Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 07:59 AM EDT

PDB ID	:	6E47
Title	:	Crystal Structure of the Murine Norovirus VP1 P domain in complex with the CD300lf Receptor and Glycochenodeoxycholic Acid
Authors	:	Nelson, C.A.; Fremont, D.H.
Deposited on	:	2018-07-16
Resolution	:	1.95 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 (i) 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 (i)) were used in the production of this report:

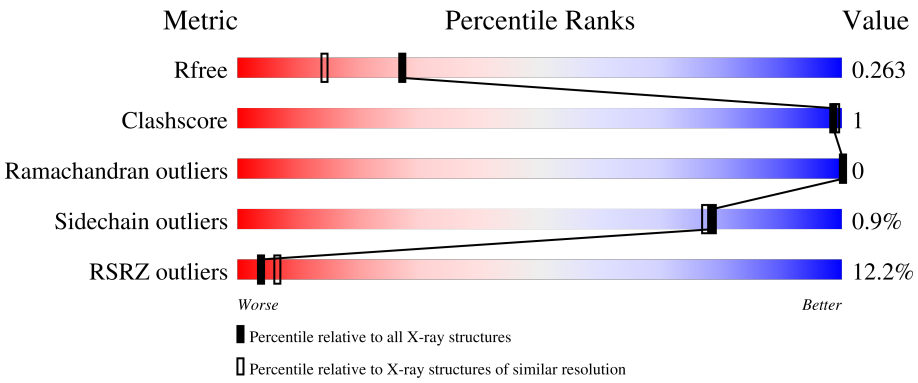
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	302	11% 97%
1	B	302	12% 98%
2	F	112	21% 96%
2	G	112	9% 96%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13508 atoms, of which 6467 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 VP1 P domain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	302	4596	1494	2273	380	442	7	0	0	0
1	B	302	4596	1494	2273	380	442	7	0	0	0

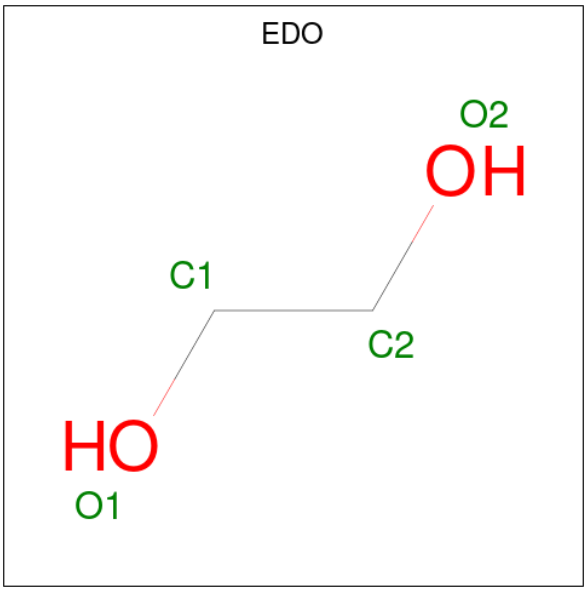
- Molecule 2 is a protein called CMRF35-like molecule 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	F	109	1704	539	841	148	169	7	0	0	0
2	G	112	1749	553	864	151	174	7	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	2	2	2	0	0
3	B	2	2	2	0	0
3	F	1	1	1	0	0
3	G	1	1	1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	10	2	6	2	0	0
			Total	C	H	O		
4	A	1	10	2	6	2	0	0
			Total	C	H	O		
4	A	1	10	2	6	2	0	0
			Total	C	H	O		
4	A	1	10	2	6	2	0	0
			Total	C	H	O		
4	A	1	10	2	6	2	0	0
			Total	C	H	O		
4	A	1	10	2	6	2	0	0
			Total	C	H	O		
4	B	1	10	2	6	2	0	0
			Total	C	H	O		
4	B	1	10	2	6	2	0	0
			Total	C	H	O		
4	B	1	10	2	6	2	0	0
			Total	C	H	O		
4	B	1	10	2	6	2	0	0
			Total	C	H	O		
4	B	1	10	2	6	2	0	0
			Total	C	H	O		
4	B	1	10	2	6	2	0	0
			Total	C	H	O		
4	F	1	10	2	6	2	0	0
			Total	C	H	O		
4	F	1	10	2	6	2	0	0

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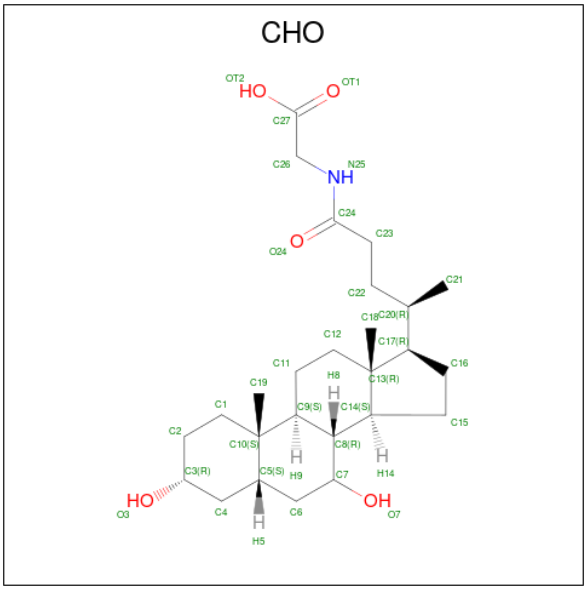
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	F	1	10	2	6	2	0	0
			Total	C	H	O		
4	F	1	10	2	6	2	0	0
			Total	C	H	O		
4	F	1	10	2	6	2	0	0
			Total	C	H	O		
4	F	1	10	2	6	2	0	0
			Total	C	H	O		
4	F	1	10	2	6	2	0	0
			Total	C	H	O		
4	G	1	10	2	6	2	0	0
			Total	C	H	O		
4	G	1	10	2	6	2	0	0
			Total	C	H	O		
4	G	1	10	2	6	2	0	0

- Molecule 5 is GLYCOCHENODEOXYCHOLIC ACID (three-letter code: CHO) (formula: $C_{26}H_{43}NO_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
5	B	1	74	26	42	1	5	0	0
			Total	C	H	N	O		
5	B	1	74	26	42	1	5	0	0

- Molecule 6 is water.

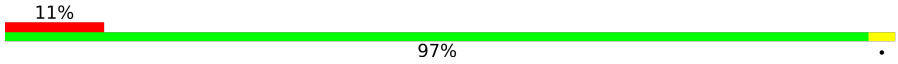
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	191	191	191	0	0
			Total	O		
6	B	178	178	178	0	0
			Total	O		
6	F	45	45	45	0	0
			Total	O		
6	G	75	75	75	0	0

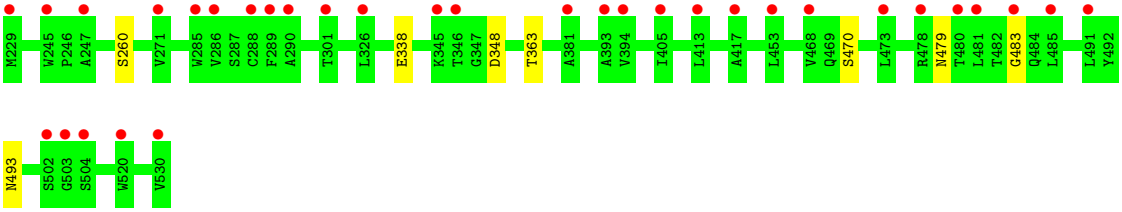
3 Residue-property plots (i)

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: VP1 P domain

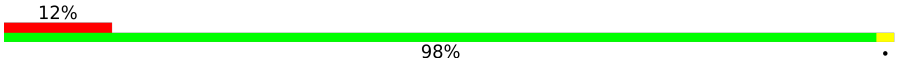
Chain A:

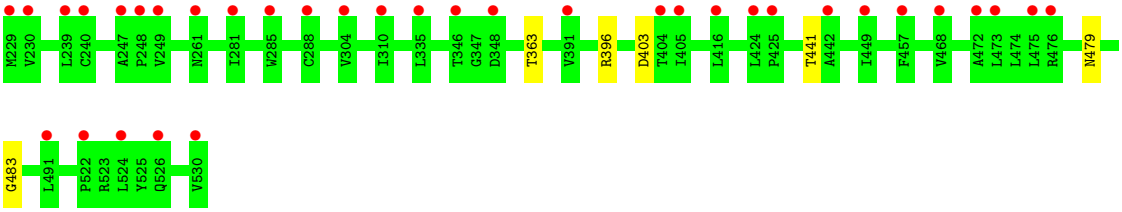




- Molecule 1: VP1 P domain

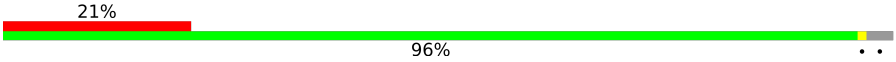
Chain B:

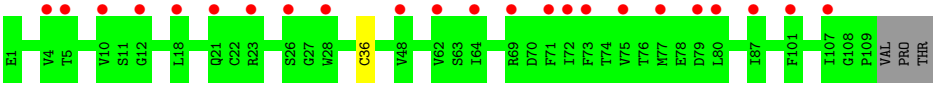




- Molecule 2: CMRF35-like molecule 1

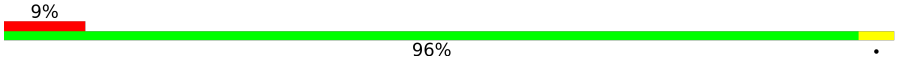
Chain F:

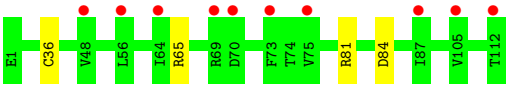




- Molecule 2: CMRF35-like molecule 1

Chain G:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.10Å 134.82Å 139.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.70 – 1.95 48.49 – 2.14	Depositor EDS
% Data completeness (in resolution range)	87.0 (60.70-1.95) 95.9 (48.49-2.14)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.208 , 0.257 0.220 , 0.263	Depositor DCC
R_{free} test set	2587 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13508	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 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, CHO, MG

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	0.25	0/2386	0.46	0/3269
1	B	0.25	0/2386	0.46	0/3269
2	F	0.25	0/880	0.48	0/1189
2	G	0.24	0/903	0.47	0/1221
All	All	0.25	0/6555	0.46	0/8948

There are no bond length outliers.

There are no bond angle outliers.

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	2323	2273	2273	4	0
1	B	2323	2273	2273	4	0
2	F	863	841	841	0	0
2	G	885	864	864	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	24	36	36	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	36	36	1	0
4	F	28	42	42	0	0
4	G	12	18	18	0	0
5	B	64	84	76	0	0
6	A	191	0	0	0	1
6	B	178	0	0	0	0
6	F	45	0	0	0	0
6	G	75	0	0	0	1
All	All	7041	6467	6459	7	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (7) 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:A:470:SER:O	1:A:493:ASN:ND2	2.31	0.60
1:B:403:ASP:OD1	4:B:609:EDO:O2	2.17	0.57
1:A:479:ASN:O	1:A:483:GLY:N	2.43	0.49
1:B:479:ASN:O	1:B:483:GLY:N	2.45	0.49
2:G:81:ARG:N	2:G:84:ASP:OD1	2.40	0.48
1:A:338:GLU:OE2	1:B:396:ARG:NE	2.38	0.42
1:A:348:ASP:HA	1:B:441:THR:HA	2.01	0.42

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:872:HOH:O	6:G:335:HOH:O[3_454]	2.08	0.12

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	300/302 (99%)	288 (96%)	12 (4%)	0	100	100
1	B	300/302 (99%)	289 (96%)	11 (4%)	0	100	100
2	F	107/112 (96%)	103 (96%)	4 (4%)	0	100	100
2	G	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
All	All	817/828 (99%)	786 (96%)	31 (4%)	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	249/249 (100%)	247 (99%)	2 (1%)	81	80
1	B	249/249 (100%)	248 (100%)	1 (0%)	91	90
2	F	97/100 (97%)	96 (99%)	1 (1%)	76	74
2	G	100/100 (100%)	98 (98%)	2 (2%)	55	48
All	All	695/698 (100%)	689 (99%)	6 (1%)	78	77

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	SER
1	A	363	THR
1	B	363	THR
2	F	36	CYS
2	G	36	CYS
2	G	65	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 30 ligands modelled in this entry, 6 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
4	EDO	B	606	-	3,3,3	0.46	0	2,2,2	0.33	0
5	CHO	B	602	-	35,35,35	5.87	20 (57%)	54,54,54	1.85	15 (27%)
4	EDO	B	607	-	3,3,3	0.47	0	2,2,2	0.36	0
4	EDO	B	610	-	3,3,3	0.47	0	2,2,2	0.35	0
4	EDO	F	202	-	3,3,3	0.48	0	2,2,2	0.30	0
5	CHO	B	601	-	35,35,35	5.86	21 (60%)	54,54,54	1.75	13 (24%)
4	EDO	A	605	-	3,3,3	0.47	0	2,2,2	0.37	0
4	EDO	B	608	-	3,3,3	0.47	0	2,2,2	0.33	0
4	EDO	A	604	-	3,3,3	0.48	0	2,2,2	0.34	0
4	EDO	F	207	-	3,3,3	0.47	0	2,2,2	0.35	0
4	EDO	A	603	-	3,3,3	0.48	0	2,2,2	0.31	0
4	EDO	G	202	-	3,3,3	0.47	0	2,2,2	0.31	0
4	EDO	A	606	-	3,3,3	0.48	0	2,2,2	0.29	0
4	EDO	F	203	-	3,3,3	0.48	0	2,2,2	0.35	0
4	EDO	A	608	-	3,3,3	0.48	0	2,2,2	0.36	0
4	EDO	F	204	-	3,3,3	0.47	0	2,2,2	0.35	0
4	EDO	F	205	-	3,3,3	0.47	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	B	605	-	3,3,3	0.47	0	2,2,2	0.33	0
4	EDO	A	607	-	3,3,3	0.48	0	2,2,2	0.34	0
4	EDO	F	208	-	3,3,3	0.47	0	2,2,2	0.31	0
4	EDO	G	204	-	3,3,3	0.48	0	2,2,2	0.31	0
4	EDO	B	609	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	F	206	-	3,3,3	0.47	0	2,2,2	0.36	0
4	EDO	G	203	-	3,3,3	0.47	0	2,2,2	0.34	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
4	EDO	B	606	-	-	0/1/1/1	-
5	CHO	B	602	-	-	9/14/75/75	0/4/4/4
4	EDO	B	607	-	-	1/1/1/1	-
4	EDO	B	610	-	-	0/1/1/1	-
4	EDO	F	202	-	-	1/1/1/1	-
5	CHO	B	601	-	-	8/14/75/75	0/4/4/4
4	EDO	A	605	-	-	1/1/1/1	-
4	EDO	B	608	-	-	0/1/1/1	-
4	EDO	A	604	-	-	0/1/1/1	-
4	EDO	F	207	-	-	0/1/1/1	-
4	EDO	A	603	-	-	0/1/1/1	-
4	EDO	G	202	-	-	1/1/1/1	-
4	EDO	A	606	-	-	0/1/1/1	-
4	EDO	F	203	-	-	1/1/1/1	-
4	EDO	A	608	-	-	1/1/1/1	-
4	EDO	F	204	-	-	0/1/1/1	-
4	EDO	F	205	-	-	0/1/1/1	-
4	EDO	B	605	-	-	1/1/1/1	-
4	EDO	A	607	-	-	0/1/1/1	-
4	EDO	F	208	-	-	0/1/1/1	-
4	EDO	G	204	-	-	0/1/1/1	-
4	EDO	B	609	-	-	0/1/1/1	-
4	EDO	F	206	-	-	0/1/1/1	-
4	EDO	G	203	-	-	0/1/1/1	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	CHO	C12-C13	-17.35	1.23	1.54
5	B	602	CHO	C12-C13	-17.35	1.23	1.54
5	B	602	CHO	C13-C17	-16.49	1.23	1.55
5	B	601	CHO	C13-C17	-16.46	1.23	1.55
5	B	601	CHO	C11-C9	-13.89	1.30	1.53
5	B	602	CHO	C11-C9	-13.64	1.30	1.53
5	B	601	CHO	C16-C15	-9.50	1.27	1.54
5	B	602	CHO	C16-C15	-9.50	1.28	1.54
5	B	602	CHO	C20-C17	7.86	1.68	1.54
5	B	602	CHO	C13-C14	-7.80	1.40	1.55
5	B	601	CHO	C13-C14	-7.66	1.40	1.55
5	B	601	CHO	C20-C17	7.64	1.67	1.54
5	B	602	CHO	C24-N25	7.22	1.49	1.33
5	B	601	CHO	C24-N25	7.07	1.49	1.33
5	B	602	CHO	C8-C9	-5.96	1.42	1.53
5	B	601	CHO	C8-C9	-5.88	1.42	1.53
5	B	602	CHO	C10-C9	5.02	1.65	1.56
5	B	601	CHO	C10-C9	4.80	1.64	1.56
5	B	601	CHO	C6-C7	3.98	1.59	1.52
5	B	602	CHO	C6-C7	3.91	1.59	1.52
5	B	602	CHO	C8-C14	3.82	1.61	1.53
5	B	601	CHO	C8-C14	3.68	1.61	1.53
5	B	602	CHO	C21-C20	-3.55	1.44	1.53
5	B	601	CHO	C21-C20	-3.51	1.44	1.53
5	B	601	CHO	O7-C7	-3.15	1.36	1.43
5	B	602	CHO	O7-C7	-3.14	1.36	1.43
5	B	602	CHO	C23-C24	3.14	1.57	1.51
5	B	601	CHO	C23-C24	3.13	1.57	1.51
5	B	601	CHO	C8-C7	3.03	1.58	1.53
5	B	602	CHO	C8-C7	2.79	1.58	1.53
5	B	601	CHO	C6-C5	-2.60	1.49	1.53
5	B	602	CHO	C16-C17	2.56	1.59	1.54
5	B	602	CHO	C6-C5	-2.50	1.49	1.53
5	B	602	CHO	C18-C13	2.49	1.58	1.54
5	B	601	CHO	C16-C17	2.46	1.59	1.54
5	B	601	CHO	C18-C13	2.42	1.58	1.54
5	B	602	CHO	C4-C5	2.25	1.57	1.53
5	B	601	CHO	C4-C5	2.19	1.57	1.53
5	B	601	CHO	O24-C24	-2.15	1.18	1.23
5	B	602	CHO	O24-C24	-2.14	1.18	1.23
5	B	601	CHO	C12-C11	2.08	1.57	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	601	CHO	C12-C13-C17	5.13	124.25	116.57
5	B	602	CHO	C12-C13-C17	4.95	123.97	116.57
5	B	602	CHO	C23-C24-N25	3.76	122.74	116.42
5	B	602	CHO	C6-C5-C4	-3.65	106.99	111.19
5	B	601	CHO	C18-C13-C12	-3.62	104.86	110.59
5	B	601	CHO	C21-C20-C17	-3.44	107.66	112.92
5	B	601	CHO	C23-C24-N25	3.35	122.06	116.42
5	B	602	CHO	C18-C13-C12	-3.24	105.47	110.59
5	B	602	CHO	C9-C10-C5	3.12	112.97	108.58
5	B	601	CHO	C9-C8-C7	3.02	115.49	111.88
5	B	602	CHO	C21-C20-C17	-3.02	108.30	112.92
5	B	602	CHO	C18-C13-C14	-2.93	106.24	111.71
5	B	601	CHO	C18-C13-C14	-2.86	106.38	111.71
5	B	602	CHO	C9-C8-C7	2.79	115.21	111.88
5	B	601	CHO	C6-C5-C4	-2.78	107.99	111.19
5	B	602	CHO	C11-C12-C13	2.69	117.39	112.78
5	B	601	CHO	C12-C13-C14	2.67	111.42	107.27
5	B	601	CHO	C11-C12-C13	2.65	117.33	112.78
5	B	602	CHO	C13-C17-C20	-2.61	115.40	119.49
5	B	602	CHO	C18-C13-C17	-2.42	107.20	111.71
5	B	602	CHO	O24-C24-N25	-2.36	118.56	123.01
5	B	602	CHO	C12-C13-C14	2.34	110.89	107.27
5	B	602	CHO	C19-C10-C5	-2.27	106.51	110.36
5	B	601	CHO	C13-C17-C20	-2.26	115.95	119.49
5	B	601	CHO	O24-C24-N25	-2.18	118.90	123.01
5	B	601	CHO	C18-C13-C17	-2.17	107.66	111.71
5	B	602	CHO	OT2-C27-C26	2.15	120.21	112.74
5	B	601	CHO	OT2-C27-C26	2.02	119.76	112.74

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	601	CHO	C13-C17-C20-C22
5	B	601	CHO	N25-C26-C27-OT1
5	B	601	CHO	N25-C26-C27-OT2
5	B	602	CHO	C13-C17-C20-C21
5	B	602	CHO	C13-C17-C20-C22
5	B	602	CHO	N25-C26-C27-OT1
5	B	602	CHO	N25-C26-C27-OT2
5	B	601	CHO	C16-C17-C20-C21
5	B	602	CHO	C16-C17-C20-C21
5	B	601	CHO	C13-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
5	B	601	CHO	C16-C17-C20-C22
5	B	602	CHO	C16-C17-C20-C22
5	B	601	CHO	C23-C24-N25-C26
5	B	602	CHO	C23-C24-N25-C26
5	B	601	CHO	O24-C24-N25-C26
5	B	602	CHO	O24-C24-N25-C26
4	B	607	EDO	O1-C1-C2-O2
4	A	608	EDO	O1-C1-C2-O2
4	A	605	EDO	O1-C1-C2-O2
4	F	202	EDO	O1-C1-C2-O2
4	G	202	EDO	O1-C1-C2-O2
5	B	602	CHO	C27-C26-N25-C24
4	B	605	EDO	O1-C1-C2-O2
4	F	203	EDO	O1-C1-C2-O2

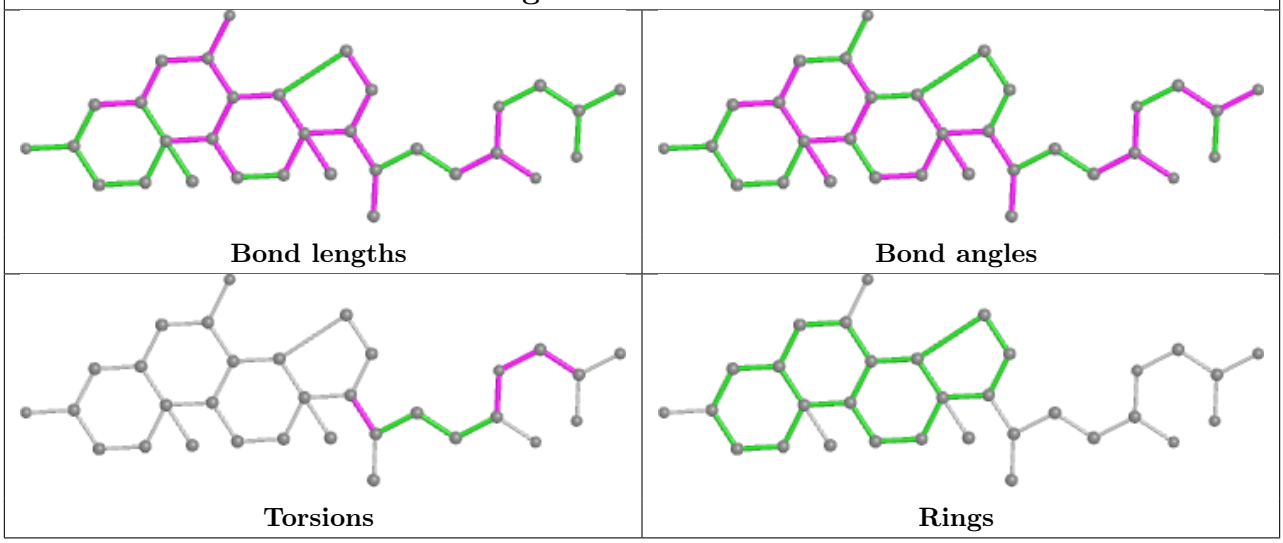
There are no ring outliers.

1 monomer is involved in 1 short contact:

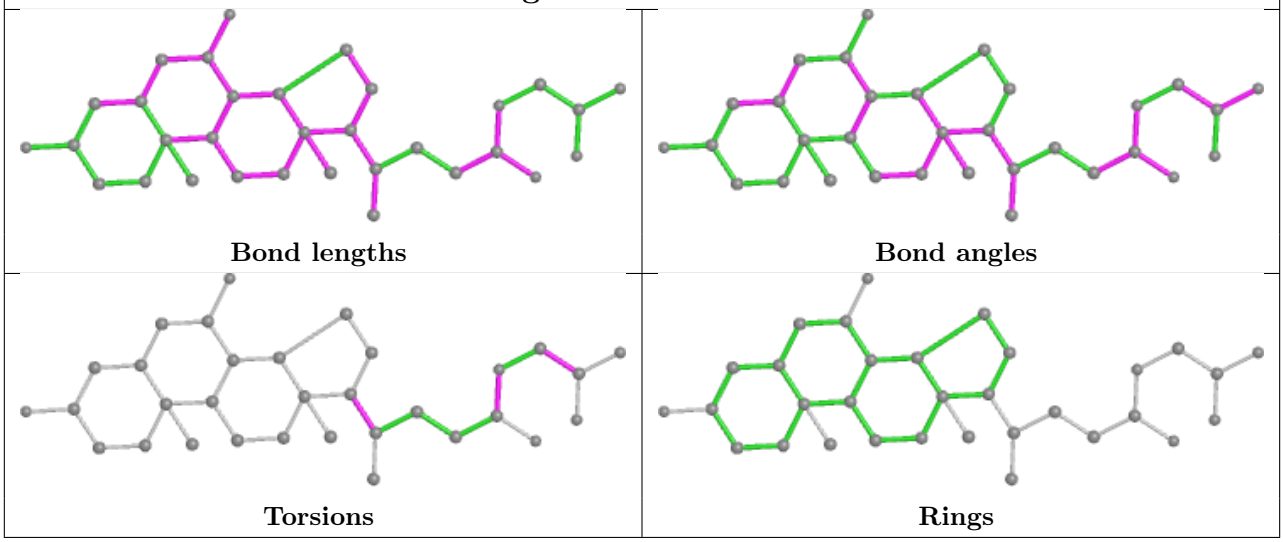
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	609	EDO	1	0

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 then 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 CHO B 602



Ligand CHO B 601



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)

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	302/302 (100%)	1.08	33 (10%)	5	9	21, 30, 49, 82	0
1	B	302/302 (100%)	1.16	35 (11%)	4	8	21, 30, 50, 66	0
2	F	109/112 (97%)	1.38	23 (21%)	1	1	28, 38, 63, 81	0
2	G	112/112 (100%)	1.02	10 (8%)	9	15	23, 33, 49, 89	0
All	All	825/828 (99%)	1.14	101 (12%)	4	6	21, 32, 53, 89	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	72	ILE	4.7
2	F	28	TRP	4.5
1	A	480	THR	4.2
1	A	481	LEU	3.9
2	F	23	ARG	3.8
1	A	485	LEU	3.8
1	A	502	SER	3.7
1	B	310	ILE	3.5
2	G	64	ILE	3.5
1	A	381	ALA	3.4
2	G	73	PHE	3.4
2	G	56	LEU	3.2
1	B	468	VAL	3.2
1	B	472	ALA	3.2
2	F	71	PHE	3.1
1	B	247	ALA	3.1
1	A	491	LEU	3.1
1	A	345	LYS	3.1
1	B	424	LEU	3.0
1	B	230	VAL	3.0
2	F	79	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	12	GLY	3.0
1	A	413	LEU	2.9
2	F	80	LEU	2.9
2	F	107	ILE	2.9
1	A	301	THR	2.9
2	F	69	ARG	2.9
2	F	62	VAL	2.9
2	F	64	ILE	2.8
1	A	394	VAL	2.8
2	G	48	VAL	2.8
1	B	346	THR	2.8
1	B	475	LEU	2.8
1	A	483	GLY	2.8
2	G	87	ILE	2.7
1	A	478	ARG	2.7
2	F	73	PHE	2.7
1	A	468	VAL	2.7
1	A	285	TRP	2.7
1	A	473	LEU	2.7
1	A	453	LEU	2.6
2	G	112	THR	2.6
1	A	288	CYS	2.5
1	A	247	ALA	2.5
1	A	504	SER	2.5
2	F	10	VAL	2.5
1	B	404	THR	2.5
1	B	304	VAL	2.4
1	B	476	ARG	2.4
1	B	524	LEU	2.4
2	F	18	LEU	2.4
2	F	101	PHE	2.4
1	B	229	MET	2.4
2	F	4	VAL	2.4
1	B	285	TRP	2.4
1	B	425	PRO	2.4
1	B	522	PRO	2.3
1	B	526	GLN	2.3
1	A	520	TRP	2.3
2	F	75	VAL	2.3
2	F	87	ILE	2.3
1	B	473	LEU	2.3
1	A	393	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	503	GLY	2.3
1	A	229	MET	2.3
1	B	348	ASP	2.3
1	B	249	VAL	2.2
1	B	261	ASN	2.2
2	G	69	ARG	2.2
1	B	391	VAL	2.2
2	G	70	ASP	2.2
2	G	75	VAL	2.2
1	B	240	CYS	2.2
1	A	326	LEU	2.2
1	B	491	LEU	2.2
1	B	457	PHE	2.2
2	F	48	VAL	2.2
2	G	105	VAL	2.2
2	F	77	MET	2.2
1	A	346	THR	2.2
1	A	286	VAL	2.2
1	B	248	PRO	2.1
2	F	26	SER	2.1
1	B	405	ILE	2.1
1	A	245	TRP	2.1
1	A	405	ILE	2.1
2	F	5	THR	2.1
1	B	239	LEU	2.1
1	A	289	PHE	2.1
1	A	530	VAL	2.1
1	B	281	ILE	2.1
2	F	21	GLN	2.1
1	A	271	VAL	2.1
1	B	442	ALA	2.1
1	A	417	ALA	2.1
1	B	449	ILE	2.1
1	B	288	CYS	2.1
1	B	530	VAL	2.0
1	A	290	ALA	2.0
1	B	416	LEU	2.0
1	B	335	LEU	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 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, 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.

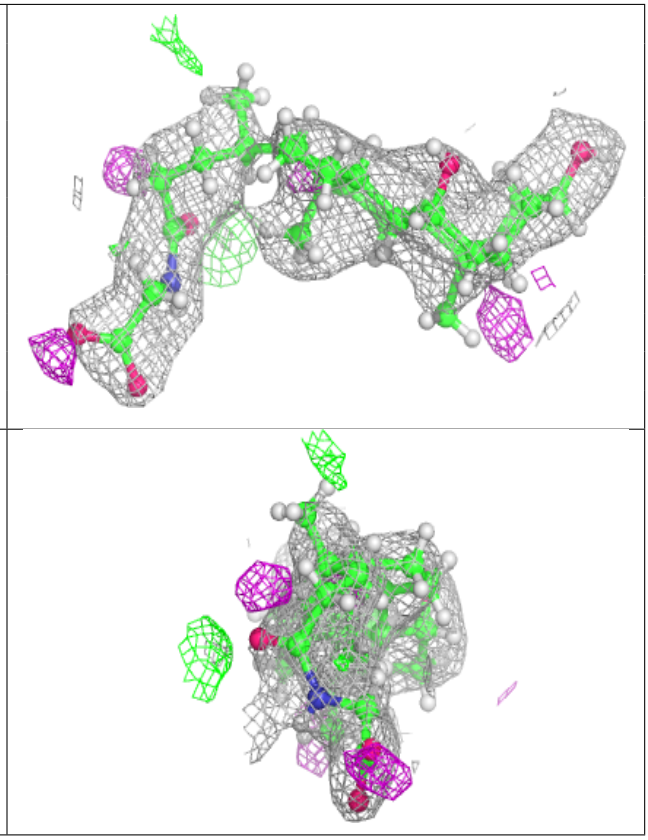
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	605	4/4	0.73	0.24	46,55,58,69	0
4	EDO	F	208	4/4	0.75	0.31	47,58,70,70	0
4	EDO	A	604	4/4	0.76	0.25	40,50,60,72	0
4	EDO	F	206	4/4	0.80	0.22	39,53,64,64	0
5	CHO	B	602	32/32	0.80	0.22	35,50,63,67	0
4	EDO	A	605	4/4	0.82	0.17	24,42,51,56	0
4	EDO	A	608	4/4	0.82	0.20	46,55,56,59	0
4	EDO	A	603	4/4	0.82	0.21	28,35,45,55	0
4	EDO	G	203	4/4	0.83	0.14	34,41,47,57	0
4	EDO	B	610	4/4	0.83	0.29	65,78,84,84	0
4	EDO	A	606	4/4	0.84	0.20	33,44,51,61	0
4	EDO	F	205	4/4	0.84	0.30	37,66,76,84	0
4	EDO	A	607	4/4	0.84	0.17	39,58,64,69	0
3	MG	B	603	1/1	0.85	0.10	34,34,34,34	0
4	EDO	F	204	4/4	0.85	0.16	50,60,64,64	0
4	EDO	F	207	4/4	0.85	0.15	43,52,62,62	0
4	EDO	B	606	4/4	0.86	0.17	40,52,63,63	0
5	CHO	B	601	32/32	0.86	0.18	33,48,60,65	0
4	EDO	B	609	4/4	0.86	0.19	26,39,46,55	0
4	EDO	F	202	4/4	0.87	0.19	32,44,60,60	0
4	EDO	G	204	4/4	0.87	0.17	38,47,52,61	0
3	MG	B	604	1/1	0.88	0.09	27,27,27,27	0
4	EDO	B	607	4/4	0.88	0.22	27,42,50,60	0
4	EDO	G	202	4/4	0.90	0.27	41,49,55,62	0
4	EDO	B	608	4/4	0.91	0.16	40,56,59,69	0
3	MG	A	602	1/1	0.92	0.07	32,32,32,32	0
4	EDO	F	203	4/4	0.92	0.17	39,46,53,53	0
3	MG	G	201	1/1	0.92	0.15	25,25,25,25	0
3	MG	A	601	1/1	0.94	0.12	35,35,35,35	0
3	MG	F	201	1/1	0.95	0.16	25,25,25,25	0

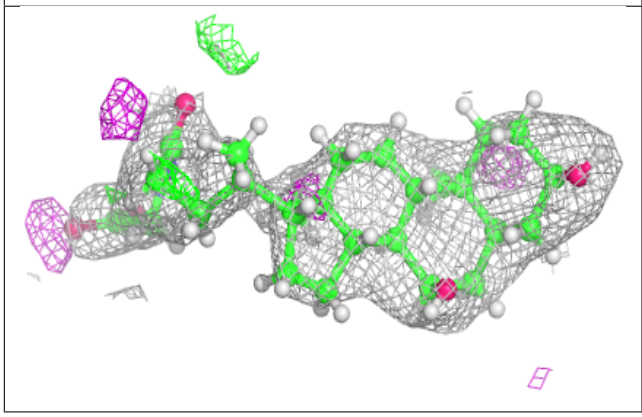
The following is a graphical depiction of the model fit to experimental electron density of all

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 CHO B 602:

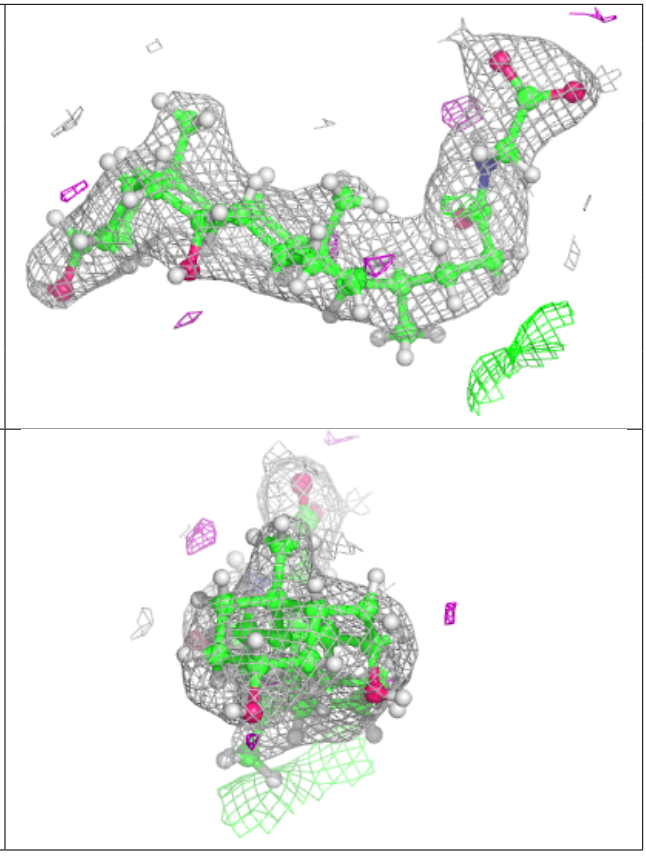
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around CHO B 601:

$2mF_o$-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.