



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 01:49 am BST

PDB ID : 1HBU
Title : METHYL-COENZYME M REDUCTASE IN THE MCR-RED1-SILENT
STATE IN COMPLEX with COENZYME M
Authors : Ermler, U.; Grabarse, W.
Deposited on : 2001-04-20
Resolution : 1.90 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

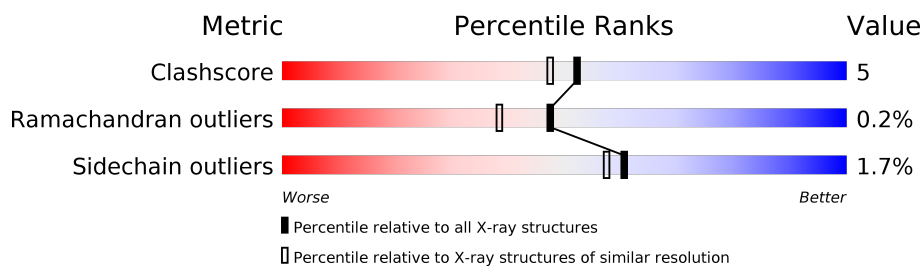
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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	85% 14% .
1	D	549	86% 13% .
2	B	442	87% 12% .
2	E	442	87% 12% .
3	C	248	81% 18% .
3	F	248	80% 16% .

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
7	GOL	B	1444	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 21670 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	24	10	0
			4284	2708	723	833	20			
1	D	548	Total	C	N	O	S	23	13	0
			4289	2710	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

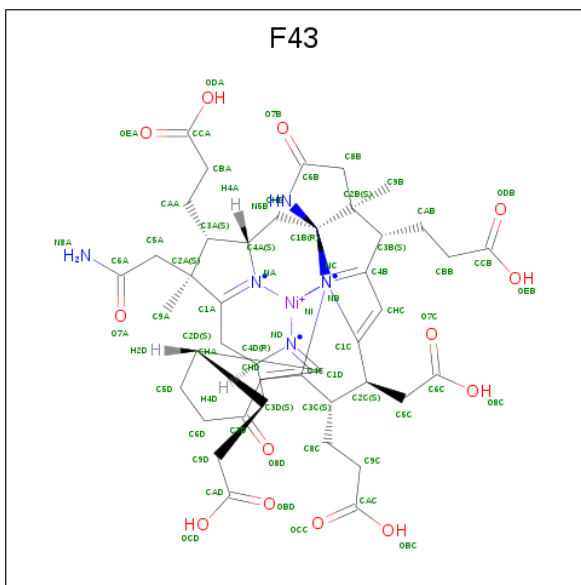
- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE I BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	26	13	0
			3344	2113	556	654	21			
2	E	442	Total	C	N	O	S	41	11	0
			3333	2108	551	653	21			

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

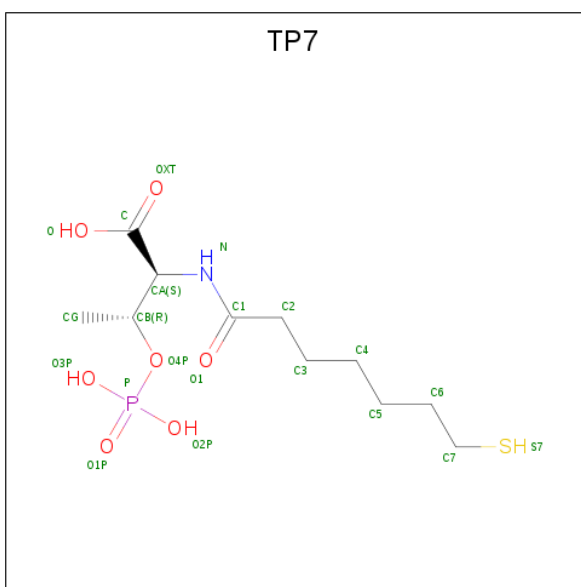
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total 2007	C 1242	N 355	O 398	S 12	39	5	0
3	F	247	Total 2006	C 1242	N 354	O 398	S 12	44	5	0

- Molecule 4 is FACTOR 430 (three-letter code: F43) (formula: $\text{C}_{42}\text{H}_{51}\text{N}_6\text{NiO}_{13}$).



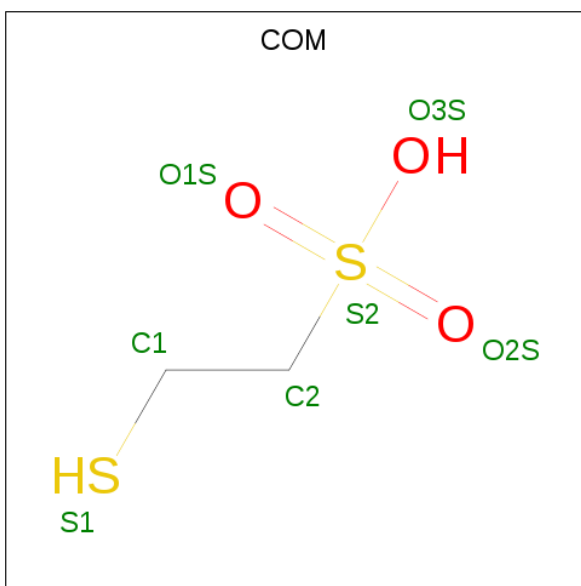
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 62	C 42	N 6	Ni 1	O 13	0	0
4	D	1	Total 62	C 42	N 6	Ni 1	O 13	0	0

- Molecule 5 is Coenzyme B (three-letter code: TP7) (formula: $\text{C}_{11}\text{H}_{22}\text{NO}_7\text{PS}$).



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	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	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 1	Zn 1	0	1

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total 1	Mg 1	0	0
9	E	3	Total 3	Mg 3	0	0
9	B	2	Total 2	Mg 2	0	0
9	C	1	Total 1	Mg 1	0	0
9	A	5	Total 5	Mg 5	0	0
9	F	1	Total 1	Mg 1	0	0

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	2	Total 2	Na 2	0	0
10	A	4	Total 4	Na 4	0	0
10	D	3	Total 3	Na 3	0	0

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

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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	444	Total 444	O 444	0	27

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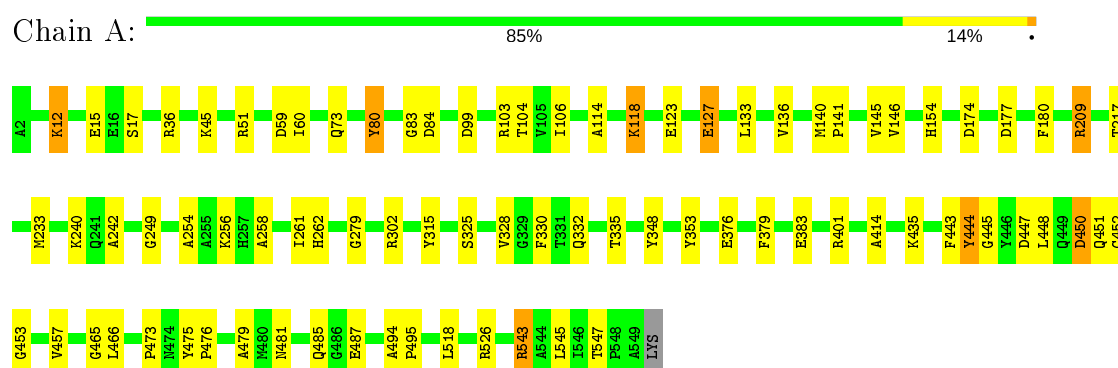
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	385	Total 385	O 385	0	23
12	C	254	Total 254	O 254	0	23
12	D	440	Total 440	O 440	0	32
12	E	360	Total 360	O 360	0	23
12	F	253	Total 253	O 253	0	13

3 Residue-property plots

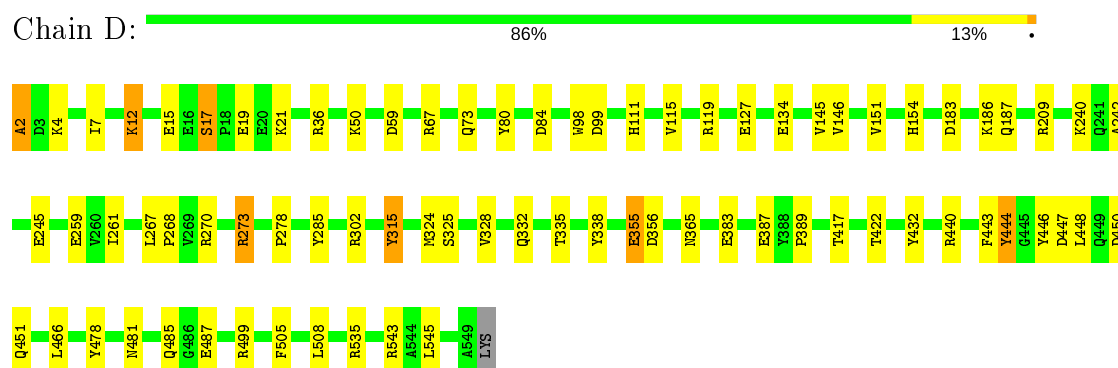
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

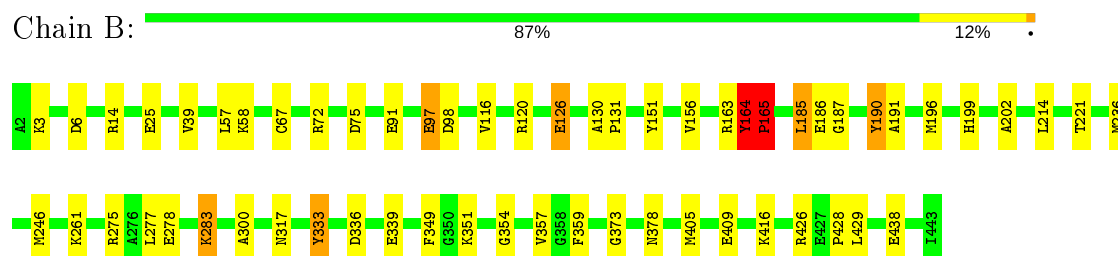
• Molecule 1: METHYL-COENZYME M REDUCTASE I ALPHA SUBUNIT




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

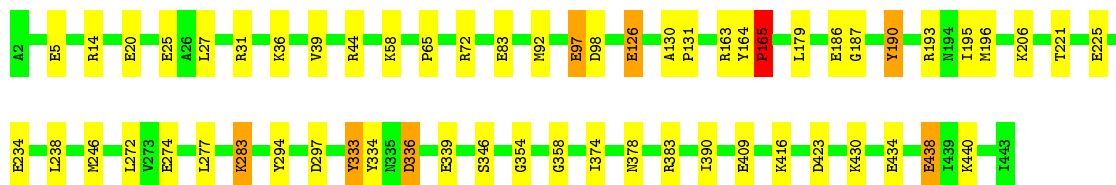


• Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT




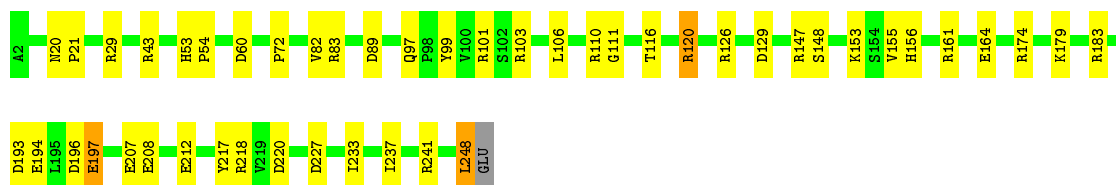
• Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT

Chain E:  87% 12% .




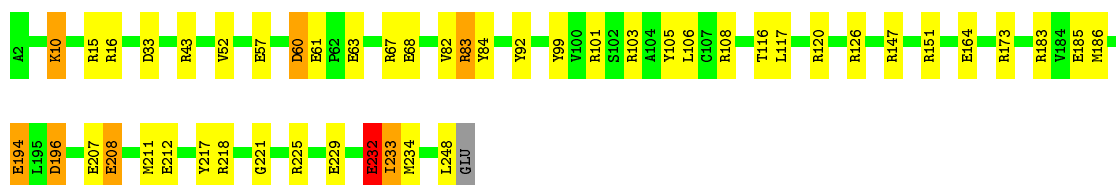
• Molecule 3: METHYL-COENZYME M REDUCTASE I GAMMA SUBUNIT

Chain C:  81% 18% .



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

Chain F:  80% 16% .



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	81.10 Å 116.50 Å 121.80 Å 90.00° 91.80° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90	Depositor
% Data completeness (in resolution range)	94.3 (10.00-1.90)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.162 , 0.211	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21670	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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	1.04	6/4389 (0.1%)	1.25	22/5956 (0.4%)
1	D	1.15	8/4410 (0.2%)	1.37	44/5984 (0.7%)
2	B	1.00	6/3476 (0.2%)	1.27	28/4703 (0.6%)
2	E	2.03	8/3447 (0.2%)	1.30	29/4666 (0.6%)
3	C	1.43	4/2072 (0.2%)	1.37	32/2790 (1.1%)
3	F	2.38	11/2070 (0.5%)	1.58	45/2789 (1.6%)
All	All	1.49	43/19864 (0.2%)	1.34	200/26888 (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	A	0	1
1	D	0	3
2	B	0	2
2	E	0	3
3	C	0	1
All	All	0	10

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	438	GLU	CG-CD	90.76	2.88	1.51
3	F	207	GLU	CG-CD	53.45	2.32	1.51
1	A	127	GLU	CG-CD	49.49	2.26	1.51
3	F	164	GLU	CB-CG	45.51	2.38	1.52
3	F	194	GLU	CB-CG	42.64	2.33	1.52
1	D	355	GLU	CG-CD	42.48	2.15	1.51
3	F	212	GLU	CB-CG	40.24	2.28	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	179	LYS	CD-CE	39.55	2.50	1.51
2	E	83	GLU	CG-CD	38.63	2.09	1.51
3	C	164	GLU	CG-CD	37.61	2.08	1.51
3	F	57	GLU	CG-CD	34.72	2.04	1.51
2	E	297	ASP	CB-CG	31.81	2.18	1.51
2	B	438	GLU	CG-CD	-31.72	1.04	1.51
2	E	274	GLU	CB-CG	31.61	2.12	1.52
3	F	208	GLU	CB-CG	31.11	2.11	1.52
2	B	91	GLU	CG-CD	28.29	1.94	1.51
1	D	50	LYS	CD-CE	-27.32	0.82	1.51
1	D	240	LYS	CE-NZ	-24.16	0.88	1.49
2	E	58	LYS	CG-CD	23.40	2.32	1.52
2	E	416	LYS	CD-CE	21.06	2.03	1.51
1	D	2	ALA	CA-C	17.43	1.98	1.52
3	C	208	GLU	CB-CG	-15.55	1.22	1.52
3	F	196	ASP	CB-CG	-14.42	1.21	1.51
2	E	20	GLU	CB-CG	13.76	1.78	1.52
1	D	186	LYS	CD-CE	13.44	1.84	1.51
1	D	12	LYS	CD-CE	10.65	1.77	1.51
2	B	97	GLU	CB-CG	10.47	1.72	1.52
3	C	212	GLU	CG-CD	-10.46	1.36	1.51
3	F	164	GLU	CG-CD	10.00	1.67	1.51
1	A	45	LYS	CE-NZ	9.98	1.74	1.49
2	E	5	GLU	CG-CD	9.72	1.66	1.51
1	D	127	GLU	CG-CD	-9.68	1.37	1.51
1	A	118	LYS	CD-CE	-9.65	1.27	1.51
3	F	232	GLU	CA-CB	8.71	1.73	1.53
2	B	278	GLU	CG-CD	-8.62	1.39	1.51
1	A	123	GLU	CB-CG	8.27	1.67	1.52
1	A	240	LYS	CE-NZ	8.16	1.69	1.49
1	A	12	LYS	CG-CD	7.17	1.76	1.52
2	B	283	LYS	CG-CD	6.78	1.75	1.52
1	D	15	GLU	CB-CG	-6.65	1.39	1.52
3	F	61	GLU	CB-CG	5.92	1.63	1.52
3	F	10	LYS	CG-CD	5.75	1.72	1.52
2	B	98	ASP	CB-CG	-5.26	1.40	1.51

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	438	GLU	CB-CG-CD	-22.34	53.90	114.20
3	F	10	LYS	CB-CG-CD	17.37	156.75	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	232	GLU	O-C-N	16.81	149.60	122.70
1	D	15	GLU	CA-CB-CG	16.76	150.27	113.40
3	F	196	ASP	CB-CG-OD1	15.76	132.48	118.30
1	D	270	ARG	NE-CZ-NH2	15.06	127.83	120.30
3	F	232	GLU	CA-C-N	-13.43	87.65	117.20
3	F	196	ASP	CB-CG-OD2	-13.37	106.26	118.30
1	D	499	ARG	NE-CZ-NH2	13.33	126.96	120.30
1	A	12	LYS	CG-CD-CE	12.87	150.50	111.90
3	F	183	ARG	NE-CZ-NH2	12.69	126.65	120.30
3	F	60	ASP	CB-CG-OD2	-12.28	107.25	118.30
2	E	58	LYS	CB-CG-CD	-12.01	80.39	111.60
2	B	98	ASP	CA-CB-CG	-11.93	87.16	113.40
3	C	208	GLU	CA-CB-CG	11.36	138.40	113.40
3	C	207	GLU	CA-CB-CG	10.81	137.18	113.40
1	D	127	GLU	CG-CD-OE1	10.53	139.36	118.30
3	C	220	ASP	CB-CG-OD2	10.26	127.53	118.30
3	C	197	GLU	CB-CG-CD	10.17	141.67	114.20
2	B	165	PRO	N-CA-CB	10.16	115.50	103.30
1	D	499	ARG	NE-CZ-NH1	-10.07	115.26	120.30
3	F	232	GLU	CB-CA-C	-9.94	90.51	110.40
1	D	440	ARG	NE-CZ-NH2	-9.89	115.35	120.30
1	D	273	ARG	NE-CZ-NH2	-9.88	115.36	120.30
3	F	232	GLU	N-CA-CB	9.84	128.31	110.60
2	E	83	GLU	CB-CG-CD	-9.81	87.71	114.20
1	D	209[A]	ARG	CD-NE-CZ	9.66	137.12	123.60
1	D	209[B]	ARG	CD-NE-CZ	9.66	137.12	123.60
2	B	165	PRO	CA-N-CD	-9.57	98.11	111.50
2	B	120	ARG	NE-CZ-NH1	-9.49	115.56	120.30
1	A	51	ARG	NE-CZ-NH1	-9.43	115.58	120.30
1	D	444	TYR	CB-CG-CD1	-9.42	115.35	121.00
3	C	179	LYS	CG-CD-CE	-9.39	83.71	111.90
3	F	10	LYS	CG-CD-CE	9.14	139.34	111.90
2	B	275	ARG	NE-CZ-NH2	9.05	124.82	120.30
2	B	426	ARG	NE-CZ-NH2	8.89	124.75	120.30
2	E	97	GLU	CG-CD-OE2	-8.87	100.57	118.30
3	F	60	ASP	CB-CG-OD1	8.87	126.28	118.30
2	B	98	ASP	CB-CG-OD1	8.84	126.26	118.30
1	D	127	GLU	CG-CD-OE2	-8.60	101.10	118.30
1	D	535	ARG	NE-CZ-NH2	8.57	124.58	120.30
2	E	44	ARG	NE-CZ-NH2	8.48	124.54	120.30
1	D	355	GLU	CG-CD-OE2	-8.39	101.51	118.30
3	F	61	GLU	CA-CB-CG	8.32	131.71	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	183	ARG	NE-CZ-NH1	-8.26	116.17	120.30
1	D	240	LYS	CD-CE-NZ	8.24	130.64	111.70
2	E	165	PRO	CA-N-CD	-8.11	100.15	111.50
2	B	409	GLU	OE1-CD-OE2	-7.99	113.71	123.30
3	C	161	ARG	NE-CZ-NH1	-7.98	116.31	120.30
3	F	67	ARG	NE-CZ-NH1	-7.91	116.34	120.30
2	E	165	PRO	N-CA-CB	7.85	112.72	103.30
2	B	438	GLU	CB-CG-CD	7.68	134.93	114.20
3	F	33	ASP	CB-CG-OD2	7.63	125.16	118.30
1	A	401	ARG	NE-CZ-NH1	7.59	124.09	120.30
2	B	336[A]	ASP	CB-CG-OD1	7.51	125.06	118.30
2	B	336[B]	ASP	CB-CG-OD1	7.51	125.06	118.30
1	D	2	ALA	N-CA-C	-7.48	90.80	111.00
2	B	359	PHE	CB-CG-CD2	7.43	126.00	120.80
3	C	89	ASP	CB-CG-OD2	7.41	124.97	118.30
1	A	80	TYR	CB-CG-CD2	-7.38	116.57	121.00
3	C	101	ARG	NE-CZ-NH2	7.35	123.97	120.30
2	B	14	ARG	NE-CZ-NH1	-7.28	116.66	120.30
1	A	487	GLU	OE1-CD-OE2	-7.20	114.66	123.30
2	E	193	ARG	NE-CZ-NH1	-7.18	116.71	120.30
3	F	232	GLU	N-CA-C	7.13	130.25	111.00
3	C	43	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	D	59	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	A	302	ARG	NE-CZ-NH1	-7.08	116.76	120.30
3	C	212	GLU	CG-CD-OE1	7.07	132.44	118.30
1	D	355	GLU	CB-CG-CD	-7.07	95.11	114.20
2	B	426	ARG	NE-CZ-NH1	-7.05	116.77	120.30
3	C	60	ASP	CB-CG-OD1	-7.04	111.96	118.30
3	F	232	GLU	OE1-CD-OE2	-7.04	114.85	123.30
1	D	444	TYR	CB-CG-CD2	7.03	125.22	121.00
3	F	43	ARG	NE-CZ-NH1	-6.97	116.81	120.30
3	C	126	ARG	NE-CZ-NH1	-6.97	116.82	120.30
2	B	275	ARG	NE-CZ-NH1	-6.95	116.82	120.30
1	D	2	ALA	CA-C-O	-6.88	105.64	120.10
3	C	207	GLU	CB-CG-CD	6.86	132.73	114.20
2	B	163	ARG	NE-CZ-NH1	-6.85	116.87	120.30
3	F	16	ARG	NE-CZ-NH2	6.79	123.70	120.30
2	B	98	ASP	CB-CG-OD2	-6.79	112.19	118.30
3	F	207	GLU	CG-CD-OE1	6.79	131.88	118.30
3	F	207	GLU	CB-CG-CD	-6.78	95.89	114.20
2	B	261	LYS	CB-CG-CD	6.66	128.91	111.60
3	C	110	ARG	NE-CZ-NH2	6.64	123.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	447	ASP	CB-CG-OD2	-6.61	112.35	118.30
2	B	278	GLU	CB-CG-CD	6.61	132.04	114.20
1	A	118	LYS	CD-CE-NZ	-6.58	96.57	111.70
3	F	151	ARG	NE-CZ-NH1	-6.57	117.02	120.30
3	F	208	GLU	CA-CB-CG	6.54	127.79	113.40
3	F	83	ARG	NE-CZ-NH2	6.54	123.57	120.30
3	C	129	ASP	CB-CG-OD1	6.54	124.18	118.30
1	D	302[A]	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	D	302[B]	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	D	183	ASP	CB-CG-OD1	6.46	124.11	118.30
3	F	126	ARG	NE-CZ-NH2	6.44	123.52	120.30
3	F	207	GLU	CG-CD-OE2	-6.39	105.52	118.30
3	F	232	GLU	CG-CD-OE1	6.34	130.97	118.30
3	C	218	ARG	NE-CZ-NH1	-6.33	117.14	120.30
2	E	333	TYR	CA-CB-CG	-6.31	101.41	113.40
1	D	273	ARG	NH1-CZ-NH2	6.31	126.34	119.40
1	D	302[A]	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	D	302[B]	ARG	NE-CZ-NH1	-6.30	117.15	120.30
2	E	92	MET	CG-SD-CE	6.25	110.20	100.20
1	D	99	ASP	CB-CG-OD2	6.22	123.90	118.30
3	F	185	GLU	OE1-CD-OE2	6.19	130.73	123.30
2	B	164	TYR	CA-C-O	-6.19	107.10	120.10
2	B	333	TYR	CA-CB-CG	-6.15	101.72	113.40
3	C	101	ARG	NE-CZ-NH1	-6.15	117.23	120.30
2	B	97	GLU	CB-CG-CD	-6.13	97.64	114.20
2	E	336[A]	ASP	CB-CG-OD1	6.07	123.77	118.30
2	E	336[B]	ASP	CB-CG-OD1	6.07	123.77	118.30
2	E	297	ASP	CA-CB-CG	-5.98	100.25	113.40
1	D	50	LYS	CD-CE-NZ	5.97	125.42	111.70
2	E	72	ARG	CD-NE-CZ	5.97	131.95	123.60
1	D	446	TYR	CB-CG-CD2	5.96	124.58	121.00
2	B	72	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	D	355	GLU	CG-CD-OE1	5.90	130.11	118.30
1	D	478	TYR	CB-CG-CD2	5.90	124.54	121.00
3	C	241	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	330	PHE	CB-CG-CD1	5.87	124.91	120.80
3	F	233	ILE	N-CA-C	-5.86	95.18	111.00
1	D	446	TYR	CB-CG-CD1	-5.85	117.49	121.00
2	E	336[A]	ASP	CB-CG-OD2	-5.85	113.04	118.30
2	E	336[B]	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	A	80	TYR	CB-CG-CD1	5.79	124.48	121.00
1	D	36	ARG	NE-CZ-NH1	-5.79	117.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	15	ARG	NE-CZ-NH1	-5.79	117.41	120.30
2	E	283	LYS	CG-CD-CE	-5.75	94.64	111.90
3	C	212	GLU	CG-CD-OE2	-5.72	106.86	118.30
2	B	190	TYR	CB-CG-CD2	-5.71	117.57	121.00
1	A	543	ARG	NE-CZ-NH2	5.66	123.13	120.30
2	E	165	PRO	N-CD-CG	5.66	111.69	103.20
1	A	36	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	209[A]	ARG	CD-NE-CZ	5.59	131.43	123.60
1	A	209[B]	ARG	CD-NE-CZ	5.59	131.43	123.60
3	C	147	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	D	119	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	D	338	TYR	CB-CG-CD1	5.55	124.33	121.00
3	C	120	ARG	CD-NE-CZ	5.55	131.37	123.60
2	E	383	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	D	270	ARG	NE-CZ-NH1	-5.54	117.53	120.30
2	E	31	ARG	NE-CZ-NH1	5.54	123.07	120.30
3	C	103	ARG	NE-CZ-NH2	5.53	123.07	120.30
1	A	84	ASP	CB-CG-OD1	-5.53	113.32	118.30
3	C	217	TYR	CA-CB-CG	5.52	123.89	113.40
3	F	63	GLU	CA-CB-CG	5.52	125.54	113.40
2	B	6	ASP	CB-CG-OD1	5.51	123.26	118.30
2	E	163	ARG	NE-CZ-NH1	-5.50	117.55	120.30
2	E	334	TYR	CB-CG-CD2	5.50	124.30	121.00
3	C	193	ASP	CB-CG-OD1	5.49	123.24	118.30
2	E	423	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	D	183	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	401	ARG	CD-NE-CZ	5.45	131.23	123.60
2	E	44	ARG	CD-NE-CZ	5.43	131.21	123.60
2	E	440	LYS	CA-CB-CG	5.42	125.33	113.40
3	F	232	GLU	CB-CG-CD	5.42	128.82	114.20
3	C	174	ARG	NE-CZ-NH2	-5.41	117.59	120.30
3	F	173	ARG	NE-CZ-NH1	-5.41	117.59	120.30
2	B	165	PRO	N-CD-CG	5.41	111.31	103.20
2	E	72	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	D	12	LYS	CD-CE-NZ	5.40	124.12	111.70
2	E	83	GLU	CG-CD-OE2	-5.39	107.52	118.30
1	A	99	ASP	CB-CG-OD1	5.38	123.14	118.30
3	F	61	GLU	CB-CG-CD	5.37	128.69	114.20
3	F	147	ARG	NE-CZ-NH1	-5.36	117.62	120.30
3	F	248	LEU	CB-CA-C	-5.36	100.01	110.20
2	B	151	TYR	CB-CG-CD2	-5.33	117.80	121.00
3	C	227	ASP	CB-CG-OD2	5.33	123.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ASP	CB-CG-OD1	5.33	123.09	118.30
1	A	240	LYS	CD-CE-NZ	5.32	123.94	111.70
2	B	190	TYR	CB-CG-CD1	5.32	124.19	121.00
2	E	190	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	A	526	ARG	NE-CZ-NH1	5.32	122.96	120.30
3	F	101	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	D	487	GLU	OE1-CD-OE2	-5.30	116.94	123.30
3	C	126	ARG	NE-CZ-NH2	5.28	122.94	120.30
3	C	29	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	127	GLU	CB-CG-CD	5.23	128.31	114.20
2	E	225	GLU	OE1-CD-OE2	-5.22	117.04	123.30
1	A	444	TYR	CB-CG-CD2	5.22	124.13	121.00
3	F	16	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	D	315	TYR	CA-CB-CG	5.20	123.28	113.40
3	C	97	GLN	CA-CB-CG	5.17	124.78	113.40
3	F	151	ARG	NH1-CZ-NH2	5.17	125.08	119.40
1	D	440	ARG	CG-CD-NE	5.15	122.62	111.80
3	F	126	ARG	NE-CZ-NH1	-5.15	117.72	120.30
3	F	196	ASP	CA-CB-CG	5.14	124.72	113.40
1	A	103	ARG	NE-CZ-NH1	5.13	122.87	120.30
3	C	212	GLU	CB-CG-CD	5.13	128.04	114.20
3	F	92	TYR	CA-CB-CG	-5.11	103.69	113.40
1	D	285	TYR	CB-CG-CD1	-5.11	117.94	121.00
3	C	183	ARG	CD-NE-CZ	5.09	130.72	123.60
1	D	67	ARG	NE-CZ-NH2	5.07	122.83	120.30
3	C	183	ARG	NE-CZ-NH2	5.05	122.82	120.30
3	F	108	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	A	118	LYS	CG-CD-CE	-5.04	96.79	111.90
3	F	105	TYR	CB-CG-CD2	5.03	124.02	121.00
3	F	217	TYR	CA-CB-CG	5.01	122.92	113.40

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	547	THR	Mainchain
2	B	164	TYR	Mainchain,Peptide
3	C	197	GLU	Sidechain
1	D	2	ALA	Mainchain,Peptide
1	D	355	GLU	Sidechain
2	E	164	TYR	Mainchain,Peptide
2	E	97	GLU	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4284	0	4085	52	0
1	D	4289	0	4091	40	0
2	B	3344	0	3329	62	0
2	E	3333	0	3320	34	0
3	C	2007	0	1937	23	0
3	F	2006	0	1937	23	0
4	A	62	0	43	4	0
4	D	62	0	43	2	0
5	A	21	0	19	4	0
5	D	21	0	19	6	0
6	A	7	0	5	3	0
6	D	7	0	5	1	0
7	A	24	0	31	5	0
7	B	6	0	8	6	0
7	C	6	0	8	0	0
7	D	24	0	31	1	0
7	E	6	0	8	1	0
8	A	1	0	0	0	0
9	A	5	0	0	0	0
9	B	2	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	3	0	0	0	0
9	F	1	0	0	0	0
10	A	4	0	0	0	0
10	B	2	0	0	0	0
10	D	3	0	0	0	0
11	B	1	0	0	0	0
11	E	1	0	0	0	0
12	A	444	0	0	5	0
12	B	385	0	0	6	0
12	C	254	0	0	2	0
12	D	440	0	0	7	0
12	E	360	0	0	6	0
12	F	253	0	0	5	0
All	All	21670	0	18919	209	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 5.

All (209) 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)
2:B:185[B]:LEU:HD22	2:B:190:TYR:CB	1.26	1.62
2:B:236[B]:MET:CE	2:B:236[B]:MET:SD	2.14	1.36
2:B:185[B]:LEU:CD2	2:B:190:TYR:CB	2.02	1.36
2:B:185[B]:LEU:HD21	2:B:190:TYR:C	1.48	1.33
3:F:232:GLU:CA	12:F:2241:HOH:O	1.75	1.27
2:B:351[B]:LYS:NZ	12:B:2332[B]:HOH:O	1.73	1.18
3:F:232:GLU:CB	12:F:2241:HOH:O	1.89	1.17
2:B:185[B]:LEU:CD2	2:B:190:TYR:HB2	1.68	1.14
2:B:277[B]:LEU:HD13	12:B:2293:HOH:O	1.48	1.13
2:B:185[B]:LEU:HD21	2:B:191:ALA:N	1.73	1.04
2:B:185[B]:LEU:HD21	2:B:190:TYR:CA	1.87	1.03
2:B:185[B]:LEU:CD2	2:B:190:TYR:C	2.26	1.03
2:B:277[B]:LEU:HD22	12:B:2136:HOH:O	1.60	1.02
5:A:1551:TP7:O2P	5:A:1551:TP7:HG2C	1.60	1.00
2:B:185[B]:LEU:HD22	2:B:190:TYR:HB3	1.40	0.99
2:B:185[B]:LEU:CD2	2:B:190:TYR:CA	2.41	0.98
3:C:153[B]:LYS:NZ	12:C:2155[B]:HOH:O	1.79	0.97
2:B:185[B]:LEU:CD2	2:B:190:TYR:HB3	1.91	0.96
1:A:466[B]:LEU:CD1	2:E:165:PRO:HD2	1.95	0.96
3:F:232:GLU:CG	12:F:2241:HOH:O	2.10	0.93
1:A:466[B]:LEU:HD12	2:E:165:PRO:HD2	1.49	0.93
1:A:262[B]:HIS:ND1	12:A:2252[B]:HOH:O	2.08	0.84
3:F:232:GLU:HA	12:F:2241:HOH:O	1.48	0.84
1:A:466[A]:LEU:HD22	2:E:165:PRO:HD2	1.60	0.81
5:D:1551:TP7:HG2C	5:D:1551:TP7:O1P	1.84	0.78
2:B:185[B]:LEU:HD22	2:B:190:TYR:HB2	0.75	0.75
1:A:256:LYS:O	7:A:1553:GOL:H31	1.88	0.73
2:B:58[A]:LYS:HE3	2:B:75:ASP:OD1	1.87	0.73
2:B:236[B]:MET:CE	2:B:236[B]:MET:CG	2.67	0.72
2:B:339:GLU:HB3	3:C:237[B]:ILE:HD13	1.72	0.72
2:B:277[B]:LEU:CD2	12:B:2136:HOH:O	2.28	0.70
7:B:1444:GOL:O3	7:B:1444:GOL:O1	1.98	0.70
2:E:206[B]:LYS:NZ	2:E:409:GLU:OE1	2.19	0.69
7:B:1444:GOL:H31	12:B:2051:HOH:O	1.92	0.69
2:E:234:GLU:HG2	12:E:2247:HOH:O	1.92	0.69
1:A:466[B]:LEU:HD11	2:E:165:PRO:HD2	1.75	0.69
2:B:236[B]:MET:HB2	3:C:248:LEU:CD1	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236[A]:MET:HB2	3:C:248:LEU:CD1	2.23	0.68
2:B:165:PRO:HD2	1:D:466[B]:LEU:CD1	2.24	0.67
1:D:187:GLN:HA	1:D:187:GLN:HE21	1.60	0.66
2:E:234:GLU:CG	12:E:2247:HOH:O	2.43	0.65
2:B:236[A]:MET:HB2	3:C:248:LEU:HD12	1.80	0.64
1:A:127:GLU:HG3	12:A:2169:HOH:O	1.97	0.63
1:D:268:PRO:HG3	12:D:2370:HOH:O	1.96	0.63
2:B:300:ALA:HB2	3:C:248:LEU:HD13	1.81	0.63
1:D:328:VAL:HB	4:D:1550:F43:H9A1	1.81	0.62
2:E:27:LEU:HD22	2:E:246[B]:MET:SD	2.39	0.62
2:B:236[B]:MET:HB2	3:C:248:LEU:HD12	1.81	0.61
2:B:25:GLU:OE1	7:B:1444:GOL:H32	2.00	0.61
1:A:328:VAL:HB	4:A:1550:F43:H9A1	1.83	0.59
2:B:236[B]:MET:CE	2:B:236[B]:MET:HG2	2.33	0.59
2:B:25:GLU:HG2	7:B:1444:GOL:H32	1.84	0.58
2:B:165:PRO:HD2	1:D:466[A]:LEU:HD22	1.86	0.58
2:E:277[B]:LEU:HD21	2:E:294:TYR:CE2	2.39	0.57
2:B:405:MET:HG3	1:D:115:VAL:HG22	1.88	0.56
1:D:261[B]:ILE:HD12	1:D:508:LEU:HD12	1.86	0.56
1:D:187:GLN:HA	1:D:187:GLN:NE2	2.21	0.55
2:B:126:GLU:HB3	2:E:126:GLU:HB3	1.89	0.55
2:B:339:GLU:HB3	3:C:237[A]:ILE:HD12	1.89	0.55
2:B:214:LEU:HB2	2:B:428:PRO:HG3	1.88	0.55
2:B:25:GLU:CG	7:B:1444:GOL:H32	2.36	0.55
3:F:229:GLU:O	3:F:232:GLU:HB2	2.07	0.55
1:D:21:LYS:HE3	12:D:2339[B]:HOH:O	2.06	0.55
1:A:466[B]:LEU:CD1	2:E:165:PRO:CD	2.79	0.54
2:E:196[B]:MET:SD	2:E:374:ILE:O	2.55	0.54
3:F:232:GLU:HB3	3:F:233:ILE:CG1	2.37	0.54
1:A:447:ASP:HA	1:A:450:ASP:OD1	2.08	0.53
2:B:3:LYS:HG3	7:B:1444:GOL:H2	1.90	0.53
1:D:315:TYR:HB3	1:D:485:GLN:HE21	1.73	0.53
1:D:387[B]:GLU:HG3	12:D:2341:HOH:O	2.09	0.53
1:D:383[A]:GLU:OE2	3:F:225:ARG:NH2	2.41	0.53
2:B:246:MET:CE	2:B:429:LEU:HD12	2.39	0.52
2:B:246:MET:HE3	2:B:429:LEU:HD12	1.91	0.52
3:C:99:TYR:CD2	3:C:116:THR:HG21	2.45	0.52
7:D:1556:GOL:H11	12:D:2001:HOH:O	2.08	0.52
1:A:451:GLN:HB2	2:B:354:GLY:HA2	1.92	0.52
3:F:232:GLU:HB3	3:F:233:ILE:CA	2.31	0.52
1:A:279:GLY:HA2	1:A:473:PRO:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:VAL:HG21	2:B:221:THR:HG21	1.90	0.52
2:E:336[B]:ASP:OD1	3:F:103:ARG:NE	2.39	0.52
1:A:465:GLY:O	1:A:466[B]:LEU:HG	2.10	0.51
1:A:73:GLN:HB2	1:A:80:TYR:CE2	2.45	0.51
7:A:1555:GOL:H12	12:A:2408:HOH:O	2.10	0.51
1:A:466[B]:LEU:HD11	2:E:165:PRO:CD	2.40	0.51
3:F:232:GLU:HB3	3:F:233:ILE:HG12	1.92	0.51
2:B:300:ALA:HB2	3:C:248:LEU:CD1	2.41	0.51
1:A:249:GLY:HA3	12:E:2316:HOH:O	2.11	0.51
2:B:202:ALA:HB1	2:B:416:LYS:HB2	1.92	0.51
2:E:430:LYS:O	2:E:434:GLU:HG3	2.10	0.51
4:A:1550:F43:C1C	6:A:1552:COM:H12	2.40	0.50
1:D:242:ALA:HB3	1:D:245:GLU:HB3	1.93	0.50
1:A:383[B]:GLU:HG3	12:A:2332:HOH:O	2.11	0.50
1:D:17:SER:OG	1:D:19:GLU:OE2	2.29	0.50
1:A:332:GLN:HA	1:A:335:THR:OG1	2.10	0.50
2:B:165:PRO:HD2	1:D:466[B]:LEU:HD11	1.94	0.49
2:E:187:GLY:O	2:E:190:TYR:HB2	2.13	0.49
2:B:186:GLU:HG3	2:B:378:ASN:O	2.13	0.49
2:B:236[B]:MET:HB2	3:C:248:LEU:HD11	1.93	0.49
2:E:179[B]:LEU:CD1	2:E:195:ILE:HD11	2.43	0.49
1:D:451:GLN:HB2	2:E:354:GLY:HA2	1.94	0.48
1:A:60:ILE:HD11	1:D:134:GLU:HG2	1.94	0.48
1:D:154:HIS:CE1	1:D:545:LEU:HD21	2.48	0.48
1:D:332:GLN:HA	1:D:335:THR:OG1	2.12	0.48
1:D:365:ASN:HD22	1:D:417:THR:HB	1.78	0.48
2:E:238:LEU:HD11	12:E:2247:HOH:O	2.14	0.48
2:E:186:GLU:HG3	2:E:378:ASN:O	2.14	0.48
5:A:1551:TP7:O2P	5:A:1551:TP7:CG	2.38	0.48
1:A:104:THR:HG21	1:A:209[B]:ARG:HH21	1.79	0.48
1:D:267:LEU:HD12	1:D:273:ARG:HB2	1.95	0.48
1:A:451:GLN:HB2	2:B:354:GLY:CA	2.43	0.48
7:A:1556:GOL:H11	12:A:2007:HOH:O	2.13	0.47
1:D:73:GLN:HB2	1:D:80:TYR:CE2	2.49	0.47
2:B:236[A]:MET:HB2	3:C:248:LEU:HD11	1.94	0.47
1:A:104:THR:CG2	1:A:209[B]:ARG:HH21	2.28	0.47
1:A:154:HIS:CE1	1:A:545:LEU:HD21	2.50	0.47
1:A:145:VAL:HG23	1:A:146:VAL:HG23	1.96	0.47
1:D:324:MET:HB3	5:D:1551:TP7:H31C	1.96	0.47
1:D:443:PHE:HB2	6:D:1552:COM:O1S	2.15	0.47
1:A:494:ALA:N	1:A:495:PRO:HD2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:ASN:O	3:C:111:GLY:HA2	2.14	0.47
5:D:1551:TP7:CG	5:D:1551:TP7:O1P	2.60	0.47
3:F:82:VAL:O	3:F:83:ARG:HD2	2.15	0.47
2:B:333:TYR:HB2	3:C:106:LEU:HD22	1.97	0.46
1:A:242:ALA:HB2	3:F:84:TYR:CE2	2.51	0.46
2:E:277[B]:LEU:HD21	2:E:294:TYR:HE2	1.81	0.46
1:A:106:ILE:HB	1:A:261:ILE:HB	1.98	0.46
5:D:1551:TP7:H42C	5:D:1551:TP7:H72C	1.43	0.46
5:D:1551:TP7:H21C	5:D:1551:TP7:H51C	1.72	0.46
1:A:414:ALA:HB1	1:A:495:PRO:HD3	1.98	0.46
1:A:473:PRO:O	1:A:479:ALA:HA	2.16	0.46
2:B:164:TYR:CD1	2:B:165:PRO:HA	2.51	0.46
1:D:481:ASN:HA	5:D:1551:TP7:S7	2.56	0.45
1:A:254:ALA:HA	1:A:258:ALA:HB3	1.98	0.45
1:A:379:PHE:O	1:A:383[B]:GLU:HG3	2.17	0.45
1:A:315:TYR:HB3	1:A:485:GLN:HE21	1.81	0.45
3:F:117:LEU:HD22	3:F:120:ARG:HD3	1.98	0.45
1:A:209[B]:ARG:CZ	1:A:518:LEU:HD21	2.46	0.44
1:A:481:ASN:HA	5:A:1551:TP7:S7	2.58	0.44
2:E:272:LEU:C	2:E:272:LEU:HD13	2.38	0.44
2:E:36:LYS:HB2	12:E:2034:HOH:O	2.16	0.44
2:E:39:VAL:HG21	2:E:221:THR:HG21	1.98	0.44
3:F:117:LEU:HB2	3:F:120:ARG:HG3	2.00	0.44
1:A:453:GLY:O	1:A:457:VAL:HG23	2.18	0.44
1:D:451:GLN:HB2	2:E:354:GLY:CA	2.48	0.44
1:A:114:ALA:HB1	1:A:118:LYS:HD2	1.99	0.44
1:A:445:GL3:HA2	2:B:357:VAL:HG12	1.99	0.44
2:E:390:ILE:HG21	12:E:2324[B]:HOH:O	2.18	0.44
1:A:443:PHE:HB2	6:A:1552:COM:O1S	2.18	0.44
1:D:356:ASP:HB3	12:D:2313:HOH:O	2.17	0.44
1:A:140:MET:HB3	1:A:141:PRO:HD3	2.00	0.43
3:C:194:GLU:HG3	12:C:2194:HOH:O	2.17	0.43
2:B:116:VAL:HG21	2:B:130:ALA:HA	1.99	0.43
2:B:67:CYS:HB3	1:D:505:PHE:CE1	2.53	0.43
2:E:374:ILE:HD12	2:E:374:ILE:C	2.39	0.43
1:A:217:THR:HG23	12:D:2132:HOH:O	2.18	0.43
3:C:155:VAL:O	3:C:156:HIS:C	2.57	0.43
1:D:154:HIS:NE2	1:D:545:LEU:HD21	2.33	0.43
2:B:349:PHE:HZ	3:C:248:LEU:HD21	1.83	0.43
1:A:348:TYR:CB	7:A:1556:GOL:H31	2.49	0.43
1:A:435:LYS:HG3	3:C:99:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:HIS:HB2	1:D:259[B]:GLU:OE2	2.18	0.43
3:F:211:MET:HE1	3:F:221:GLY:HA2	2.00	0.43
1:A:348:TYR:HB3	7:A:1556:GOL:H31	2.00	0.42
1:A:448:LEU:O	1:A:452:SMC:HCS2	2.19	0.42
1:D:98:TRP:CZ2	1:D:278:PRO:HD3	2.54	0.42
1:D:387[B]:GLU:CG	12:D:2341:HOH:O	2.67	0.42
1:D:432:TYR:HB3	3:F:234:MET:SD	2.60	0.42
2:E:130:ALA:HB3	2:E:131:PRO:CD	2.49	0.42
1:A:104:THR:HG21	1:A:209[B]:ARG:NH2	2.35	0.42
2:B:57:LEU:HD21	2:B:156:VAL:HA	2.01	0.42
2:B:185[B]:LEU:HD13	2:B:187:GLY:O	2.20	0.42
1:D:145:VAL:HG23	1:D:146:VAL:HG23	2.01	0.42
1:A:209[A]:ARG:CZ	1:A:518:LEU:HD21	2.49	0.42
2:B:130:ALA:HB3	2:B:131:PRO:CD	2.50	0.42
5:A:1551:TP7:H42C	5:A:1551:TP7:H72C	1.53	0.42
1:A:353:TYR:CE1	1:A:376:GLU:HG2	2.55	0.42
1:D:21:LYS:HG3	1:D:389:PRO:HG2	2.01	0.42
2:E:339:GLU:HG3	2:E:346:SER:HB3	2.01	0.42
2:E:333:TYR:HB2	3:F:106:LEU:HD22	2.02	0.42
3:F:232:GLU:CB	3:F:233:ILE:HG12	2.50	0.42
2:E:14:ARG:NH1	3:F:68:GLU:OE2	2.51	0.42
4:A:1550:F43:C9A	4:A:1550:F43:CBA	2.98	0.41
3:C:20:ASN:HA	3:C:21:PRO:HD3	1.91	0.41
3:C:82:VAL:O	3:C:83:ARG:HD2	2.20	0.41
3:F:52[A]:VAL:HG11	12:F:2111:HOH:O	2.21	0.41
2:B:165:PRO:HD2	1:D:466[B]:LEU:HD12	1.99	0.41
2:B:196[A]:MET:HG2	2:B:373:GLY:O	2.19	0.41
1:A:133:LEU:HA	1:A:136:VAL:HG12	2.02	0.41
2:B:185[B]:LEU:HD23	2:B:190:TYR:HB3	1.93	0.41
1:A:475:TYR:HA	1:A:476:PRO:HD3	1.99	0.41
1:D:448:LEU:HD12	2:E:358:GLY:HA3	2.03	0.41
1:A:83:GLY:HA3	1:D:151:VAL:HG11	2.00	0.41
1:D:4:LYS:HB2	1:D:7:ILE:HG12	2.03	0.41
2:E:25:GLU:OE1	7:E:1444:GOL:H12	2.21	0.41
3:F:232:GLU:HB3	3:F:233:ILE:HD13	2.03	0.41
4:A:1550:F43:CHC	6:A:1552:COM:H12	2.51	0.41
3:C:53:HIS:HB2	3:C:54:PRO:HD2	2.03	0.41
1:A:177:ASP:HB3	1:A:180:PHE:CD1	2.56	0.41
1:A:233:MET:SD	4:D:1550:F43:HBB1	2.61	0.40
1:D:365:ASN:ND2	1:D:422:THR:OG1	2.53	0.40
3:F:99:TYR:CD2	3:F:116:THR:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:333:TYR:HA	2:E:336[B]:ASP:HB3	2.03	0.40
3:C:233:ILE:HA	3:C:233:ILE:HD13	1.95	0.40
3:C:53:HIS:HB2	3:C:54:PRO:CD	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/549 (100%)	532 (97%)	18 (3%)	1 (0%)	47	38
1	D	554/549 (101%)	530 (96%)	23 (4%)	1 (0%)	47	38
2	B	454/442 (103%)	441 (97%)	12 (3%)	1 (0%)	47	38
2	E	451/442 (102%)	438 (97%)	12 (3%)	1 (0%)	47	38
3	C	250/248 (101%)	242 (97%)	8 (3%)	0	100	100
3	F	250/248 (101%)	240 (96%)	9 (4%)	1 (0%)	34	24
All	All	2510/2478 (101%)	2423 (96%)	82 (3%)	5 (0%)	47	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	165	PRO
2	B	165	PRO
3	F	232	GLU
1	A	325	SER
1	D	325	SER

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	443/434 (102%)	436 (98%)	7 (2%)	62	60
1	D	446/434 (103%)	440 (99%)	6 (1%)	69	68
2	B	355/341 (104%)	350 (99%)	5 (1%)	67	65
2	E	352/341 (103%)	347 (99%)	5 (1%)	67	65
3	C	220/216 (102%)	214 (97%)	6 (3%)	44	38
3	F	220/216 (102%)	213 (97%)	7 (3%)	39	30
All	All	2036/1982 (103%)	2000 (98%)	36 (2%)	60	55

All (36) 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	174	ASP
1	A	444	TYR
1	A	450	ASP
1	A	543	ARG
2	B	97	GLU
2	B	126	GLU
2	B	185[A]	LEU
2	B	185[B]	LEU
2	B	283	LYS
3	C	72	PRO
3	C	120	ARG
3	C	148[A]	SER
3	C	148[B]	SER
3	C	196	ASP
3	C	248	LEU
1	D	12	LYS
1	D	17	SER
1	D	84	ASP
1	D	444	TYR

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Mol	Chain	Res	Type
1	D	450	ASP
1	D	543	ARG
2	E	65	PRO
2	E	98	ASP
2	E	126	GLU
2	E	283	LYS
2	E	438	GLU
3	F	10	LYS
3	F	60	ASP
3	F	186	MET
3	F	194	GLU
3	F	196	ASP
3	F	208	GLU
3	F	232	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	485	GLN
1	D	42	ASN
1	D	111	HIS
1	D	187	GLN
1	D	365	ASN
1	D	485	GLN
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	GL3	A	445	1	2,3,4	3.31	1 (50%)	1,2,4	0.44	0
1	MHS	D	257	1	7,11,12	1.72	1 (14%)	6,14,16	1.16	1 (16%)
1	GL3	D	445	1	2,3,4	3.18	1 (50%)	1,2,4	0.44	0
1	SMC	D	452	1	5,6,7	0.78	0	2,6,8	0.88	0
1	SMC	A	452	1	5,6,7	1.26	1 (20%)	2,6,8	1.73	1 (50%)
1	MHS	A	257	1	7,11,12	1.78	1 (14%)	6,14,16	1.56	1 (16%)
1	MGN	D	400	1	6,9,10	1.00	0	5,12,14	2.48	1 (20%)
1	MGN	A	400	1	6,9,10	1.08	1 (16%)	5,12,14	2.51	1 (20%)
1	AGM	A	271	1	10,11,12	0.89	0	6,13,15	1.99	3 (50%)
1	AGM	D	271	1	10,11,12	0.79	0	6,13,15	0.52	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	GL3	A	445	1	-	1/1/1/2	-
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1
1	GL3	D	445	1	-	1/1/1/2	-
1	SMC	D	452	1	-	1/3/5/7	-
1	SMC	A	452	1	-	1/3/5/7	-
1	MHS	A	257	1	-	0/5/6/8	0/1/1/1
1	MGN	D	400	1	-	0/7/9/12	-
1	MGN	A	400	1	-	0/7/9/12	-
1	AGM	A	271	1	-	2/10/11/13	-
1	AGM	D	271	1	-	2/10/11/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	445	GL3	C-S	-4.66	1.64	1.80
1	D	445	GL3	C-S	-4.49	1.65	1.80
1	A	257	MHS	CM-ND1	4.25	1.57	1.47
1	D	257	MHS	CM-ND1	3.95	1.56	1.47
1	A	452	SMC	CB-SG	-2.37	1.77	1.80
1	A	400	MGN	CB1-CA	2.21	1.57	1.55

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	400	MGN	CB2-CA-CB1	-5.00	102.20	111.00
1	A	400	MGN	CB2-CA-CB1	-4.97	102.24	111.00
1	A	271	AGM	NE1-CZ-NH2	-2.99	115.36	120.59
1	A	271	AGM	NH1-CZ-NE1	2.59	125.33	119.55
1	A	257	MHS	CD2-NE2-CE1	2.46	109.62	105.78
1	A	452	SMC	CA-CB-SG	-2.43	110.12	114.04
1	A	271	AGM	CG-CD-NE1	-2.33	106.38	110.49
1	D	257	MHS	CB-CA-C	-2.06	107.61	111.47

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	445	GL3	1	0
1	A	452	SMC	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 42 ligands modelled in this entry, 25 are monoatomic - leaving 17 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
5	TP7	A	1551	-	16,20,20	2.21	5 (31%)	18,26,26	2.01	6 (33%)
7	GOL	D	1554	10	5,5,5	0.52	0	5,5,5	1.21	1 (20%)
7	GOL	A	1556	-	5,5,5	0.63	0	5,5,5	0.92	0
6	COM	A	1552	4	6,6,6	1.72	1 (16%)	7,8,8	1.34	1 (14%)
7	GOL	B	1444	-	5,5,5	0.81	0	5,5,5	1.30	1 (20%)
7	GOL	C	1249	-	5,5,5	0.61	0	5,5,5	0.47	0
6	COM	D	1552	4	6,6,6	1.61	1 (16%)	7,8,8	1.86	1 (14%)
7	GOL	A	1553	10	5,5,5	0.68	0	5,5,5	1.25	0
7	GOL	D	1553	-	5,5,5	0.86	0	5,5,5	0.73	0
7	GOL	D	1556	-	5,5,5	0.72	0	5,5,5	0.86	0
7	GOL	A	1554	-	5,5,5	0.64	0	5,5,5	1.01	0
5	TP7	D	1551	-	16,20,20	2.14	5 (31%)	18,26,26	1.96	5 (27%)
7	GOL	E	1444	-	5,5,5	0.62	0	5,5,5	0.87	0
7	GOL	D	1555	-	5,5,5	0.65	0	5,5,5	0.70	0
4	F43	A	1550	1,6	46,71,71	3.43	16 (34%)	48,118,118	2.57	20 (41%)
4	F43	D	1550	1,6	46,71,71	3.58	17 (36%)	48,118,118	2.15	20 (41%)
7	GOL	A	1555	-	5,5,5	0.77	0	5,5,5	0.91	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
5	TP7	A	1551	-	-	6/20/24/24	-
7	GOL	D	1554	10	-	2/4/4/4	-
7	GOL	A	1556	-	-	2/4/4/4	-
6	COM	A	1552	4	-	0/4/4/4	-
7	GOL	B	1444	-	-	2/4/4/4	-
7	GOL	C	1249	-	-	0/4/4/4	-
6	COM	D	1552	4	-	1/4/4/4	-
7	GOL	A	1553	10	-	2/4/4/4	-
7	GOL	D	1553	-	-	0/4/4/4	-
7	GOL	D	1556	-	-	4/4/4/4	-
7	GOL	A	1554	-	-	0/4/4/4	-

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

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1550	F43	NI-NA	16.80	2.25	1.89
4	D	1550	F43	NI-NB	12.35	2.16	1.89
4	D	1550	F43	NI-NA	8.88	2.08	1.89
4	D	1550	F43	NI-ND	8.65	2.08	1.89
4	D	1550	F43	C9D-C3D	-6.19	1.46	1.54
4	A	1550	F43	C4A-NA	-6.17	1.39	1.49
4	D	1550	F43	C4A-NA	-5.88	1.40	1.49
4	A	1550	F43	NI-ND	5.76	2.01	1.89
5	A	1551	TP7	C2-C1	-5.69	1.40	1.51
4	D	1550	F43	CHA-C4D	5.62	1.58	1.53
4	A	1550	F43	C9D-C3D	-5.54	1.47	1.54
4	D	1550	F43	C6D-C7D	5.17	1.57	1.50
4	D	1550	F43	C1C-NC	5.17	1.48	1.37
5	D	1551	TP7	C2-C1	-5.03	1.41	1.51
4	A	1550	F43	C6D-C7D	5.00	1.57	1.50
4	D	1550	F43	C9B-C2B	-4.85	1.44	1.54
4	A	1550	F43	CAA-C3A	4.34	1.61	1.53
4	D	1550	F43	C5D-C2D	-4.30	1.45	1.53
4	A	1550	F43	CHB-C1B	3.92	1.56	1.53
6	A	1552	COM	C2-S2	3.70	1.82	1.77
5	D	1551	TP7	P-O4P	3.36	1.65	1.59
6	D	1552	COM	C2-S2	3.36	1.82	1.77
4	A	1550	F43	C1C-NC	3.33	1.44	1.37
5	A	1551	TP7	P-O4P	3.23	1.65	1.59
4	D	1550	F43	C9A-C2A	3.16	1.60	1.54
4	D	1550	F43	CAA-C3A	3.14	1.59	1.53
5	A	1551	TP7	C1-N	2.95	1.40	1.34
5	D	1551	TP7	C1-N	2.87	1.40	1.34
4	A	1550	F43	C5D-C2D	-2.84	1.48	1.53
5	D	1551	TP7	CA-N	-2.80	1.41	1.46
4	A	1550	F43	NI-NB	2.71	1.95	1.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1550	F43	C3D-C4D	-2.70	1.48	1.53
5	D	1551	TP7	CB-CA	-2.65	1.47	1.53
5	A	1551	TP7	CA-N	-2.57	1.41	1.46
5	A	1551	TP7	CB-CA	-2.51	1.48	1.53
4	D	1550	F43	C2B-C3B	2.48	1.64	1.57
4	D	1550	F43	C4D-ND	-2.44	1.45	1.49
4	A	1550	F43	C5A-C2A	-2.41	1.48	1.56
4	A	1550	F43	C9B-C2B	-2.35	1.49	1.54
4	D	1550	F43	O7A-C6A	2.28	1.30	1.24
4	D	1550	F43	CHB-C1B	2.25	1.54	1.53
4	A	1550	F43	C5C-C2C	2.25	1.57	1.54
4	A	1550	F43	C6A-N8A	-2.17	1.25	1.32
4	A	1550	F43	CHC-C4B	2.11	1.45	1.39
4	D	1550	F43	CHD-C7D	2.01	1.50	1.46

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1550	F43	C2B-C1B-NB	5.60	110.22	101.84
4	A	1550	F43	C4A-NA-C1A	5.35	115.45	108.97
4	A	1550	F43	C5D-C2D-C1D	5.28	117.55	110.45
4	A	1550	F43	C3D-C4D-ND	5.13	110.32	102.34
4	D	1550	F43	O8D-C7D-C6D	-5.05	112.59	120.86
4	D	1550	F43	C4B-CHC-C1C	4.98	134.00	125.84
4	A	1550	F43	CAB-C3B-C4B	4.91	119.84	111.19
4	A	1550	F43	CAB-C3B-C2B	-4.67	109.21	119.09
4	A	1550	F43	C3B-C4B-CHC	-4.50	113.61	123.32
5	D	1551	TP7	CG-CB-CA	4.24	121.56	113.17
4	D	1550	F43	C5D-C2D-C1D	3.93	115.74	110.45
5	D	1551	TP7	C5-C6-C7	-3.88	106.19	113.09
4	D	1550	F43	CAB-C3B-C2B	-3.85	110.94	119.09
5	A	1551	TP7	CG-CB-CA	3.80	120.70	113.17
4	A	1550	F43	C9A-C2A-C5A	3.65	116.83	110.80
6	D	1552	COM	C2-C1-S1	-3.65	103.85	113.10
4	A	1550	F43	C5C-C2C-C3C	-3.52	105.91	114.94
4	D	1550	F43	CAB-C3B-C4B	3.33	117.06	111.19
5	A	1551	TP7	O1-C1-N	-3.32	117.35	122.95
4	D	1550	F43	C5C-C2C-C3C	-3.24	106.64	114.94
4	A	1550	F43	O7A-C6A-C5A	-3.22	111.80	121.99
4	A	1550	F43	C6D-C7D-CHD	3.17	122.91	116.95
5	A	1551	TP7	C5-C6-C7	-3.10	107.56	113.09
4	D	1550	F43	C3D-C4D-ND	3.04	107.07	102.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1550	F43	C5A-C6A-N8A	2.94	125.83	116.52
4	A	1550	F43	C2A-C3A-C4A	-2.89	97.95	102.36
4	D	1550	F43	C6D-C5D-C2D	2.89	117.28	111.46
4	D	1550	F43	O7A-C6A-N8A	-2.87	114.66	122.50
4	A	1550	F43	O8D-C7D-C6D	-2.84	116.20	120.86
5	A	1551	TP7	P-O4P-CB	-2.82	114.68	123.21
5	D	1551	TP7	O1-C1-N	-2.78	118.26	122.95
4	A	1550	F43	C4D-ND-C1D	-2.77	104.88	108.51
4	D	1550	F43	O7B-C6B-C8B	-2.60	123.42	126.59
4	D	1550	F43	C6D-C7D-CHD	2.59	121.82	116.95
4	A	1550	F43	O8D-C7D-CHD	-2.57	118.36	122.75
4	A	1550	F43	C2B-C3B-C4B	-2.51	98.80	101.63
4	D	1550	F43	CBB-CAB-C3B	-2.50	107.45	114.69
4	D	1550	F43	C3B-C4B-CHC	-2.43	118.07	123.32
4	D	1550	F43	C4D-ND-C1D	2.36	111.61	108.51
5	D	1551	TP7	C4-C3-C2	2.34	121.60	113.19
4	A	1550	F43	O7B-C6B-N5B	-2.29	122.16	125.13
4	D	1550	F43	C3A-C4A-NA	2.29	105.78	102.30
4	D	1550	F43	C2A-C3A-C4A	-2.26	98.91	102.36
4	D	1550	F43	C9A-C2A-C1A	2.23	113.36	107.65
4	D	1550	F43	C9B-C2B-C3B	2.22	118.64	112.96
5	D	1551	TP7	O4P-P-O1P	-2.19	100.93	109.39
4	D	1550	F43	C3C-C4C-NC	2.18	113.41	110.05
4	A	1550	F43	C8C-C3C-C4C	-2.17	105.04	112.19
5	A	1551	TP7	C4-C3-C2	2.17	120.97	113.19
4	A	1550	F43	C9B-C2B-C3B	2.15	118.47	112.96
4	A	1550	F43	C9B-C2B-C8B	-2.07	105.21	110.45
6	A	1552	COM	O2S-S2-O1S	2.04	120.99	113.95
7	B	1444	GOL	C3-C2-C1	-2.02	103.85	111.70
7	D	1554	GOL	O3-C3-C2	-2.01	100.54	110.20
5	A	1551	TP7	C6-C7-S7	2.00	119.39	112.96

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	1554	GOL	O2-C2-C3-O3
7	D	1556	GOL	O1-C1-C2-C3
7	D	1556	GOL	C1-C2-C3-O3
7	D	1556	GOL	O2-C2-C3-O3
7	D	1555	GOL	O1-C1-C2-C3
7	D	1555	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	A	1556	GOL	C1-C2-C3-O3
7	A	1556	GOL	O2-C2-C3-O3
7	A	1555	GOL	O1-C1-C2-C3
7	B	1444	GOL	O1-C1-C2-C3
7	A	1553	GOL	C1-C2-C3-O3
4	D	1550	F43	C3A-CAA-CBA-CCA
5	D	1551	TP7	C2-C3-C4-C5
4	A	1550	F43	C3A-CAA-CBA-CCA
7	A	1555	GOL	O1-C1-C2-O2
5	D	1551	TP7	O1-C1-N-CA
7	D	1554	GOL	C1-C2-C3-O3
5	A	1551	TP7	C2-C3-C4-C5
7	D	1555	GOL	O1-C1-C2-O2
7	D	1555	GOL	O2-C2-C3-O3
7	E	1444	GOL	O2-C2-C3-O3
7	B	1444	GOL	O1-C1-C2-O2
5	D	1551	TP7	C3-C4-C5-C6
5	A	1551	TP7	C-CA-CB-O4P
5	A	1551	TP7	C3-C4-C5-C6
7	D	1556	GOL	O1-C1-C2-O2
7	A	1553	GOL	O2-C2-C3-O3
7	E	1444	GOL	C1-C2-C3-O3
6	D	1552	COM	C1-C2-S2-O2S
5	A	1551	TP7	C4-C5-C6-C7
5	D	1551	TP7	C4-C5-C6-C7
5	A	1551	TP7	C-CA-CB-CG
7	E	1444	GOL	O1-C1-C2-C3
5	A	1551	TP7	CB-O4P-P-O3P

There are no ring outliers.

12 monomers are involved in 31 short contacts:

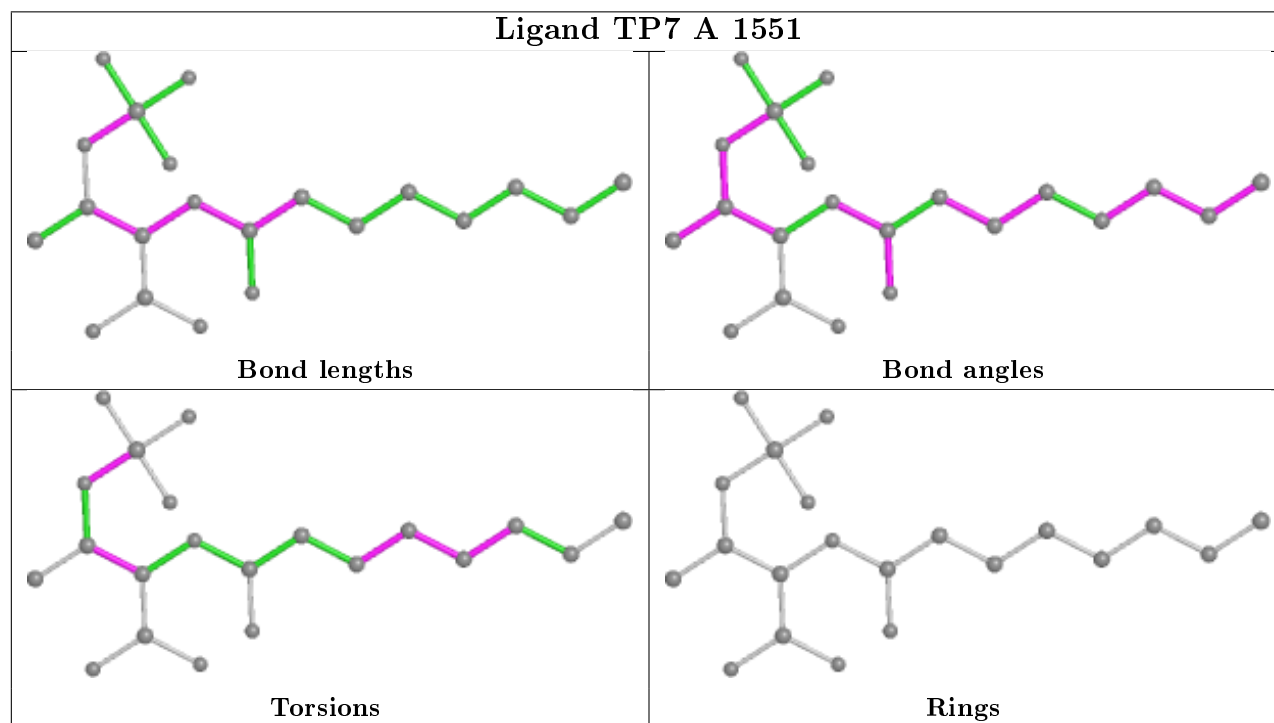
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1551	TP7	4	0
7	A	1556	GOL	3	0
6	A	1552	COM	3	0
7	B	1444	GOL	6	0
6	D	1552	COM	1	0
7	A	1553	GOL	1	0
7	D	1556	GOL	1	0
5	D	1551	TP7	6	0
7	E	1444	GOL	1	0

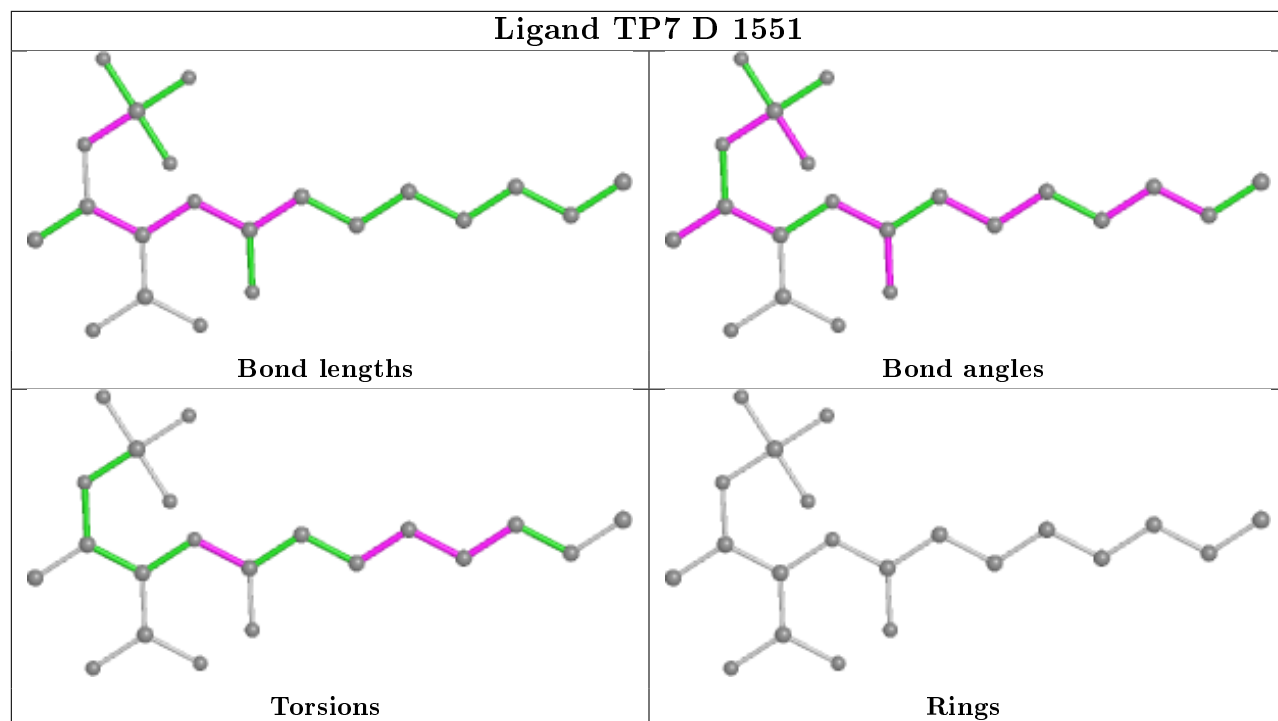
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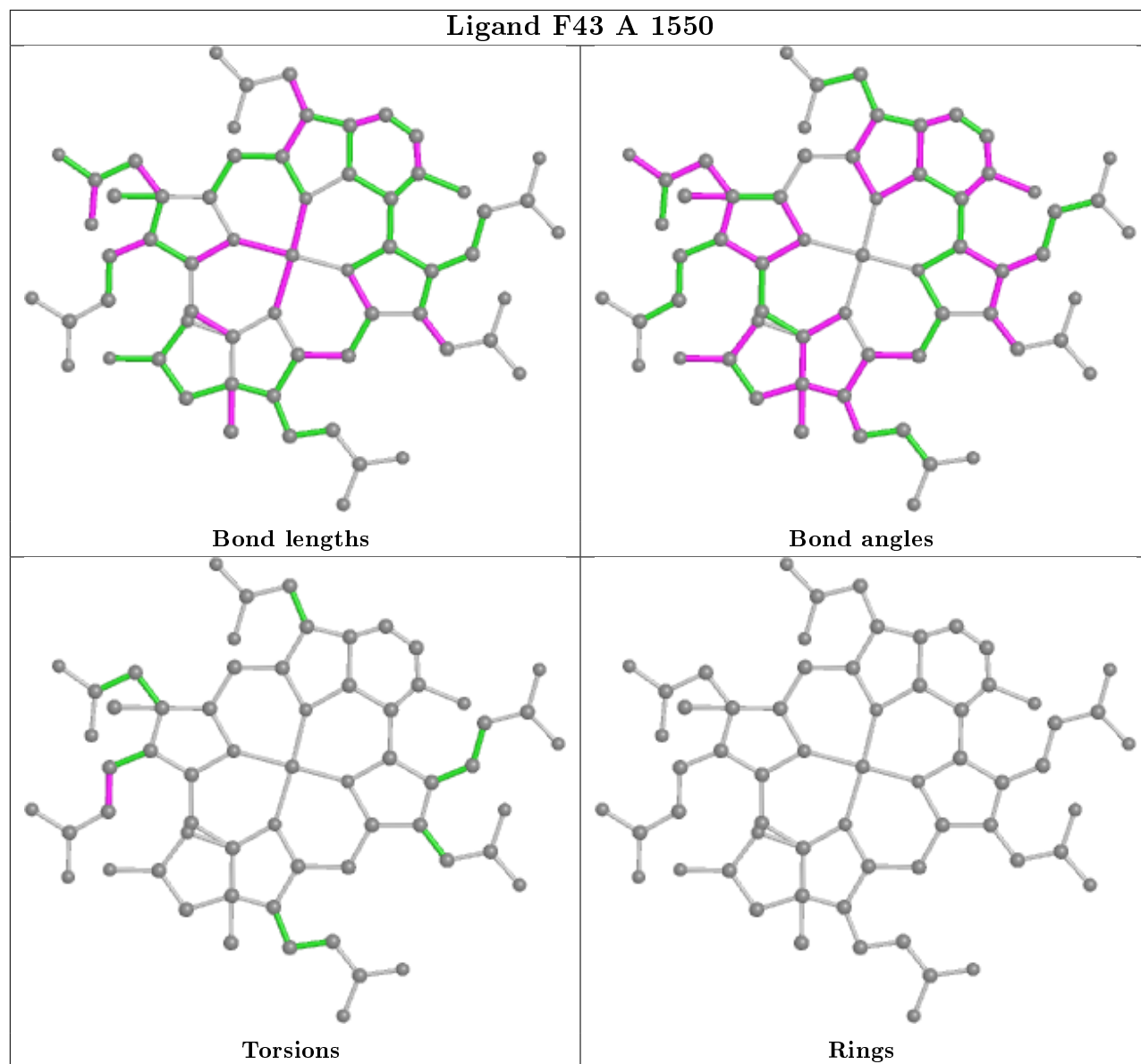
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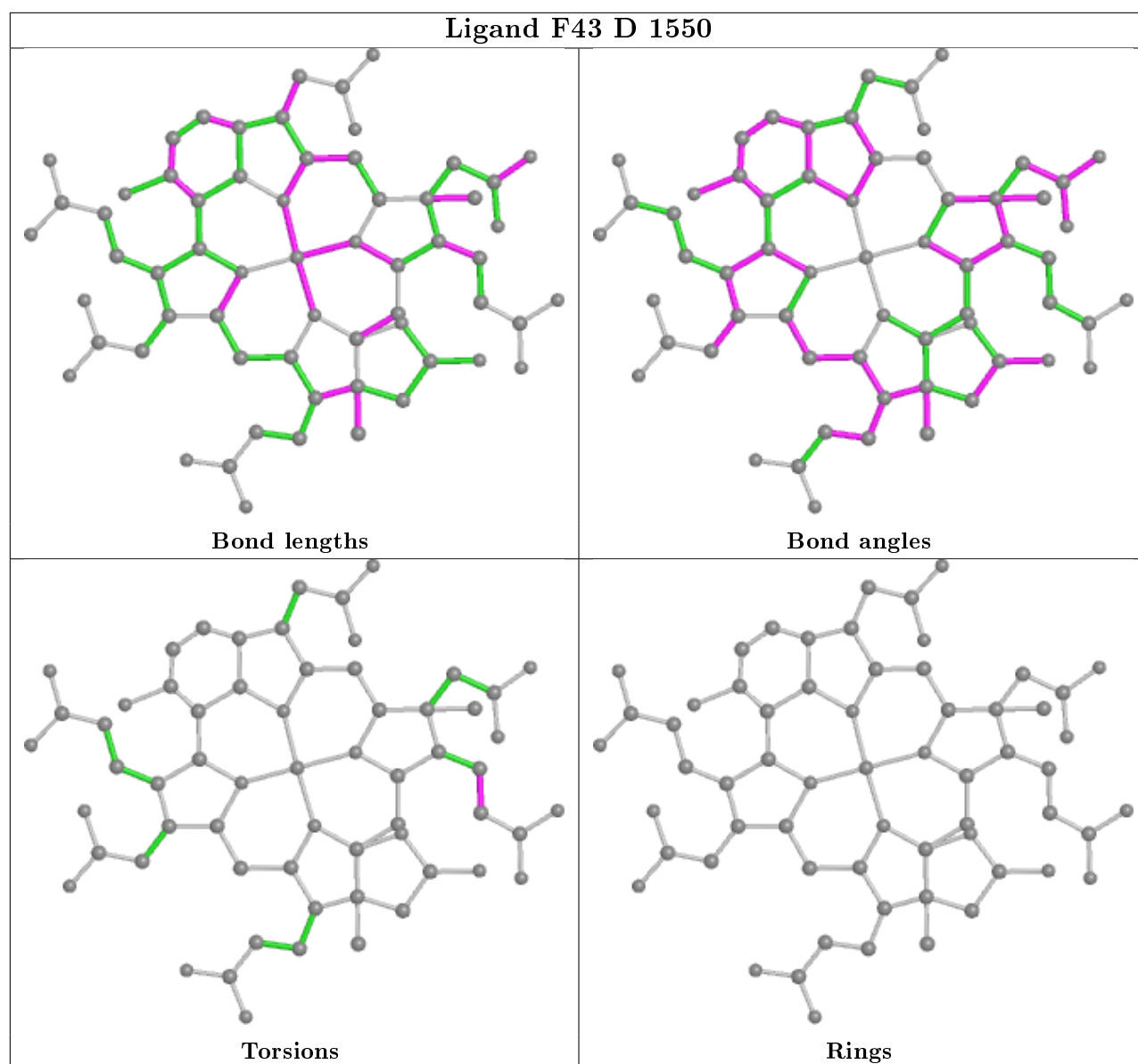
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1550	F43	4	0
4	D	1550	F43	2	0
7	A	1555	GOL	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.