Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 04:39 pm GMT

PDB ID	:	6H6M
Title	:	CR10 murine norovirus protruding domain in complex with the CD300lf receptor and glycochenodeoxycholate (GCDCA)
Authors	:	Kilic, T.; Hansman, G.S.
Deposited on	:	2018-07-27
Resolution	:	2.38 Å(reported)

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

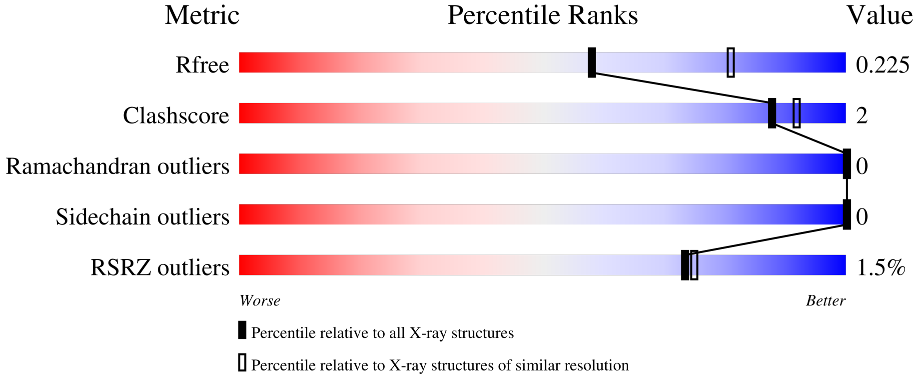
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

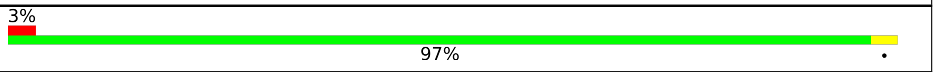
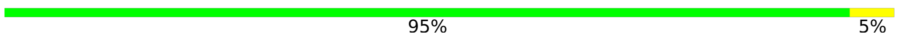
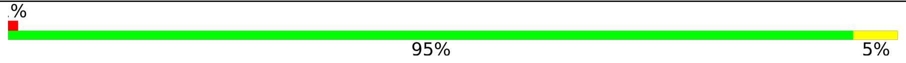
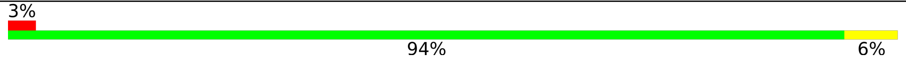
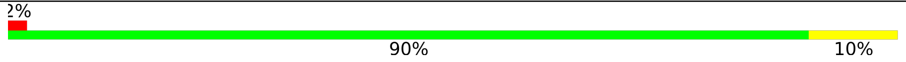
The reported resolution of this entry is 2.38 Å.

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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	303	
1	B	303	
1	C	303	
1	D	303	
2	E	111	

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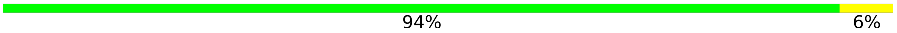
Mol	Chain	Length	Quality of chain
2	F	111	

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 11579 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.

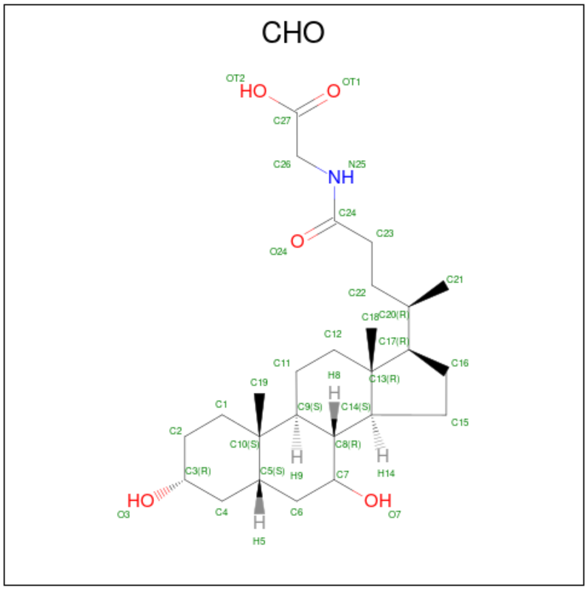
- Molecule 1 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	303	2284	1475	373	429	7	0	0	0
1	B	303	2298	1485	374	432	7	0	0	0
1	C	303	2304	1487	374	436	7	0	1	0
1	D	303	2262	1461	371	423	7	0	0	0

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

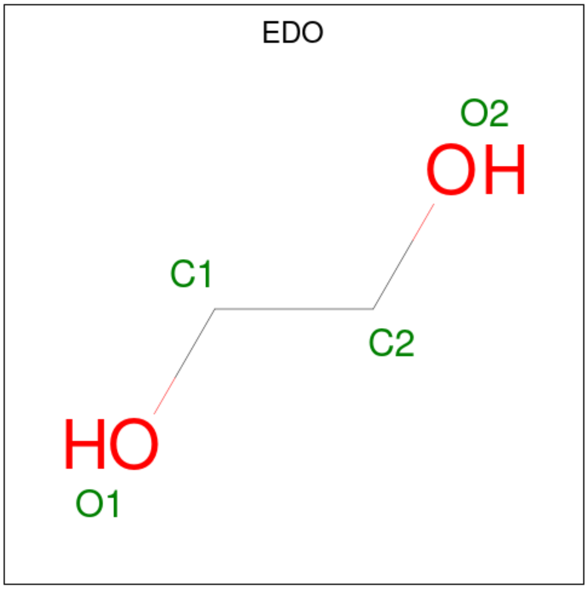
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	111	841	530	138	166	7	0	0	0
2	F	111	870	547	144	171	8	0	1	0

- Molecule 3 is GLYCOCHENODEOXYCHOLIC ACID (three-letter code: CHO) (formula: $C_{26}H_{43}NO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 32 26 1 5	0	0
3	B	1	Total C N O 32 26 1 5	0	0
3	C	1	Total C N O 32 26 1 5	0	0
3	D	1	Total C N O 32 26 1 5	0	0

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

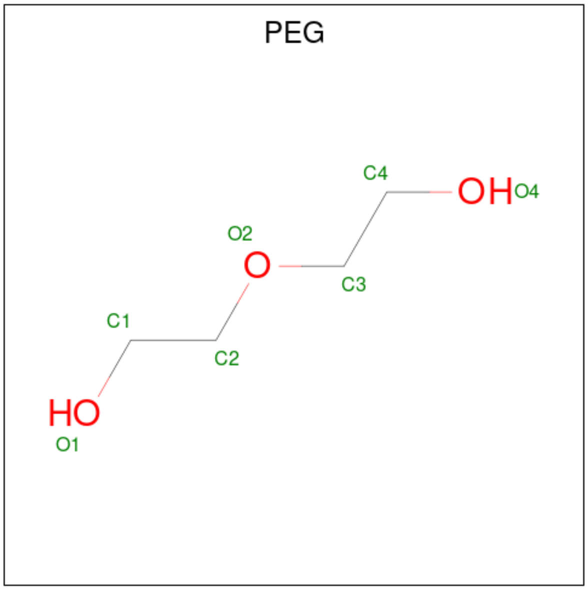


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

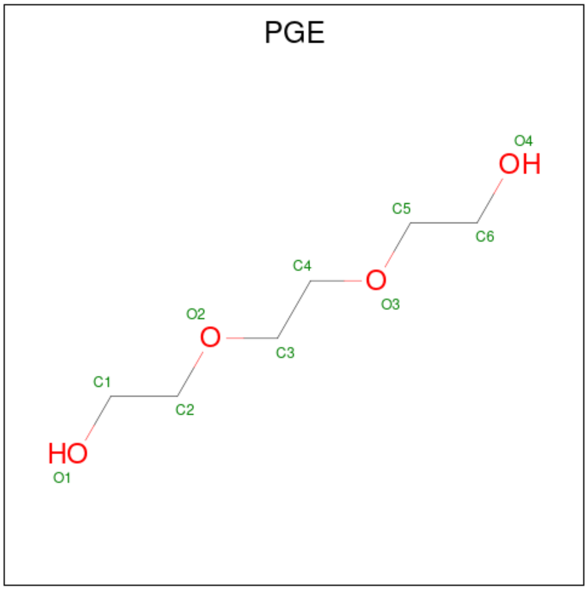
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C O 7 4 3	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total C O 10 6 4	0	0

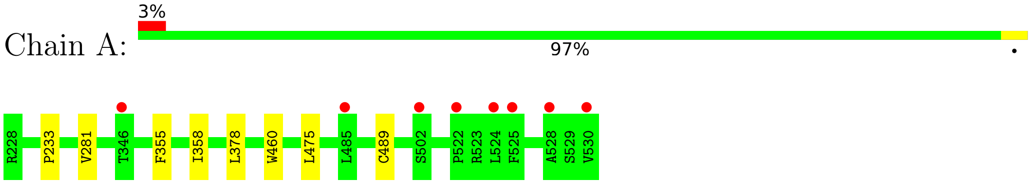
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	98	Total O 98 98	0	0
8	B	119	Total O 119 119	0	0
8	C	128	Total O 128 128	0	0
8	D	97	Total O 97 97	0	0
8	E	28	Total O 28 28	0	0
8	F	41	Total O 41 41	0	0

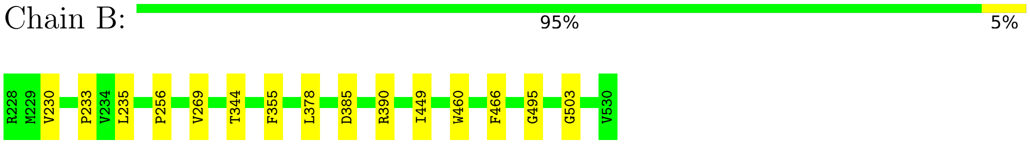
3 Residue-property plots ⓘ

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.

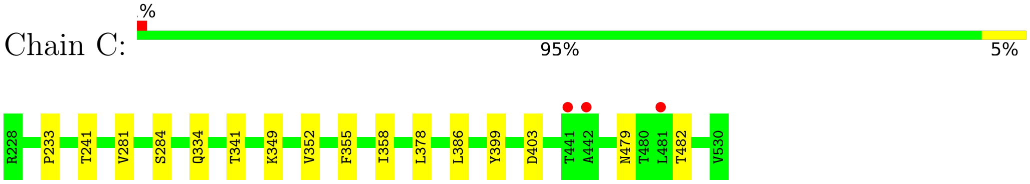
- Molecule 1: Capsid protein



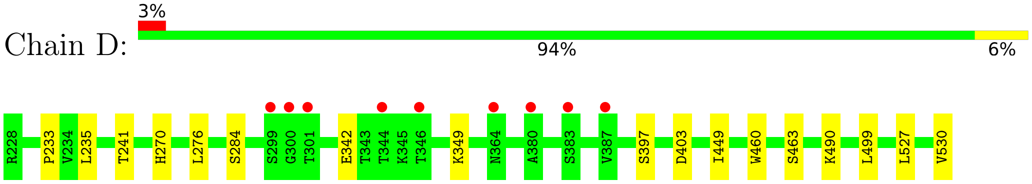
- Molecule 1: Capsid protein



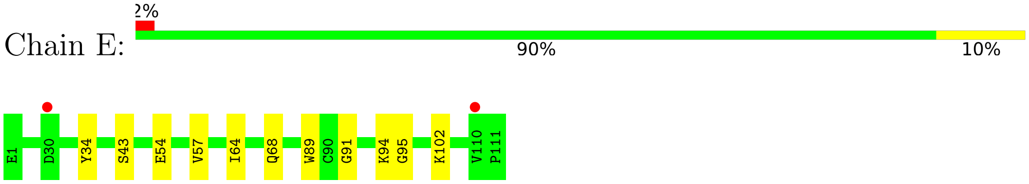
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

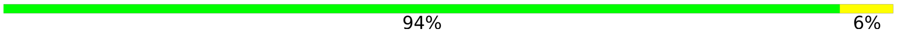


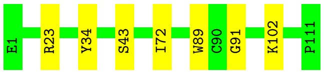
- Molecule 2: CMRF35-like molecule 1



- Molecule 2: CMRF35-like molecule 1

Chain F:





4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.94Å 137.55Å 93.80Å 90.00° 95.84° 90.00°	Depositor
Resolution (Å)	46.66 – 2.38 46.66 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.0 (46.66-2.38) 98.0 (46.66-2.38)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.186 , 0.225 0.186 , 0.225	Depositor DCC
R_{free} test set	3751 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11579	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: PEG, EDO, NA, CHO, PGE

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	0.28	0/2348	0.47	0/3224
1	B	0.28	0/2362	0.47	0/3240
1	C	0.28	0/2371	0.48	0/3252
1	D	0.27	0/2325	0.48	0/3193
2	E	0.27	0/859	0.51	0/1170
2	F	0.27	0/891	0.51	0/1207
All	All	0.28	0/11156	0.48	0/15286

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	2284	0	2169	5	0
1	B	2298	0	2212	10	0
1	C	2304	0	2217	12	0
1	D	2262	0	2148	12	0
2	E	841	0	786	6	0
2	F	870	0	844	4	0
3	A	32	0	42	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	32	0	42	0	0
3	C	32	0	42	1	0
3	D	32	0	42	0	0
4	A	16	0	24	0	0
4	B	16	0	24	1	0
4	C	12	0	18	1	0
4	D	8	0	12	2	0
4	E	4	0	6	0	0
4	F	4	0	6	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	E	7	0	10	0	0
7	F	10	0	14	0	0
8	A	98	0	0	0	0
8	B	119	0	0	0	0
8	C	128	0	0	0	0
8	D	97	0	0	0	0
8	E	28	0	0	0	0
8	F	41	0	0	0	0
All	All	11579	0	10658	43	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 2.

All (43) 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:449:ILE:HA	4:B:602:EDO:H12	1.68	0.74
1:D:449:ILE:HA	4:D:603:EDO:H21	1.73	0.69
1:A:281:VAL:HG11	1:B:235:LEU:HD21	1.83	0.61
2:E:54:GLU:HG2	2:E:68:GLN:HG3	1.86	0.57
1:B:355:PHE:CD2	1:B:378:LEU:HD23	2.39	0.57
1:C:479:ASN:OD1	1:C:482:THR:N	2.34	0.56
2:E:57:VAL:HB	2:E:64:ILE:HG22	1.91	0.52
3:A:601:CHO:H21	1:B:390:ARG:HB3	1.91	0.52
1:A:355:PHE:CE2	1:A:378:LEU:HD23	2.46	0.51
1:A:358:ILE:HD11	2:E:43:SER:HB3	1.93	0.51
1:B:233:PRO:HD3	1:B:460:TRP:CE2	2.46	0.50
2:F:23:ARG:HG2	2:F:72:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:PHE:CE2	1:C:378:LEU:HD23	2.49	0.48
1:C:403:ASP:HB2	4:C:603:EDO:H22	1.95	0.48
1:D:499:LEU:HD23	1:D:530:VAL:HG11	1.95	0.48
1:D:270:HIS:CD2	1:D:276:LEU:HD11	2.49	0.47
1:D:403:ASP:O	4:D:602:EDO:H22	2.13	0.47
1:C:352:VAL:HG21	1:D:397:SER:HB3	1.97	0.47
2:E:34:TYR:CZ	2:E:91:GLY:HA3	2.50	0.46
1:C:281:VAL:HG11	1:D:235:LEU:HD22	1.98	0.46
3:C:601:CHO:H222	3:C:601:CHO:H162	1.66	0.45
1:C:349:LYS:HA	1:C:349:LYS:HD3	1.82	0.44
1:C:284:SER:HB3	1:D:241:THR:HG23	1.99	0.43
2:E:89:TRP:CZ3	2:E:102:LYS:HB2	2.54	0.43
1:B:256:PRO:HG2	1:B:503:GLY:O	2.18	0.43
1:C:233:PRO:HB3	1:D:463:SER:HB3	2.00	0.43
1:C:334:GLN:HB3	1:C:399:TYR:HB3	2.01	0.43
1:C:241:THR:HG23	1:D:284:SER:HB3	2.01	0.43
3:A:601:CHO:H222	3:A:601:CHO:H162	1.83	0.42
1:D:233:PRO:HG3	1:D:460:TRP:CE3	2.54	0.42
2:F:34:TYR:CZ	2:F:91:GLY:HA3	2.54	0.42
1:A:475:LEU:HB2	1:A:489:CYS:SG	2.60	0.42
1:D:342:GLU:HA	1:D:349:LYS:O	2.19	0.41
2:F:89:TRP:CZ3	2:F:102:LYS:HB2	2.55	0.41
1:D:490:LYS:HG3	1:D:527:LEU:HD21	2.02	0.41
1:A:233:PRO:HD3	1:A:460:TRP:CE2	2.55	0.41
1:B:230:VAL:HG22	1:B:466:PHE:CB	2.51	0.41
1:C:341:THR:HB	1:C:386:LEU:HD22	2.01	0.41
2:E:94:LYS:HG2	2:E:95:GLY:N	2.35	0.41
1:B:344:THR:OG1	1:B:385:ASP:HB3	2.21	0.41
1:C:358:ILE:HD11	2:F:43:SER:HB3	2.03	0.41
1:B:230:VAL:HG22	1:B:466:PHE:HB3	2.03	0.40
1:B:269:VAL:O	1:B:495:GLY:HA3	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	301/303 (99%)	290 (96%)	11 (4%)	0	100	100
1	B	301/303 (99%)	287 (95%)	14 (5%)	0	100	100
1	C	302/303 (100%)	290 (96%)	12 (4%)	0	100	100
1	D	301/303 (99%)	288 (96%)	13 (4%)	0	100	100
2	E	109/111 (98%)	106 (97%)	3 (3%)	0	100	100
2	F	110/111 (99%)	107 (97%)	3 (3%)	0	100	100
All	All	1424/1434 (99%)	1368 (96%)	56 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	232/252 (92%)	232 (100%)	0	100	100
1	B	239/252 (95%)	239 (100%)	0	100	100
1	C	241/252 (96%)	241 (100%)	0	100	100
1	D	228/252 (90%)	228 (100%)	0	100	100
2	E	90/99 (91%)	90 (100%)	0	100	100
2	F	98/99 (99%)	98 (100%)	0	100	100
All	All	1128/1206 (94%)	1128 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	HIS
2	E	68	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 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	E	201	-	3,3,3	0.48	0	2,2,2	0.29	0
3	CHO	A	601	-	35,35,35	0.46	0	54,54,54	0.68	0
4	EDO	A	604	-	3,3,3	0.49	0	2,2,2	0.27	0
4	EDO	C	603	-	3,3,3	0.47	0	2,2,2	0.17	0
4	EDO	B	602	-	3,3,3	0.48	0	2,2,2	0.26	0
4	EDO	B	603	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	D	602	-	3,3,3	0.45	0	2,2,2	0.41	0
4	EDO	A	603	-	3,3,3	0.46	0	2,2,2	0.24	0
4	EDO	A	602	-	3,3,3	0.48	0	2,2,2	0.29	0
4	EDO	D	603	-	3,3,3	0.49	0	2,2,2	0.11	0
7	PGE	F	202	-	9,9,9	0.52	0	8,8,8	0.18	0
4	EDO	F	201	-	3,3,3	0.50	0	2,2,2	0.34	0
3	CHO	B	600	-	35,35,35	0.48	0	54,54,54	0.71	0
4	EDO	B	604	-	3,3,3	0.45	0	2,2,2	0.40	0
4	EDO	C	602	-	3,3,3	0.48	0	2,2,2	0.46	0
4	EDO	C	604	-	3,3,3	0.46	0	2,2,2	0.24	0
4	EDO	A	605	-	3,3,3	0.46	0	2,2,2	0.28	0
4	EDO	B	605	-	3,3,3	0.47	0	2,2,2	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	CHO	C	601	-	35,35,35	0.45	0	54,54,54	0.61	0
3	CHO	D	600	-	35,35,35	0.44	0	54,54,54	0.67	0
6	PEG	E	202	-	6,6,6	0.49	0	5,5,5	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
4	EDO	E	201	-	-	0/1/1/1	-
3	CHO	A	601	-	-	4/14/75/75	0/4/4/4
4	EDO	A	604	-	-	1/1/1/1	-
4	EDO	C	603	-	-	1/1/1/1	-
4	EDO	B	602	-	-	1/1/1/1	-
4	EDO	B	603	-	-	1/1/1/1	-
4	EDO	D	602	-	-	1/1/1/1	-
4	EDO	A	603	-	-	1/1/1/1	-
4	EDO	A	602	-	-	0/1/1/1	-
4	EDO	D	603	-	-	1/1/1/1	-
7	PGE	F	202	-	-	2/7/7/7	-
4	EDO	F	201	-	-	0/1/1/1	-
3	CHO	B	600	-	-	4/14/75/75	0/4/4/4
4	EDO	B	604	-	-	0/1/1/1	-
4	EDO	C	602	-	-	0/1/1/1	-
4	EDO	C	604	-	-	1/1/1/1	-
4	EDO	A	605	-	-	0/1/1/1	-
4	EDO	B	605	-	-	0/1/1/1	-
3	CHO	C	601	-	-	5/14/75/75	0/4/4/4
3	CHO	D	600	-	-	4/14/75/75	0/4/4/4
6	PEG	E	202	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	CHO	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
3	D	600	CHO	C16-C17-C20-C21
3	C	601	CHO	C16-C17-C20-C21
3	A	601	CHO	C13-C17-C20-C21
3	C	601	CHO	C13-C17-C20-C21
3	D	600	CHO	C13-C17-C20-C21
3	A	601	CHO	C16-C17-C20-C22
3	B	600	CHO	C16-C17-C20-C21
3	A	601	CHO	C13-C17-C20-C22
3	C	601	CHO	C13-C17-C20-C22
3	D	600	CHO	C13-C17-C20-C22
3	B	600	CHO	C13-C17-C20-C21
3	D	600	CHO	C16-C17-C20-C22
3	B	600	CHO	C13-C17-C20-C22
3	C	601	CHO	C16-C17-C20-C22
4	A	603	EDO	O1-C1-C2-O2
4	B	602	EDO	O1-C1-C2-O2
4	C	603	EDO	O1-C1-C2-O2
4	D	602	EDO	O1-C1-C2-O2
3	B	600	CHO	C16-C17-C20-C22
6	E	202	PEG	O1-C1-C2-O2
6	E	202	PEG	O2-C3-C4-O4
7	F	202	PGE	C6-C5-O3-C4
4	A	604	EDO	O1-C1-C2-O2
4	C	604	EDO	O1-C1-C2-O2
4	D	603	EDO	O1-C1-C2-O2
3	C	601	CHO	C17-C20-C22-C23
4	B	603	EDO	O1-C1-C2-O2
7	F	202	PGE	C3-C4-O3-C5

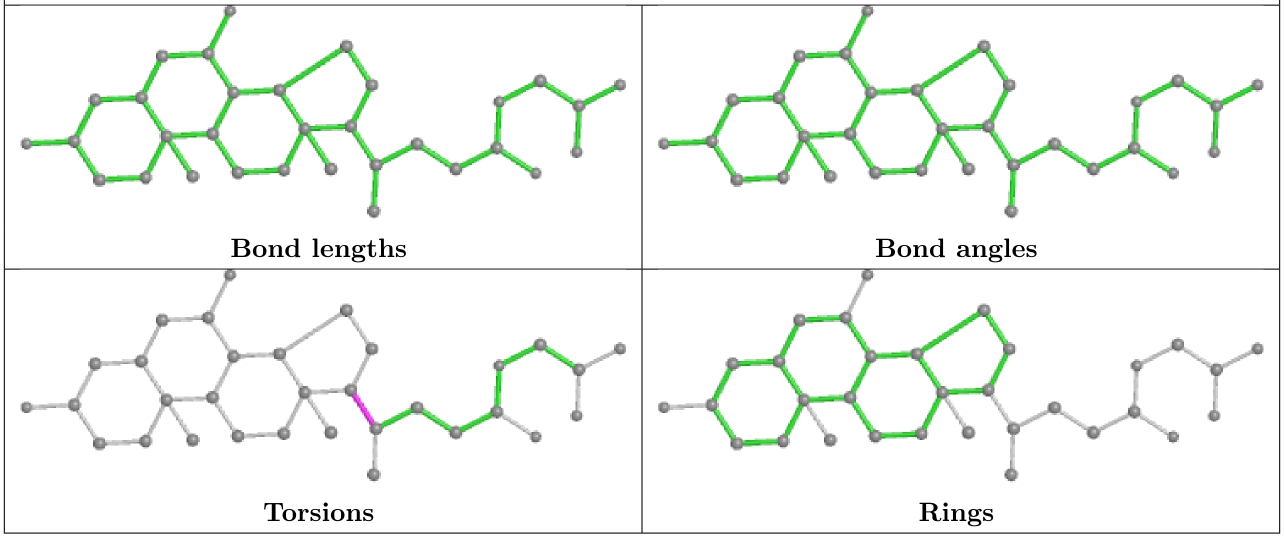
There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	CHO	2	0
4	C	603	EDO	1	0
4	B	602	EDO	1	0
4	D	602	EDO	1	0
4	D	603	EDO	1	0
3	C	601	CHO	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 A 601



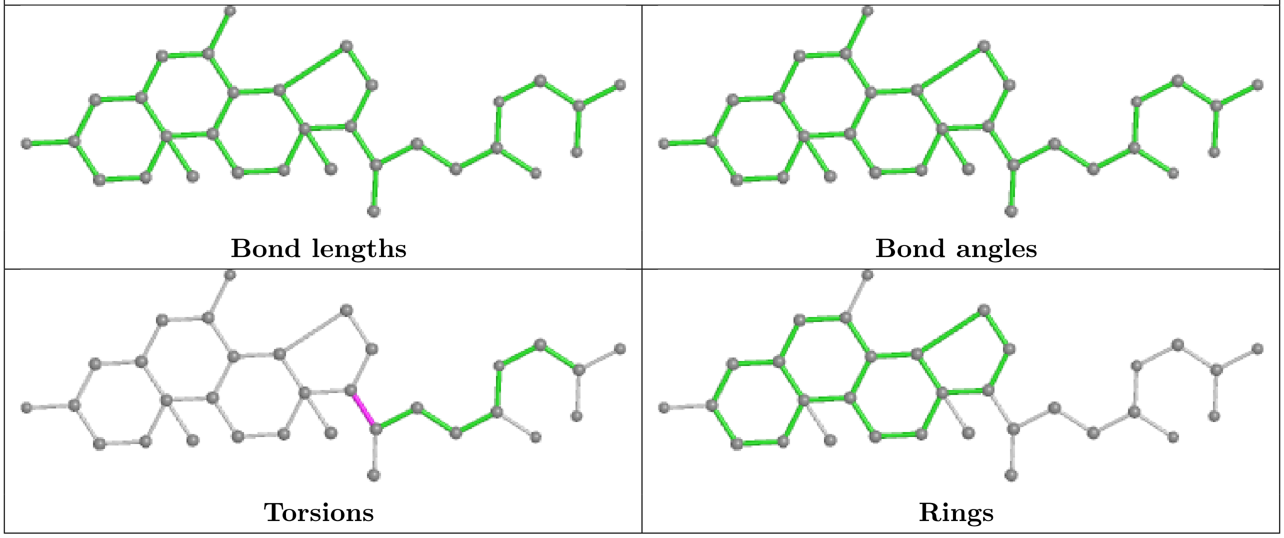
Bond lengths

Bond angles

Torsions

Rings

Ligand CHO B 600



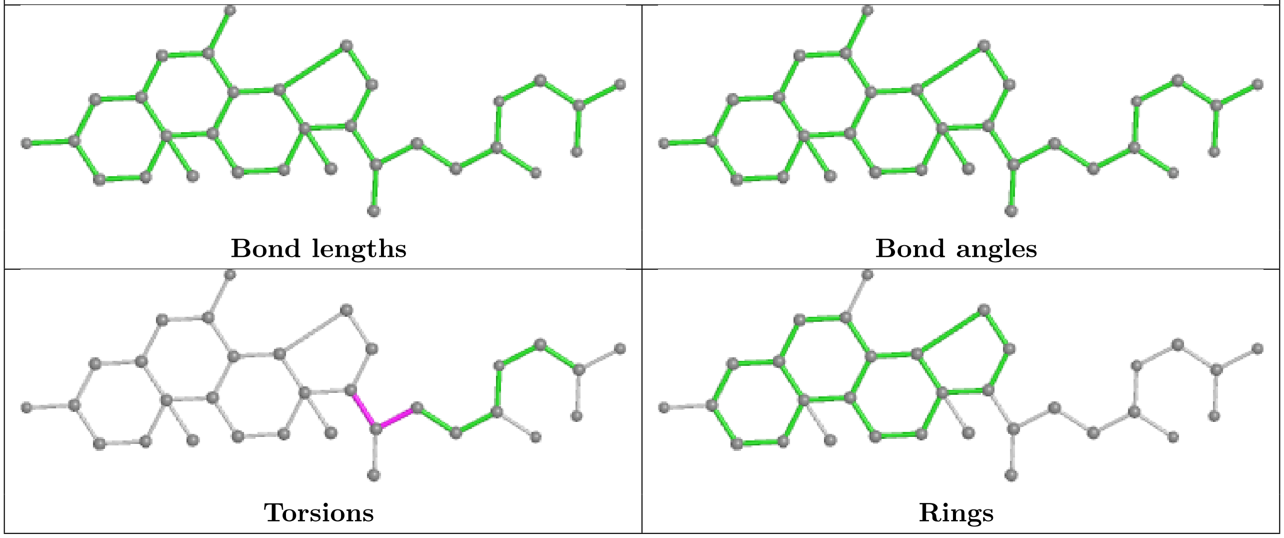
Bond lengths

Bond angles

Torsions

Rings

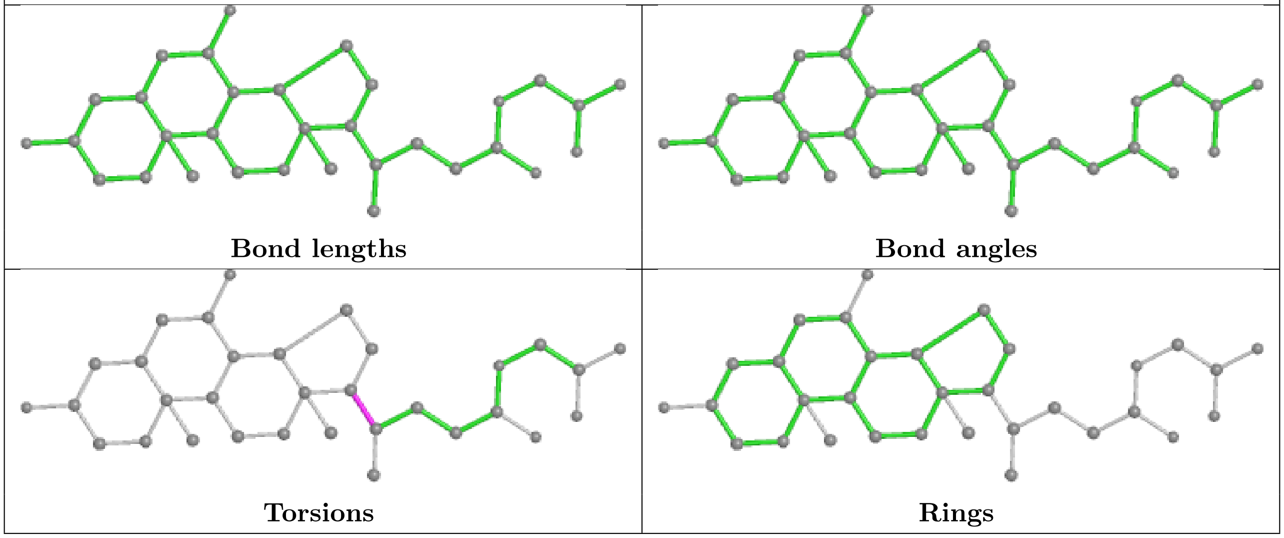
Ligand CHO C 601



Bond lengths Bond angles

Torsions Rings

Ligand CHO D 600



Bond lengths Bond angles

Torsions Rings

5.7 Other polymers ⓘ

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, 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	303/303 (100%)	0.02	8 (2%)	56	57	24, 38, 66, 79	0
1	B	303/303 (100%)	-0.19	0	100	100	22, 31, 50, 75	0
1	C	303/303 (100%)	-0.20	3 (0%)	82	83	23, 32, 49, 72	0
1	D	303/303 (100%)	0.01	9 (2%)	50	53	23, 36, 66, 83	0
2	E	111/111 (100%)	0.06	2 (1%)	68	70	27, 39, 56, 67	0
2	F	111/111 (100%)	0.00	0	100	100	27, 35, 47, 64	0
All	All	1434/1434 (100%)	-0.07	22 (1%)	73	75	22, 34, 60, 83	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	364	ASN	3.9
1	C	442	ALA	3.7
1	D	344	THR	3.7
1	D	300	GLY	3.3
1	D	346	THR	2.8
1	A	485	LEU	2.8
1	A	346	THR	2.7
1	D	387	VAL	2.6
1	C	441	THR	2.6
2	E	30	ASP	2.5
1	D	299	SER	2.5
1	A	522	PRO	2.5
1	A	502	SER	2.5
1	A	528	ALA	2.5
1	D	380	ALA	2.4
1	C	481	LEU	2.4
2	E	110	VAL	2.4
1	A	530	VAL	2.3
1	A	524	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	525	PHE	2.2
1	D	301	THR	2.1
1	D	383	SER	2.1

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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^{th} 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	A	604	4/4	0.77	0.31	40,41,43,44	0
3	CHO	C	601	32/32	0.80	0.23	56,59,61,61	0
4	EDO	C	604	4/4	0.82	0.18	34,36,39,42	0
4	EDO	B	602	4/4	0.84	0.19	40,40,41,41	0
6	PEG	E	202	7/7	0.84	0.20	67,67,67,67	0
7	PGE	F	202	10/10	0.84	0.22	60,60,60,60	0
4	EDO	F	201	4/4	0.89	0.18	34,34,35,36	0
5	NA	B	601	1/1	0.89	0.15	45,45,45,45	0
4	EDO	A	602	4/4	0.91	0.17	44,44,44,45	0
5	NA	D	601	1/1	0.92	0.06	44,44,44,44	0
4	EDO	A	603	4/4	0.92	0.11	45,45,45,45	0
3	CHO	D	600	32/32	0.92	0.13	32,35,37,37	0
5	NA	C	605	1/1	0.93	0.07	42,42,42,42	0
4	EDO	D	603	4/4	0.93	0.20	41,43,43,44	0
4	EDO	C	603	4/4	0.93	0.16	43,44,45,45	0
3	CHO	A	601	32/32	0.93	0.16	37,38,41,42	0
4	EDO	B	603	4/4	0.94	0.13	36,36,37,38	0
4	EDO	B	605	4/4	0.95	0.12	30,32,33,33	0
4	EDO	E	201	4/4	0.95	0.23	35,37,37,37	0
3	CHO	B	600	32/32	0.95	0.12	28,30,34,35	0

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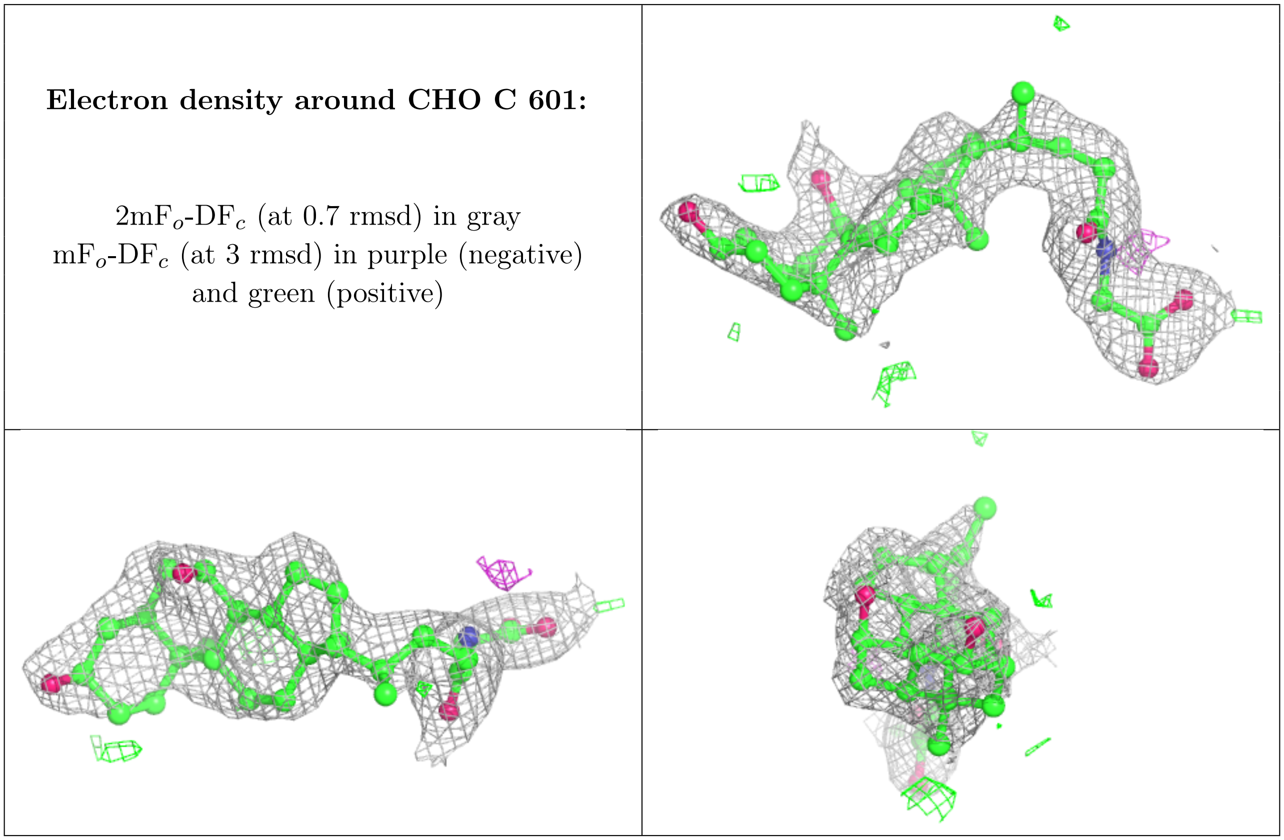
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
4	EDO	B	604	4/4	0.95	0.15	29,31,33,35	0
4	EDO	C	602	4/4	0.96	0.09	26,27,28,28	0
4	EDO	D	602	4/4	0.96	0.13	34,34,35,35	0
4	EDO	A	605	4/4	0.98	0.18	34,34,34,35	0
5	NA	A	606	1/1	0.99	0.07	36,36,36,36	0

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.

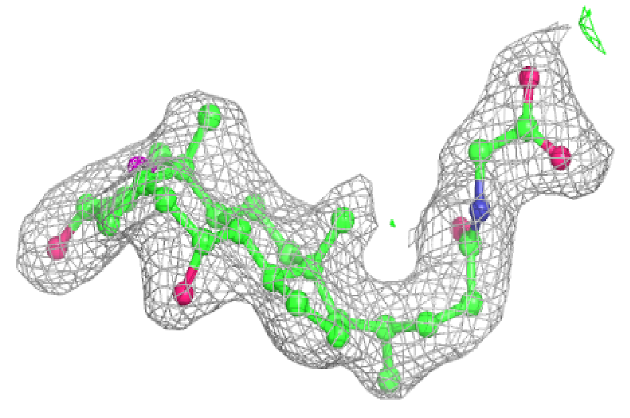


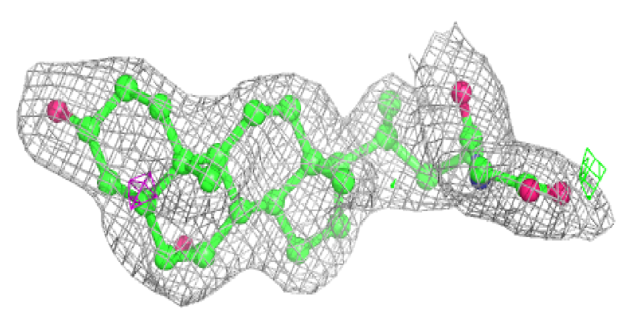
Electron density around CHO C 601:

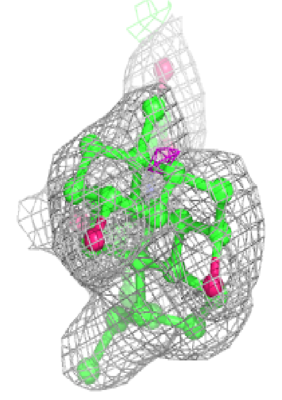
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around CHO D 600:

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

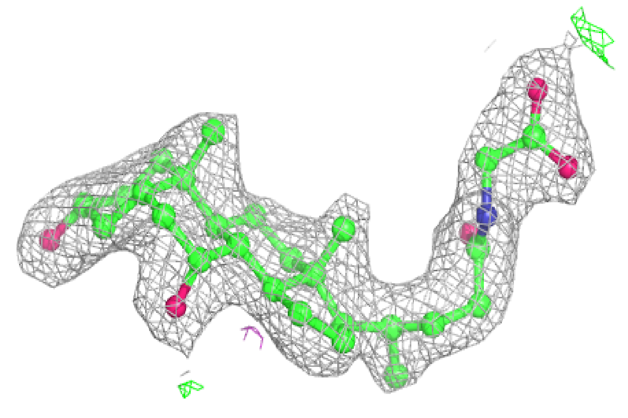


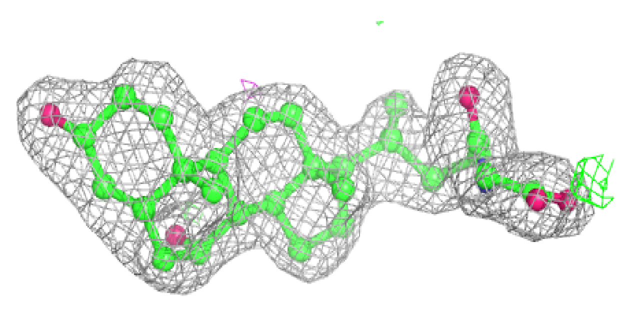


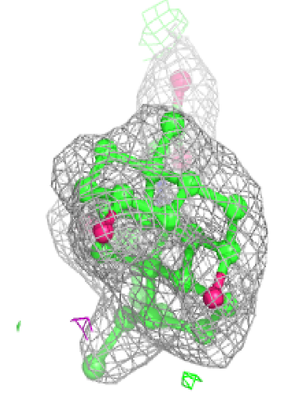


Electron density around CHO A 601:

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

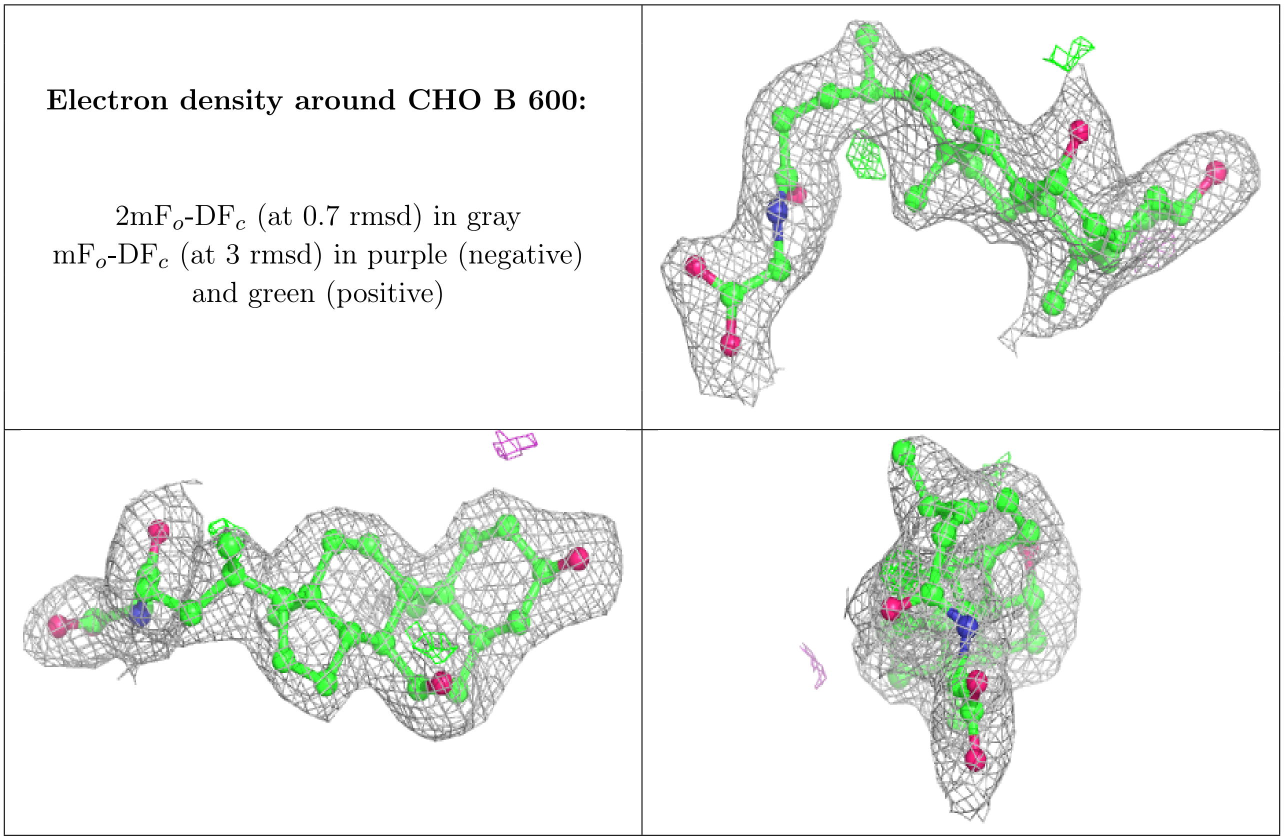






Electron density around CHO B 600:

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.