



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 02:02 PM EDT

PDB ID : 3G4L  
Title : Crystal structure of human phosphodiesterase 4d with roflumilast  
Authors : Staker, B.L.  
Deposited on : 2009-02-03  
Resolution : 2.50 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](mailto: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.

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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) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

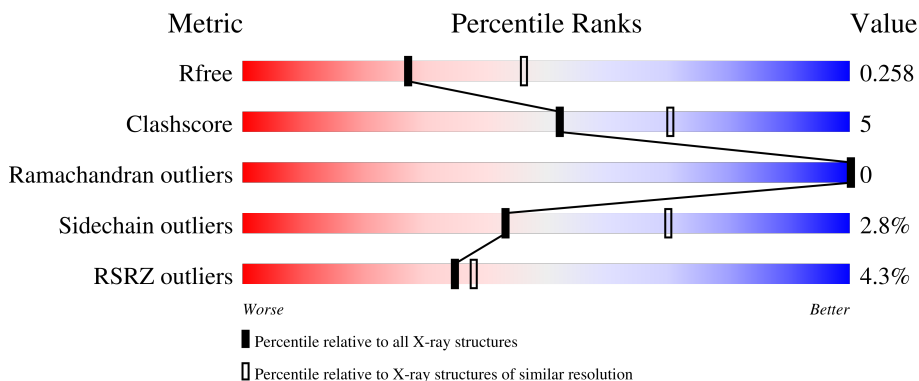
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	381	 3% 75% 9% • 14%
1	B	381	 4% 72% 13% • 14%
1	C	381	 3% 72% 12% • 14%
1	D	381	 4% 81% 7% • 12%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10942 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
			Total	C	N	O	S			
1	A	327	Total 2642	C 1673	N 451	O 504	S 14	0	0	0
1	B	326	Total 2615	C 1653	N 445	O 504	S 13	0	0	0
1	C	326	Total 2638	C 1668	N 450	O 506	S 14	0	0	0
1	D	334	Total 2694	C 1707	N 459	O 514	S 14	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	MET	-	expression tag	UNP Q08499
A	579	ALA	SER	engineered mutation	UNP Q08499
A	581	ALA	SER	engineered mutation	UNP Q08499
A	618	HIS	-	expression tag	UNP Q08499
A	619	HIS	-	expression tag	UNP Q08499
A	620	HIS	-	expression tag	UNP Q08499
A	621	HIS	-	expression tag	UNP Q08499
A	622	HIS	-	expression tag	UNP Q08499
A	623	HIS	-	expression tag	UNP Q08499
B	243	MET	-	expression tag	UNP Q08499
B	579	ALA	SER	engineered mutation	UNP Q08499
B	581	ALA	SER	engineered mutation	UNP Q08499
B	618	HIS	-	expression tag	UNP Q08499
B	619	HIS	-	expression tag	UNP Q08499
B	620	HIS	-	expression tag	UNP Q08499
B	621	HIS	-	expression tag	UNP Q08499
B	622	HIS	-	expression tag	UNP Q08499
B	623	HIS	-	expression tag	UNP Q08499
C	243	MET	-	expression tag	UNP Q08499
C	579	ALA	SER	engineered mutation	UNP Q08499
C	581	ALA	SER	engineered mutation	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
C	618	HIS	-	expression tag	UNP Q08499
C	619	HIS	-	expression tag	UNP Q08499
C	620	HIS	-	expression tag	UNP Q08499
C	621	HIS	-	expression tag	UNP Q08499
C	622	HIS	-	expression tag	UNP Q08499
C	623	HIS	-	expression tag	UNP Q08499
D	243	MET	-	expression tag	UNP Q08499
D	579	ALA	SER	engineered mutation	UNP Q08499
D	581	ALA	SER	engineered mutation	UNP Q08499
D	618	HIS	-	expression tag	UNP Q08499
D	619	HIS	-	expression tag	UNP Q08499
D	620	HIS	-	expression tag	UNP Q08499
D	621	HIS	-	expression tag	UNP Q08499
D	622	HIS	-	expression tag	UNP Q08499
D	623	HIS	-	expression tag	UNP Q08499

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

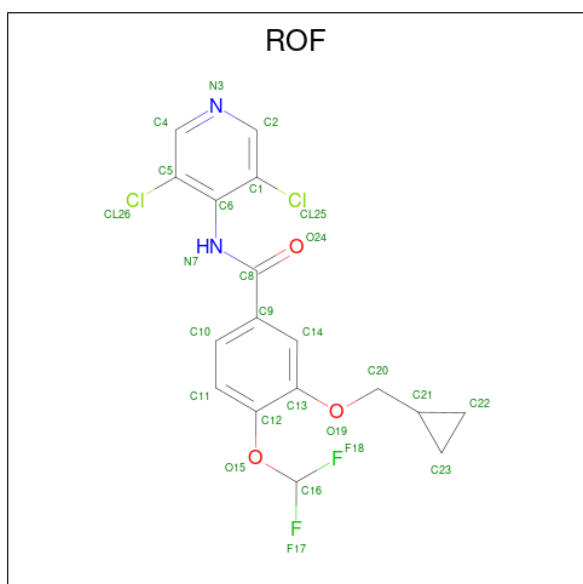
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



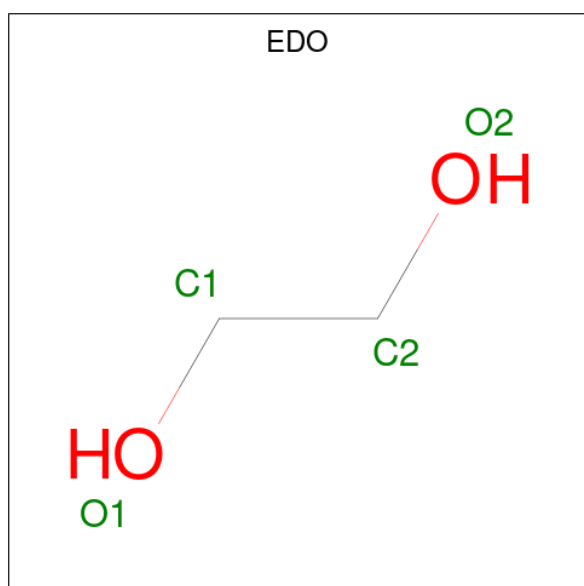
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is 3-(CYCLOPROPYLMETHOXY)-N-(3,5-DICHLOROPYRIDIN-4-YL)-4-(DIFLUOROMETHOXY)BENZAMIDE (three-letter code: ROF) (formula:  $C_{17}H_{14}Cl_2F_2N_2O_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	Cl	F	N	O	0	0
			26	17	2	2	2	3		
5	B	1	Total	C	Cl	F	N	O	0	0
			26	17	2	2	2	3		
5	C	1	Total	C	Cl	F	N	O	0	0
			26	17	2	2	2	3		
5	D	1	Total	C	Cl	F	N	O	0	0
			26	17	2	2	2	3		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

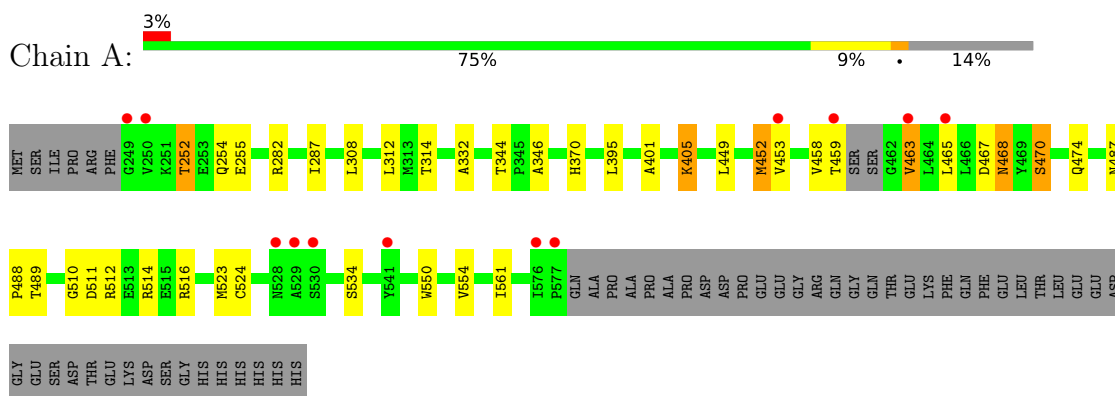
- Molecule 7 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	A	54	Total 54	O 54	0	0
7	B	38	Total 38	O 38	0	0
7	C	36	Total 36	O 36	0	0
7	D	61	Total 61	O 61	0	0

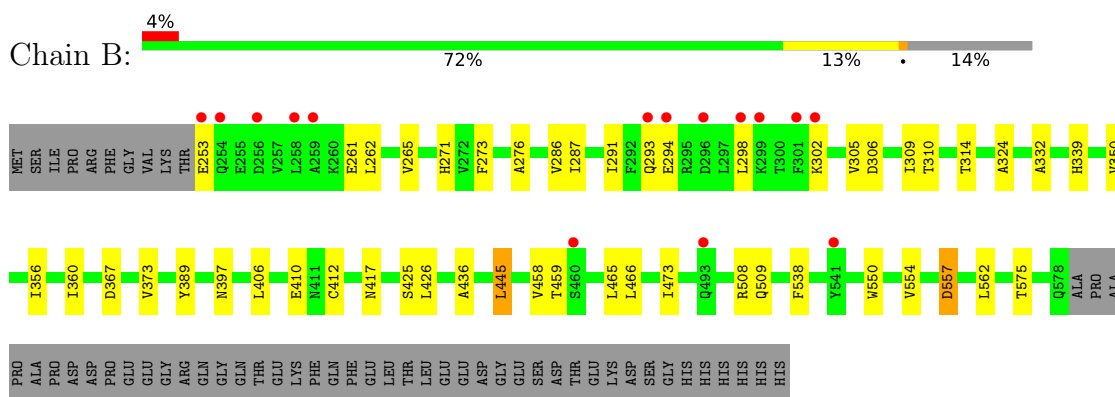
### 3 Residue-property plots [i](#)

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.

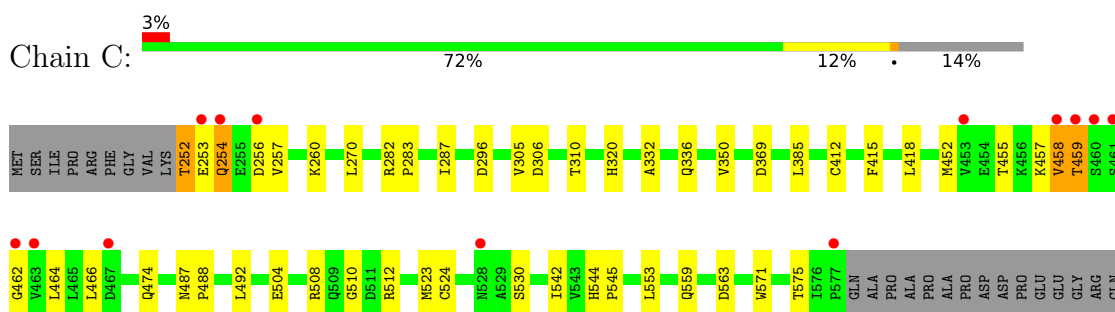
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



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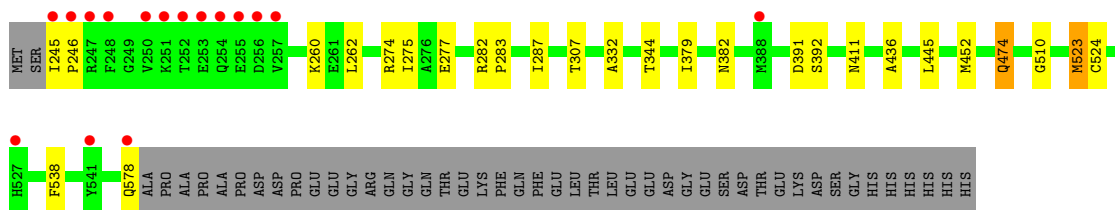




GLY  
GLN  
THR  
GLU  
LYS  
PHE  
GLN  
PHE  
GLU  
THR  
LEU  
LEU  
GLU  
GLU  
ASP  
GLY  
GLU  
SER  
SER  
ASP  
THR  
GLU  
LYS  
ASP  
SER  
GLY  
HIS  
HIS  
HIS  
HIS  
HIS

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

Chain D: 4% 81% 7% 12%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.67Å 111.95Å 161.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 48.56 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 99.4 (48.56-2.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.214 , 0.259 0.218 , 0.258	Depositor DCC
$R_{free}$ test set	3187 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtrriage
Anisotropy	0.077	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10942	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, MG, ZN, ROF, SO4

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	0.49	0/2695	0.57	0/3660
1	B	0.53	0/2669	0.63	1/3633 (0.0%)
1	C	0.49	0/2692	0.58	0/3658
1	D	0.51	0/2750	0.60	0/3737
All	All	0.51	0/10806	0.60	1/14688 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	ASP	CB-CG-OD1	6.74	124.36	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2642	0	2599	36	0
1	B	2615	0	2537	35	0
1	C	2638	0	2591	26	0
1	D	2694	0	2647	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	26	0	14	2	0
5	B	26	0	13	2	0
5	C	26	0	14	1	0
5	D	26	0	13	4	0
6	A	12	0	18	1	0
6	B	8	0	12	0	0
6	C	4	0	6	0	0
6	D	8	0	12	0	0
7	A	54	0	0	4	0
7	B	38	0	0	1	0
7	C	36	0	0	0	0
7	D	61	0	0	0	0
All	All	10942	0	10476	116	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 (116) 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:B:262:LEU:O	1:B:265:VAL:HG23	1.72	0.88
1:A:452:MET:CE	1:A:474:GLN:HE21	1.97	0.77
1:B:410:GLU:HB3	7:B:113:HOH:O	1.87	0.73
5:D:904:ROF:CL25	5:D:904:ROF:O24	2.43	0.73
5:A:901:ROF:CL25	5:A:901:ROF:O24	2.45	0.72
1:B:356:ILE:O	1:B:360:ILE:HD12	1.89	0.72
1:B:459:THR:HG22	1:B:465:LEU:HD13	1.71	0.72
1:A:452:MET:HE1	1:A:474:GLN:HE21	1.55	0.71
1:B:554:VAL:O	1:B:557:ASP:OD1	2.09	0.70
1:A:452:MET:HE1	1:A:474:GLN:HB3	1.76	0.68
1:A:523:MET:CE	1:A:534:SER:OG	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:MET:HE1	1:A:534:SER:OG	1.98	0.63
1:A:252:THR:CG2	1:A:255:GLU:H	2.12	0.62
1:C:464:LEU:HD21	1:C:553:LEU:HD11	1.82	0.61
7:A:47:HOH:O	1:C:512:ARG:HD2	2.01	0.60
1:B:287:ILE:HD12	1:B:332:ALA:HB1	1.82	0.60
1:B:550:TRP:O	1:B:554:VAL:HG22	2.03	0.59
1:B:350:VAL:HG11	1:B:466:LEU:HD12	1.84	0.58
1:D:538:PHE:CG	5:D:904:ROF:H202	2.38	0.58
5:C:903:ROF:O24	5:C:903:ROF:CL25	2.60	0.56
1:A:452:MET:HE2	1:A:474:GLN:HE21	1.71	0.56
1:B:262:LEU:O	1:B:265:VAL:CG2	2.50	0.56
1:A:523:MET:HE2	1:A:534:SER:CB	2.36	0.56
1:B:436:ALA:HB1	1:B:445:LEU:HD21	1.88	0.55
1:D:262:LEU:HD23	1:D:275:ILE:HD13	1.87	0.55
1:C:504:GLU:OE2	1:C:508:ARG:NH2	2.39	0.55
1:C:459:THR:O	1:C:462:GLY:N	2.40	0.55
1:A:308:LEU:O	1:A:312:LEU:HG	2.07	0.54
1:B:314:THR:HG22	1:B:406:LEU:HD22	1.89	0.54
1:A:516:ARG:HD3	7:A:138:HOH:O	2.08	0.53
1:A:252:THR:HG22	1:A:255:GLU:H	1.73	0.53
1:A:523:MET:HE1	7:A:86:HOH:O	2.08	0.53
1:B:262:LEU:HD11	1:B:286:VAL:CG1	2.39	0.53
1:B:291:ILE:HD13	1:B:339:HIS:HB2	1.92	0.52
1:B:324:ALA:HB2	1:B:508:ARG:HH21	1.73	0.52
1:B:305:VAL:O	1:B:309:ILE:HD12	2.11	0.51
1:A:252:THR:HG22	1:A:255:GLU:CG	2.41	0.51
1:C:252:THR:HG22	1:C:254:GLN:HE22	1.76	0.51
1:A:510:GLY:HA3	1:A:524:CYS:O	2.11	0.50
1:B:309:ILE:HD12	1:B:309:ILE:H	1.77	0.50
1:B:538:PHE:CG	5:B:902:ROF:H202	2.47	0.50
1:C:492:LEU:HD21	1:C:571:TRP:CD2	2.47	0.50
1:C:510:GLY:HA3	1:C:524:CYS:O	2.12	0.50
1:C:287:ILE:HD12	1:C:332:ALA:HB1	1.93	0.50
1:D:379:ILE:HG23	1:D:391:ASP:OD1	2.12	0.49
1:B:262:LEU:HD11	1:B:286:VAL:HG12	1.95	0.49
1:D:523:MET:HG2	5:D:904:ROF:C22	2.42	0.49
1:D:262:LEU:CD2	1:D:275:ILE:HD13	2.43	0.49
1:A:252:THR:HG22	1:A:255:GLU:HG3	1.95	0.48
1:C:350:VAL:CG1	1:C:466:LEU:HD12	2.44	0.48
1:B:310:THR:HG22	1:B:412:CYS:SG	2.53	0.48
1:B:305:VAL:HG13	1:B:306:ASP:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:PHE:O	1:B:276:ALA:HB3	2.13	0.47
1:D:245:ILE:N	1:D:246:PRO:CD	2.78	0.47
1:A:252:THR:HG23	1:A:255:GLU:H	1.80	0.47
1:A:512:ARG:O	1:A:516:ARG:HD2	2.14	0.46
1:B:350:VAL:CG1	1:B:466:LEU:HD12	2.45	0.46
1:B:309:ILE:HD12	1:B:309:ILE:N	2.30	0.46
1:C:270:LEU:HD22	1:C:336:GLN:HG3	1.96	0.46
1:A:287:ILE:HD12	1:A:332:ALA:HB1	1.98	0.46
1:D:287:ILE:HD12	1:D:332:ALA:HB1	1.98	0.46
5:B:902:ROF:CL25	5:B:902:ROF:O24	2.71	0.46
1:D:274:ARG:NH1	1:D:277:GLU:OE1	2.49	0.46
1:A:449:LEU:O	1:A:453:VAL:HG23	2.16	0.45
1:B:314:THR:CG2	1:B:406:LEU:HD22	2.46	0.45
1:B:324:ALA:HB2	1:B:508:ARG:NH2	2.31	0.45
1:C:575:THR:O	1:C:575:THR:HG22	2.17	0.45
1:A:314:THR:HG23	6:A:6:EDO:H12	1.97	0.44
1:B:426:LEU:C	1:B:426:LEU:HD23	2.37	0.44
1:B:261:GLU:OE1	1:B:271:HIS:ND1	2.50	0.44
1:C:282:ARG:N	1:C:283:PRO:CD	2.81	0.44
1:A:487:ASN:HB2	1:A:488:PRO:HD3	2.00	0.44
1:A:523:MET:CE	7:A:86:HOH:O	2.66	0.44
1:C:415:PHE:HA	1:C:418:LEU:HD13	1.99	0.44
1:C:320:HIS:HE1	1:C:369:ASP:OD1	2.01	0.43
1:C:542:ILE:HD12	1:C:542:ILE:N	2.33	0.43
1:C:559:GLN:HE21	1:C:563:ASP:CG	2.21	0.43
1:C:310:THR:HG22	1:C:412:CYS:SG	2.58	0.43
1:C:457:LYS:O	1:C:464:LEU:HD12	2.19	0.43
1:B:305:VAL:HG13	1:B:306:ASP:H	1.84	0.43
1:D:510:GLY:HA3	1:D:524:CYS:O	2.19	0.43
1:A:489:THR:HB	1:A:561:ILE:HG23	2.00	0.43
1:C:253:GLU:O	1:C:257:VAL:HG23	2.19	0.43
1:C:487:ASN:HB2	1:C:488:PRO:HD3	2.00	0.43
1:A:346:ALA:O	1:A:463:VAL:HG22	2.19	0.43
1:C:350:VAL:HG11	1:C:466:LEU:HD12	2.01	0.43
1:C:452:MET:HE1	1:C:474:GLN:CB	2.48	0.43
1:C:544:HIS:HB3	1:C:545:PRO:HD3	2.00	0.43
1:A:523:MET:HG3	5:A:901:ROF:H221	2.01	0.43
1:C:458:VAL:HG23	1:C:459:THR:C	2.39	0.43
1:B:298:LEU:O	1:B:302:LYS:N	2.52	0.42
1:D:245:ILE:N	1:D:246:PRO:HD2	2.33	0.42
1:C:305:VAL:HG13	1:C:306:ASP:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:MET:HE2	1:A:534:SER:HB3	2.00	0.42
1:D:452:MET:CE	1:D:474:GLN:HE21	2.33	0.42
5:D:904:ROF:CL25	5:D:904:ROF:C8	3.04	0.42
1:C:492:LEU:HD21	1:C:571:TRP:CE2	2.54	0.42
1:A:370:HIS:NE2	1:A:395:LEU:HD13	2.34	0.42
1:A:252:THR:HG23	1:A:254:GLN:N	2.35	0.42
1:A:550:TRP:O	1:A:554:VAL:HG22	2.20	0.41
1:B:293:GLN:O	1:B:294:GLU:C	2.58	0.41
1:B:473:ILE:HD12	1:B:473:ILE:HA	1.87	0.41
1:A:401:ALA:O	1:A:405:LYS:HB2	2.19	0.41
1:D:436:ALA:HB1	1:D:445:LEU:HD11	2.01	0.41
1:A:458:VAL:HG23	1:A:459:THR:N	2.36	0.41
1:A:470:SER:O	1:A:474:GLN:HB2	2.21	0.41
1:A:452:MET:HE2	1:A:474:GLN:NE2	2.34	0.41
1:B:302:LYS:O	1:B:417:ASN:ND2	2.41	0.41
1:B:389:TYR:CE2	1:B:397:ASN:HB3	2.56	0.41
1:D:282:ARG:N	1:D:283:PRO:CD	2.84	0.41
1:A:467:ASP:HB2	1:A:468:ASN:HD22	1.86	0.41
1:A:511:ASP:OD1	1:A:514:ARG:NH2	2.54	0.41
1:A:523:MET:HB3	1:A:523:MET:HE3	1.72	0.41
1:B:373:VAL:HA	1:B:509:GLN:OE1	2.21	0.40
1:D:307:THR:HG23	1:D:411:ASN:O	2.22	0.40
1:B:575:THR:O	1:B:575:THR:HG22	2.22	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	323/381 (85%)	317 (98%)	6 (2%)	0	100	100
1	B	324/381 (85%)	309 (95%)	15 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	324/381 (85%)	315 (97%)	9 (3%)	0	100	100
1	D	332/381 (87%)	326 (98%)	6 (2%)	0	100	100
All	All	1303/1524 (86%)	1267 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	297/345 (86%)	288 (97%)	9 (3%)	41	68
1	B	292/345 (85%)	286 (98%)	6 (2%)	53	78
1	C	298/345 (86%)	287 (96%)	11 (4%)	34	60
1	D	303/345 (88%)	296 (98%)	7 (2%)	50	76
All	All	1190/1380 (86%)	1157 (97%)	33 (3%)	43	70

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

Mol	Chain	Res	Type
1	A	252	THR
1	A	282	ARG
1	A	344	THR
1	A	405	LYS
1	A	452	MET
1	A	463	VAL
1	A	465	LEU
1	A	468	ASN
1	A	470	SER
1	B	253	GLU
1	B	425	SER
1	B	445	LEU
1	B	458	VAL
1	B	557	ASP

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Mol	Chain	Res	Type
1	B	562	LEU
1	C	252	THR
1	C	254	GLN
1	C	256	ASP
1	C	260	LYS
1	C	296	ASP
1	C	385	LEU
1	C	455	THR
1	C	458	VAL
1	C	459	THR
1	C	523	MET
1	C	530	SER
1	D	260	LYS
1	D	344	THR
1	D	382	ASN
1	D	392	SER
1	D	474	GLN
1	D	523	MET
1	D	578	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	411	ASN
1	A	474	GLN
1	B	289	HIS
1	B	411	ASN
1	B	416	GLN
1	C	320	HIS
1	C	411	ASN
1	C	424	GLN
1	C	444	ASN
1	C	559	GLN
1	D	289	HIS
1	D	293	GLN
1	D	411	ASN
1	D	416	GLN
1	D	474	GLN

### 5.3.3 RNA [i](#)

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	B	624	-	3,3,3	0.45	0	2,2,2	0.30	0
6	EDO	C	5	-	3,3,3	0.46	0	2,2,2	0.38	0
6	EDO	A	9	-	3,3,3	0.42	0	2,2,2	0.39	0
4	SO4	B	3	-	4,4,4	0.12	0	6,6,6	0.32	0
4	SO4	C	2	-	4,4,4	0.13	0	6,6,6	0.33	0
5	ROF	C	903	-	28,28,28	1.30	3 (10%)	39,39,39	1.83	10 (25%)
5	ROF	A	901	-	28,28,28	1.03	2 (7%)	39,39,39	1.89	9 (23%)
5	ROF	B	902	-	28,28,28	1.01	2 (7%)	39,39,39	1.66	11 (28%)
5	ROF	D	904	-	28,28,28	1.07	2 (7%)	39,39,39	2.08	15 (38%)
6	EDO	A	6	-	3,3,3	0.44	0	2,2,2	0.30	0
4	SO4	A	4	-	4,4,4	0.19	0	6,6,6	0.26	0
6	EDO	D	10	-	3,3,3	0.43	0	2,2,2	0.25	0
4	SO4	D	1	-	4,4,4	0.11	0	6,6,6	0.54	0
6	EDO	D	2	-	3,3,3	0.50	0	2,2,2	0.21	0
6	EDO	B	8	-	3,3,3	0.48	0	2,2,2	0.22	0
6	EDO	A	7	-	3,3,3	0.52	0	2,2,2	0.26	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	B	624	-	-	1/1/1/1	-
6	EDO	C	5	-	-	0/1/1/1	-
6	EDO	A	9	-	-	0/1/1/1	-
5	ROF	C	903	-	-	5/17/19/19	0/3/3/3
5	ROF	A	901	-	-	5/17/19/19	0/3/3/3
5	ROF	B	902	-	-	5/17/19/19	0/3/3/3
5	ROF	D	904	-	-	6/17/19/19	0/3/3/3
6	EDO	A	6	-	-	1/1/1/1	-
6	EDO	D	10	-	-	1/1/1/1	-
6	EDO	D	2	-	-	0/1/1/1	-
6	EDO	B	8	-	-	0/1/1/1	-
6	EDO	A	7	-	-	0/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	903	ROF	C1-CL25	3.21	1.81	1.73
5	C	903	ROF	C6-N7	-3.08	1.37	1.43
5	B	902	ROF	C6-N7	-3.03	1.37	1.43
5	D	904	ROF	C6-N7	-2.86	1.38	1.43
5	C	903	ROF	C5-CL26	2.86	1.80	1.73
5	A	901	ROF	C1-CL25	2.62	1.79	1.73
5	D	904	ROF	C1-CL25	2.61	1.79	1.73
5	A	901	ROF	C6-N7	-2.42	1.38	1.43
5	B	902	ROF	C5-CL26	2.31	1.79	1.73

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	ROF	C1-C6-N7	5.37	127.56	121.14
5	D	904	ROF	C1-C6-N7	5.04	127.17	121.14
5	C	903	ROF	C5-C6-N7	-4.60	115.64	121.14
5	C	903	ROF	C1-C6-N7	4.44	126.45	121.14
5	A	901	ROF	O24-C8-C9	-4.38	113.13	120.94
5	D	904	ROF	C5-C6-N7	-4.07	116.28	121.14
5	D	904	ROF	O24-C8-C9	-3.99	113.83	120.94
5	C	903	ROF	C6-C1-CL25	3.97	123.82	119.27
5	A	901	ROF	C5-C6-N7	-3.92	116.45	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	904	ROF	C22-C21-C20	3.86	140.47	119.43
5	A	901	ROF	C6-C1-CL25	3.75	123.57	119.27
5	D	904	ROF	C23-C21-C20	3.69	139.57	119.43
5	C	903	ROF	O24-C8-C9	-3.65	114.43	120.94
5	A	901	ROF	C9-C8-N7	3.47	123.56	115.92
5	C	903	ROF	C9-C8-N7	3.44	123.50	115.92
5	D	904	ROF	C9-C8-N7	3.42	123.44	115.92
5	B	902	ROF	C2-C1-C6	3.40	122.03	120.16
5	B	902	ROF	C23-C21-C20	3.38	137.86	119.43
5	B	902	ROF	C1-C2-N3	-3.33	119.94	122.85
5	A	901	ROF	C4-C5-C6	3.20	121.91	120.16
5	B	902	ROF	O24-C8-C9	-3.14	115.34	120.94
5	B	902	ROF	C22-C21-C20	3.05	136.05	119.43
5	D	904	ROF	C4-C5-C6	3.04	121.83	120.16
5	D	904	ROF	C5-C4-N3	-2.70	120.50	122.85
5	D	904	ROF	C6-C1-CL25	2.67	122.33	119.27
5	B	902	ROF	C1-C6-N7	2.66	124.32	121.14
5	A	901	ROF	C20-O19-C13	2.59	124.02	118.27
5	C	903	ROF	C4-C5-CL26	2.58	122.10	118.60
5	B	902	ROF	C5-C4-N3	-2.47	120.70	122.85
5	D	904	ROF	C6-C5-CL26	-2.39	116.54	119.27
5	A	901	ROF	C1-C2-N3	-2.38	120.77	122.85
5	D	904	ROF	C12-O15-C16	2.36	127.12	118.77
5	B	902	ROF	C2-N3-C4	2.36	120.71	117.48
5	A	901	ROF	C2-C1-CL25	-2.36	115.38	118.60
5	C	903	ROF	C1-C2-N3	-2.35	120.80	122.85
5	C	903	ROF	C20-O19-C13	2.33	123.45	118.27
5	D	904	ROF	O19-C13-C14	-2.32	118.25	123.58
5	B	902	ROF	C9-C8-N7	2.26	120.89	115.92
5	D	904	ROF	O19-C13-C12	2.25	120.37	115.73
5	D	904	ROF	C4-C5-CL26	2.23	121.63	118.60
5	C	903	ROF	C5-C4-N3	-2.21	120.92	122.85
5	B	902	ROF	C4-C5-CL26	2.18	121.56	118.60
5	C	903	ROF	C2-N3-C4	2.11	120.35	117.48
5	D	904	ROF	C1-C2-N3	-2.10	121.01	122.85
5	B	902	ROF	C5-C6-N7	-2.05	118.69	121.14

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	901	ROF	C5-C6-N7-C8

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Mol	Chain	Res	Type	Atoms
5	A	901	ROF	C1-C6-N7-C8
5	B	902	ROF	O19-C20-C21-C23
5	B	902	ROF	C1-C6-N7-C8
5	C	903	ROF	C1-C6-N7-C8
5	D	904	ROF	O19-C20-C21-C22
5	D	904	ROF	C5-C6-N7-C8
5	D	904	ROF	C1-C6-N7-C8
5	C	903	ROF	C5-C6-N7-C8
6	A	6	EDO	O1-C1-C2-O2
5	C	903	ROF	C21-C20-O19-C13
5	C	903	ROF	C12-C13-O19-C20
5	A	901	ROF	O19-C20-C21-C23
5	D	904	ROF	O19-C20-C21-C23
5	A	901	ROF	C21-C20-O19-C13
5	D	904	ROF	C12-C13-O19-C20
5	B	902	ROF	C12-C13-O19-C20
5	C	903	ROF	C14-C13-O19-C20
6	B	624	EDO	O1-C1-C2-O2
6	D	10	EDO	O1-C1-C2-O2
5	D	904	ROF	C14-C13-O19-C20
5	B	902	ROF	C14-C13-O19-C20
5	A	901	ROF	O19-C20-C21-C22
5	B	902	ROF	O19-C20-C21-C22

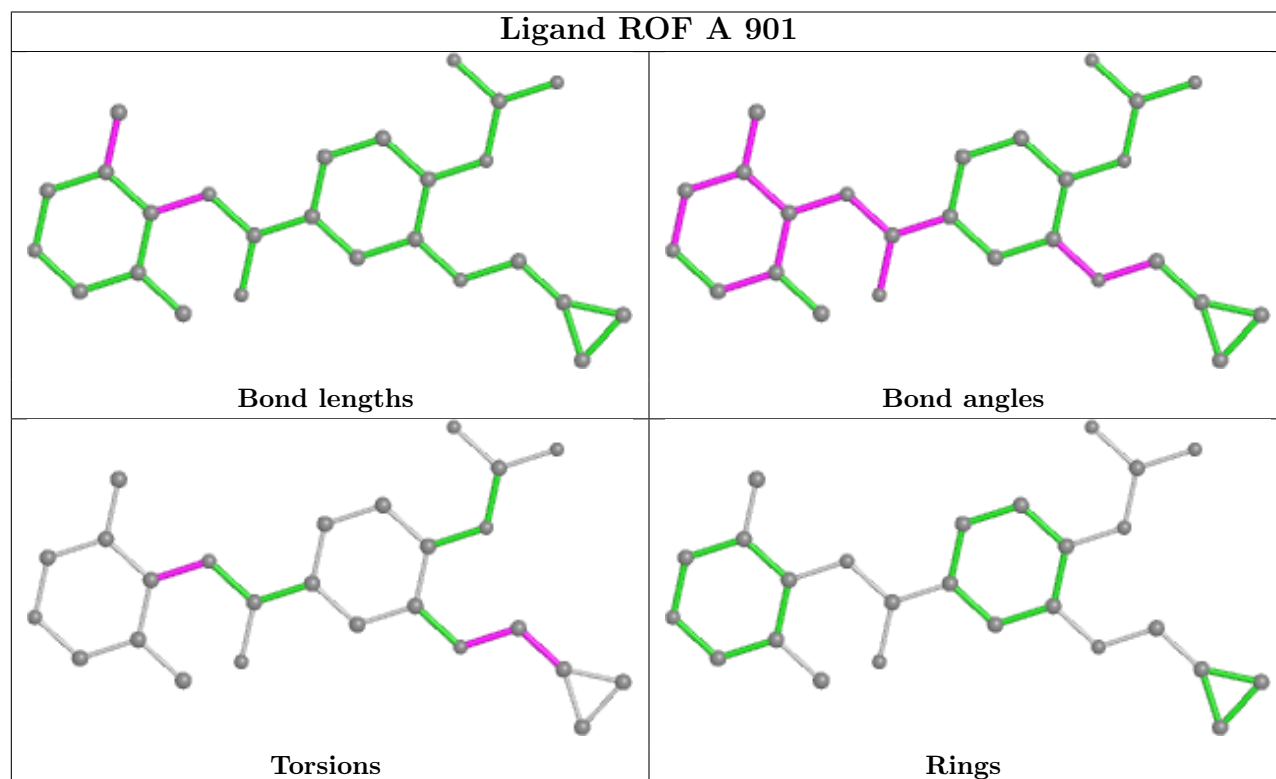
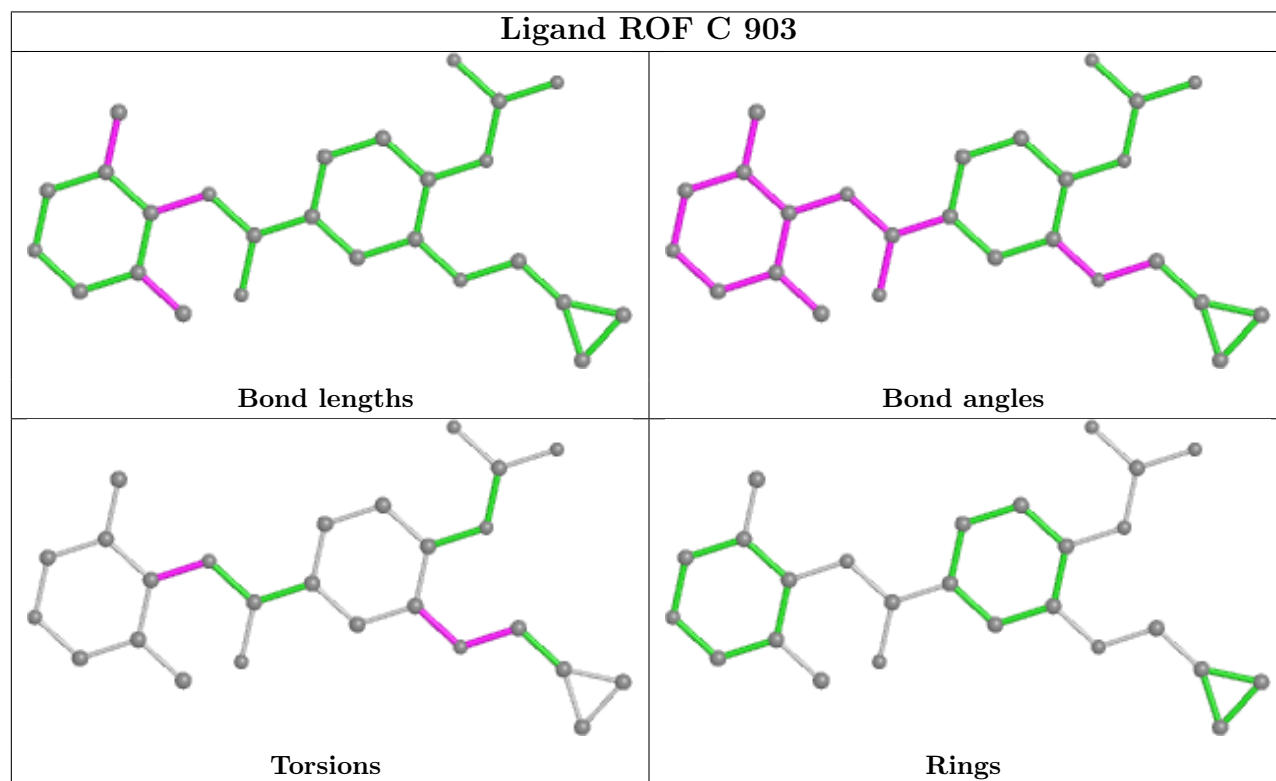
There are no ring outliers.

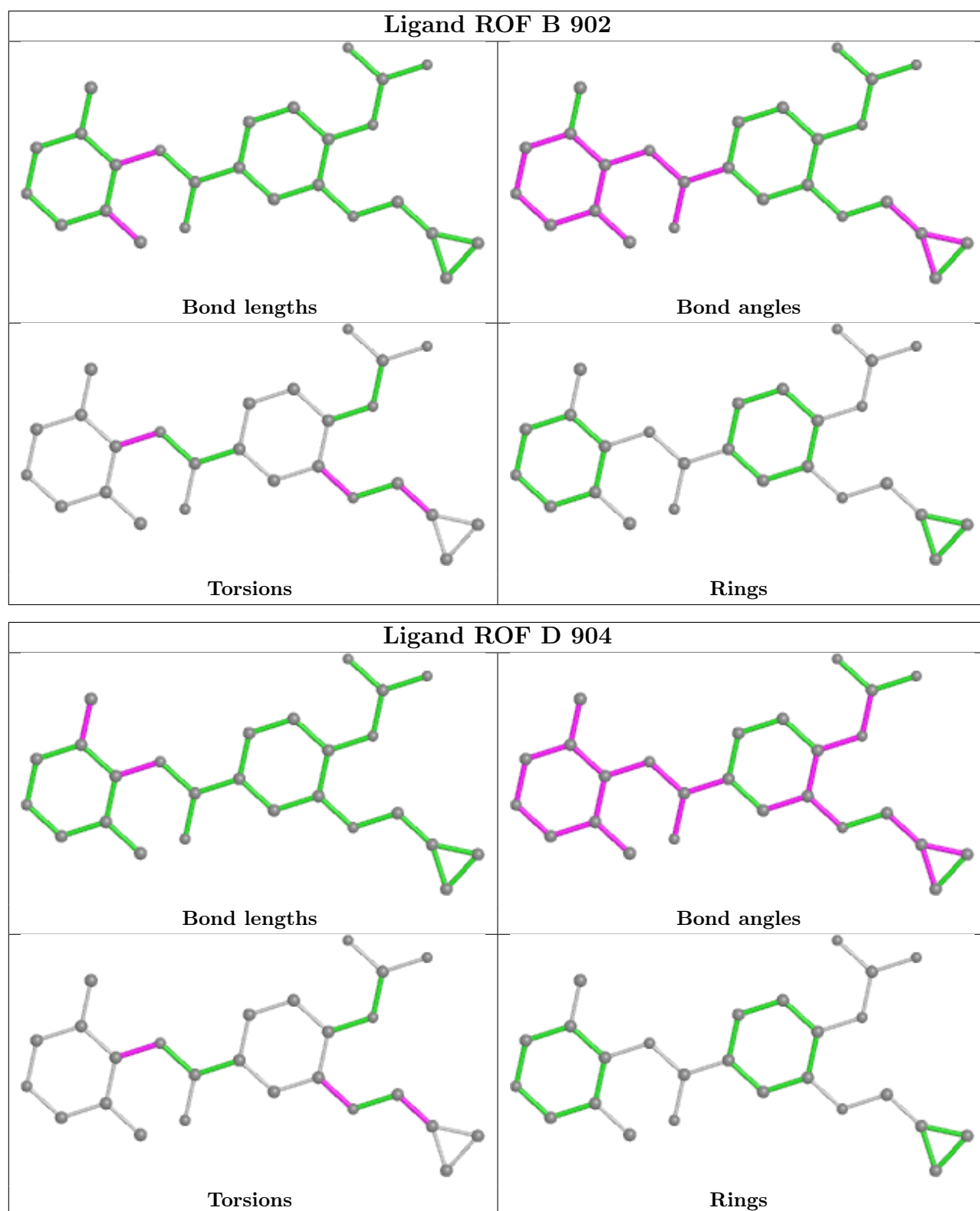
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	903	ROF	1	0
5	A	901	ROF	2	0
5	B	902	ROF	2	0
5	D	904	ROF	4	0
6	A	6	EDO	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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	327/381 (85%)	0.24	12 (3%) 41 45	18, 30, 47, 55	0
1	B	326/381 (85%)	0.23	15 (4%) 32 34	19, 31, 48, 75	0
1	C	326/381 (85%)	0.17	13 (3%) 38 41	19, 31, 49, 69	0
1	D	334/381 (87%)	0.23	16 (4%) 30 32	18, 30, 49, 88	0
All	All	1313/1524 (86%)	0.22	56 (4%) 35 38	18, 31, 48, 88	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	460	SER	7.4
1	D	245	ILE	5.4
1	D	252	THR	5.4
1	D	253	GLU	5.0
1	D	250	VAL	4.9
1	A	577	PRO	4.8
1	D	248	PHE	4.2
1	C	254	GLN	4.0
1	C	528	ASN	3.7
1	A	249	GLY	3.7
1	B	254	GLN	3.6
1	B	258	LEU	3.6
1	C	463	VAL	3.5
1	D	255	GLU	3.5
1	D	251	LYS	3.4
1	D	246	PRO	3.3
1	C	461	SER	3.2
1	D	247	ARG	3.2
1	C	459	THR	3.2
1	B	302	LYS	3.1
1	D	254	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	250	VAL	3.0
1	A	576	ILE	3.0
1	B	299	LYS	2.9
1	A	453	VAL	2.9
1	D	256	ASP	2.8
1	C	462	GLY	2.8
1	B	296	ASP	2.8
1	B	256	ASP	2.8
1	A	530	SER	2.7
1	B	253	GLU	2.7
1	B	301	PHE	2.6
1	D	578	GLN	2.6
1	D	541	TYR	2.6
1	A	459	THR	2.6
1	C	256	ASP	2.6
1	C	467	ASP	2.6
1	A	541	TYR	2.5
1	D	388	MET	2.4
1	B	298	LEU	2.4
1	B	293	GLN	2.4
1	A	465	LEU	2.4
1	C	253	GLU	2.4
1	C	577	PRO	2.3
1	C	458	VAL	2.3
1	A	463	VAL	2.3
1	B	541	TYR	2.3
1	C	453	VAL	2.3
1	A	529	ALA	2.3
1	A	528	ASN	2.2
1	B	460	SER	2.2
1	B	259	ALA	2.2
1	B	294	GLU	2.1
1	B	493	GLN	2.1
1	D	527	HIS	2.0
1	D	257	VAL	2.0

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

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

### 6.3 Carbohydrates [i](#)

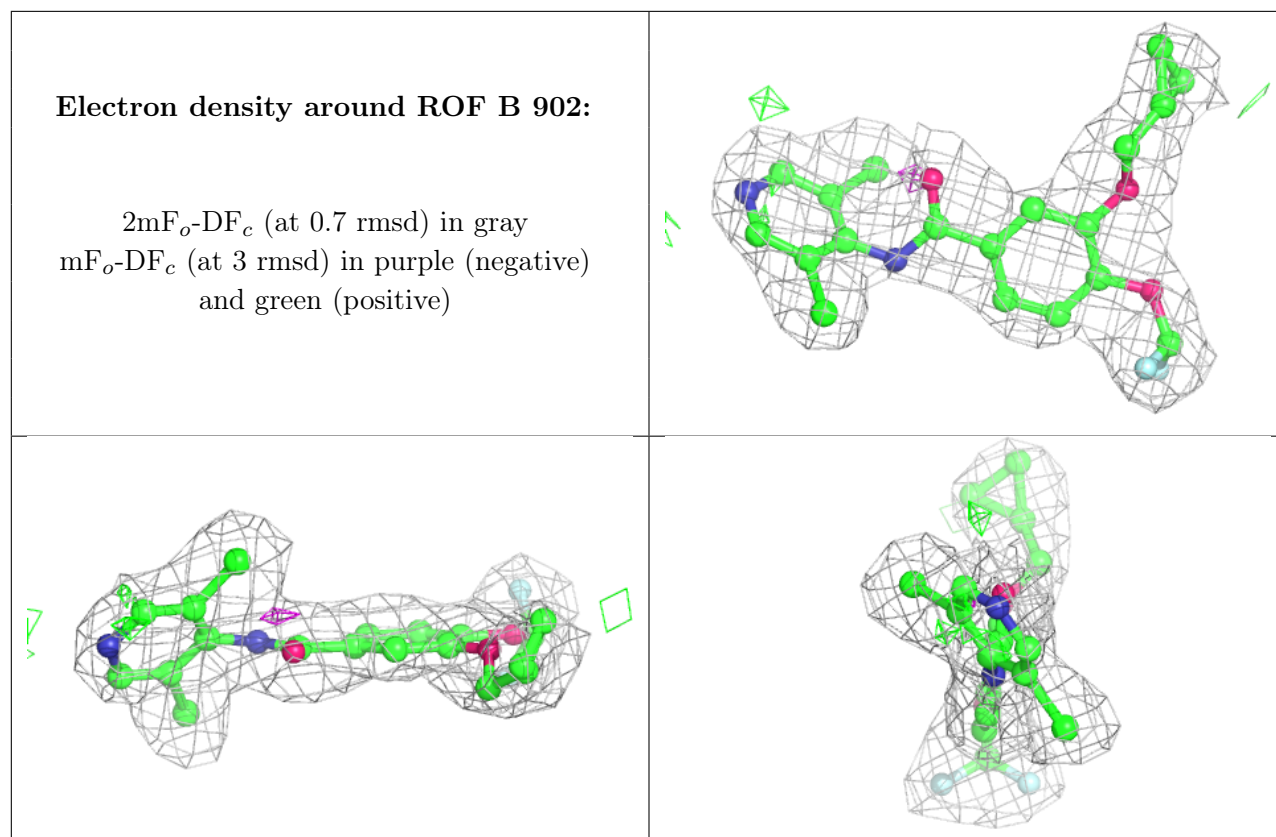
There are no monosaccharides in this entry.

### 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, 95<sup>th</sup> 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.

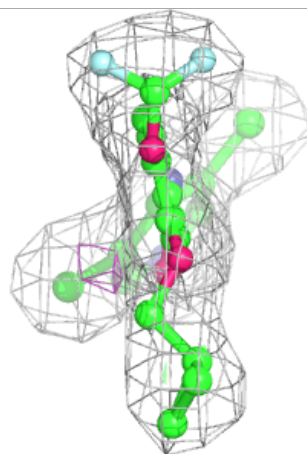
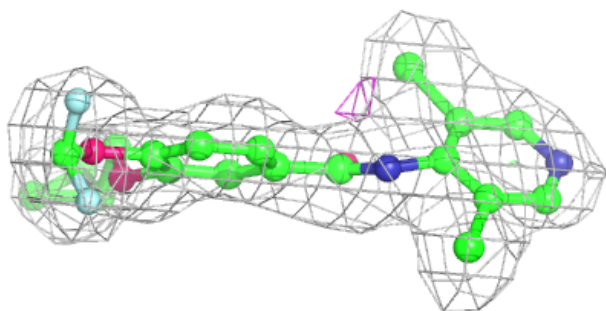
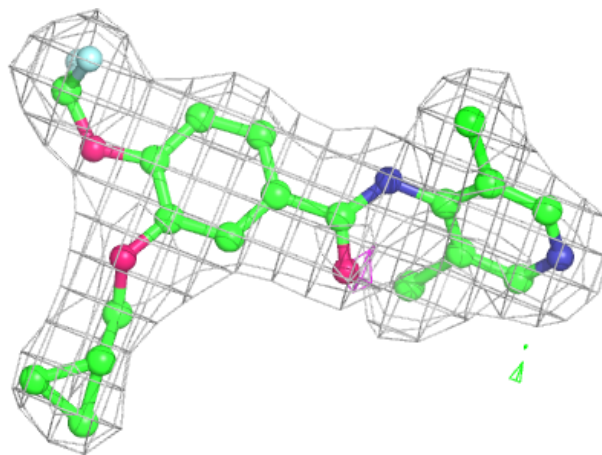
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	EDO	A	7	4/4	0.81	0.34	41,42,42,44	0
6	EDO	C	5	4/4	0.89	0.20	41,41,42,43	0
3	MG	B	804	1/1	0.91	0.18	27,27,27,27	0
5	ROF	B	902	26/26	0.92	0.17	35,37,43,46	0
6	EDO	B	624	4/4	0.92	0.22	37,38,38,38	0
6	EDO	B	8	4/4	0.92	0.19	47,47,47,47	0
5	ROF	C	903	26/26	0.92	0.19	34,35,41,41	0
5	ROF	A	901	26/26	0.93	0.20	34,36,40,40	0
6	EDO	A	6	4/4	0.93	0.23	31,32,33,33	0
6	EDO	D	2	4/4	0.93	0.16	34,36,37,37	0
6	EDO	A	9	4/4	0.94	0.24	49,50,50,50	0
5	ROF	D	904	26/26	0.95	0.17	28,33,38,40	0
4	SO4	B	3	5/5	0.95	0.18	67,68,69,69	0
6	EDO	D	10	4/4	0.96	0.23	31,32,32,34	0
4	SO4	D	1	5/5	0.97	0.16	50,51,52,53	0
4	SO4	C	2	5/5	0.98	0.14	54,54,55,55	0
4	SO4	A	4	5/5	0.98	0.18	48,49,50,50	0
3	MG	A	802	1/1	0.99	0.10	19,19,19,19	0
2	ZN	B	803	1/1	0.99	0.09	25,25,25,25	0
3	MG	C	806	1/1	0.99	0.13	18,18,18,18	0
3	MG	D	808	1/1	0.99	0.10	16,16,16,16	0
2	ZN	D	807	1/1	1.00	0.12	20,20,20,20	0
2	ZN	A	801	1/1	1.00	0.11	20,20,20,20	0
2	ZN	C	805	1/1	1.00	0.11	21,21,21,21	0

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.



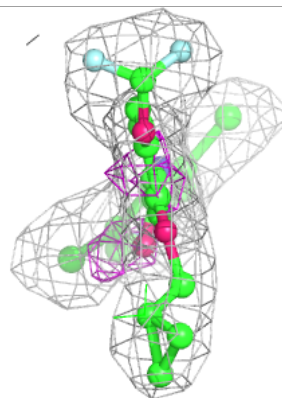
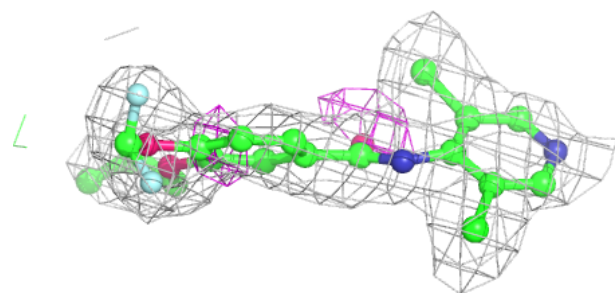
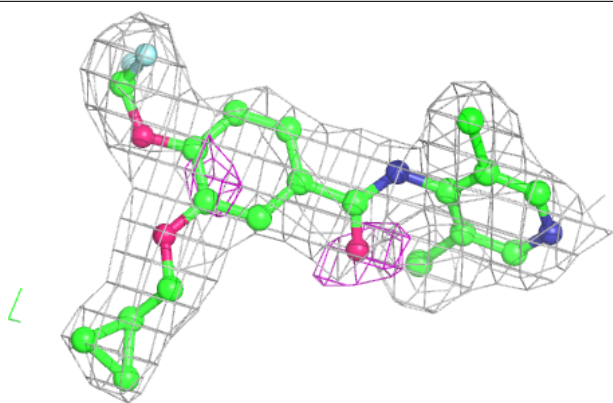
**Electron density around ROF C 903:**

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

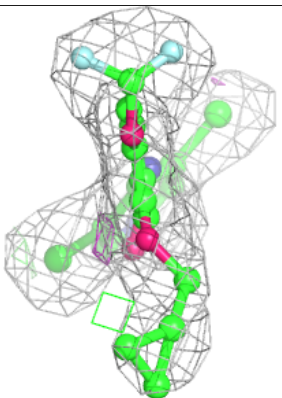
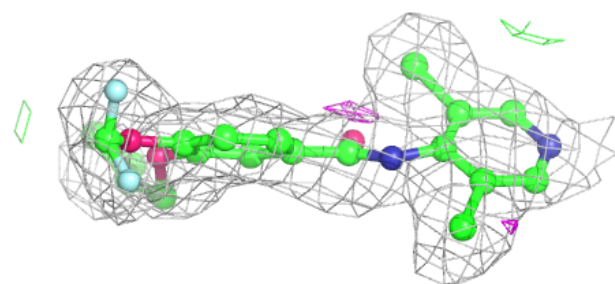
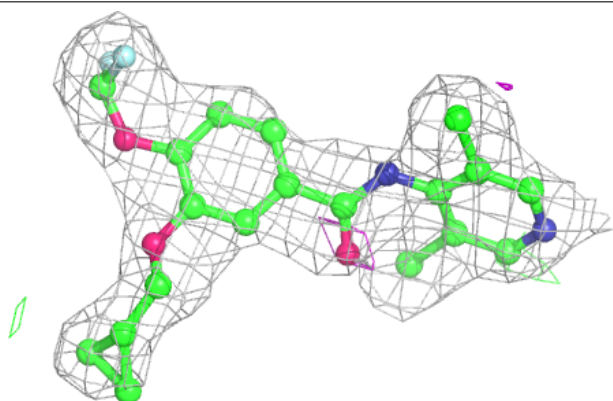


**Electron density around ROF A 901:**

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

**Electron density around ROF D 904:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.