



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:21 AM UTC

PDB ID : 4OGB / pdb_00004ogb
Title : Crystal structure of the catalytic domain of PDE4D2 with compound 2
Authors : Feil, S.C.; Parker, M.W.
Deposited on : 2014-01-15
Resolution : 2.03 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 : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

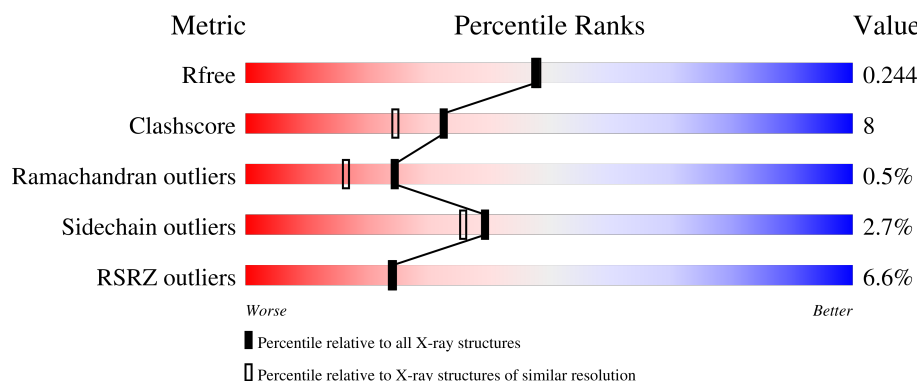
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	361	 4% 76% 12% • 9%
1	B	361	 12% 76% 12% • 11%
1	C	361	 4% 73% 15% • 10%
1	D	361	 4% 78% 11% 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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	B	507	-	-	X	-
3	EDO	C	512	-	-	X	-
4	PEG	D	516	-	-	X	-
6	DMS	A	513	-	-	X	-
6	DMS	B	510	-	-	X	-

2 Entry composition [i](#)

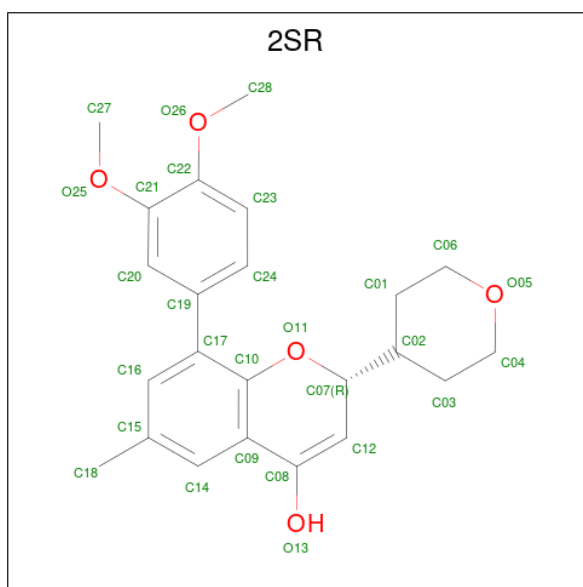
There are 8 unique types of molecules in this entry. The entry contains 11286 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2651	1676	453	508	14			
1	B	321	Total	C	N	O	S	0	1	0
			2606	1649	447	496	14			
1	C	325	Total	C	N	O	S	0	1	0
			2642	1669	453	506	14			
1	D	324	Total	C	N	O	S	0	2	0
			2640	1669	452	505	14			

- Molecule 2 is (2R)-8-(3,4-dimethoxyphenyl)-6-methyl-2-(tetrahydro-2H-pyran-4-yl)-2H-chromen-4-ol (CCD ID: 2SR) (formula: C₂₃H₂₆O₅).



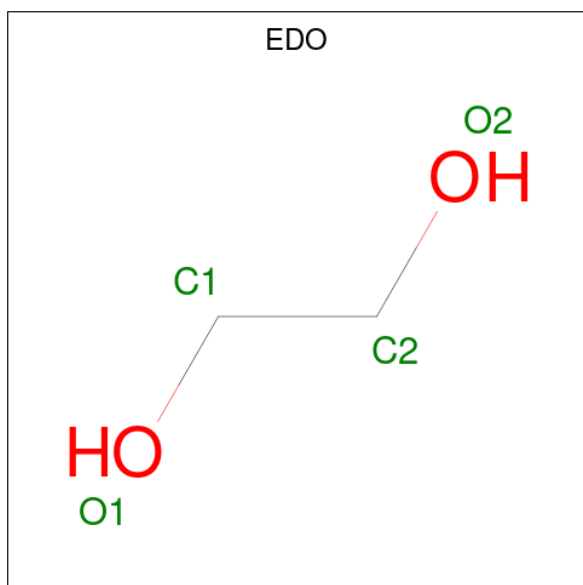
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			28	23	5		
2	B	1	Total	C	O	0	0
			28	23	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			28	23	5		
2	D	1	Total	C	O	0	0
			28	23	5		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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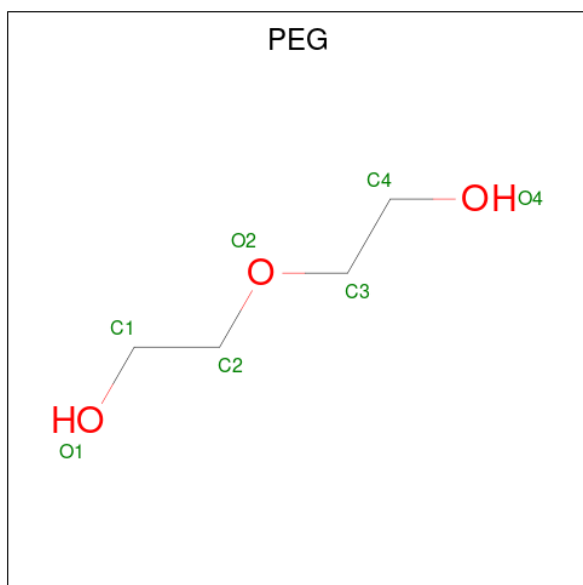
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

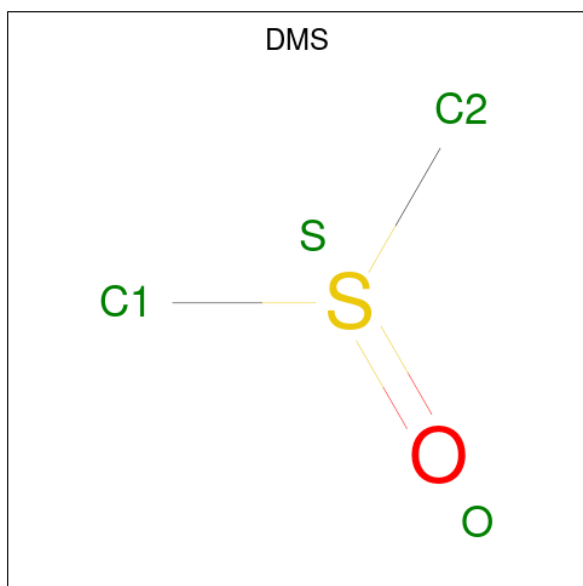
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		
5	B	2	Total	Zn	0	0
			2	2		
5	C	2	Total	Zn	0	0
			2	2		

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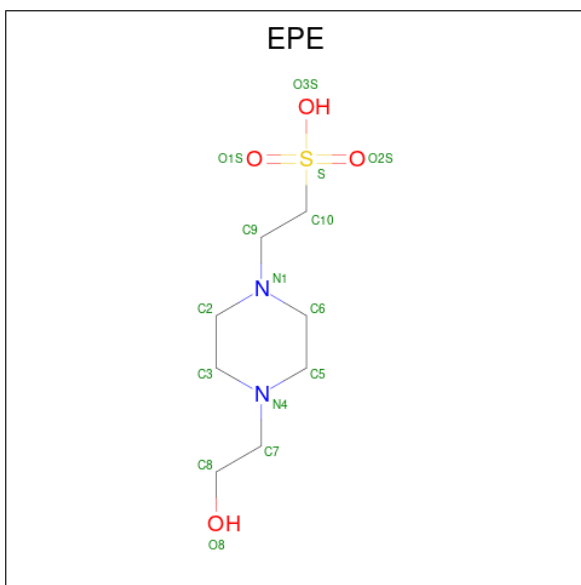
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	2	Total	Zn	0	0
			2	2		

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

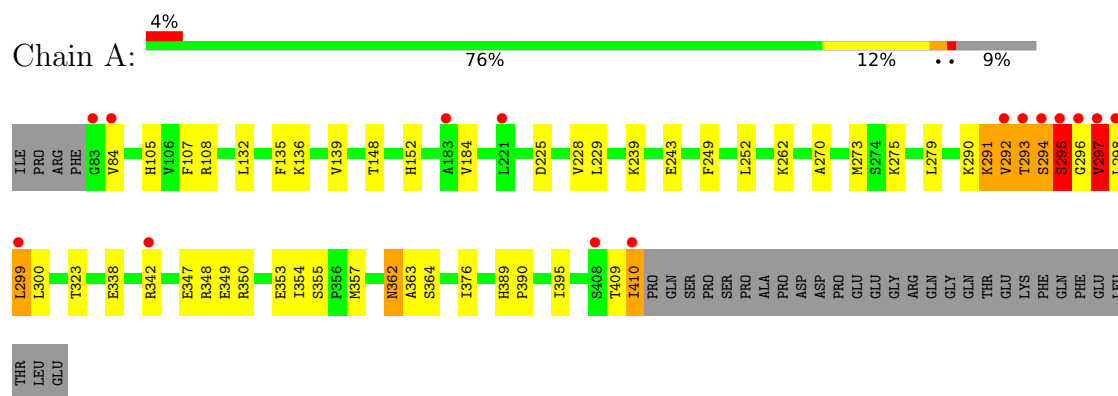
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	120	Total	O	0	0
			120	120		
8	B	104	Total	O	0	0
			104	104		
8	C	77	Total	O	0	0
			77	77		
8	D	131	Total	O	0	0
			131	131		

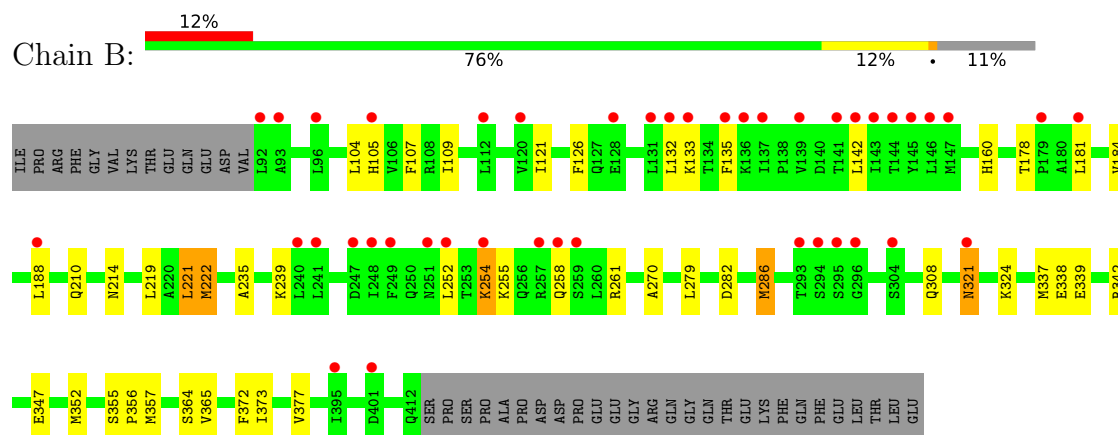
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

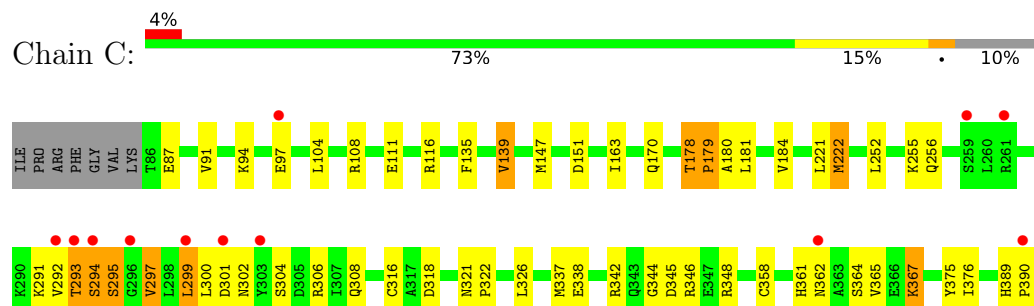
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

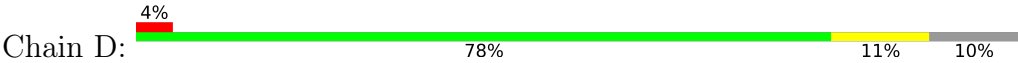


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



PRO
GLN
SER
PRO
SER
PRO
ALA
PRO
ASP
ASP
PRO
GLU
GLU
GLY
ARG
GLN
GLY
GLN
THR
GLU
LYS
PHE
GLN
PHE
GLU
LEU
THR
LEU
GLU

● Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



ILE
PRO
ARG
PHE
GLY
VAL
LYS
THR
GLU
Q88
E89
D90
V91
W102
G103
L104
H105
V106
F107
V120
H123
D140
I143
E150
N162
Q170
L219
A220
L221
M222
S226
S227
V228
L229
K262
A270
M273
L279
M286
N302
R306
I307
Q308

N321
P322
Q327
F340
F341
R342
R348
E349
R350
G351
F352
E353
I354
K357
C358
D359
N362
A363
K367
Y375
I376
V377
H378
I410
P411
GLN
SER
PRO
SER
SER
PRO
ALA
PRO
ASP
ASP
PRO
GLU
GLU
GLY
ARG
GLN
GLY
GLN
THR
LYS
PHE
GLN
PHE
GLU
LEU
THR

LEU
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.84Å 111.55Å 160.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.22 – 2.03 47.22 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.22-2.03) 99.8 (47.22-2.03)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.03Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.202 , 0.243 0.206 , 0.244	Depositor DCC
R_{free} test set	5713 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11286	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, ZN, EPE, DMS, 2SR, PEG

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	0.69	1/2704 (0.0%)	0.77	1/3672 (0.0%)
1	B	0.63	1/2660 (0.0%)	0.83	2/3615 (0.1%)
1	C	0.79	4/2695 (0.1%)	0.84	3/3660 (0.1%)
1	D	0.72	5/2695 (0.2%)	0.80	1/3662 (0.0%)
All	All	0.71	11/10754 (0.1%)	0.81	7/14609 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	378	HIS	C-O	-6.56	1.18	1.24
1	D	226	SER	C-O	-6.24	1.16	1.24
1	B	355	SER	C-N	5.92	1.41	1.33
1	C	318	ASP	C-O	-5.60	1.17	1.24
1	D	308	GLN	C-O	-5.26	1.17	1.24
1	C	316	CYS	C-O	-5.24	1.18	1.24
1	D	307	ILE	C-O	-5.19	1.17	1.24
1	A	228	VAL	C-O	-5.11	1.18	1.24
1	C	163	ILE	C-O	-5.09	1.18	1.24
1	C	179	PRO	N-CD	5.04	1.54	1.47
1	D	367	LYS	CA-C	-5.00	1.46	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	355	SER	CA-C-N	-6.09	113.69	119.90
1	B	355	SER	C-N-CA	-6.09	113.69	119.90
1	D	367	LYS	CB-CA-C	-5.82	100.05	110.70
1	C	294	SER	CA-C-N	5.34	127.44	120.28
1	C	294	SER	C-N-CA	5.34	127.44	120.28
1	C	139	VAL	CB-CA-C	-5.13	105.40	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	ALA	N-CA-C	5.01	117.92	109.95

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	2651	0	2609	48	0
1	B	2606	0	2565	39	0
1	C	2642	0	2596	47	0
1	D	2640	0	2587	39	0
2	A	28	0	26	3	0
2	B	28	0	26	2	0
2	C	28	0	26	0	0
2	D	28	0	26	3	0
3	A	32	0	48	6	0
3	B	28	0	42	7	0
3	C	36	0	54	8	0
3	D	32	0	48	2	0
4	A	7	0	10	0	0
4	D	21	0	30	7	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	8	0	12	4	0
6	B	8	0	12	7	0
6	D	8	0	12	2	0
7	C	15	0	17	0	0
8	A	120	0	0	3	0
8	B	104	0	0	5	0
8	C	77	0	0	1	0
8	D	131	0	0	2	0
All	All	11286	0	10746	170	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 8.

All (170) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:MET:HE1	1:D:222:MET:SD	1.67	1.32
1:C:222:MET:CE	1:D:222:MET:SD	2.25	1.25
1:C:222:MET:HG3	3:C:512:EDO:H21	1.18	1.17
1:D:286:MET:HE3	1:D:308:GLN:HE22	1.05	1.10
1:D:286:MET:HE3	1:D:308:GLN:NE2	1.65	1.10
1:C:222:MET:HG3	3:C:512:EDO:C2	1.85	1.05
1:A:290:LYS:O	1:A:291:LYS:HD2	1.70	0.92
1:D:286:MET:CE	1:D:308:GLN:NE2	2.35	0.89
1:C:361:HIS:O	1:C:362:ASN:ND2	2.04	0.89
1:C:222:MET:CG	3:C:512:EDO:H21	2.03	0.88
1:A:290:LYS:C	1:A:291:LYS:HD2	2.01	0.85
1:C:361:HIS:C	1:C:362:ASN:HD22	1.89	0.81
1:C:222:MET:HE2	1:D:222:MET:SD	2.21	0.80
1:D:102:TRP:H	4:D:516:PEG:H11	1.48	0.78
1:A:292:VAL:HG13	1:A:293:THR:N	2.01	0.75
1:B:104:LEU:HB3	3:B:509:EDO:H21	1.69	0.73
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.71	0.73
1:D:286:MET:CE	1:D:308:GLN:HE22	1.92	0.73
1:C:180:ALA:C	1:C:297:VAL:HG22	2.16	0.71
1:A:292:VAL:HG13	1:A:293:THR:H	1.54	0.70
1:A:299:LEU:C	1:A:299:LEU:HD12	2.17	0.70
1:A:409:THR:O	1:A:410:ILE:HG22	1.93	0.69
1:A:107:PHE:HB2	6:A:513:DMS:H21	1.75	0.68
1:C:338:GLU:OE2	1:C:342:ARG:NH2	2.26	0.68
1:C:345:ASP:OD1	1:C:348:ARG:NH2	2.27	0.68
1:A:292:VAL:HG22	1:A:297:VAL:H	1.59	0.67
1:C:375:TYR:O	1:C:376:ILE:HD12	1.95	0.67
1:C:116:ARG:NE	8:C:644:HOH:O	2.28	0.66
1:B:337:MET:HE2	1:B:365:VAL:HG22	1.78	0.65
1:A:132:LEU:HD22	1:A:139:VAL:HG12	1.78	0.65
1:B:308:GLN:HG3	8:B:605:HOH:O	1.97	0.63
1:C:337:MET:HE2	1:C:365:VAL:HG22	1.79	0.63
1:B:254:LYS:HE3	1:B:258:GLN:HE22	1.63	0.62
1:C:180:ALA:O	1:C:297:VAL:HG22	2.00	0.61
1:A:299:LEU:HD12	1:A:300:LEU:N	2.14	0.61
1:A:362:ASN:OD1	1:A:362:ASN:N	2.34	0.61
1:C:289:THR:O	1:C:289:THR:HG22	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:TYR:C	1:C:376:ILE:HD12	2.26	0.60
1:D:88:GLN:HG3	1:D:90:ASP:H	1.66	0.60
1:B:210:GLN:HE21	1:B:214:ASN:HD21	1.48	0.60
1:A:239:LYS:HZ2	3:A:508:EDO:H22	1.65	0.60
1:A:292:VAL:CG2	1:A:297:VAL:H	2.14	0.60
1:C:292:VAL:O	1:C:292:VAL:HG23	2.00	0.60
1:A:296:GLY:O	1:A:297:VAL:HB	2.02	0.59
1:B:105:HIS:CE1	1:B:107:PHE:HB2	2.36	0.59
1:C:302:ASN:O	1:C:306:ARG:HG3	2.03	0.58
1:B:352:MET:HB3	3:B:507:EDO:H22	1.84	0.58
1:C:255:LYS:HG2	3:C:505:EDO:H11	1.85	0.58
1:C:302:ASN:ND2	1:C:302:ASN:H	2.01	0.57
1:D:102:TRP:H	4:D:516:PEG:C1	2.18	0.56
1:A:295:SER:OG	1:A:296:GLY:N	2.37	0.56
1:B:135:PHE:HB3	1:B:252:LEU:HD11	1.87	0.56
1:A:338:GLU:OE2	1:A:342:ARG:NH2	2.37	0.56
1:A:296:GLY:O	1:A:297:VAL:CB	2.54	0.56
1:B:356:PRO:O	1:B:357:MET:HB2	2.06	0.56
1:A:249:PHE:CD2	3:A:506:EDO:H22	2.42	0.55
1:B:372:PHE:HE2	6:B:510:DMS:H21	1.70	0.55
1:D:102:TRP:HB2	4:D:516:PEG:H32	1.88	0.55
1:C:151:ASP:HA	3:C:509:EDO:H21	1.89	0.54
1:D:102:TRP:N	4:D:516:PEG:H11	2.20	0.54
1:C:364:SER:HB2	1:C:367:LYS:HB3	1.89	0.54
1:A:108:ARG:H	6:A:513:DMS:C2	2.20	0.54
1:B:181:LEU:HD23	1:B:184:VAL:HG21	1.89	0.54
1:B:321[B]:ASN:HB2	6:B:510:DMS:H23	1.89	0.53
1:C:108:ARG:NH1	1:C:111:GLU:OE1	2.40	0.53
1:A:349:GLU:HB3	1:C:147:MET:SD	2.49	0.53
1:B:126:PHE:HB3	1:B:132:LEU:HD11	1.91	0.53
1:B:338:GLU:OE2	1:B:342:ARG:NH2	2.42	0.53
1:A:108:ARG:H	6:A:513:DMS:H23	1.74	0.53
8:A:627:HOH:O	1:B:222:MET:HG3	2.09	0.52
1:C:293:THR:O	1:C:295:SER:N	2.44	0.51
1:D:105[A]:HIS:HE1	1:D:107:PHE:HB2	1.76	0.51
1:C:184:VAL:HG11	1:C:300:LEU:HD12	1.93	0.51
1:B:235:ALA:O	1:B:239:LYS:HD3	2.10	0.51
1:C:222:MET:HG3	3:C:512:EDO:C1	2.41	0.51
1:D:220:ALA:HA	1:D:228:VAL:HG21	1.93	0.51
1:B:105:HIS:HE1	1:B:107:PHE:HB2	1.75	0.50
1:B:254:LYS:HE3	1:B:258:GLN:NE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:GLU:CD	1:A:342:ARG:HH21	2.18	0.50
1:A:376:ILE:HD13	2:A:501:2SR:H20	1.92	0.50
1:D:123:HIS:HD1	3:D:505:EDO:H11	1.75	0.50
1:A:239:LYS:NZ	3:A:508:EDO:H22	2.27	0.50
1:A:376:ILE:CD1	2:A:501:2SR:H20	2.41	0.50
1:A:323:THR:HB	1:A:395:ILE:HG23	1.92	0.50
1:B:221:LEU:HG	8:B:698:HOH:O	2.12	0.49
1:A:270:ALA:HB1	1:A:279:LEU:HD11	1.94	0.49
1:A:347:GLU:OE2	1:A:355:SER:OG	2.30	0.49
1:A:293:THR:O	1:A:294:SER:C	2.56	0.49
1:D:105[A]:HIS:CE1	1:D:107:PHE:HB2	2.47	0.49
1:C:178:THR:HG22	1:C:181:LEU:HD12	1.95	0.49
1:D:273:MET:HG3	2:D:502:2SR:H22	1.94	0.49
1:C:282:ASP:HB3	1:C:308:GLN:NE2	2.28	0.49
1:A:299:LEU:C	1:A:299:LEU:CD1	2.85	0.48
1:A:350:ARG:NH1	8:A:644:HOH:O	2.47	0.47
1:B:214:ASN:OD1	3:B:507:EDO:H21	2.14	0.47
1:B:347:GLU:HG2	3:B:507:EDO:H12	1.96	0.47
1:D:262:LYS:HG3	4:D:507:PEG:H32	1.97	0.47
1:B:178:THR:CG2	1:B:181:LEU:HB2	2.45	0.47
1:D:229:LEU:HD23	1:D:229:LEU:HA	1.72	0.47
1:B:321[A]:ASN:CG	6:B:510:DMS:H23	2.40	0.46
1:C:135:PHE:HA	3:C:504:EDO:H21	1.97	0.46
1:C:293:THR:C	1:C:295:SER:N	2.72	0.46
1:C:293:THR:HG23	1:C:299:LEU:HB2	1.98	0.46
1:D:162:ASN:CG	6:D:508:DMS:H22	2.41	0.46
1:D:262:LYS:HA	4:D:507:PEG:H41	1.97	0.46
1:D:88:GLN:NE2	8:D:626:HOH:O	2.49	0.46
1:A:348:ARG:HB2	1:A:354:ILE:HD11	1.97	0.46
6:B:512:DMS:H13	1:D:143:ILE:HB	1.97	0.46
1:C:304:SER:O	1:C:308:GLN:HB2	2.16	0.46
1:D:342:ARG:HG2	8:D:667:HOH:O	2.16	0.46
1:D:348:ARG:HB3	1:D:354:ILE:HD11	1.98	0.45
1:C:104:LEU:HD22	1:C:170:GLN:HG3	1.98	0.45
1:A:273:MET:HG3	2:A:501:2SR:H22	1.99	0.45
1:D:350:ARG:HH11	1:D:350:ARG:HG3	1.80	0.45
1:A:148:THR:O	1:A:152:HIS:HD2	2.00	0.45
1:B:282:ASP:HB3	1:B:308:GLN:OE1	2.17	0.45
1:C:252:LEU:HD12	1:C:256:GLN:HB3	1.98	0.44
1:C:344:GLY:HA3	1:C:358:CYS:O	2.17	0.44
1:C:179:PRO:HD2	1:C:391:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:2SR:H9	8:B:613:HOH:O	2.18	0.44
1:B:255:LYS:HA	1:B:258:GLN:OE1	2.17	0.44
1:A:262:LYS:NZ	8:A:700:HOH:O	2.50	0.44
1:B:252:LEU:HD23	8:B:671:HOH:O	2.18	0.44
1:B:324:LYS:HZ3	3:B:509:EDO:H11	1.82	0.44
1:C:94:LYS:O	1:C:97:GLU:HG2	2.17	0.44
1:D:376:ILE:CD1	2:D:502:2SR:H20	2.48	0.44
1:C:222:MET:CB	3:C:512:EDO:H21	2.46	0.43
1:D:359:ASP:HB3	1:D:362:ASN:OD1	2.17	0.43
1:A:225:ASP:OD1	1:B:261:ARG:NH2	2.48	0.43
1:B:286:MET:HB3	1:B:286:MET:HE2	1.80	0.43
1:D:357:MET:HE3	1:D:357:MET:HB2	1.87	0.43
1:C:179:PRO:HD2	1:C:391:ASP:CG	2.43	0.43
1:B:160:HIS:ND1	1:B:339:GLU:OE2	2.40	0.43
1:C:221:LEU:HD23	1:C:221:LEU:O	2.17	0.43
1:D:150:GLU:O	6:D:508:DMS:H23	2.18	0.43
1:A:184:VAL:HG11	1:A:300:LEU:HD12	2.01	0.43
1:A:357:MET:HE3	1:A:357:MET:HB2	1.81	0.43
1:C:87:GLU:O	1:C:91:VAL:HG23	2.19	0.43
1:B:373:ILE:HA	1:B:377:VAL:HB	2.01	0.42
1:A:136:LYS:HA	3:A:503:EDO:H21	2.01	0.42
1:A:243:GLU:HG2	3:A:508:EDO:H12	2.00	0.42
1:A:132:LEU:CD2	1:A:139:VAL:HG12	2.49	0.42
1:C:321:ASN:HB2	1:C:322:PRO:HD3	2.01	0.42
4:D:507:PEG:H41	4:D:507:PEG:H21	1.89	0.42
1:A:105:HIS:C	6:A:513:DMS:H22	2.44	0.42
6:B:512:DMS:H12	1:D:140[A]:ASP:HA	2.02	0.42
6:B:512:DMS:H12	1:D:140[B]:ASP:HA	2.02	0.42
1:D:123:HIS:HD1	3:D:505:EDO:C1	2.33	0.42
1:B:188:LEU:HD12	1:B:188:LEU:HA	1.86	0.41
1:C:326:LEU:HD21	1:C:405:TRP:CE2	2.55	0.41
1:D:340:PHE:HZ	2:D:502:2SR:H10	1.84	0.41
1:A:389:HIS:HA	1:A:390:PRO:HA	1.77	0.41
1:B:352:MET:HE2	3:B:507:EDO:H22	2.02	0.41
1:C:389:HIS:CD2	1:C:390:PRO:HA	2.55	0.41
1:D:321:ASN:HB2	1:D:322:PRO:HD3	2.01	0.41
1:A:229:LEU:HA	1:A:229:LEU:HD23	1.88	0.41
1:A:275:LYS:HB3	3:A:507:EDO:H21	2.02	0.41
2:B:501:2SR:H11	6:B:510:DMS:H11	2.03	0.41
1:B:133:LYS:HD3	1:B:133:LYS:HA	1.86	0.41
1:D:104:LEU:HD22	1:D:170:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:MET:HE2	3:B:507:EDO:C2	2.50	0.41
1:A:296:GLY:O	1:A:297:VAL:HG23	2.21	0.41
1:B:252:LEU:HB3	8:B:671:HOH:O	2.19	0.41
1:D:219:LEU:HD12	1:D:219:LEU:HA	1.95	0.41
1:A:225:ASP:CG	1:B:261:ARG:HH21	2.29	0.41
1:C:181:LEU:O	1:C:184:VAL:HG23	2.21	0.40
1:D:270:ALA:HB1	1:D:279:LEU:HD11	2.03	0.40
1:B:132:LEU:HD21	1:B:142:LEU:HD22	2.02	0.40
1:A:135:PHE:HB3	1:A:252:LEU:HD11	2.02	0.40
1:D:302:ASN:O	1:D:306:ARG:HG3	2.21	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	326/361 (90%)	312 (96%)	10 (3%)	4 (1%)	10	4
1	B	320/361 (89%)	310 (97%)	10 (3%)	0	100	100
1	C	324/361 (90%)	313 (97%)	9 (3%)	2 (1%)	21	13
1	D	324/361 (90%)	318 (98%)	6 (2%)	0	100	100
All	All	1294/1444 (90%)	1253 (97%)	35 (3%)	6 (0%)	24	16

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	VAL
1	C	294	SER
1	A	295	SER
1	A	292	VAL
1	A	294	SER

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Mol	Chain	Res	Type
1	C	293	THR

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	299/329 (91%)	288 (96%)	11 (4%)	30	25
1	B	294/329 (89%)	284 (97%)	10 (3%)	32	27
1	C	298/329 (91%)	288 (97%)	10 (3%)	32	27
1	D	298/329 (91%)	296 (99%)	2 (1%)	76	80
All	All	1189/1316 (90%)	1156 (97%)	33 (3%)	39	34

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	291	LYS
1	A	293	THR
1	A	295	SER
1	A	297	VAL
1	A	298	LEU
1	A	299	LEU
1	A	353	GLU
1	A	362	ASN
1	A	364	SER
1	A	410	ILE
1	B	109	ILE
1	B	121	ILE
1	B	219	LEU
1	B	221	LEU
1	B	222	MET
1	B	254	LYS
1	B	286	MET
1	B	321[A]	ASN
1	B	321[B]	ASN

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Mol	Chain	Res	Type
1	B	364	SER
1	C	139	VAL
1	C	178	THR
1	C	222	MET
1	C	291	LYS
1	C	295	SER
1	C	297	VAL
1	C	299	LEU
1	C	301	ASP
1	C	346	ARG
1	C	367	LYS
1	D	120	VAL
1	D	308	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	250	GLN
1	B	210	GLN
1	B	250	GLN
1	B	369	GLN
1	C	152	HIS
1	C	210	GLN
1	C	250	GLN
1	C	308	GLN
1	C	312	ASN
1	C	362	ASN
1	C	389	HIS
1	C	407	GLN
1	D	127	GLN
1	D	152	HIS
1	D	250	GLN
1	D	258	GLN
1	D	308	GLN
1	D	312	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 8 are monoatomic - leaving 47 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	EPE	C	506	-	15,15,15	0.82	1 (6%)	19,20,20	1.97	5 (26%)
3	EDO	D	511	-	3,3,3	0.49	0	2,2,2	0.30	0
6	DMS	B	512	-	3,3,3	0.63	0	3,3,3	0.52	0
6	DMS	D	504	-	3,3,3	0.70	0	3,3,3	0.63	0
3	EDO	C	504	-	3,3,3	0.43	0	2,2,2	0.61	0
4	PEG	D	507	-	6,6,6	0.41	0	5,5,5	0.38	0
3	EDO	C	512	-	3,3,3	0.51	0	2,2,2	0.30	0
3	EDO	D	509	-	3,3,3	0.47	0	2,2,2	0.30	0
3	EDO	B	505	-	3,3,3	0.47	0	2,2,2	0.36	0
3	EDO	C	505	-	3,3,3	0.46	0	2,2,2	0.49	0
3	EDO	A	514	-	3,3,3	0.60	0	2,2,2	0.37	0
3	EDO	B	508	-	3,3,3	0.43	0	2,2,2	0.37	0
2	2SR	A	501	-	29,31,31	3.06	10 (34%)	41,44,44	1.62	7 (17%)
3	EDO	D	503	-	3,3,3	0.33	0	2,2,2	0.45	0
6	DMS	B	510	-	3,3,3	0.66	0	3,3,3	0.64	0
3	EDO	A	506	-	3,3,3	0.34	0	2,2,2	0.66	0
3	EDO	B	511	-	3,3,3	0.43	0	2,2,2	0.44	0
3	EDO	C	508	-	3,3,3	0.42	0	2,2,2	0.45	0
3	EDO	B	507	-	3,3,3	0.48	0	2,2,2	0.09	0
2	2SR	B	501	-	29,31,31	3.11	12 (41%)	41,44,44	1.72	8 (19%)
6	DMS	D	508	-	3,3,3	0.66	0	3,3,3	0.73	0
2	2SR	D	502	-	29,31,31	2.99	12 (41%)	41,44,44	1.81	11 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	D	505	-	3,3,3	0.50	0	2,2,2	0.29	0
3	EDO	C	507	-	3,3,3	0.51	0	2,2,2	0.30	0
3	EDO	C	513	-	3,3,3	0.45	0	2,2,2	0.26	0
3	EDO	A	505	-	3,3,3	0.39	0	2,2,2	0.53	0
3	EDO	D	501	-	3,3,3	0.45	0	2,2,2	0.66	0
3	EDO	B	506	-	3,3,3	0.48	0	2,2,2	0.15	0
3	EDO	A	502	-	3,3,3	0.45	0	2,2,2	0.58	0
3	EDO	C	503	-	3,3,3	0.39	0	2,2,2	0.54	0
6	DMS	A	513	-	3,3,3	0.53	0	3,3,3	0.58	0
3	EDO	A	508	-	3,3,3	0.44	0	2,2,2	0.32	0
3	EDO	A	507	-	3,3,3	0.51	0	2,2,2	0.29	0
3	EDO	B	504	-	3,3,3	0.45	0	2,2,2	0.55	0
3	EDO	D	514	-	3,3,3	0.54	0	2,2,2	0.17	0
3	EDO	B	509	-	3,3,3	0.46	0	2,2,2	0.28	0
3	EDO	D	510	-	3,3,3	0.46	0	2,2,2	0.48	0
6	DMS	A	511	-	3,3,3	0.67	0	3,3,3	0.75	0
3	EDO	A	503	-	3,3,3	0.50	0	2,2,2	0.40	0
3	EDO	C	509	-	3,3,3	0.47	0	2,2,2	0.45	0
4	PEG	A	504	-	6,6,6	0.27	0	5,5,5	0.53	0
2	2SR	C	502	-	29,31,31	3.12	12 (41%)	41,44,44	1.82	12 (29%)
4	PEG	D	516	-	6,6,6	0.35	0	5,5,5	0.56	0
3	EDO	D	506	-	3,3,3	0.53	0	2,2,2	0.18	0
3	EDO	A	512	-	3,3,3	0.46	0	2,2,2	0.43	0
4	PEG	D	515	-	6,6,6	0.32	0	5,5,5	0.32	0
3	EDO	C	501	-	3,3,3	0.66	0	2,2,2	0.04	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
7	EPE	C	506	-	-	6/9/19/19	0/1/1/1
3	EDO	D	511	-	-	0/1/1/1	-
3	EDO	C	504	-	-	1/1/1/1	-
4	PEG	D	507	-	-	3/4/4/4	-
3	EDO	C	512	-	-	1/1/1/1	-
3	EDO	D	509	-	-	0/1/1/1	-
3	EDO	B	505	-	-	1/1/1/1	-
3	EDO	C	505	-	-	0/1/1/1	-
3	EDO	A	514	-	-	0/1/1/1	-
3	EDO	B	508	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2SR	A	501	-	-	8/12/32/32	0/4/4/4
3	EDO	D	503	-	-	1/1/1/1	-
3	EDO	A	506	-	-	1/1/1/1	-
3	EDO	B	511	-	-	0/1/1/1	-
3	EDO	C	508	-	-	0/1/1/1	-
3	EDO	B	507	-	-	0/1/1/1	-
2	2SR	B	501	-	-	8/12/32/32	1/4/4/4
2	2SR	D	502	-	-	4/12/32/32	1/4/4/4
3	EDO	D	505	-	-	1/1/1/1	-
3	EDO	C	507	-	-	1/1/1/1	-
3	EDO	C	513	-	-	0/1/1/1	-
3	EDO	A	505	-	-	1/1/1/1	-
3	EDO	D	501	-	-	0/1/1/1	-
3	EDO	B	506	-	-	0/1/1/1	-
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	C	503	-	-	1/1/1/1	-
3	EDO	A	508	-	-	1/1/1/1	-
3	EDO	A	507	-	-	0/1/1/1	-
3	EDO	B	504	-	-	0/1/1/1	-
3	EDO	D	514	-	-	0/1/1/1	-
3	EDO	B	509	-	-	1/1/1/1	-
3	EDO	D	510	-	-	0/1/1/1	-
3	EDO	A	503	-	-	1/1/1/1	-
3	EDO	C	509	-	-	0/1/1/1	-
4	PEG	A	504	-	-	3/4/4/4	-
2	2SR	C	502	-	-	7/12/32/32	0/4/4/4
4	PEG	D	516	-	-	3/4/4/4	-
3	EDO	D	506	-	-	1/1/1/1	-
3	EDO	A	512	-	-	0/1/1/1	-
4	PEG	D	515	-	-	2/4/4/4	-
3	EDO	C	501	-	-	0/1/1/1	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	2SR	O11-C10	11.21	1.54	1.37
2	C	502	2SR	O11-C10	11.19	1.54	1.37
2	B	501	2SR	O11-C10	10.72	1.53	1.37
2	D	502	2SR	O11-C10	10.44	1.53	1.37
2	B	501	2SR	C14-C09	6.67	1.50	1.39
2	D	502	2SR	C14-C09	6.51	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	2SR	C14-C09	6.43	1.49	1.39
2	A	501	2SR	C14-C09	6.31	1.49	1.39
2	C	502	2SR	C17-C10	5.51	1.51	1.41
2	B	501	2SR	C17-C10	5.16	1.50	1.41
2	A	501	2SR	C17-C10	5.13	1.50	1.41
2	D	502	2SR	C17-C10	4.61	1.49	1.41
2	B	501	2SR	O13-C08	4.23	1.41	1.31
2	C	502	2SR	O13-C08	4.17	1.40	1.31
2	D	502	2SR	O13-C08	4.16	1.40	1.31
2	A	501	2SR	O13-C08	4.07	1.40	1.31
2	B	501	2SR	O25-C21	3.68	1.43	1.37
2	C	502	2SR	O11-C07	3.56	1.48	1.45
2	B	501	2SR	C17-C19	3.43	1.55	1.49
2	C	502	2SR	O25-C21	3.38	1.42	1.37
2	A	501	2SR	O11-C07	3.33	1.48	1.45
2	D	502	2SR	C17-C19	3.13	1.55	1.49
2	D	502	2SR	O25-C21	3.10	1.42	1.37
2	A	501	2SR	C17-C19	3.04	1.54	1.49
2	C	502	2SR	C17-C19	3.02	1.54	1.49
2	A	501	2SR	O25-C21	2.93	1.41	1.37
2	B	501	2SR	O11-C07	2.91	1.48	1.45
2	B	501	2SR	C16-C15	2.86	1.43	1.39
2	D	502	2SR	C16-C15	2.82	1.43	1.39
7	C	506	EPE	C10-S	2.69	1.81	1.77
2	D	502	2SR	C09-C10	-2.56	1.35	1.40
2	A	501	2SR	C16-C15	2.55	1.43	1.39
2	D	502	2SR	C14-C15	2.52	1.42	1.39
2	B	501	2SR	C14-C15	2.47	1.42	1.39
2	C	502	2SR	C16-C15	2.42	1.42	1.39
2	B	501	2SR	C09-C10	-2.42	1.35	1.40
2	D	502	2SR	C03-C02	-2.41	1.47	1.53
2	A	501	2SR	C09-C10	-2.34	1.35	1.40
2	C	502	2SR	C14-C15	2.29	1.42	1.39
2	D	502	2SR	O11-C07	2.29	1.47	1.45
2	D	502	2SR	C01-C02	-2.23	1.47	1.53
2	C	502	2SR	C09-C10	-2.22	1.36	1.40
2	C	502	2SR	C03-C02	-2.10	1.48	1.53
2	C	502	2SR	O26-C22	2.07	1.40	1.37
2	B	501	2SR	O26-C22	2.07	1.40	1.37
2	A	501	2SR	C03-C02	-2.04	1.48	1.53
2	B	501	2SR	C01-C02	-2.02	1.48	1.53

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	2SR	O25-C21-C22	4.90	122.05	115.40
2	B	501	2SR	O26-C22-C21	4.63	121.68	115.40
7	C	506	EPE	C5-N4-C3	4.42	118.35	108.84
2	D	502	2SR	C06-C01-C02	-4.40	105.07	110.73
2	A	501	2SR	O26-C22-C21	4.26	121.18	115.40
2	C	502	2SR	O25-C21-C22	4.22	121.12	115.40
7	C	506	EPE	C7-N4-C5	4.12	122.23	111.24
2	C	502	2SR	O26-C22-C21	4.09	120.95	115.40
2	D	502	2SR	O26-C22-C21	4.07	120.93	115.40
2	D	502	2SR	C04-C03-C02	-4.02	105.56	110.73
2	A	501	2SR	O25-C21-C22	3.87	120.66	115.40
2	C	502	2SR	O13-C08-C12	-3.78	118.22	121.64
2	B	501	2SR	O26-C22-C23	-3.37	118.63	124.30
2	C	502	2SR	C06-C01-C02	3.36	115.05	110.73
2	B	501	2SR	C02-C07-C12	3.31	118.60	113.12
2	A	501	2SR	O26-C22-C23	-3.27	118.79	124.30
2	C	502	2SR	O26-C22-C23	-3.07	119.13	124.30
7	C	506	EPE	C7-N4-C3	3.06	119.41	111.24
7	C	506	EPE	O2S-S-C10	3.03	111.30	106.73
2	B	501	2SR	O25-C21-C20	-3.00	118.91	124.08
2	D	502	2SR	O25-C21-C22	2.97	119.44	115.40
7	C	506	EPE	C6-N1-C2	2.97	115.23	108.84
2	D	502	2SR	O26-C22-C23	-2.96	119.31	124.30
2	C	502	2SR	C04-C03-C02	2.83	114.37	110.73
2	C	502	2SR	O11-C07-C12	2.81	113.91	109.32
2	A	501	2SR	O25-C21-C20	-2.76	119.32	124.08
2	A	501	2SR	O11-C07-C12	2.73	113.78	109.32
2	C	502	2SR	O25-C21-C20	-2.61	119.57	124.08
2	D	502	2SR	C02-C07-C12	2.58	117.39	113.12
2	C	502	2SR	C03-C02-C01	2.45	113.63	109.43
2	D	502	2SR	C27-O25-C21	-2.45	113.92	117.51
2	C	502	2SR	C10-C09-C08	2.26	120.16	116.78
2	B	501	2SR	C18-C15-C16	-2.22	117.92	120.92
2	D	502	2SR	O11-C07-C02	-2.21	103.22	107.40
2	B	501	2SR	C16-C15-C14	2.20	120.56	118.11
2	A	501	2SR	C28-O26-C22	-2.20	114.29	117.51
2	D	502	2SR	O25-C21-C20	-2.17	120.34	124.08
2	A	501	2SR	C10-C09-C08	2.15	119.99	116.78
2	C	502	2SR	C18-C15-C16	-2.12	118.05	120.92
2	D	502	2SR	O13-C08-C12	-2.11	119.73	121.64
2	D	502	2SR	C16-C15-C14	2.10	120.44	118.11
2	C	502	2SR	C16-C15-C14	2.07	120.42	118.11
2	B	501	2SR	O11-C07-C12	2.06	112.68	109.32

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	2SR	C01-C02-C07-O11
2	A	501	2SR	C01-C02-C07-C12
2	A	501	2SR	C03-C02-C07-O11
2	A	501	2SR	C03-C02-C07-C12
2	B	501	2SR	C01-C02-C07-O11
2	B	501	2SR	C01-C02-C07-C12
2	B	501	2SR	C03-C02-C07-O11
2	B	501	2SR	C03-C02-C07-C12
2	C	502	2SR	C01-C02-C07-O11
2	C	502	2SR	C01-C02-C07-C12
2	C	502	2SR	C03-C02-C07-O11
2	C	502	2SR	C03-C02-C07-C12
7	C	506	EPE	C8-C7-N4-C5
7	C	506	EPE	C9-C10-S-O1S
7	C	506	EPE	C9-C10-S-O3S
4	A	504	PEG	C1-C2-O2-C3
2	B	501	2SR	C21-C22-O26-C28
2	B	501	2SR	C23-C22-O26-C28
2	D	502	2SR	C23-C22-O26-C28
4	D	507	PEG	C4-C3-O2-C2
2	A	501	2SR	C21-C22-O26-C28
3	A	505	EDO	O1-C1-C2-O2
3	D	505	EDO	O1-C1-C2-O2
2	B	501	2SR	C20-C21-O25-C27
2	C	502	2SR	C23-C22-O26-C28
2	D	502	2SR	C21-C22-O26-C28
2	A	501	2SR	C22-C21-O25-C27
2	D	502	2SR	C22-C21-O25-C27
2	B	501	2SR	C22-C21-O25-C27
2	A	501	2SR	C23-C22-O26-C28
3	B	509	EDO	O1-C1-C2-O2
3	C	503	EDO	O1-C1-C2-O2
2	C	502	2SR	C21-C22-O26-C28
3	C	504	EDO	O1-C1-C2-O2
3	C	512	EDO	O1-C1-C2-O2
2	A	501	2SR	C20-C21-O25-C27
4	A	504	PEG	O1-C1-C2-O2
4	D	515	PEG	O2-C3-C4-O4
2	D	502	2SR	C20-C21-O25-C27
4	D	516	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
7	C	506	EPE	C9-C10-S-O2S
4	D	507	PEG	O1-C1-C2-O2
4	D	507	PEG	C1-C2-O2-C3
7	C	506	EPE	S-C10-C9-N1
3	B	505	EDO	O1-C1-C2-O2
4	A	504	PEG	C4-C3-O2-C2
4	D	516	PEG	C1-C2-O2-C3
3	A	508	EDO	O1-C1-C2-O2
3	C	507	EDO	O1-C1-C2-O2
7	C	506	EPE	C10-C9-N1-C2
4	D	516	PEG	C4-C3-O2-C2
3	D	503	EDO	O1-C1-C2-O2
3	A	503	EDO	O1-C1-C2-O2
3	A	502	EDO	O1-C1-C2-O2
2	C	502	2SR	C22-C21-O25-C27
3	D	506	EDO	O1-C1-C2-O2
4	D	515	PEG	C4-C3-O2-C2
3	A	506	EDO	O1-C1-C2-O2

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	2SR	C01-C02-C03-C04-C06-O05
2	D	502	2SR	C01-C02-C03-C04-C06-O05

20 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	512	DMS	3	0
3	C	504	EDO	1	0
4	D	507	PEG	3	0
3	C	512	EDO	5	0
3	C	505	EDO	1	0
2	A	501	2SR	3	0
6	B	510	DMS	4	0
3	A	506	EDO	1	0
3	B	507	EDO	5	0
2	B	501	2SR	2	0
6	D	508	DMS	2	0
2	D	502	2SR	3	0
3	D	505	EDO	2	0
6	A	513	DMS	4	0

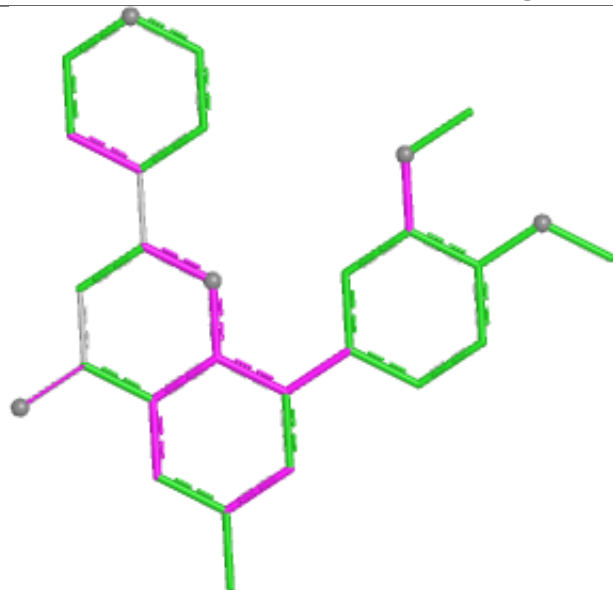
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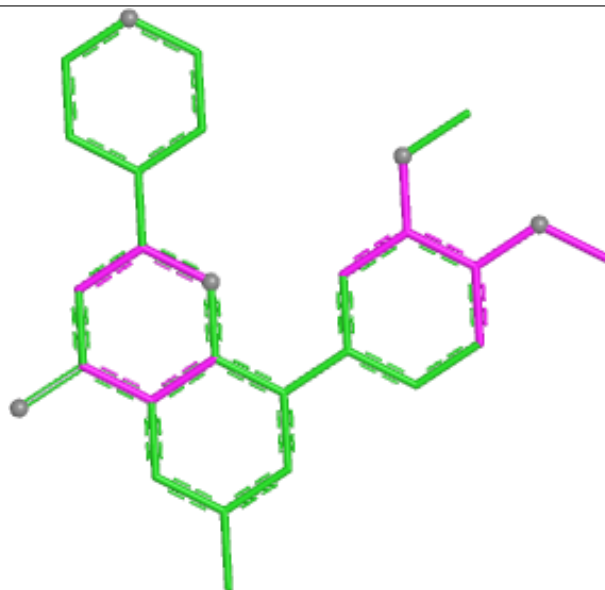
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	508	EDO	3	0
3	A	507	EDO	1	0
3	B	509	EDO	2	0
3	A	503	EDO	1	0
3	C	509	EDO	1	0
4	D	516	PEG	4	0

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.

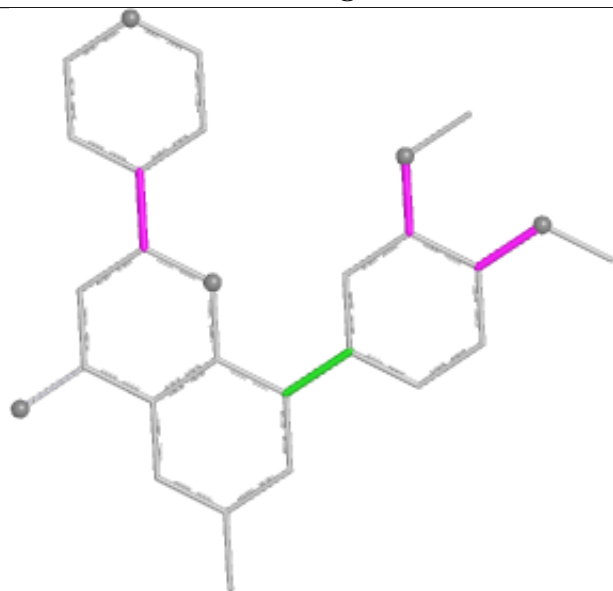
Ligand 2SR A 501



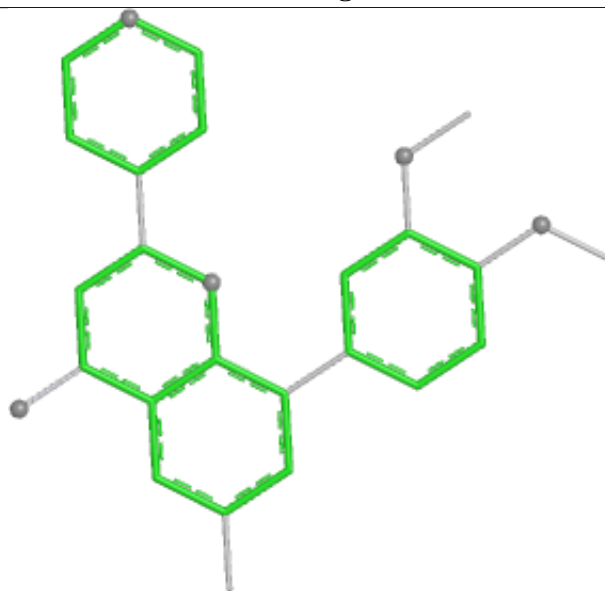
Bond lengths



Bond angles

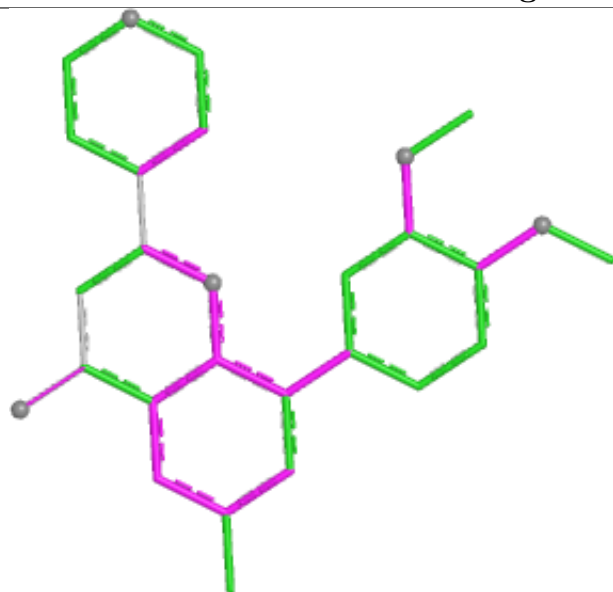


Torsions

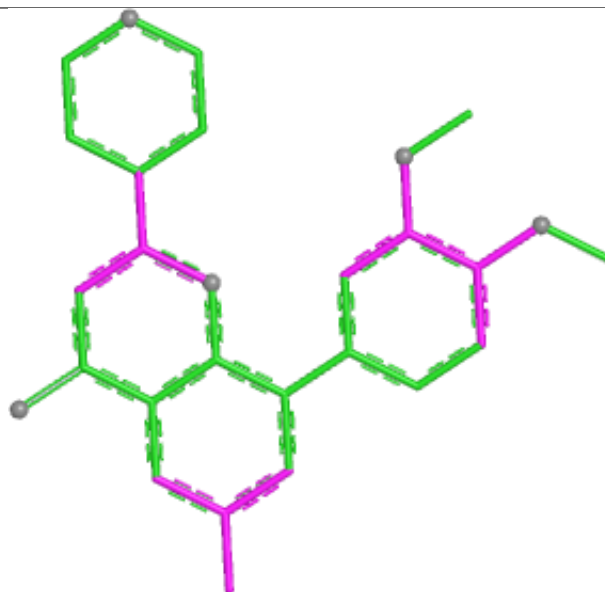


Rings

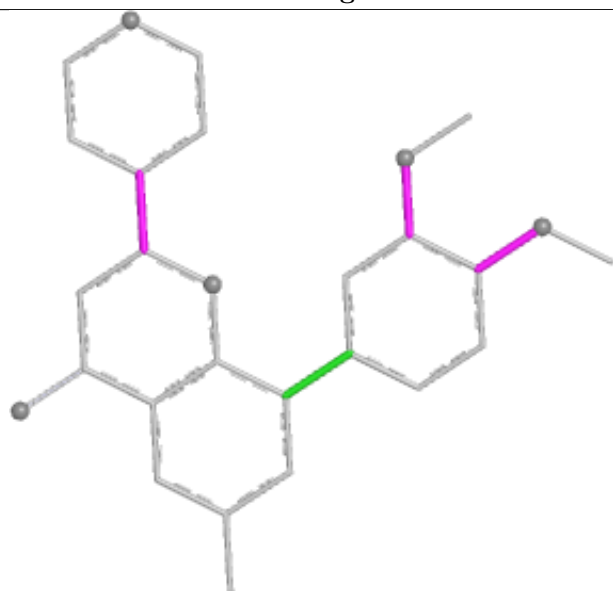
Ligand 2SR B 501



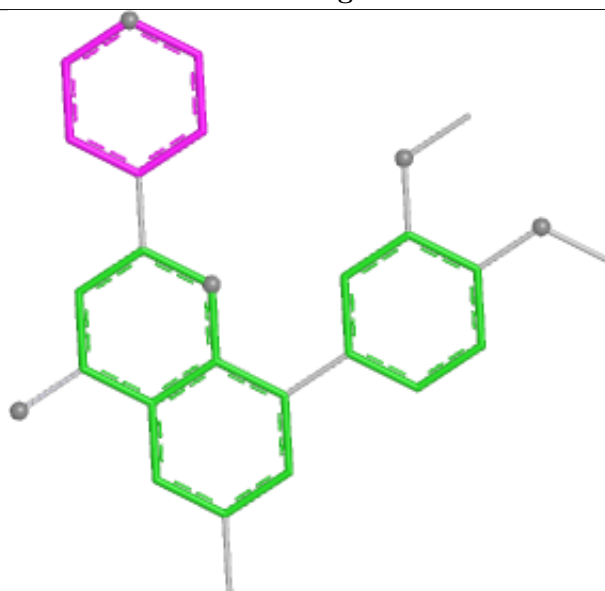
Bond lengths



Bond angles

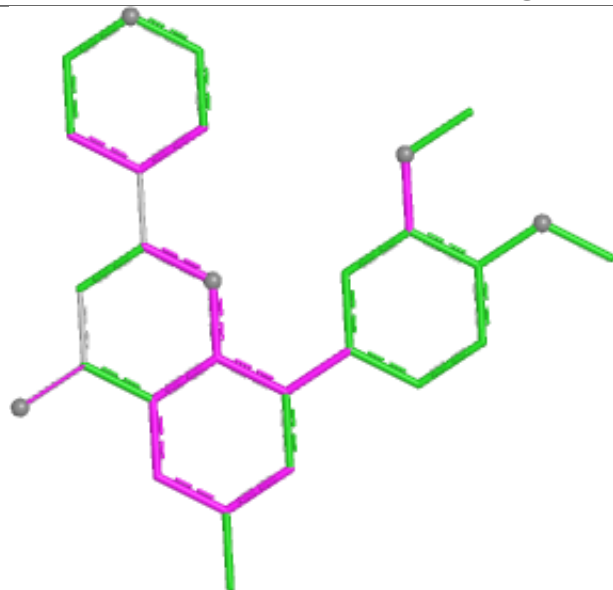


Torsions

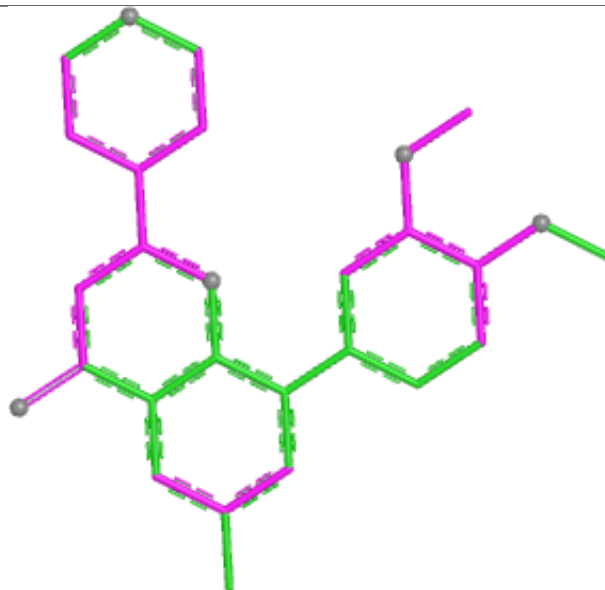


Rings

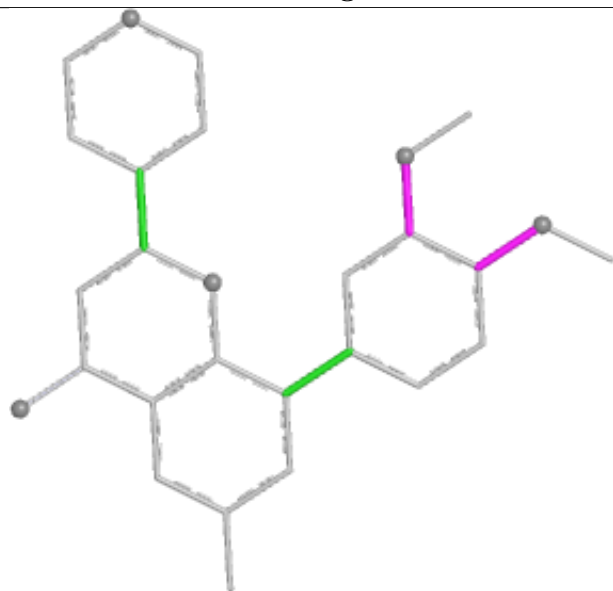
Ligand 2SR D 502



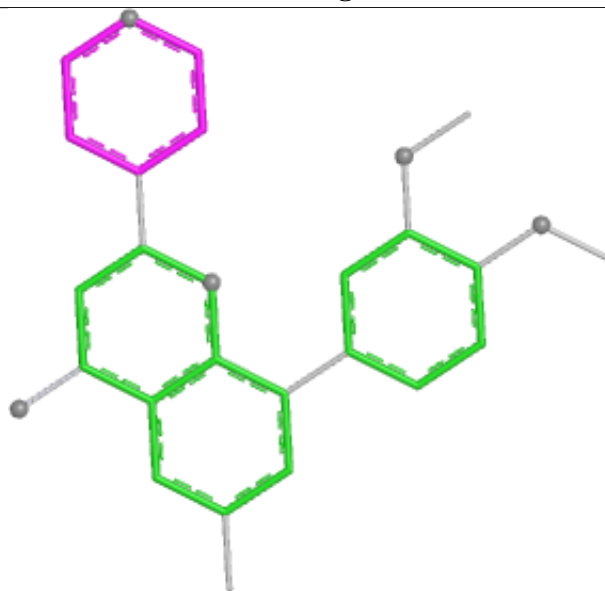
Bond lengths



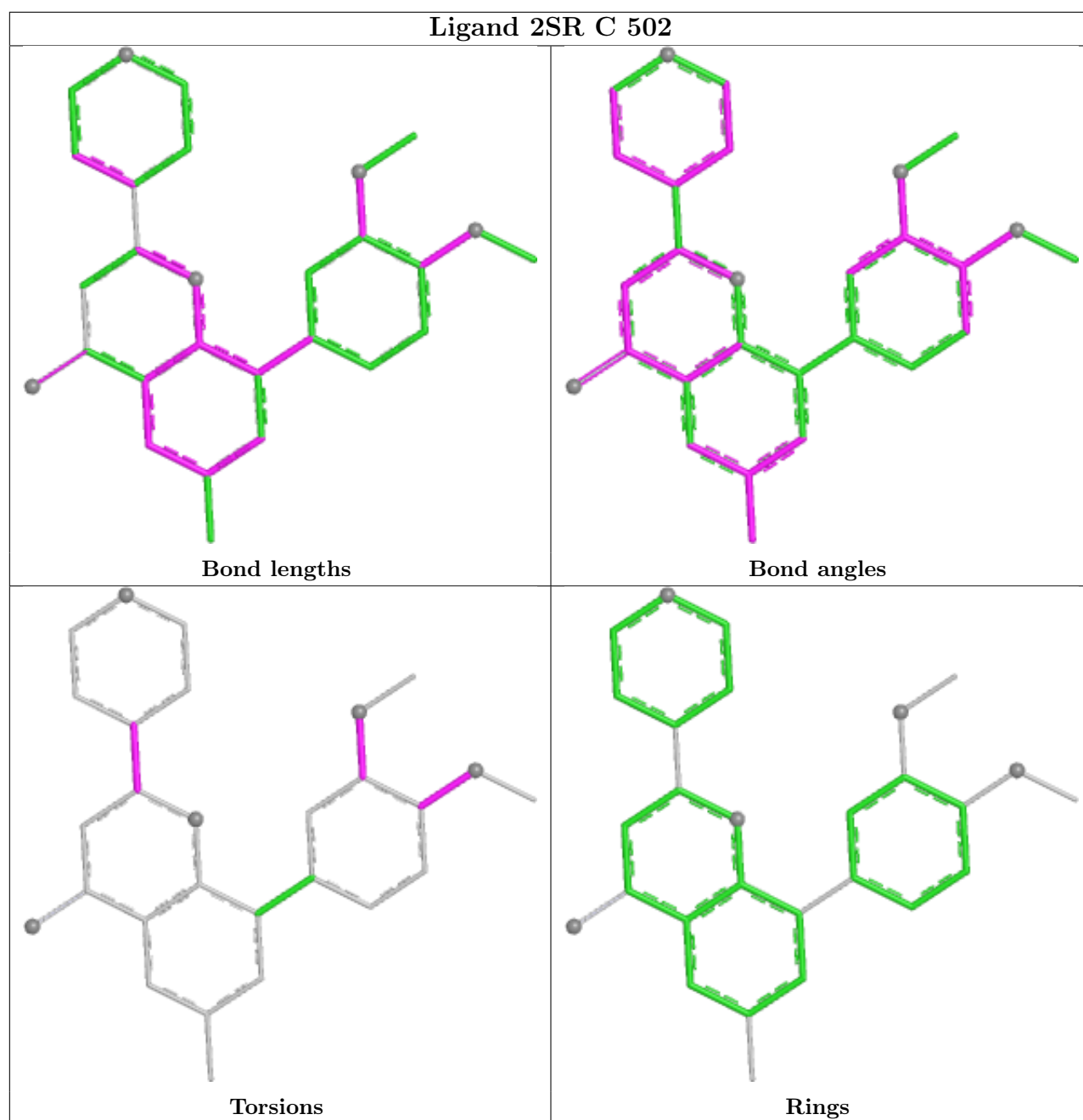
Bond angles



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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	328/361 (90%)	0.18	15 (4%) 37 37	17, 32, 59, 115	0
1	B	321/361 (88%)	0.90	43 (13%) 7 6	18, 43, 61, 77	1 (0%)
1	C	325/361 (90%)	0.51	15 (4%) 37 37	16, 39, 66, 106	1 (0%)
1	D	324/361 (89%)	0.13	13 (4%) 42 42	12, 29, 56, 75	2 (0%)
All	All	1298/1444 (89%)	0.43	86 (6%) 24 24	12, 36, 61, 115	4 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	THR	5.6
1	A	410	ILE	5.2
1	D	362	ASN	4.3
1	B	92	LEU	4.2
1	B	295	SER	4.0
1	D	351	GLY	3.9
1	B	147	MET	3.7
1	D	363	ALA	3.6
1	B	93	ALA	3.6
1	A	83	GLY	3.5
1	D	410	ILE	3.4
1	A	295	SER	3.4
1	A	342	ARG	3.3
1	C	294	SER	3.2
1	A	296	GLY	3.2
1	A	292	VAL	3.1
1	D	222	MET	3.1
1	D	342	ARG	3.0
1	A	298	LEU	3.0
1	A	297	VAL	3.0
1	B	188	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	294	SER	3.0
1	B	258	GLN	3.0
1	B	132	LEU	2.9
1	B	146	LEU	2.9
1	A	299	LEU	2.9
1	A	294	SER	2.9
1	D	105[A]	HIS	2.9
1	B	139	VAL	2.8
1	C	303	TYR	2.8
1	B	143	ILE	2.8
1	B	135	PHE	2.8
1	B	145	TYR	2.7
1	B	251	ASN	2.7
1	B	112	LEU	2.7
1	C	299	LEU	2.7
1	B	128	GLU	2.7
1	B	141	THR	2.6
1	B	321[A]	ASN	2.6
1	B	241	LEU	2.6
1	B	248	ILE	2.5
1	C	410	ILE	2.5
1	B	296	GLY	2.5
1	B	395	ILE	2.5
1	A	408	SER	2.5
1	B	144	THR	2.5
1	B	252	LEU	2.5
1	D	352	MET	2.5
1	B	249	PHE	2.5
1	C	97	GLU	2.4
1	B	131	LEU	2.4
1	D	91	VAL	2.4
1	B	142	LEU	2.4
1	B	257	ARG	2.4
1	C	261[A]	ARG	2.4
1	D	350	ARG	2.4
1	B	240	LEU	2.4
1	C	292	VAL	2.4
1	B	401	ASP	2.3
1	C	293	THR	2.3
1	D	354	ILE	2.3
1	C	362	ASN	2.3
1	B	120	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	293	THR	2.2
1	A	183	ALA	2.2
1	C	301	ASP	2.2
1	B	259	SER	2.2
1	B	179	PRO	2.1
1	A	84	VAL	2.1
1	B	181	LEU	2.1
1	C	390	PRO	2.1
1	B	137	ILE	2.1
1	C	296	GLY	2.1
1	D	375	TYR	2.1
1	B	105	HIS	2.1
1	B	254	LYS	2.1
1	B	133	LYS	2.1
1	C	287	VAL	2.1
1	B	304	SER	2.1
1	C	259	SER	2.1
1	B	247	ASP	2.0
1	C	289	THR	2.0
1	A	221	LEU	2.0
1	B	96	LEU	2.0
1	D	327	GLN	2.0
1	B	136	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2SR	B	501	28/28	0.67	0.23	45,56,68,76	0
2	2SR	A	501	28/28	0.72	0.20	51,62,70,72	0
3	EDO	B	511	4/4	0.72	0.18	58,58,58,66	0
4	PEG	D	515	7/7	0.72	0.29	53,67,90,105	0
2	2SR	C	502	28/28	0.75	0.19	46,58,63,67	0
3	EDO	A	503	4/4	0.75	0.24	40,40,48,51	0
3	EDO	A	507	4/4	0.77	0.17	46,49,53,54	0
6	DMS	B	512	4/4	0.78	0.23	33,45,52,66	0
3	EDO	D	511	4/4	0.79	0.17	49,49,50,55	0
3	EDO	A	514	4/4	0.79	0.17	27,38,38,45	0
2	2SR	D	502	28/28	0.79	0.17	47,54,58,59	0
3	EDO	C	512	4/4	0.80	0.26	43,45,52,54	0
3	EDO	B	509	4/4	0.80	0.27	40,46,48,54	0
6	DMS	D	508	4/4	0.80	0.21	38,42,53,61	0
4	PEG	D	516	7/7	0.82	0.16	36,44,59,69	0
3	EDO	C	503	4/4	0.82	0.17	39,41,44,55	0
3	EDO	A	502	4/4	0.82	0.16	52,52,53,54	0
3	EDO	C	508	4/4	0.83	0.17	57,57,60,60	0
3	EDO	D	510	4/4	0.84	0.18	38,40,45,52	0
3	EDO	C	507	4/4	0.84	0.14	45,46,47,48	0
3	EDO	D	509	4/4	0.84	0.15	38,47,49,52	0
6	DMS	A	513	4/4	0.85	0.19	29,46,51,55	0
3	EDO	C	504	4/4	0.85	0.18	45,45,50,53	0
3	EDO	C	509	4/4	0.85	0.14	34,41,43,47	0
6	DMS	A	511	4/4	0.86	0.17	45,59,63,71	0
3	EDO	D	506	4/4	0.86	0.13	41,42,43,48	0
3	EDO	A	508	4/4	0.87	0.21	30,31,36,51	0
6	DMS	D	504	4/4	0.87	0.25	41,42,55,63	0
3	EDO	C	501	4/4	0.87	0.14	35,38,41,43	0
3	EDO	B	505	4/4	0.88	0.16	45,46,49,54	0
4	PEG	A	504	7/7	0.88	0.12	33,36,46,51	0
6	DMS	B	510	4/4	0.88	0.22	59,64,73,74	0
4	PEG	D	507	7/7	0.88	0.13	29,33,37,42	0
3	EDO	A	512	4/4	0.88	0.11	28,30,30,31	0
3	EDO	D	505	4/4	0.88	0.13	41,50,51,52	0
3	EDO	C	513	4/4	0.89	0.13	41,53,55,58	0
3	EDO	B	508	4/4	0.89	0.12	55,57,63,64	0
3	EDO	A	505	4/4	0.90	0.10	27,32,36,39	0
3	EDO	C	505	4/4	0.90	0.13	44,44,52,54	0
3	EDO	B	504	4/4	0.91	0.11	35,40,40,50	0
3	EDO	A	506	4/4	0.92	0.10	31,31,32,34	0

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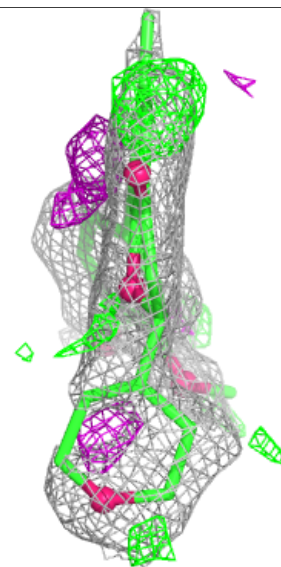
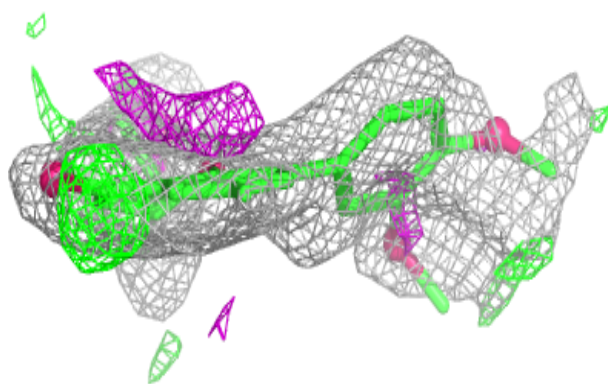
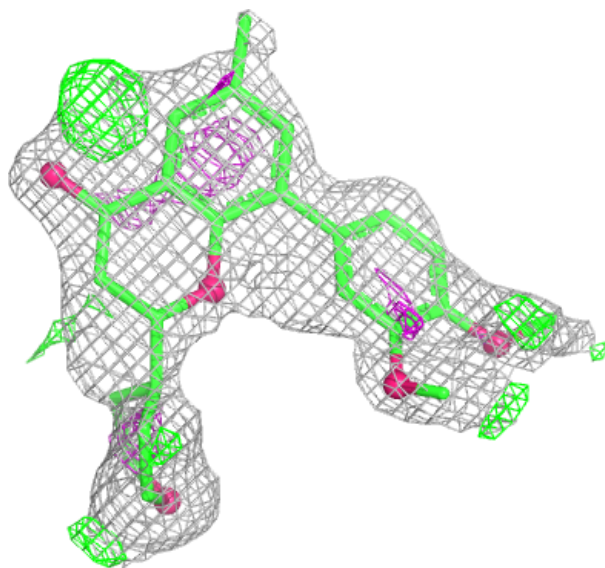
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	B	507	4/4	0.92	0.23	30,30,38,41	0
3	EDO	D	503	4/4	0.92	0.11	34,35,36,43	0
3	EDO	B	506	4/4	0.94	0.10	40,41,42,43	0
7	EPE	C	506	15/15	0.94	0.11	41,52,71,74	0
3	EDO	D	501	4/4	0.95	0.10	30,31,33,37	0
3	EDO	D	514	4/4	0.96	0.06	25,28,29,30	0
5	ZN	B	502	1/1	0.99	0.03	34,34,34,34	0
5	ZN	B	503	1/1	0.99	0.04	35,35,35,35	1
5	ZN	D	513	1/1	0.99	0.03	33,33,33,33	1
5	ZN	A	509	1/1	0.99	0.03	28,28,28,28	0
5	ZN	A	510	1/1	0.99	0.02	30,30,30,30	1
5	ZN	D	512	1/1	1.00	0.01	27,27,27,27	0
5	ZN	C	510	1/1	1.00	0.02	33,33,33,33	0
5	ZN	C	511	1/1	1.00	0.02	32,32,32,32	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

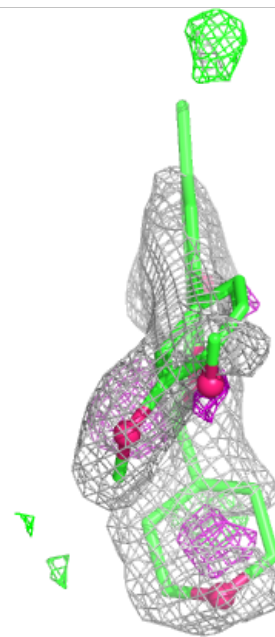
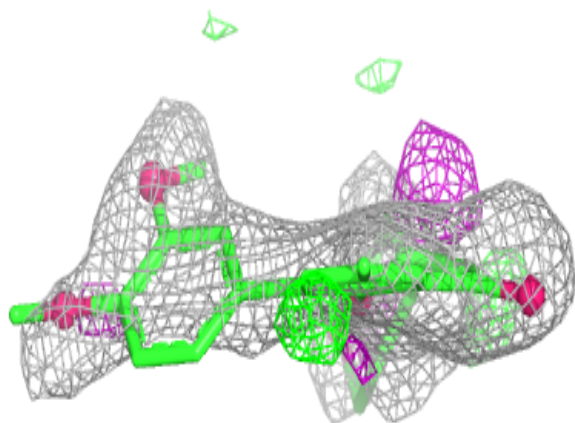
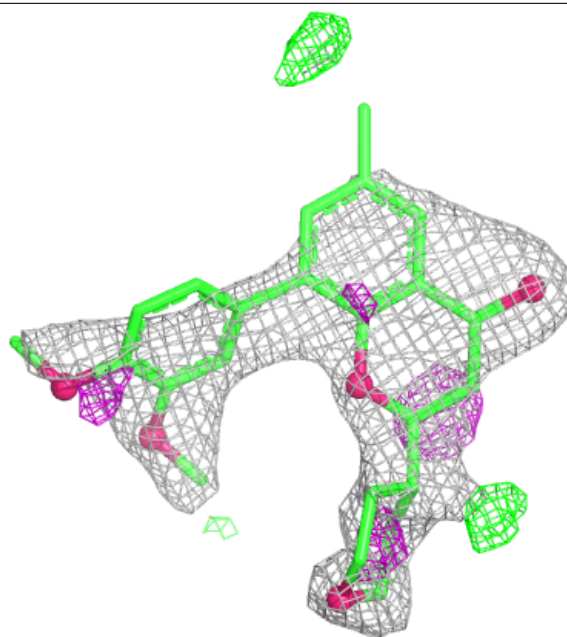
Electron density around 2SR B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



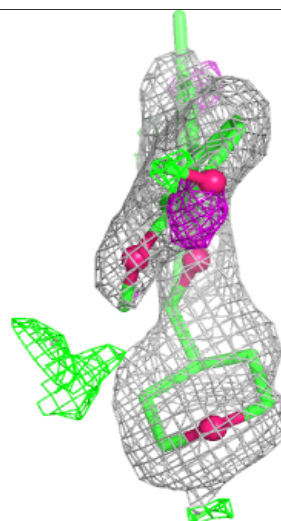
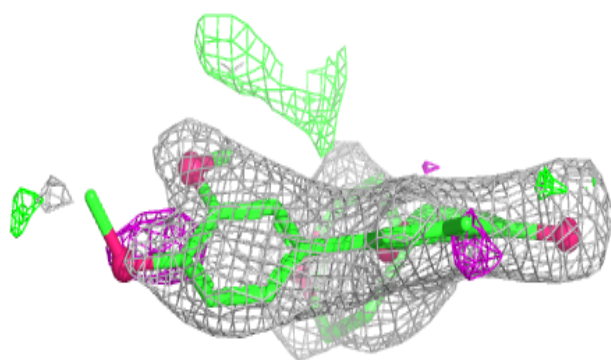
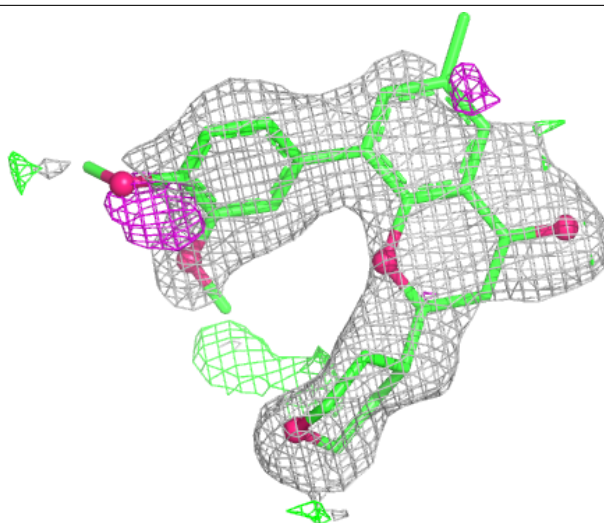
Electron density around 2SR A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



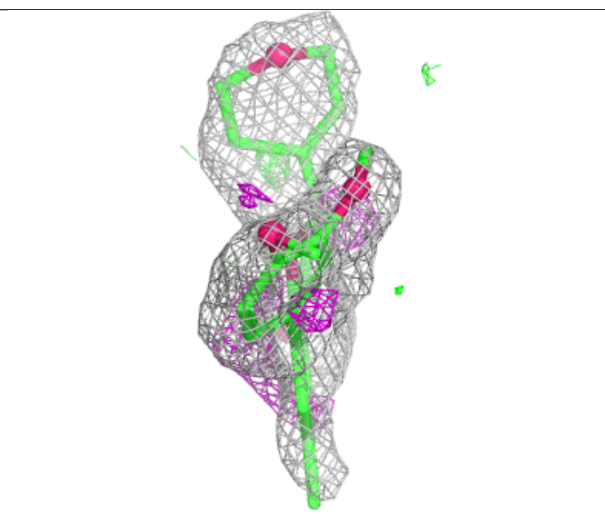
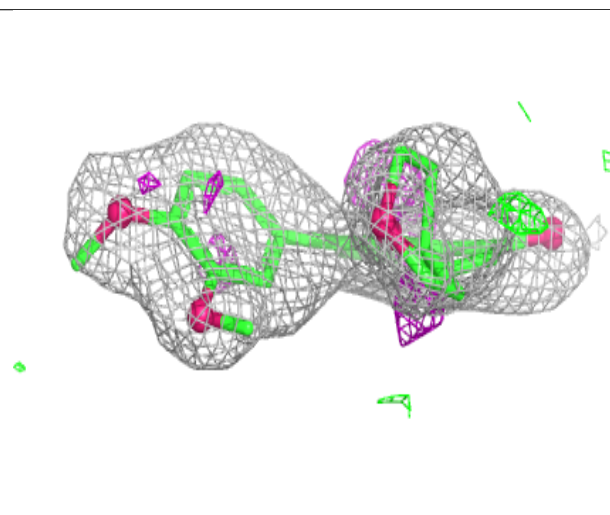
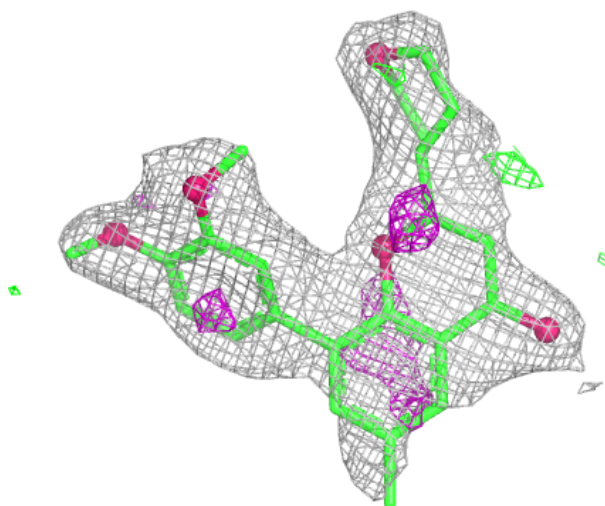
Electron density around 2SR C 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 2SR D 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.