



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:33 PM UTC

PDB ID : 6LLF / pdb_00006llf
Title : Biphenyl-2,2',3-triol-soaked resting complex of Oxy and Fd in carbazole
1,9a-dioxygenase
Authors : Wang, Y.X.; Suzuki-Minakuchi, C.; Nojiri, H.
Deposited on : 2019-12-23
Resolution : 1.93 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

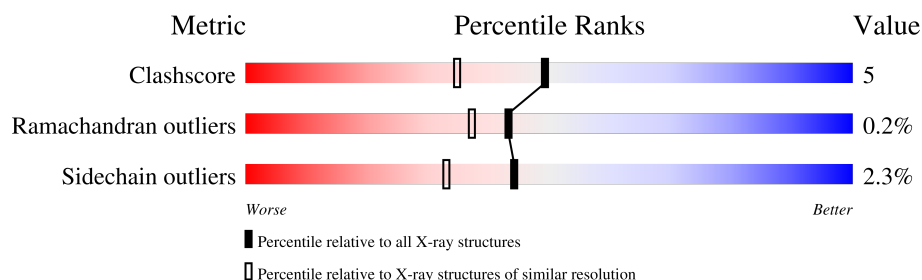
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)

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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	392	86% 13% ..
1	B	392	88% 11% .
1	C	392	89% 10% ..
2	D	115	81% 9% . 10%
2	E	115	80% 11% . 8%
2	F	115	79% 10% . 10%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDO	C	406	-	-	X	-
7	GOL	C	408	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13321 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 Terminal oxygenase component of carbazole.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	4	0
			3147	2010	537	587	13			
1	B	389	Total	C	N	O	S	0	6	0
			3168	2025	543	587	13			
1	C	388	Total	C	N	O	S	0	8	0
			3174	2029	543	589	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	385	LEU	-	expression tag	UNP Q84II6
A	386	GLU	-	expression tag	UNP Q84II6
A	387	HIS	-	expression tag	UNP Q84II6
A	388	HIS	-	expression tag	UNP Q84II6
A	389	HIS	-	expression tag	UNP Q84II6
A	390	HIS	-	expression tag	UNP Q84II6
A	391	HIS	-	expression tag	UNP Q84II6
A	392	HIS	-	expression tag	UNP Q84II6
B	385	LEU	-	expression tag	UNP Q84II6
B	386	GLU	-	expression tag	UNP Q84II6
B	387	HIS	-	expression tag	UNP Q84II6
B	388	HIS	-	expression tag	UNP Q84II6
B	389	HIS	-	expression tag	UNP Q84II6
B	390	HIS	-	expression tag	UNP Q84II6
B	391	HIS	-	expression tag	UNP Q84II6
B	392	HIS	-	expression tag	UNP Q84II6
C	385	LEU	-	expression tag	UNP Q84II6
C	386	GLU	-	expression tag	UNP Q84II6
C	387	HIS	-	expression tag	UNP Q84II6
C	388	HIS	-	expression tag	UNP Q84II6
C	389	HIS	-	expression tag	UNP Q84II6
C	390	HIS	-	expression tag	UNP Q84II6
C	391	HIS	-	expression tag	UNP Q84II6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	392	HIS	-	expression tag	UNP Q84II6

- Molecule 2 is a protein called Ferredoxin CarAc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	104	Total	C	N	O	S	0	1	0
			771	485	129	150	7			
2	E	106	Total	C	N	O	S	0	1	0
			788	496	132	153	7			
2	F	104	Total	C	N	O	S	0	2	0
			780	490	130	153	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	108	LEU	-	expression tag	UNP Q8GI16
D	109	GLU	-	expression tag	UNP Q8GI16
D	110	HIS	-	expression tag	UNP Q8GI16
D	111	HIS	-	expression tag	UNP Q8GI16
D	112	HIS	-	expression tag	UNP Q8GI16
D	113	HIS	-	expression tag	UNP Q8GI16
D	114	HIS	-	expression tag	UNP Q8GI16
D	115	HIS	-	expression tag	UNP Q8GI16
E	108	LEU	-	expression tag	UNP Q8GI16
E	109	GLU	-	expression tag	UNP Q8GI16
E	110	HIS	-	expression tag	UNP Q8GI16
E	111	HIS	-	expression tag	UNP Q8GI16
E	112	HIS	-	expression tag	UNP Q8GI16
E	113	HIS	-	expression tag	UNP Q8GI16
E	114	HIS	-	expression tag	UNP Q8GI16
E	115	HIS	-	expression tag	UNP Q8GI16
F	108	LEU	-	expression tag	UNP Q8GI16
F	109	GLU	-	expression tag	UNP Q8GI16
F	110	HIS	-	expression tag	UNP Q8GI16
F	111	HIS	-	expression tag	UNP Q8GI16
F	112	HIS	-	expression tag	UNP Q8GI16
F	113	HIS	-	expression tag	UNP Q8GI16
F	114	HIS	-	expression tag	UNP Q8GI16
F	115	HIS	-	expression tag	UNP Q8GI16

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

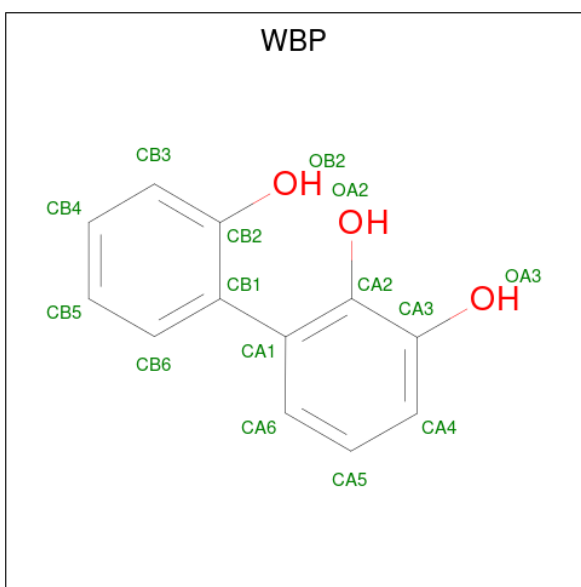


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	D	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is FE (II) ION (CCD ID: FE2) (formula: Fe).

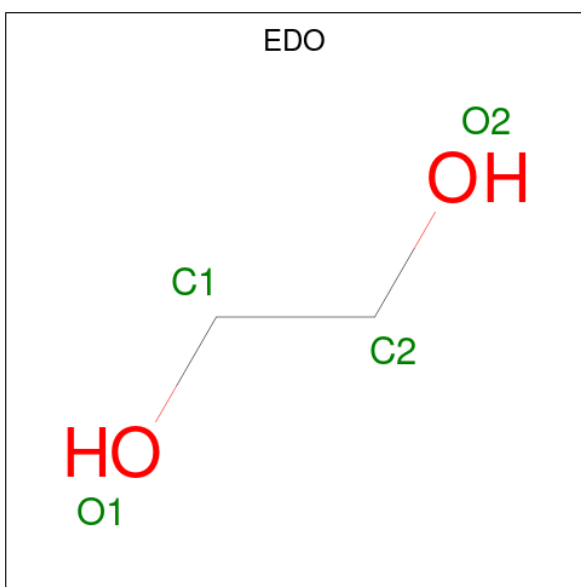
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Fe	0	0
			1	1		
4	B	1	Total	Fe	0	0
			1	1		
4	C	1	Total	Fe	0	0
			1	1		

- Molecule 5 is 3-(2-hydroxyphenyl)benzene-1,2-diol (CCD ID: WBP) (formula: C₁₂H₁₀O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	1
			30	24	6		
5	B	1	Total	C	O	0	0
			15	12	3		
5	C	1	Total	C	O	0	0
			15	12	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



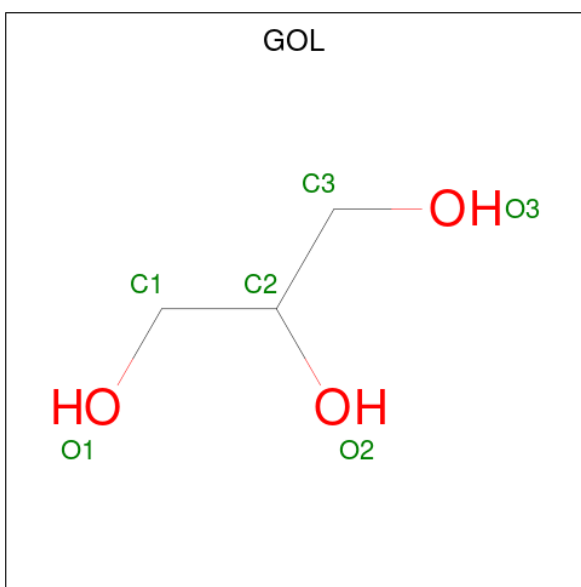
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

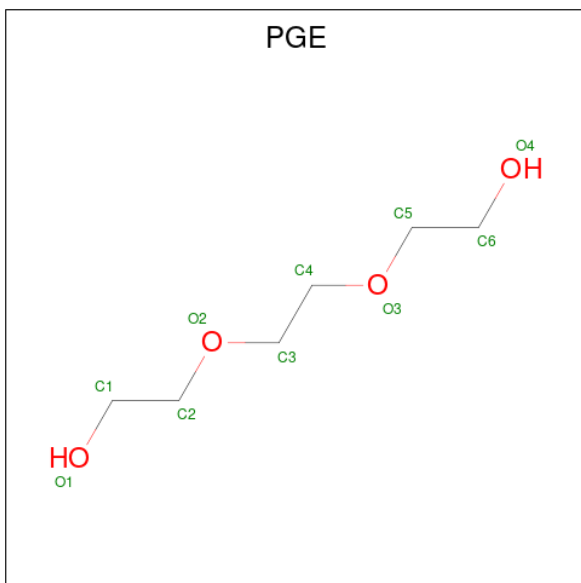
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



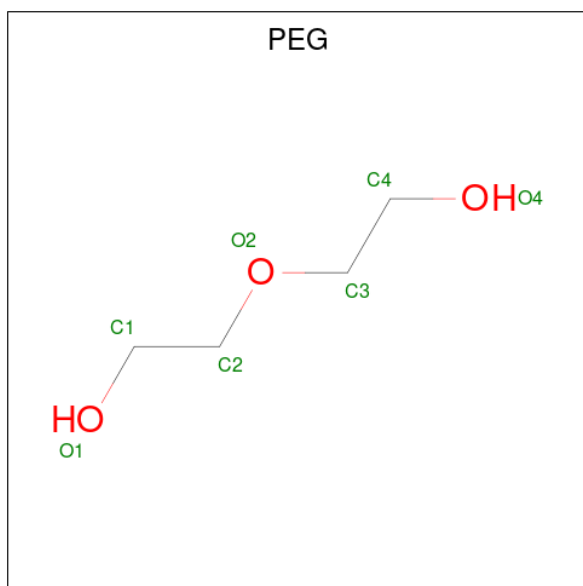
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	371	Total	O	0	0
			371	371		
10	B	378	Total	O	0	0
			378	378		
10	C	376	Total	O	0	0
			376	376		
10	D	32	Total	O	0	0
			32	32		
10	E	68	Total	O	0	0
			68	68		
10	F	72	Total	O	0	0
			72	72		

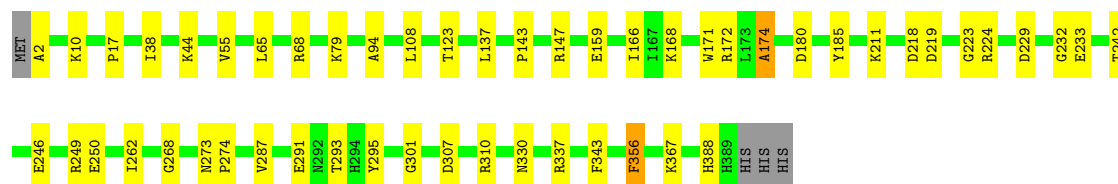
3 Residue-property plots [i](#)

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

Note EDS failed to run properly.

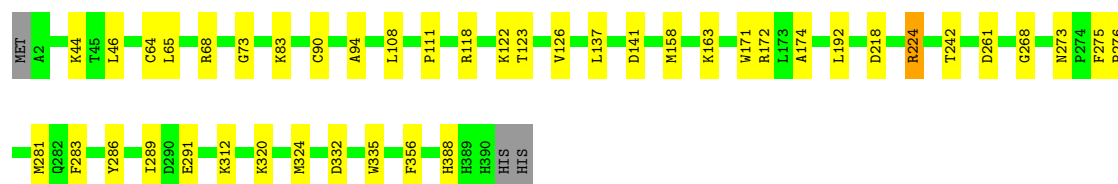
- Molecule 1: Terminal oxygenase component of carbazole

Chain A: 



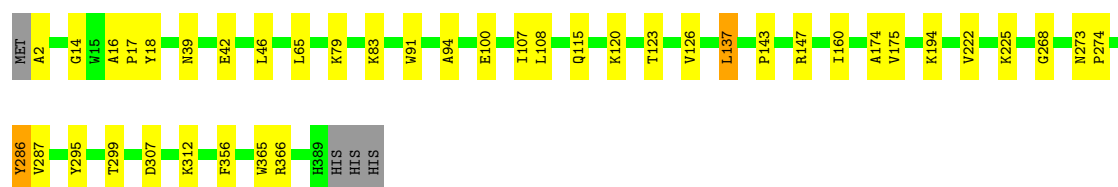
- Molecule 1: Terminal oxygenase component of carbazole

Chain B: 



- Molecule 1: Terminal oxygenase component of carbazole

Chain C: 



- Molecule 2: Ferredoxin CarAc

Chain D: 



- Molecule 2: Ferredoxin CarAc

Chain E:

80%

11%

•

8%



● Molecule 2: Ferredoxin CarAc

Chain F:

79%

10%

•

10%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.29Å 89.68Å 105.02Å 90.00° 104.08° 90.00°	Depositor
Resolution (Å)	44.88 – 1.93	Depositor
% Data completeness (in resolution range)	96.3 (44.88-1.93)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.158 , 0.200	Depositor
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.069	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13321	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FE2, FES, PEG, PGE, WBP, EDO

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	1.07	2/3246 (0.1%)	1.24	4/4406 (0.1%)
1	B	1.05	0/3276	1.24	3/4447 (0.1%)
1	C	1.07	0/3285	1.23	0/4455
2	D	1.11	0/790	1.30	2/1074 (0.2%)
2	E	1.11	0/807	1.26	0/1097
2	F	1.19	1/799 (0.1%)	1.29	0/1086
All	All	1.08	3/12203 (0.0%)	1.25	9/16565 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	48	HIS	CE1-NE2	7.82	1.40	1.32
1	A	174	ALA	C-O	5.08	1.29	1.24
1	A	17	PRO	C-O	-5.01	1.17	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	PHE	CA-CB-CG	6.48	120.28	113.80
1	B	261	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	224	ARG	CG-CD-NE	-5.42	100.08	112.00
1	A	180	ASP	CA-CB-CG	5.39	117.99	112.60
2	D	67	PHE	CA-C-O	-5.37	115.37	120.90
1	B	289	ILE	N-CA-C	-5.36	106.57	111.67
2	D	94	GLU	CB-CA-C	5.21	118.77	109.65
1	B	224	ARG	CB-CA-C	-5.20	101.34	109.70
1	A	233	GLU	CA-C-O	-5.04	115.50	120.70

There are no chirality outliers.

There are no planarity outliers.

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	3147	0	3049	32	0
1	B	3168	0	3071	33	0
1	C	3174	0	3088	28	0
2	D	771	0	750	5	0
2	E	788	0	769	11	0
2	F	780	0	755	8	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	1	0
3	F	4	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	30	0	0	3	0
5	B	15	0	0	2	0
5	C	15	0	0	3	0
6	A	24	0	36	4	0
6	B	16	0	24	6	0
6	C	16	0	24	6	0
6	D	4	0	6	1	0
6	E	4	0	6	0	0
6	F	4	0	6	0	0
7	A	12	0	16	1	0
7	B	6	0	8	0	0
7	C	6	0	8	5	0
8	A	10	0	14	3	0
9	B	7	0	10	2	0
10	A	371	0	0	10	0
10	B	378	0	0	11	0
10	C	376	0	0	8	0
10	D	32	0	0	2	0
10	E	68	0	0	1	0
10	F	72	0	0	2	0
All	All	13321	0	11640	128	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 (128) 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)
5:C:403:WBP:CA2	10:C:501:HOH:O	2.08	1.01
1:B:320:LYS:HE2	1:B:324:MET:HE1	1.48	0.91
1:B:68:ARG:HH11	6:B:405:EDO:H11	1.37	0.87
1:A:218:ASP:OD1	1:A:218:ASP:O	1.90	0.87
1:A:79:LYS:HE3	10:A:832:HOH:O	1.82	0.78
6:B:407:EDO:H21	10:B:714:HOH:O	1.82	0.77
1:B:141:ASP:OD2	10:B:501:HOH:O	2.04	0.75
2:E:3:GLN:HG2	2:E:4:ILE:H	1.51	0.74
2:F:7:LYS:HG2	2:F:101:TYR:CE2	2.24	0.72
2:E:3:GLN:NE2	10:E:301:HOH:O	2.23	0.72
6:A:406:EDO:H11	10:A:829:HOH:O	1.90	0.71
1:C:39:ASN:HB2	1:C:42[B]:GLU:CD	2.15	0.70
5:B:403:WBP:CA2	10:B:569:HOH:O	2.38	0.69
5:B:403:WBP:CA3	10:B:569:HOH:O	2.40	0.68
1:A:44:LYS:HG3	10:A:801:HOH:O	1.95	0.67
1:A:229:ASP:O	8:A:408:PGE:H4	1.97	0.65
2:F:7:LYS:HD3	2:F:101:TYR:CZ	2.32	0.65
1:C:120:LYS:H	7:C:408:GOL:H32	1.63	0.64
1:C:120:LYS:N	7:C:408:GOL:H32	2.12	0.63
2:F:7:LYS:HG2	2:F:101:TYR:CD2	2.34	0.63
1:C:120:LYS:H	7:C:408:GOL:C3	2.12	0.62
5:A:403[A]:WBP:OA2	10:A:501:HOH:O	2.11	0.62
1:B:192:LEU:HD12	1:B:324:MET:HE3	1.83	0.60
5:C:403:WBP:OA2	10:C:501:HOH:O	2.13	0.60
1:B:68:ARG:NH1	6:B:405:EDO:H11	2.14	0.59
5:C:403:WBP:CA3	10:C:501:HOH:O	2.42	0.59
1:B:320:LYS:HE2	1:B:324:MET:CE	2.29	0.59
7:C:408:GOL:H2	2:E:86:VAL:CG2	2.32	0.59
2:F:7:LYS:CG	2:F:101:TYR:CE2	2.85	0.59
1:B:291:GLU:OE2	10:B:502:HOH:O	2.17	0.58
1:A:219:ASP:OD1	1:A:223:GLY:HA2	2.03	0.57
1:C:65:LEU:HD23	1:C:123:THR:HG22	1.87	0.57
1:C:107:ILE:H	6:C:406:EDO:H12	1.70	0.57
2:E:14:MET:HE2	2:E:34:ARG:HB2	1.86	0.57
1:C:107:ILE:N	6:C:406:EDO:H12	2.20	0.56
6:D:202:EDO:C2	10:D:304:HOH:O	2.53	0.56
1:A:2:ALA:N	10:A:505:HOH:O	2.37	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:408:GOL:H2	2:E:86:VAL:HG22	1.87	0.56
5:A:403[B]:WBP:OA2	5:A:403[B]:WBP:OB2	2.24	0.55
1:C:2:ALA:CB	10:C:560:HOH:O	2.54	0.55
1:B:192:LEU:CD1	1:B:324:MET:HE3	2.38	0.54
1:C:107:ILE:H	6:C:406:EDO:C1	2.21	0.54
1:A:218:ASP:OD1	1:A:218:ASP:C	2.51	0.53
7:A:407:GOL:H12	10:A:684:HOH:O	2.08	0.53
1:C:2:ALA:HB3	10:C:560:HOH:O	2.07	0.53
1:A:232:GLY:H	8:A:408:PGE:H42	1.74	0.52
1:A:262:ILE:HD12	8:A:408:PGE:H6	1.92	0.52
1:A:168:LYS:HE2	10:A:806:HOH:O	2.08	0.52
1:B:224:ARG:NH2	10:B:518:HOH:O	2.42	0.52
1:A:38:ILE:CD1	1:A:55:VAL:HG12	2.39	0.52
1:B:68:ARG:HH11	6:B:405:EDO:C1	2.16	0.51
2:F:92:GLU:HG3	2:F:107:LYS:HE2	1.92	0.51
1:B:163:LYS:HD3	6:B:407:EDO:O2	2.11	0.51
1:A:159:GLU:CD	6:A:404:EDO:H22	2.36	0.50
1:C:83:LYS:HD3	10:C:800:HOH:O	2.11	0.50
1:C:94:ALA:HB1	1:C:108:LEU:HB2	1.93	0.49
1:C:287:VAL:HB	1:C:295:TYR:HB2	1.94	0.49
2:D:10:ALA:O	2:D:13:ASP:HB2	2.13	0.49
1:B:158:MET:HE3	1:B:281:MET:HE1	1.95	0.49
1:B:218:ASP:OD2	10:B:503:HOH:O	2.20	0.49
2:D:76:THR:OG1	10:D:301:HOH:O	2.11	0.48
1:A:68:ARG:HH11	6:A:406:EDO:C2	2.27	0.48
1:B:171:TRP:CE2	1:B:172:ARG:HG3	2.49	0.47
1:A:249:ARG:HG3	1:A:250:GLU:N	2.30	0.47
2:E:3:GLN:HG2	2:E:4:ILE:N	2.26	0.47
2:D:51:ALA:HB2	2:D:67:PHE:CG	2.50	0.47
1:A:330:ASN:HD21	5:A:403[A]:WBP:CA4	2.28	0.46
1:C:79[A]:LYS:HD3	6:C:405:EDO:H22	1.97	0.46
2:D:90:VAL:HG23	2:D:107:LYS:HG2	1.96	0.46
1:A:174:ALA:HB2	1:A:337:ARG:HD3	1.97	0.46
1:B:122:LYS:HA	6:B:409:EDO:H22	1.98	0.46
1:C:194:LYS:HB2	10:C:550:HOH:O	2.15	0.46
1:A:287:VAL:HB	1:A:295:TYR:HB2	1.98	0.45
1:B:158:MET:CE	1:B:281:MET:HE2	2.47	0.45
1:A:219:ASP:O	10:A:502:HOH:O	2.21	0.45
2:E:95:VAL:HA	2:E:99:GLU:O	2.16	0.45
1:C:225[B]:LYS:NZ	10:C:527:HOH:O	2.48	0.44
1:A:65:LEU:HD23	1:A:123:THR:HG22	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:CYS:HB2	1:B:126[A]:VAL:CG2	2.47	0.44
1:C:91:TRP:O	6:C:405:EDO:O1	2.27	0.44
1:B:320:LYS:HG2	1:B:324:MET:HE2	1.98	0.44
2:F:68:HIS:HB2	3:F:201:FES:S1	2.57	0.44
1:B:174:ALA:HB1	1:B:286:TYR:CD1	2.52	0.44
1:C:174:ALA:HB1	1:C:286:TYR:CD2	2.53	0.44
1:A:10:LYS:HG3	10:A:522:HOH:O	2.17	0.43
1:B:281:MET:HE3	1:B:283:PHE:CZ	2.52	0.43
1:C:115:GLN:HA	1:C:115:GLN:OE1	2.18	0.43
1:A:166:ILE:HG23	1:A:293[B]:THR:HG22	2.00	0.43
2:E:68:HIS:HB2	3:E:201:FES:S1	2.58	0.43
9:B:404:PEG:H41	10:B:813:HOH:O	2.18	0.43
1:A:307:ASP:OD1	1:A:310:ARG:NH1	2.51	0.43
1:B:273:ASN:OD1	1:B:281:MET:HG2	2.19	0.43
1:A:343:PHE:CG	1:B:73:GLY:HA3	2.54	0.43
1:C:175:VAL:HG11	1:C:365:TRP:CE2	2.54	0.43
1:A:143:PRO:HG3	1:A:147:ARG:CZ	2.49	0.43
1:B:332:ASP:HA	1:B:335:TRP:NE1	2.34	0.43
2:D:4:ILE:O	2:D:104:GLY:N	2.50	0.42
1:B:94:ALA:HB1	1:B:108:LEU:HB2	2.01	0.42
1:C:137:LEU:HD22	1:C:137:LEU:HA	1.93	0.42
1:A:68:ARG:HH11	6:A:406:EDO:H22	1.84	0.42
9:B:404:PEG:C4	10:B:813:HOH:O	2.68	0.42
1:C:94:ALA:CB	1:C:108:LEU:HB2	2.49	0.42
1:A:185:TYR:OH	1:B:83:LYS:HE2	2.19	0.42
1:C:143:PRO:HG3	1:C:147:ARG:CZ	2.50	0.42
1:B:158:MET:CE	1:B:281:MET:CE	2.98	0.41
1:C:18:TYR:CE2	1:C:366:ARG:HG2	2.55	0.41
1:C:14:GLY:HA3	10:F:329:HOH:O	2.20	0.41
2:F:12:SER:OG	10:F:301:HOH:O	2.21	0.41
1:B:118[B]:ARG:NE	10:B:520:HOH:O	2.46	0.41
1:B:90:CYS:O	1:B:94:ALA:HA	2.20	0.41
1:B:275:PHE:CG	1:B:276:PRO:HA	2.55	0.41
2:E:3:GLN:CG	2:E:4:ILE:H	2.28	0.41
1:B:65:LEU:HD23	1:B:123:THR:HG22	2.03	0.41
1:B:111:PRO:HG3	10:B:753:HOH:O	2.21	0.41
1:C:160:ILE:HG23	1:C:299:THR:HB	2.02	0.41
1:A:367[A]:LYS:CE	10:A:506:HOH:O	2.68	0.41
1:C:16:ALA:N	1:C:17:PRO:CD	2.84	0.41
1:A:94:ALA:HB1	1:A:108:LEU:HB2	2.03	0.41
1:A:242:THR:HA	1:A:246:GLU:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:THR:O	6:C:406:EDO:H21	2.21	0.41
1:B:281:MET:HE3	1:B:281:MET:HB2	1.85	0.41
1:C:273:ASN:HA	1:C:274:PRO:HA	1.89	0.41
2:E:19:ILE:HG21	2:E:54[A]:SER:HA	2.03	0.40
1:A:273:ASN:HA	1:A:274:PRO:HA	1.93	0.40
2:E:31:ALA:O	2:E:41:ALA:HA	2.21	0.40
1:A:159:GLU:O	1:A:301:GLY:HA2	2.22	0.40
1:A:171:TRP:CE2	1:A:172:ARG:HG3	2.56	0.40
2:F:8:VAL:CG2	2:F:102:VAL:HG12	2.50	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	390/392 (100%)	370 (95%)	19 (5%)	1 (0%)	36	30
1	B	393/392 (100%)	375 (95%)	17 (4%)	1 (0%)	36	30
1	C	394/392 (100%)	373 (95%)	20 (5%)	1 (0%)	36	30
2	D	103/115 (90%)	99 (96%)	4 (4%)	0	100	100
2	E	105/115 (91%)	103 (98%)	2 (2%)	0	100	100
2	F	104/115 (90%)	100 (96%)	4 (4%)	0	100	100
All	All	1489/1521 (98%)	1420 (95%)	66 (4%)	3 (0%)	43	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	GLY
1	A	268	GLY
1	C	268	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	339/339 (100%)	333 (98%)	6 (2%)	51	43
1	B	342/339 (101%)	336 (98%)	6 (2%)	51	43
1	C	343/339 (101%)	334 (97%)	9 (3%)	40	28
2	D	83/93 (89%)	82 (99%)	1 (1%)	63	57
2	E	85/93 (91%)	82 (96%)	3 (4%)	32	18
2	F	84/93 (90%)	79 (94%)	5 (6%)	17	5
All	All	1276/1296 (98%)	1246 (98%)	30 (2%)	44	31

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LEU
1	A	211	LYS
1	A	291[A]	GLU
1	A	291[B]	GLU
1	A	356	PHE
1	A	388	HIS
1	B	44	LYS
1	B	46	LEU
1	B	137	LEU
1	B	312	LYS
1	B	356	PHE
1	B	388	HIS
1	C	46	LEU
1	C	100	GLU
1	C	126	VAL
1	C	137	LEU
1	C	222	VAL
1	C	286	TYR
1	C	307	ASP
1	C	312	LYS
1	C	356	PHE
2	D	6	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	6	LEU
2	E	19	ILE
2	E	107	LYS
2	F	6	LEU
2	F	7	LYS
2	F	19	ILE
2	F	93	VAL
2	F	105	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	213	GLN
1	A	282	GLN
1	A	330	ASN
1	B	119	GLN
1	B	127	GLN
1	B	213	GLN
1	B	282	GLN
1	B	298	GLN
1	B	330	ASN
1	B	388	HIS
1	B	389	HIS
1	C	127	GLN
1	C	177	ASN
1	C	213	GLN
1	C	388	HIS
2	D	15	GLN
2	F	38	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 3 are monoatomic - leaving 33 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	EDO	A	406	-	3,3,3	0.25	0	2,2,2	0.26	0
9	PEG	B	404	-	6,6,6	0.19	0	5,5,5	0.43	0
6	EDO	A	411	-	3,3,3	0.18	0	2,2,2	0.18	0
6	EDO	A	409	-	3,3,3	0.13	0	2,2,2	0.25	0
6	EDO	B	405	-	3,3,3	0.35	0	2,2,2	0.11	0
6	EDO	C	407	-	3,3,3	0.16	0	2,2,2	0.26	0
3	FES	D	201	2	0,4,4	-	-	-		
3	FES	E	201	2	0,4,4	-	-	-		
6	EDO	E	202	-	3,3,3	0.17	0	2,2,2	0.27	0
7	GOL	B	406	-	5,5,5	0.10	0	5,5,5	0.21	0
6	EDO	A	405	-	3,3,3	0.11	0	2,2,2	0.10	0
6	EDO	A	410	-	3,3,3	0.12	0	2,2,2	0.19	0
6	EDO	B	407	-	3,3,3	0.39	0	2,2,2	0.28	0
6	EDO	B	408	-	3,3,3	0.05	0	2,2,2	0.36	0
6	EDO	A	404	-	3,3,3	0.29	0	2,2,2	0.62	0
7	GOL	A	407	-	5,5,5	0.11	0	5,5,5	0.37	0
5	WBP	C	403	-	16,16,16	2.74	3 (18%)	22,22,22	0.97	1 (4%)
7	GOL	C	408	-	5,5,5	0.21	0	5,5,5	0.66	0
6	EDO	F	202	-	3,3,3	0.12	0	2,2,2	0.18	0
7	GOL	A	412	-	5,5,5	0.12	0	5,5,5	0.31	0
5	WBP	B	403	-	16,16,16	2.85	3 (18%)	22,22,22	0.90	2 (9%)
6	EDO	D	202	-	3,3,3	0.36	0	2,2,2	0.15	0
6	EDO	C	406	-	3,3,3	0.65	0	2,2,2	0.46	0
3	FES	C	401	1	0,4,4	-	-	-		
5	WBP	A	403[A]	-	16,16,16	2.45	3 (18%)	22,22,22	1.22	3 (13%)
3	FES	B	401	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	WBP	A	403[B]	-	16,16,16	2.41	3 (18%)	22,22,22	1.04	1 (4%)
8	PGE	A	408	-	9,9,9	0.34	0	8,8,8	0.20	0
3	FES	A	401	1	0,4,4	-	-	-	-	-
6	EDO	B	409	-	3,3,3	0.26	0	2,2,2	0.55	0
6	EDO	C	405	-	3,3,3	0.42	0	2,2,2	0.52	0
3	FES	F	201	2	0,4,4	-	-	-	-	-
6	EDO	C	404	-	3,3,3	0.20	0	2,2,2	0.25	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	EDO	A	406	-	-	1/1/1/1	-
9	PEG	B	404	-	-	1/4/4/4	-
6	EDO	A	411	-	-	1/1/1/1	-
6	EDO	A	409	-	-	0/1/1/1	-
6	EDO	B	405	-	-	1/1/1/1	-
6	EDO	C	407	-	-	0/1/1/1	-
3	FES	D	201	2	-	-	0/1/1/1
3	FES	E	201	2	-	-	0/1/1/1
6	EDO	E	202	-	-	1/1/1/1	-
7	GOL	B	406	-	-	4/4/4/4	-
6	EDO	A	405	-	-	0/1/1/1	-
6	EDO	A	410	-	-	0/1/1/1	-
6	EDO	B	407	-	-	1/1/1/1	-
6	EDO	B	408	-	-	0/1/1/1	-
6	EDO	A	404	-	-	1/1/1/1	-
7	GOL	A	407	-	-	2/4/4/4	-
5	WBP	C	403	-	-	0/4/4/4	0/2/2/2
7	GOL	C	408	-	-	0/4/4/4	-
6	EDO	F	202	-	-	0/1/1/1	-
7	GOL	A	412	-	-	1/4/4/4	-
5	WBP	B	403	-	-	1/4/4/4	0/2/2/2
6	EDO	D	202	-	-	1/1/1/1	-
6	EDO	C	406	-	-	0/1/1/1	-
3	FES	C	401	1	-	-	0/1/1/1
5	WBP	A	403[A]	-	-	0/4/4/4	0/2/2/2
3	FES	B	401	1	-	-	0/1/1/1
5	WBP	A	403[B]	-	-	1/4/4/4	0/2/2/2
8	PGE	A	408	-	-	4/7/7/7	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FES	A	401	1	-	-	0/1/1/1
6	EDO	B	409	-	-	1/1/1/1	-
6	EDO	C	405	-	-	0/1/1/1	-
3	FES	F	201	2	-	-	0/1/1/1
6	EDO	C	404	-	-	0/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	403	WBP	CA3-CA2	9.08	1.50	1.40
5	C	403	WBP	CA3-CA2	8.01	1.49	1.40
5	A	403[A]	WBP	CA3-CA2	7.59	1.48	1.40
5	A	403[B]	WBP	CA3-CA2	6.82	1.47	1.40
5	C	403	WBP	CA1-CA2	6.06	1.51	1.40
5	A	403[B]	WBP	CA1-CA2	5.73	1.50	1.40
5	B	403	WBP	CA1-CA2	5.27	1.50	1.40
5	A	403[A]	WBP	CA1-CA2	4.87	1.49	1.40
5	B	403	WBP	CB1-CB2	3.76	1.50	1.40
5	C	403	WBP	CB1-CB2	3.56	1.50	1.40
5	A	403[A]	WBP	CB1-CB2	3.00	1.48	1.40
5	A	403[B]	WBP	CB1-CB2	2.67	1.47	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	403[A]	WBP	CB6-CB1-CA1	3.19	125.18	118.74
5	A	403[A]	WBP	CA1-CB1-CB2	-2.67	117.00	123.00
5	A	403[B]	WBP	CA1-CA2-CA3	-2.46	118.51	120.03
5	A	403[A]	WBP	CA4-CA3-CA2	-2.18	117.83	120.09
5	C	403	WBP	CA1-CA2-CA3	-2.10	118.73	120.03
5	B	403	WBP	CA4-CA5-CA6	2.06	122.89	120.24
5	B	403	WBP	CB4-CB5-CB6	2.05	122.77	120.24

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	407	GOL	C1-C2-C3-O3
8	A	408	PGE	O3-C5-C6-O4
7	B	406	GOL	O1-C1-C2-C3
7	B	406	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

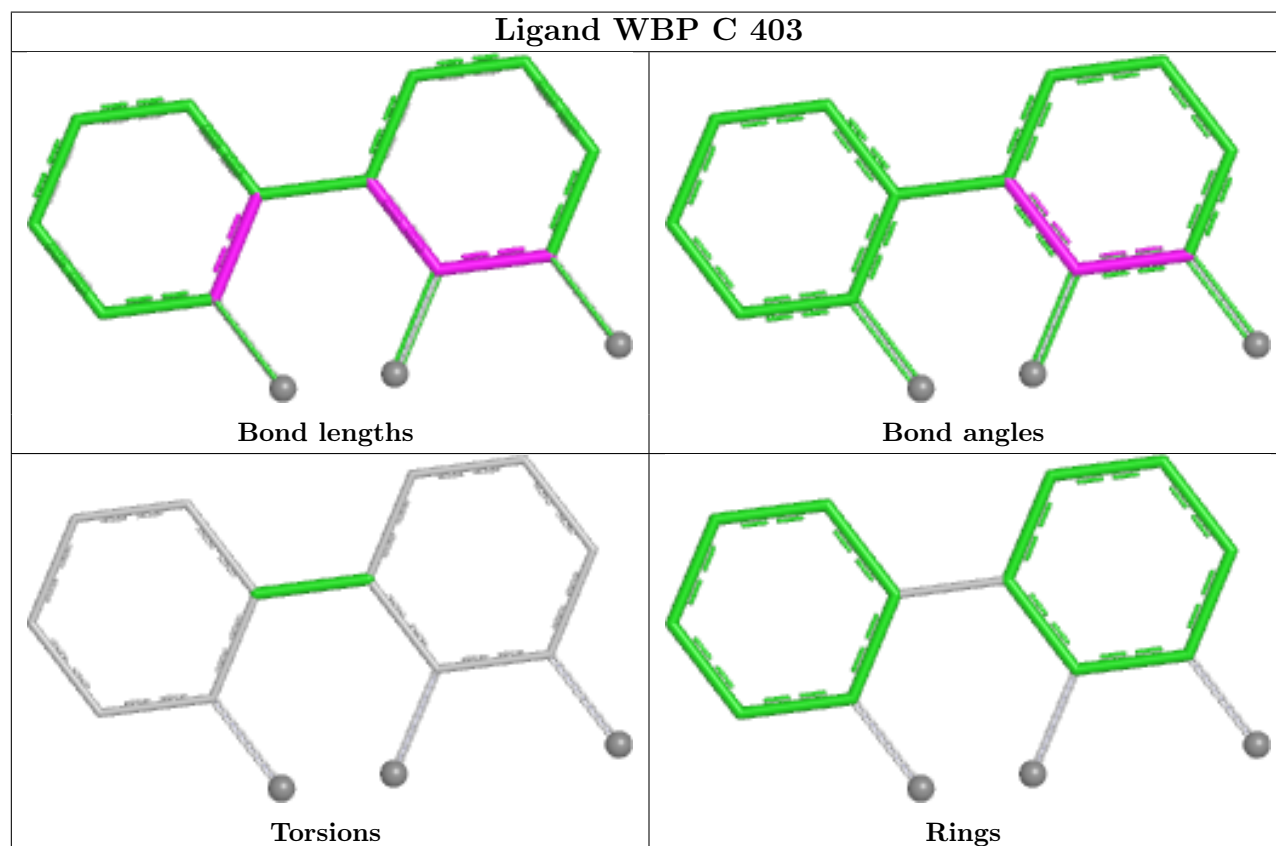
Mol	Chain	Res	Type	Atoms
7	A	407	GOL	O2-C2-C3-O3
6	A	404	EDO	O1-C1-C2-O2
7	B	406	GOL	O1-C1-C2-O2
6	B	405	EDO	O1-C1-C2-O2
7	A	412	GOL	C1-C2-C3-O3
6	A	406	EDO	O1-C1-C2-O2
6	B	409	EDO	O1-C1-C2-O2
8	A	408	PGE	C3-C4-O3-C5
8	A	408	PGE	C1-C2-O2-C3
9	B	404	PEG	C4-C3-O2-C2
6	A	411	EDO	O1-C1-C2-O2
8	A	408	PGE	C6-C5-O3-C4
5	A	403[B]	WBP	CA6-CA1-CB1-CB6
6	B	407	EDO	O1-C1-C2-O2
6	D	202	EDO	O1-C1-C2-O2
6	E	202	EDO	O1-C1-C2-O2
7	B	406	GOL	O2-C2-C3-O3
5	B	403	WBP	CA6-CA1-CB1-CB6

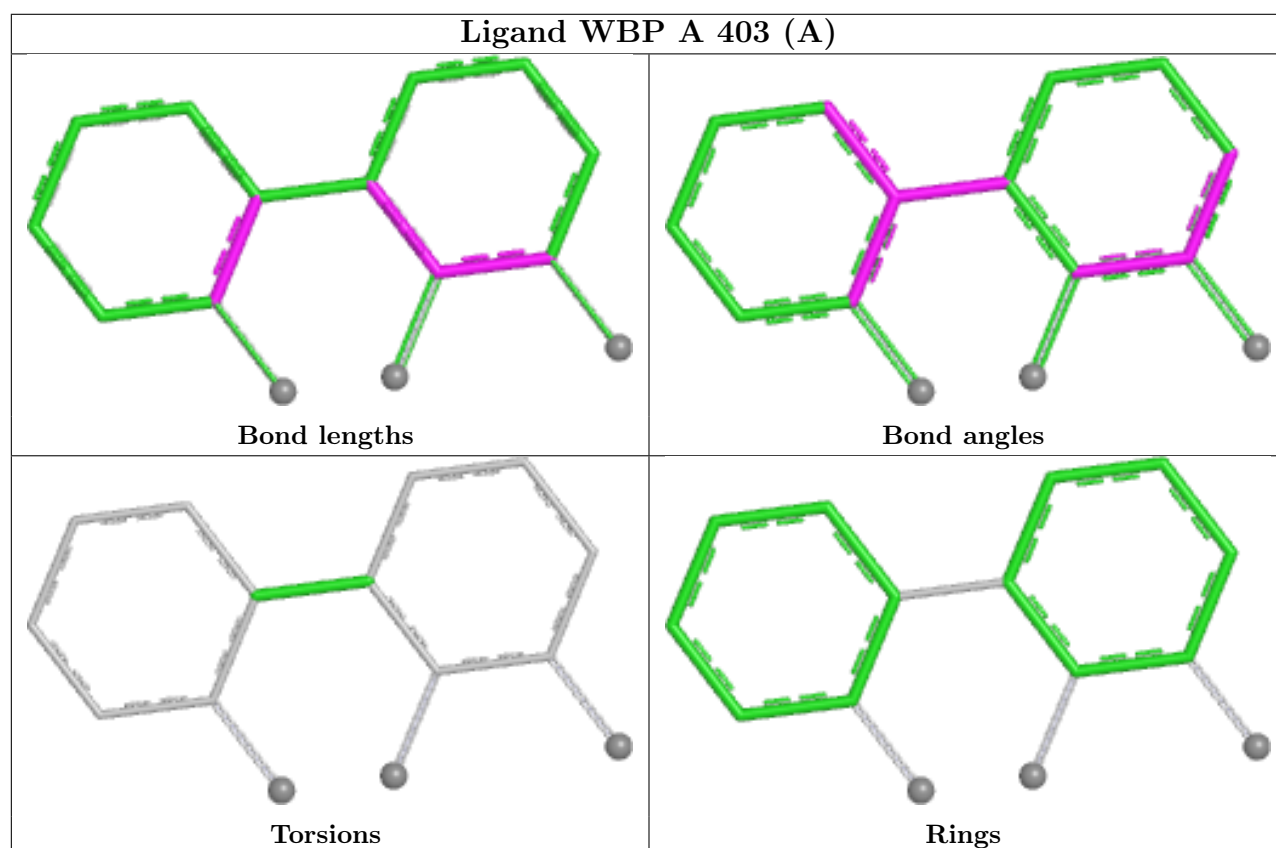
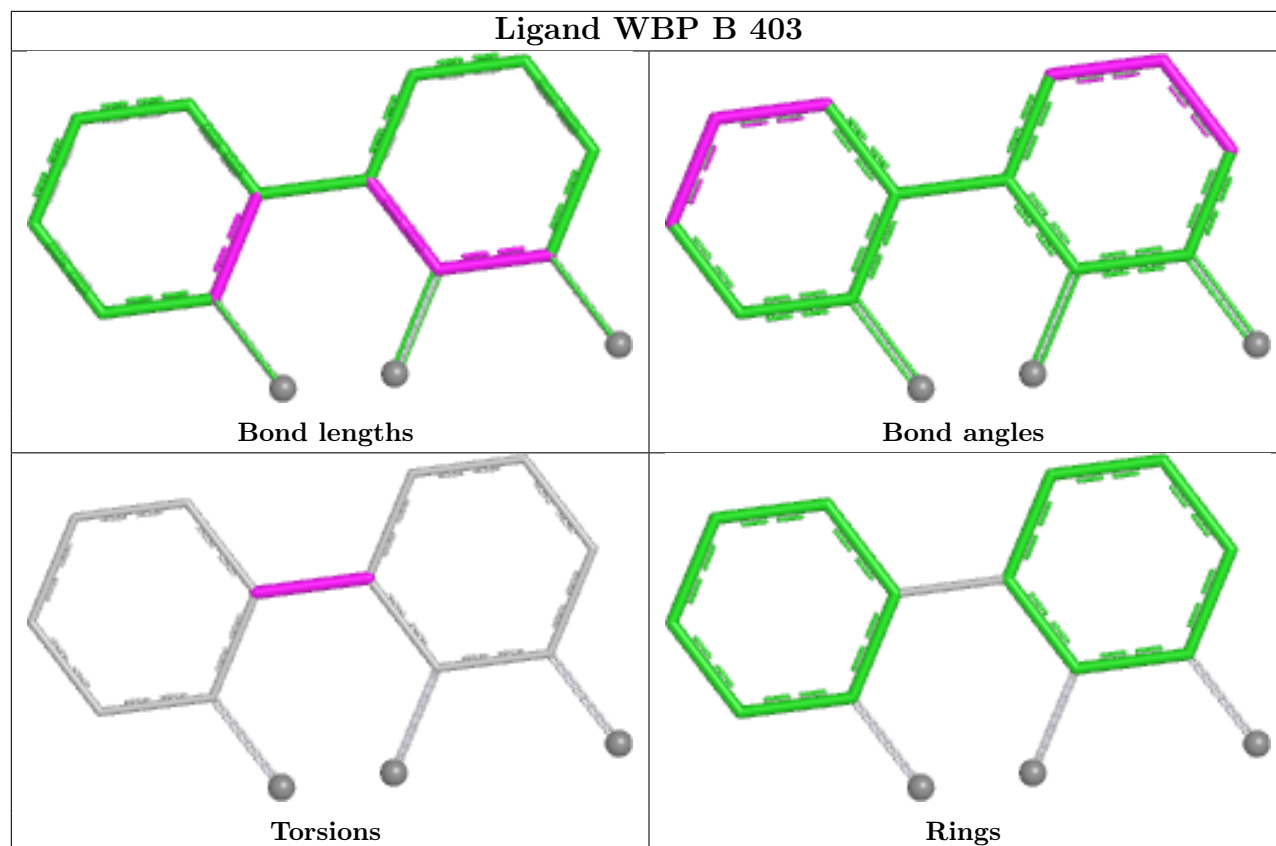
There are no ring outliers.

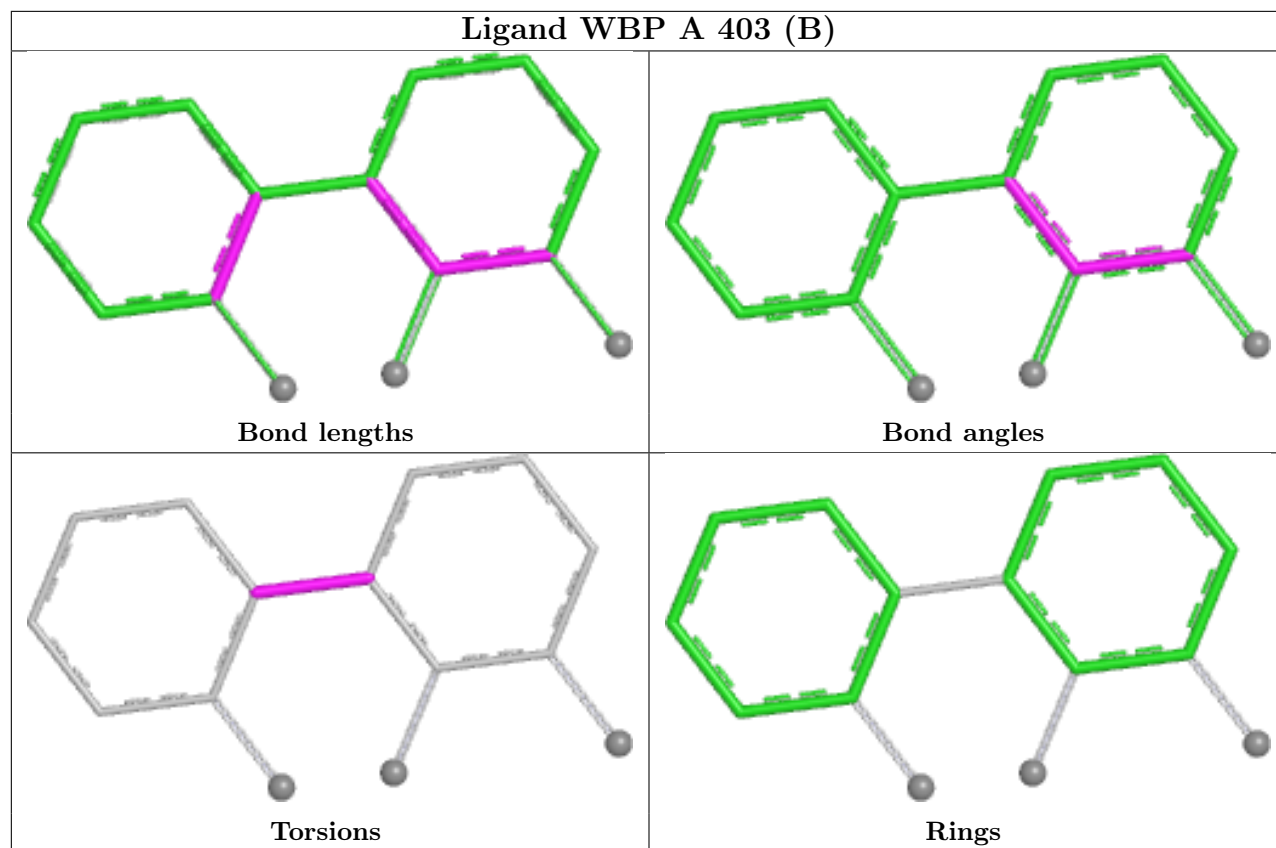
18 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	406	EDO	3	0
9	B	404	PEG	2	0
6	B	405	EDO	3	0
3	E	201	FES	1	0
6	B	407	EDO	2	0
6	A	404	EDO	1	0
7	A	407	GOL	1	0
5	C	403	WBP	3	0
7	C	408	GOL	5	0
5	B	403	WBP	2	0
6	D	202	EDO	1	0
6	C	406	EDO	4	0
5	A	403[A]	WBP	2	0
5	A	403[B]	WBP	1	0
8	A	408	PGE	3	0
6	B	409	EDO	1	0
6	C	405	EDO	2	0
3	F	201	FES	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.