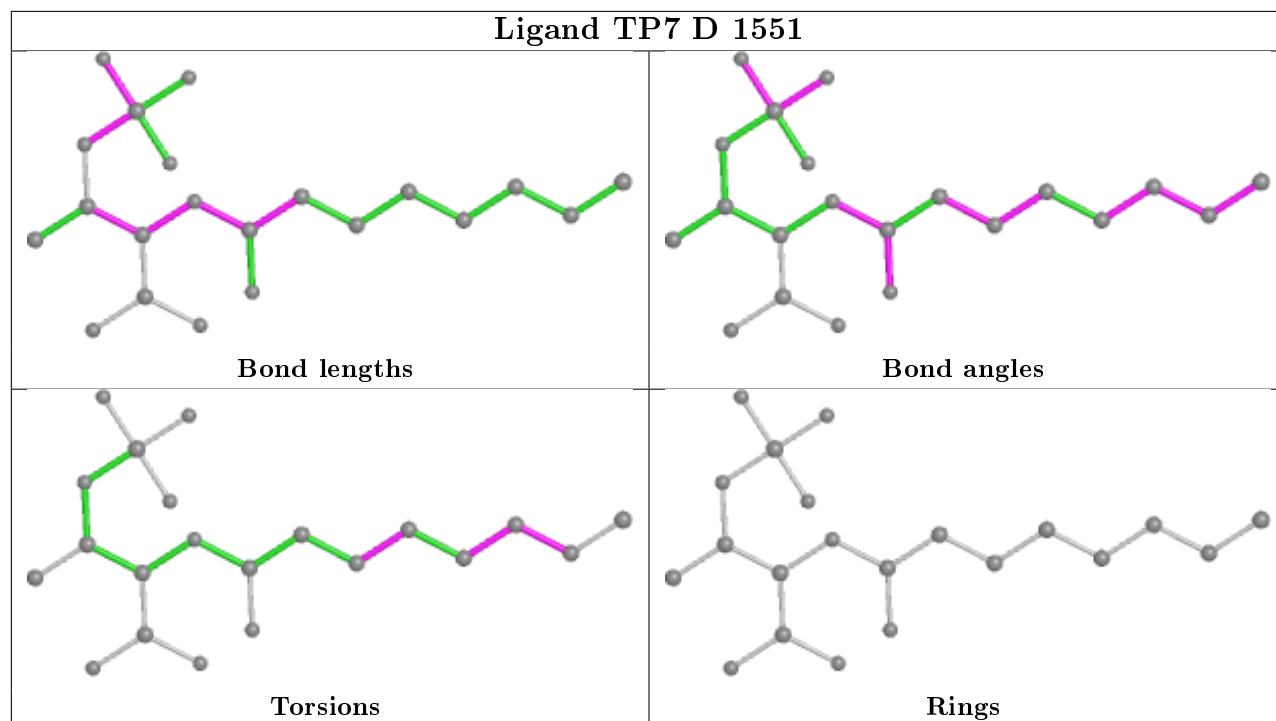


Torsions



Rings





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.