Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 10:31 AM BST

PDB ID	:	4XP4
Title	:	X-ray structure of Drosophila dopamine transporter in complex with cocaine
Authors	:	Aravind, P.; Wang, K.; Gouaux, E.
Deposited on	:	2015-01-16
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

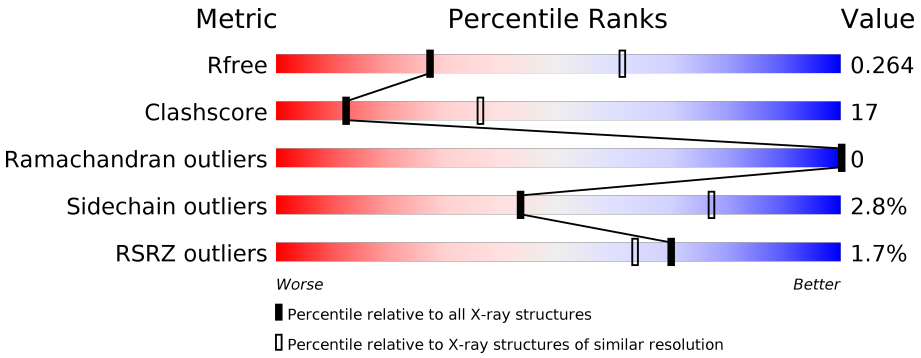
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	545	65% 31%
2	L	237	3% 65% 24% 10%
3	H	240	3% 66% 25% 9%
4	B	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	P4G	A	702	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7631 atoms, of which 58 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 Dopamine transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	1	0
			4191	2815	642	716	18			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP Q7K4Y6
A	74	ALA	VAL	engineered mutation	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	GLN	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	ALA	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	ARG	deletion	UNP Q7K4Y6
A	?	-	VAL	deletion	UNP Q7K4Y6
A	?	-	PRO	deletion	UNP Q7K4Y6
A	?	-	VAL	deletion	UNP Q7K4Y6
A	?	-	ILE	deletion	UNP Q7K4Y6
A	?	-	GLY	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	ASP	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	ALA	deletion	UNP Q7K4Y6
A	?	-	MET	deletion	UNP Q7K4Y6
A	?	-	GLY	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	GLN	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	GLU	deletion	UNP Q7K4Y6
A	?	-	THR	deletion	UNP Q7K4Y6
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	MET	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	GLY	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6
A	?	-	ASP	deletion	UNP Q7K4Y6
A	?	-	THR	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	ALA	deletion	UNP Q7K4Y6
A	?	-	VAL	deletion	UNP Q7K4Y6
A	415	ALA	LEU	engineered mutation	UNP Q7K4Y6
A	602	LEU	-	expression tag	UNP Q7K4Y6
A	603	VAL	-	expression tag	UNP Q7K4Y6
A	604	PRO	-	expression tag	UNP Q7K4Y6
A	605	ARG	-	expression tag	UNP Q7K4Y6

- Molecule 2 is a protein called ANTIBODY FRAGMENT HEAVY CHAIN-PROTEIN, 9D5-HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1619	1007	268	336	8			

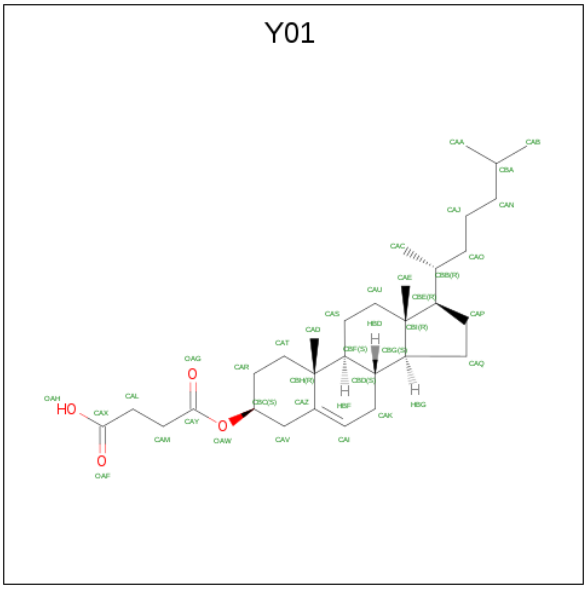
- Molecule 3 is a protein called ANTIBODY FRAGMENT HEAVY CHAIN-PROTEIN, 9D5-LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	0	0
			1618	1019	275	316	8			

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

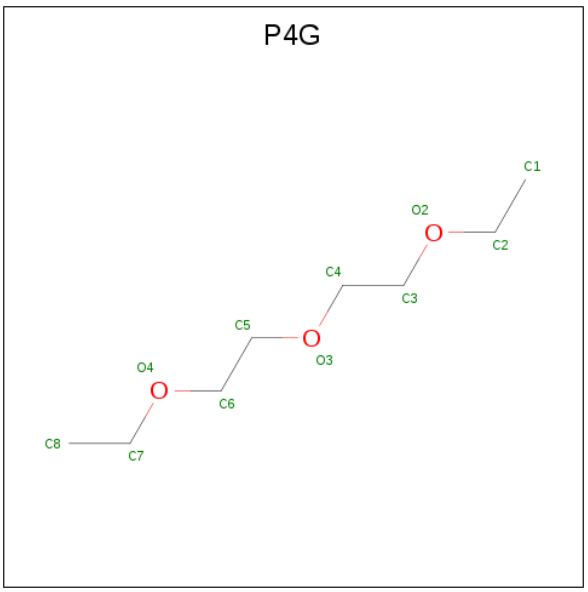
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	H	O			
4	B	2	45	12	22	11	0	0	0

- Molecule 5 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



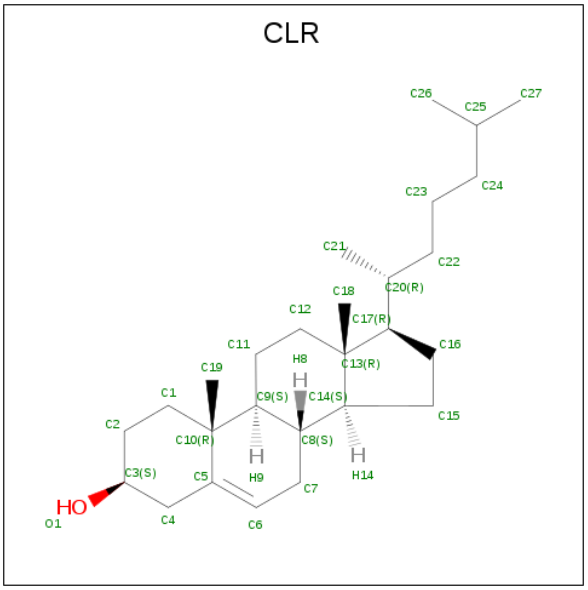
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	35	31	4	0	0

- Molecule 6 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (three-letter code: P4G) (formula: $C_8H_{18}O_3$).



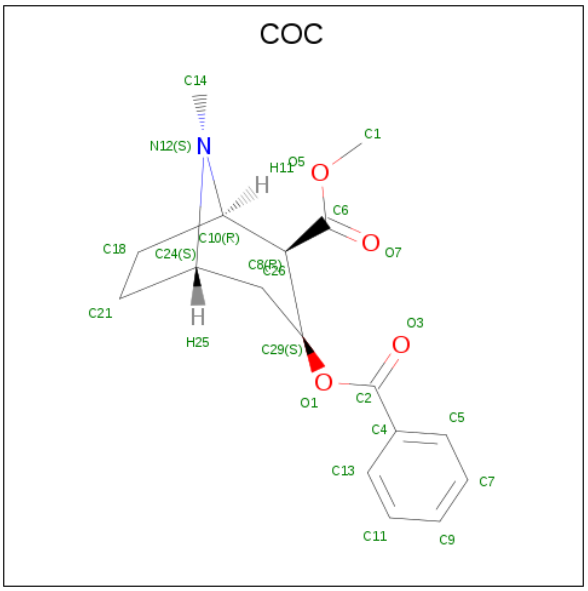
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			29	8	18	3		
6	A	1	Total	C	H	O	0	0
			29	8	18	3		

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 8 is COCAINE (three-letter code: COC) (formula: $C_{17}H_{21}NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 22 17 1 4	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total Na 2 2	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Cl 1 1	0	0

- Molecule 11 is water.

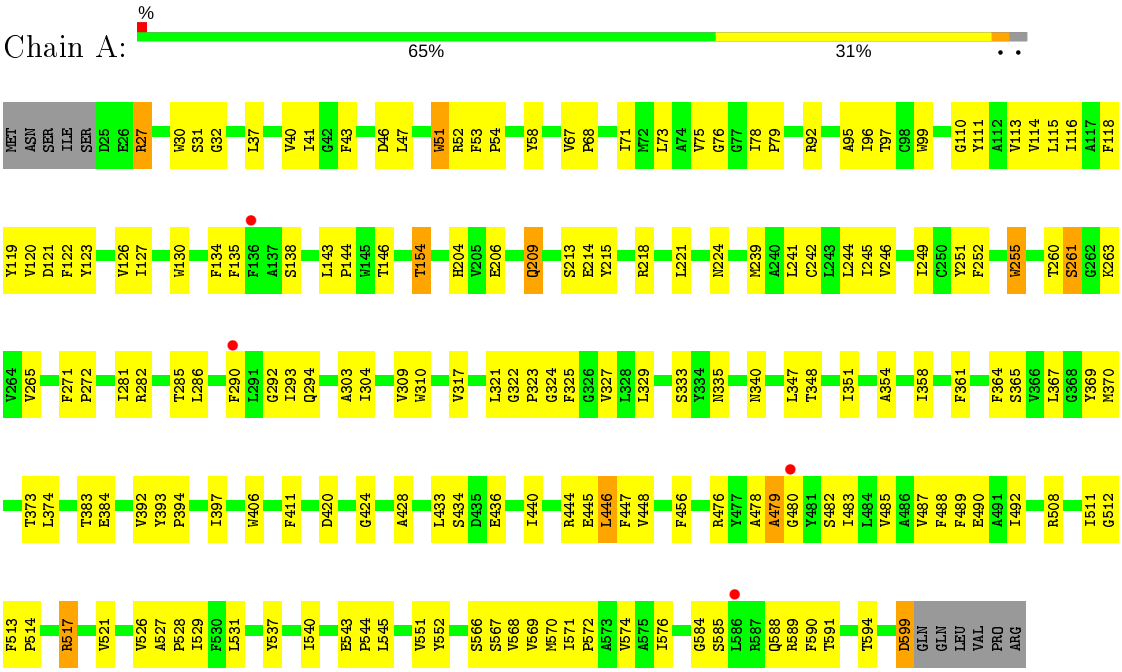
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	8	Total O 8 8	0	0
11	L	2	Total O 2 2	0	0
11	H	2	Total O 2 2	0	0

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.

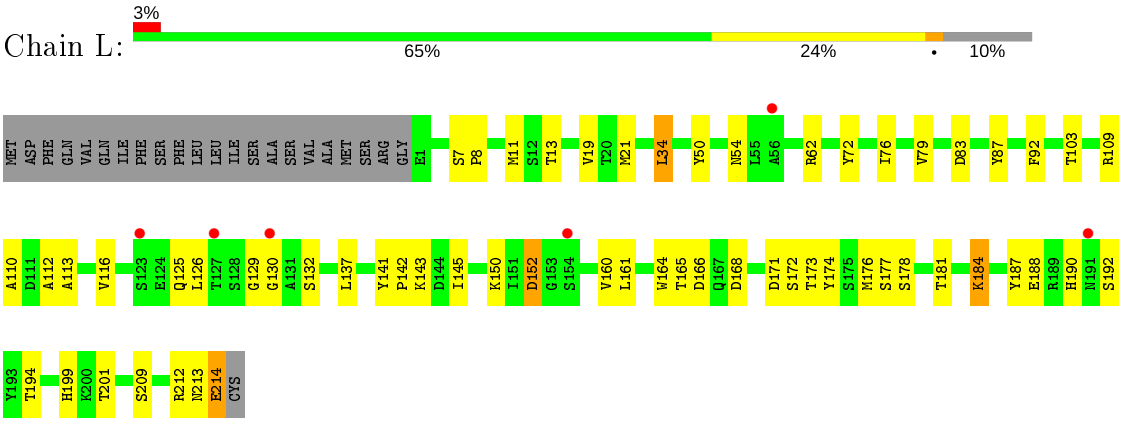
• Molecule 1: Dopamine transporter

Chain A:



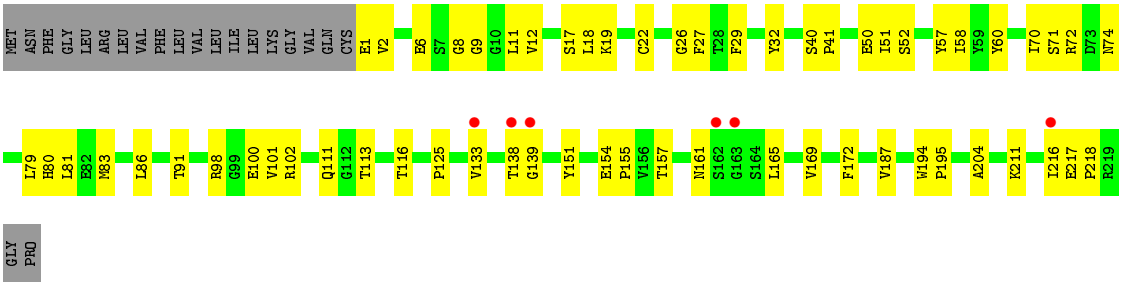
• Molecule 2: ANTIBODY FRAGMENT HEAVY CHAIN-PROTEIN, 9D5-HEAVY CHAIN

Chain L:



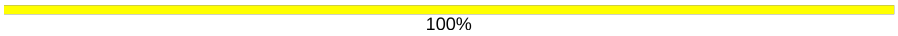
• Molecule 3: ANTIBODY FRAGMENT HEAVY CHAIN-PROTEIN, 9D5-LIGHT CHAIN

Chain H:



- Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.06Å 140.73Å 166.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.88 – 2.80 48.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.88-2.80) 98.9 (48.22-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.236 , 0.266 0.240 , 0.264	Depositor DCC
R_{free} test set	2739 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	77.6	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 57.0	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	0.90	EDS
Total number of atoms	7631	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y01, CL, P4G, NA, GLC, COC, CLR

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	0.26	0/4338	0.43	0/5940
2	L	0.23	0/1657	0.44	1/2254 (0.0%)
3	H	0.23	0/1657	0.42	0/2262
All	All	0.25	0/7652	0.43	1/10456 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
3	H	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	152	ASP	CB-CG-OD2	5.20	122.98	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	478	ALA	Peptide
1	A	479	ALA	Peptide
3	H	98	ARG	Peptide

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	4191	0	4061	157	0
2	L	1619	0	1523	52	0
3	H	1618	0	1539	42	0
4	B	23	22	21	0	0
5	A	35	0	49	6	0
6	A	22	36	36	2	0
7	A	28	0	46	2	0
8	A	22	0	21	2	0
9	A	2	0	0	0	0
10	A	1	0	0	0	0
11	A	8	0	0	0	0
11	H	2	0	0	1	0
11	L	2	0	0	0	0
All	All	7573	58	7296	251	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 17.

All (251) 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:52:ARG:NH1	1:A:384:GLU:OE2	1.74	1.20
1:A:121:ASP:HB3	8:A:706:COC:H10	1.36	1.06
1:A:78:ILE:HD12	5:A:701:Y01:HAK1	1.46	0.94
3:H:83:MET:HB3	3:H:86:LEU:HD21	1.48	0.94
2:L:129:GLY:H	2:L:184:LYS:HZ1	1.15	0.87
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.60	0.84
1:A:95:ALA:HA	1:A:329:LEU:HD23	1.65	0.78
1:A:364:PHE:HA	1:A:367:LEU:HB2	1.66	0.78
1:A:75:VAL:HB	1:A:526:VAL:HG11	1.65	0.78
1:A:53:PHE:HB3	1:A:54:PRO:HD3	1.68	0.76
2:L:129:GLY:H	2:L:184:LYS:NZ	1.84	0.76
1:A:479:ALA:CB	1:A:482:SER:HB2	2.18	0.74
2:L:129:GLY:N	2:L:184:LYS:HZ1	1.85	0.74
1:A:97:THR:HG23	1:A:436:GLU:HG2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:HD12	5:A:701:Y01:CAK	2.19	0.73
2:L:34:LEU:HD22	2:L:72:TYR:CD2	2.25	0.71
3:H:51:ILE:HD13	3:H:72:ARG:HB2	1.71	0.71
2:L:125:GLN:O	2:L:184:LYS:NZ	2.22	0.71
3:H:83:MET:CB	3:H:86:LEU:HD21	2.21	0.71
2:L:130:GLY:O	2:L:184:LYS:HE2	1.91	0.71
2:L:129:GLY:C	2:L:184:LYS:HE3	2.11	0.70
2:L:190:HIS:O	2:L:212:ARG:NH1	2.24	0.70
2:L:129:GLY:CA	2:L:184:LYS:HE3	2.22	0.70
2:L:21:MET:HE3	2:L:87:TYR:HB2	1.72	0.70
2:L:21:MET:HE3	2:L:103:THR:HB	1.74	0.69
1:A:476:ARG:HD2	1:A:545:LEU:HD13	1.73	0.69
2:L:184:LYS:HA	2:L:187:TYR:HB3	1.74	0.69
1:A:52:ARG:NH1	1:A:384:GLU:CD	2.46	0.69
3:H:51:ILE:HG13	3:H:58:ILE:CD1	2.23	0.69
2:L:213:ASN:OD1	2:L:214:GLU:N	2.25	0.69
1:A:115:LEU:HD11	1:A:567:SER:HA	1.74	0.68
1:A:252:PHE:HA	1:A:255:TRP:HB2	1.76	0.68
2:L:152:ASP:OD1	2:L:192:SER:HB3	1.94	0.68
1:A:303:ALA:HB1	1:A:309:VAL:HG21	1.76	0.67
1:A:591:THR:HA	1:A:594:THR:HG22	1.76	0.66
3:H:29:PHE:O	3:H:72:ARG:NH2	2.28	0.66
1:A:115:LEU:HA	1:A:118:PHE:HB3	1.78	0.66
1:A:251:TYR:CE1	1:A:448:VAL:HG23	2.31	0.66
1:A:75:VAL:O	1:A:79:PRO:HG2	1.95	0.65
2:L:34:LEU:HD22	2:L:72:TYR:CG	2.33	0.64
1:A:369:TYR:O	1:A:373:THR:HG22	1.96	0.64
1:A:47:LEU:HD13	1:A:127:ILE:HG21	1.80	0.63
1:A:40:VAL:CG1	1:A:348:THR:HG21	2.29	0.63
2:L:116:VAL:HG22	2:L:137:LEU:HD22	1.80	0.63
1:A:479:ALA:HB2	1:A:482:SER:HB2	1.81	0.63
2:L:113:ALA:HA	2:L:201:THR:HG21	1.80	0.63
2:L:126:LEU:C	2:L:184:LYS:HZ2	2.02	0.63
1:A:52:ARG:HH12	1:A:384:GLU:CD	2.03	0.62
1:A:71:ILE:O	1:A:75:VAL:HG22	2.00	0.62
3:H:22:CYS:HB3	3:H:79:LEU:HB3	1.81	0.62
2:L:21:MET:CE	2:L:103:THR:HB	2.29	0.62
1:A:113:VAL:HG22	1:A:324:GLY:O	2.00	0.61
1:A:143:LEU:O	1:A:146:THR:HG22	2.02	0.60
1:A:513:PHE:HB3	3:H:101:VAL:HG13	1.83	0.60
1:A:543:GLU:HG2	1:A:544:PRO:HD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.83	0.60
2:L:176:MET:HG2	2:L:177:SER:N	2.16	0.60
1:A:370:MET:HG2	1:A:374:LEU:HD12	1.84	0.59
1:A:209:GLN:HG3	1:A:213:SER:OG	2.03	0.59
1:A:286:LEU:HD23	1:A:369:TYR:CG	2.38	0.59
1:A:591:THR:HA	1:A:594:THR:CG2	2.32	0.59
1:A:116:ILE:O	1:A:120:VAL:HG23	2.02	0.59
3:H:52:SER:OG	3:H:57:TYR:HB2	2.01	0.59
1:A:433:LEU:C	1:A:440:ILE:HD11	2.24	0.58
3:H:51:ILE:HG13	3:H:58:ILE:HD11	1.85	0.58
1:A:572:PRO:O	1:A:576:ILE:HG12	2.04	0.58
1:A:245:ILE:O	1:A:249:ILE:HG13	2.04	0.58
1:A:340:ASN:HA	1:A:511:ILE:HG22	1.86	0.58
1:A:293:ILE:HD12	1:A:361:PHE:CD2	2.39	0.57
2:L:199:HIS:ND1	2:L:201:THR:HG23	2.19	0.57
1:A:135:PHE:O	1:A:138:SER:OG	2.21	0.57
1:A:393:TYR:CE2	1:A:397:ILE:HD11	2.39	0.57
2:L:199:HIS:CE1	2:L:201:THR:HG23	2.39	0.57
1:A:489:PHE:HD2	1:A:571:ILE:HD13	1.70	0.57
2:L:171:ASP:OD1	2:L:173:THR:HG22	2.04	0.57
1:A:73:LEU:HA	1:A:317:VAL:HG11	1.86	0.57
2:L:132:SER:HB3	2:L:181:THR:HG22	1.86	0.57
1:A:218:ARG:HE	1:A:224:ASN:ND2	2.03	0.57
1:A:487:VAL:HG12	1:A:531:LEU:HD11	1.87	0.57
3:H:157:THR:HB	3:H:204:ALA:HB3	1.86	0.57
1:A:369:TYR:CE1	1:A:373:THR:HG21	2.40	0.56
3:H:81:LEU:HD23	3:H:83:MET:HE3	1.86	0.56
1:A:40:VAL:HG12	1:A:348:THR:HG21	1.87	0.56
1:A:545:LEU:HG	1:A:552:TYR:CD1	2.40	0.56
2:L:116:VAL:HG22	2:L:137:LEU:CD2	2.35	0.56
1:A:292:GLY:HA3	1:A:364:PHE:O	2.06	0.56
3:H:32:TYR:O	3:H:72:ARG:NH2	2.39	0.56
1:A:209:GLN:HG3	1:A:213:SER:CB	2.36	0.56
3:H:169:VAL:HG22	3:H:187:VAL:HG23	1.88	0.56
2:L:113:ALA:CA	2:L:201:THR:HG21	2.35	0.56
1:A:479:ALA:HB1	1:A:483:ILE:H	1.71	0.55
1:A:27:ARG:HH12	1:A:333:SER:CB	2.19	0.55
3:H:9:GLY:HA2	3:H:18:LEU:HD21	1.87	0.55
2:L:109:ARG:NH1	2:L:110:ALA:O	2.39	0.55
1:A:282:ARG:HD3	1:A:406:TRP:CZ2	2.41	0.55
1:A:397:ILE:HG23	1:A:406:TRP:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:CD1	1:A:127:ILE:HG21	2.37	0.54
1:A:489:PHE:HD2	1:A:571:ILE:HG21	1.72	0.54
2:L:50:TYR:O	2:L:54:ASN:HB2	2.06	0.54
1:A:585:SER:O	1:A:589:ARG:N	2.40	0.54
2:L:109:ARG:HH12	2:L:112:ALA:HB2	1.73	0.54
3:H:40:SER:HB2	3:H:41:PRO:HD2	1.89	0.54
1:A:244:LEU:HB2	1:A:456:PHE:CE1	2.42	0.53
1:A:115:LEU:HD11	1:A:567:SER:CA	2.38	0.53
1:A:588:GLN:O	1:A:591:THR:HG22	2.08	0.53
3:H:161:ASN:HD22	3:H:165:LEU:HD23	1.73	0.53
1:A:489:PHE:CD2	1:A:571:ILE:HG21	2.43	0.53
1:A:154:THR:HG23	1:A:214:GLU:OE2	2.08	0.53
1:A:75:VAL:HG23	1:A:76:GLY:N	2.24	0.52
1:A:242:CYS:O	1:A:246:VAL:HG23	2.10	0.52
1:A:393:TYR:HE2	1:A:397:ILE:HD11	1.74	0.52
1:A:251:TYR:OH	1:A:445:GLU:O	2.26	0.52
2:L:21:MET:CE	2:L:87:TYR:HB2	2.40	0.52
1:A:433:LEU:HD12	1:A:447:PHE:CZ	2.45	0.52
1:A:218:ARG:HE	1:A:224:ASN:HD22	1.57	0.52
1:A:78:ILE:CD1	5:A:701:Y01:HAK1	2.29	0.52
1:A:115:LEU:HA	1:A:118:PHE:CB	2.40	0.51
1:A:78:ILE:HD11	5:A:701:Y01:HAQ2	1.91	0.51
1:A:75:VAL:HG23	1:A:76:GLY:H	1.75	0.51
1:A:570:MET:CE	1:A:570:MET:HA	2.41	0.51
1:A:123:TYR:O	1:A:126:VAL:HG23	2.11	0.51
1:A:154:THR:HG22	1:A:218:ARG:HH11	1.76	0.51
3:H:91:THR:HG23	3:H:116:THR:HA	1.93	0.51
2:L:168:ASP:O	2:L:172:SER:HA	2.11	0.51
2:L:62:ARG:NH1	2:L:83:ASP:OD1	2.44	0.51
1:A:370:MET:HE1	1:A:392:VAL:CG1	2.41	0.50
1:A:271:PHE:HB3	1:A:272:PRO:HD3	1.92	0.50
1:A:92:ARG:NH2	1:A:335:ASN:O	2.45	0.50
3:H:83:MET:HB3	3:H:86:LEU:CD2	2.31	0.50
2:L:126:LEU:C	2:L:184:LYS:NZ	2.64	0.50
1:A:282:ARG:O	1:A:286:LEU:HD13	2.12	0.50
1:A:40:VAL:HG11	1:A:348:THR:HG21	1.93	0.50
1:A:251:TYR:HE1	1:A:448:VAL:HG23	1.77	0.49
1:A:255:TRP:CZ3	1:A:445:GLU:HG2	2.47	0.49
1:A:480:GLY:HA3	6:A:702:P4G:H42	1.94	0.49
1:A:566:SER:O	1:A:569:VAL:HG12	2.12	0.49
1:A:393:TYR:HB3	1:A:394:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:ARG:O	1:A:521:VAL:HG23	2.12	0.48
1:A:130:TRP:HA	1:A:239:MET:HE1	1.94	0.48
1:A:574:VAL:HG13	6:A:703:P4G:H71	1.95	0.48
1:A:571:ILE:HB	1:A:572:PRO:HD3	1.94	0.48
1:A:571:ILE:HB	1:A:572:PRO:CD	2.44	0.48
3:H:60:TYR:CE1	3:H:70:ILE:HG22	2.49	0.48
1:A:43:PHE:HE2	1:A:322:GLY:HA3	1.79	0.48
1:A:293:ILE:HD12	1:A:361:PHE:HD2	1.78	0.47
3:H:81:LEU:HD23	3:H:83:MET:CE	2.43	0.47
3:H:8:GLY:O	3:H:113:THR:OG1	2.31	0.47
1:A:43:PHE:CD1	1:A:327:VAL:HG11	2.48	0.47
1:A:361:PHE:O	1:A:365:SER:HB2	2.14	0.47
1:A:383:THR:OG1	1:A:384:GLU:N	2.48	0.47
3:H:12:VAL:HG11	3:H:86:LEU:HD12	1.96	0.47
1:A:51:TRP:C	1:A:51:TRP:CD1	2.88	0.47
3:H:194:TRP:CG	3:H:195:PRO:HA	2.49	0.47
1:A:115:LEU:CD1	1:A:567:SER:HB3	2.45	0.47
5:A:701:Y01:HBB	5:A:701:Y01:HAE2	1.69	0.47
1:A:96:ILE:HD13	1:A:111:TYR:CE1	2.49	0.47
1:A:290:PHE:HD2	1:A:294:GLN:HE21	1.61	0.47
1:A:591:THR:CA	1:A:594:THR:HG22	2.43	0.47
2:L:176:MET:HE1	2:L:178:SER:HB2	1.97	0.47
1:A:113:VAL:HG13	1:A:325:PHE:C	2.36	0.46
1:A:261:SER:O	1:A:265:VAL:HG13	2.15	0.46
1:A:488:PHE:O	1:A:492:ILE:HG12	2.14	0.46
2:L:8:PRO:HD2	2:L:11:MET:CE	2.45	0.46
3:H:19:LYS:HE2	3:H:80:HIS:ND1	2.30	0.46
2:L:13:THR:HG21	2:L:19:VAL:CG1	2.44	0.46
1:A:321:LEU:O	1:A:323:PRO:HD2	2.15	0.46
1:A:281:ILE:O	1:A:285:THR:HG23	2.16	0.46
3:H:72:ARG:NE	3:H:74:ASN:OD1	2.46	0.46
2:L:141:TYR:CG	2:L:142:PRO:HA	2.51	0.46
2:L:19:VAL:HG22	2:L:76:ILE:HB	1.98	0.46
3:H:50:GLU:HG3	11:H:301:HOH:O	2.14	0.46
1:A:144:PRO:HB2	1:A:215:TYR:CE1	2.51	0.45
1:A:527:ALA:HB3	1:A:528:PRO:CD	2.41	0.45
1:A:537:TYR:O	1:A:540:ILE:HG22	2.16	0.45
1:A:67:VAL:HB	1:A:68:PRO:CD	2.46	0.45
1:A:290:PHE:O	1:A:294:GLN:HG3	2.17	0.45
1:A:434:SER:HA	1:A:440:ILE:CD1	2.46	0.45
1:A:599:ASP:N	1:A:599:ASP:OD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:21:MET:HE2	2:L:21:MET:HB3	1.86	0.45
1:A:209:GLN:HG3	1:A:213:SER:HB3	1.97	0.45
3:H:216:ILE:HD12	3:H:216:ILE:N	2.31	0.45
1:A:434:SER:HA	1:A:440:ILE:HD12	1.97	0.45
1:A:590:PHE:O	1:A:594:THR:HG22	2.16	0.45
3:H:17:SER:HB2	3:H:83:MET:O	2.17	0.45
1:A:367:LEU:HD12	1:A:370:MET:HE2	1.98	0.45
1:A:67:VAL:HB	1:A:68:PRO:HD3	1.99	0.45
3:H:217:GLU:HA	3:H:218:PRO:HD3	1.76	0.45
1:A:53:PHE:HB3	1:A:54:PRO:CD	2.44	0.45
1:A:78:ILE:HB	1:A:79:PRO:HD3	1.99	0.44
1:A:354:ALA:O	1:A:358:ILE:HG12	2.17	0.44
1:A:68:PRO:HD3	1:A:304:ILE:HD12	1.98	0.44
2:L:164:TRP:HD1	2:L:176:MET:HG3	1.82	0.44
2:L:188:GLU:HA	2:L:212:ARG:NH1	2.32	0.44
1:A:282:ARG:NH1	1:A:285:THR:OG1	2.51	0.44
7:A:705:CLR:H183	7:A:705:CLR:H212	1.98	0.44
1:A:251:TYR:O	1:A:255:TRP:N	2.50	0.44
5:A:701:Y01:HAE1	5:A:701:Y01:HAS2	1.75	0.44
2:L:19:VAL:HG13	2:L:79:VAL:HG21	1.99	0.44
1:A:110:GLY:O	1:A:114:VAL:HG23	2.18	0.43
1:A:327:VAL:HG22	1:A:424:GLY:O	2.18	0.43
1:A:476:ARG:CD	1:A:545:LEU:HD13	2.45	0.43
1:A:584:GLY:O	1:A:589:ARG:HD2	2.18	0.43
1:A:446:LEU:HD12	1:A:446:LEU:HA	1.83	0.43
1:A:260:THR:O	1:A:263:LYS:N	2.49	0.43
1:A:444:ARG:O	1:A:448:VAL:HG22	2.19	0.43
3:H:11:LEU:HD12	3:H:12:VAL:H	1.83	0.43
2:L:8:PRO:CD	2:L:11:MET:HE2	2.48	0.43
1:A:41:ILE:HD11	1:A:351:ILE:HD12	2.00	0.43
1:A:241:LEU:O	1:A:245:ILE:HG13	2.18	0.43
2:L:137:LEU:HD13	2:L:145:ILE:HD13	1.99	0.43
1:A:252:PHE:CA	1:A:255:TRP:HB2	2.46	0.42
1:A:514:PRO:HG3	3:H:100:GLU:HG2	2.00	0.42
2:L:143:LYS:HE3	2:L:174:TYR:CE1	2.54	0.42
2:L:8:PRO:HD2	2:L:11:MET:HE2	2.00	0.42
1:A:99:TRP:CZ2	1:A:490:GLU:HG2	2.54	0.42
3:H:6:GLU:N	3:H:6:GLU:OE1	2.52	0.42
3:H:71:SER:OG	3:H:80:HIS:HB2	2.18	0.42
1:A:27:ARG:HH12	1:A:333:SER:HB2	1.84	0.42
3:H:1:GLU:O	3:H:26:GLY:HA3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:ARG:HD3	1:A:508:ARG:C	2.40	0.42
1:A:485:VAL:HG21	1:A:568:VAL:HG11	2.01	0.42
2:L:130:GLY:C	2:L:184:LYS:HE2	2.40	0.42
2:L:7:SER:HA	2:L:8:PRO:C	2.40	0.42
1:A:134:PHE:HB3	1:A:411:PHE:CE2	2.55	0.41
1:A:255:TRP:CZ3	1:A:445:GLU:CG	3.02	0.41
7:A:705:CLR:H121	7:A:705:CLR:H212	2.02	0.41
2:L:165:THR:HG23	3:H:172:PHE:CD2	2.55	0.41
1:A:479:ALA:HB1	1:A:482:SER:HB2	1.96	0.41
1:A:119:TYR:O	1:A:122:PHE:HB2	2.20	0.41
2:L:150:LYS:HB2	2:L:194:THR:HB	2.02	0.41
3:H:2:VAL:HG13	3:H:27:PHE:CD1	2.55	0.41
2:L:194:THR:HG23	2:L:209:SER:OG	2.19	0.41
3:H:211:LYS:HB2	3:H:211:LYS:HE3	1.87	0.41
1:A:46:ASP:OD1	8:A:706:COC:H15	2.21	0.41
1:A:325:PHE:CZ	1:A:483:ILE:HD12	2.56	0.41
3:H:154:GLU:OE2	3:H:155:PRO:HA	2.20	0.41
1:A:304:ILE:O	1:A:310:TRP:NE1	2.41	0.41
1:A:78:ILE:N	1:A:79:PRO:CD	2.84	0.41
3:H:138:THR:HA	3:H:139:GLY:HA3	1.79	0.41
1:A:551:VAL:HG23	1:A:551:VAL:O	2.21	0.41
1:A:271:PHE:N	1:A:272:PRO:CD	2.84	0.40
1:A:30:TRP:C	1:A:32:GLY:H	2.23	0.40
1:A:43:PHE:CE1	1:A:327:VAL:HG21	2.56	0.40
1:A:37:LEU:O	1:A:41:ILE:HG12	2.21	0.40
1:A:327:VAL:HG22	1:A:428:ALA:HB2	2.03	0.40
3:H:165:LEU:HD11	3:H:187:VAL:HG21	2.04	0.40
1:A:347:LEU:O	1:A:351:ILE:HG13	2.22	0.40
1:A:489:PHE:CD2	1:A:571:ILE:HD13	2.53	0.40
2:L:160:VAL:HG12	2:L:161:LEU:N	2.36	0.40
1:A:58:TYR:HB2	1:A:364:PHE:CZ	2.56	0.40
1:A:512:GLY:HA2	3:H:102:ARG:HD2	2.03	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	533/545 (98%)	516 (97%)	17 (3%)	0	100	100
2	L	212/237 (90%)	205 (97%)	7 (3%)	0	100	100
3	H	217/240 (90%)	209 (96%)	8 (4%)	0	100	100
All	All	962/1022 (94%)	930 (97%)	32 (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	425/450 (94%)	410 (96%)	15 (4%)	36	70
2	L	182/207 (88%)	177 (97%)	5 (3%)	44	78
3	H	173/205 (84%)	171 (99%)	2 (1%)	71	92
All	All	780/862 (90%)	758 (97%)	22 (3%)	43	77

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	31	SER
1	A	51	TRP
1	A	154	THR
1	A	204	HIS
1	A	206	GLU
1	A	209	GLN
1	A	221	LEU
1	A	255	TRP
1	A	261	SER
1	A	420	ASP

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Mol	Chain	Res	Type
1	A	446	LEU
1	A	517	ARG
1	A	529	ILE
1	A	599	ASP
2	L	34	LEU
2	L	92	PHE
2	L	166	ASP
2	L	184	LYS
2	L	214	GLU
3	H	111	GLN
3	H	133	VAL

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

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

2 monosaccharides are modelled in this entry.

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	GLC	B	1	4	12,12,12	0.51	0	17,17,17	0.89	1 (5%)
4	GLC	B	2	4	11,11,12	0.54	0	15,15,17	1.19	1 (6%)

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	GLC	B	1	4	-	0/2/22/22	0/1/1/1
4	GLC	B	2	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2	GLC	C1-O5-C5	2.95	116.19	112.19
4	B	1	GLC	C3-C4-C5	-2.17	106.37	110.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2	GLC	O5-C5-C6-O6
4	B	2	GLC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
5	Y01	A	701	-	35,38,38	4.43	14 (40%)	54,57,57	2.01	18 (33%)
6	P4G	A	703	-	10,10,10	0.68	0	9,9,9	0.35	0
6	P4G	A	702	-	10,10,10	0.65	0	9,9,9	0.24	0
7	CLR	A	705	-	31,31,31	0.71	0	48,48,48	1.17	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	COC	A	706	-	24,24,24	4.44	9 (37%)	32,34,34	2.05	7 (21%)

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
5	Y01	A	701	-	-	9/17/77/77	0/4/4/4
6	P4G	A	703	-	-	5/8/8/8	-
6	P4G	A	702	-	-	5/8/8/8	-
7	CLR	A	705	-	-	0/10/68/68	0/4/4/4
8	COC	A	706	-	-	1/14/39/39	0/4/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	701	Y01	CAI-CAZ	16.92	1.70	1.33
8	A	706	COC	O1-C29	-11.25	1.26	1.46
8	A	706	COC	C24-N12	-10.82	1.32	1.48
5	A	701	Y01	CBB-CBE	-10.27	1.36	1.54
8	A	706	COC	C10-N12	-7.81	1.31	1.47
5	A	701	Y01	CBH-CBF	7.75	1.69	1.56
5	A	701	Y01	CAU-CBI	-7.23	1.41	1.54
8	A	706	COC	O1-C2	7.03	1.48	1.34
8	A	706	COC	C8-C29	5.48	1.68	1.53
5	A	701	Y01	CAP-CBE	5.44	1.65	1.54
5	A	701	Y01	CAU-CAS	5.33	1.64	1.53
8	A	706	COC	C26-C29	5.20	1.61	1.52
5	A	701	Y01	CAK-CBD	5.19	1.61	1.53
8	A	706	COC	O5-C6	4.99	1.45	1.33
8	A	706	COC	C8-C10	-4.73	1.48	1.54
5	A	701	Y01	CBI-CBE	4.66	1.63	1.55
5	A	701	Y01	CBH-CAZ	-4.59	1.43	1.52
5	A	701	Y01	OAW-CAY	3.22	1.43	1.34
5	A	701	Y01	CAQ-CBG	3.05	1.60	1.54
5	A	701	Y01	CAO-CBB	2.84	1.61	1.54
8	A	706	COC	C21-C18	-2.54	1.47	1.54
5	A	701	Y01	CBD-CBF	-2.14	1.49	1.53
5	A	701	Y01	CAE-CBI	-2.06	1.50	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	706	COC	O5-C6-C8	6.37	120.31	111.03
5	A	701	Y01	CBI-CBE-CBB	-4.58	112.31	119.49
5	A	701	Y01	CAU-CBI-CBE	4.51	123.32	116.57
8	A	706	COC	O1-C2-C4	4.46	119.12	111.92
7	A	705	CLR	C4-C5-C10	4.06	121.81	116.42
8	A	706	COC	C26-C24-N12	3.98	113.23	107.53
5	A	701	Y01	CAK-CAI-CAZ	-3.93	117.82	125.06
5	A	701	Y01	CBF-CBD-CBG	3.61	113.92	109.09
5	A	701	Y01	CAE-CBI-CBG	-3.51	105.17	111.71
5	A	701	Y01	CAU-CBI-CBG	3.48	112.67	107.27
5	A	701	Y01	OAW-CAY-CAM	3.43	118.90	111.50
8	A	706	COC	C18-C10-N12	-3.30	101.78	105.18
5	A	701	Y01	CAE-CBI-CBE	-3.30	105.56	111.71
5	A	701	Y01	CAC-CBB-CBE	-3.06	108.23	112.92
5	A	701	Y01	CAE-CBI-CAU	-3.05	105.77	110.59
8	A	706	COC	C18-C10-C8	-2.88	108.03	112.28
5	A	701	Y01	CAR-CBC-CAV	2.83	115.20	110.99
5	A	701	Y01	CBH-CAZ-CAI	-2.74	118.71	122.90
5	A	701	Y01	CAD-CBH-CBF	-2.74	108.42	111.68
5	A	701	Y01	CAV-CAZ-CBH	2.70	120.00	116.42
5	A	701	Y01	CBF-CBH-CAZ	2.47	113.52	109.65
8	A	706	COC	O5-C6-O7	-2.40	119.14	123.84
5	A	701	Y01	CBG-CBI-CBE	2.40	102.91	100.07
8	A	706	COC	O7-C6-C8	-2.39	120.55	124.99
5	A	701	Y01	CAT-CAR-CBC	2.21	114.10	110.33
7	A	705	CLR	C4-C5-C6	-2.19	117.45	120.61
7	A	705	CLR	C8-C7-C6	-2.15	109.64	112.73
7	A	705	CLR	C11-C12-C13	-2.15	109.09	112.78
5	A	701	Y01	CAP-CBE-CBI	-2.03	101.40	103.84

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	703	P4G	O2-C3-C4-O3
5	A	701	Y01	CAJ-CAO-CBB-CAC
6	A	703	P4G	O3-C5-C6-O4
5	A	701	Y01	CAJ-CAO-CBB-CBE
5	A	701	Y01	CAX-CAL-CAM-CAY
6	A	702	P4G	O2-C3-C4-O3
5	A	701	Y01	CAO-CAJ-CAN-CBA

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Mol	Chain	Res	Type	Atoms
5	A	701	Y01	CAC-CBB-CBE-CBI
5	A	701	Y01	CAJ-CAN-CBA-CAB
5	A	701	Y01	CAJ-CAN-CBA-CAA
5	A	701	Y01	CAO-CBB-CBE-CBI
6	A	702	P4G	C6-C5-O3-C4
6	A	702	P4G	O3-C5-C6-O4
6	A	703	P4G	C3-C4-O3-C5
6	A	702	P4G	C5-C6-O4-C7
6	A	703	P4G	C6-C5-O3-C4
8	A	706	COC	C8-C29-O1-C2
5	A	701	Y01	CAC-CBB-CBE-CAP
6	A	703	P4G	C5-C6-O4-C7
6	A	702	P4G	C3-C4-O3-C5

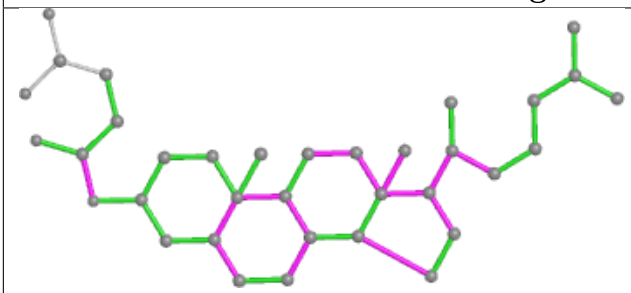
There are no ring outliers.

5 monomers are involved in 12 short contacts:

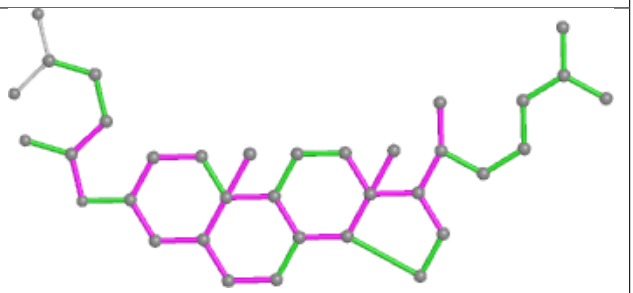
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	Y01	6	0
6	A	703	P4G	1	0
6	A	702	P4G	1	0
7	A	705	CLR	2	0
8	A	706	COC	2	0

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.

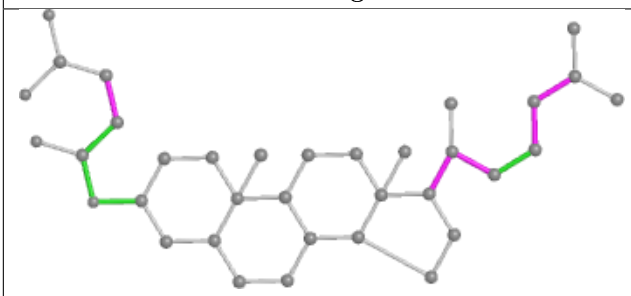
Ligand Y01 A 701



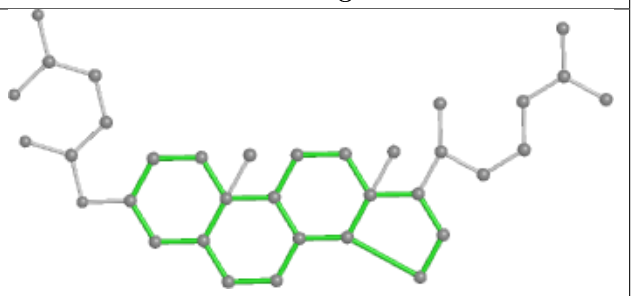
Bond lengths



Bond angles

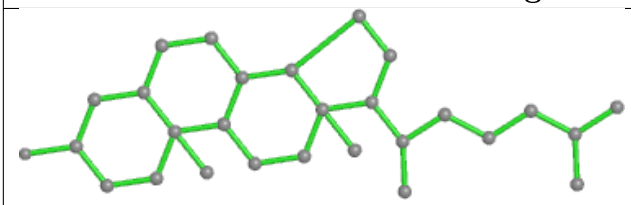


Torsions

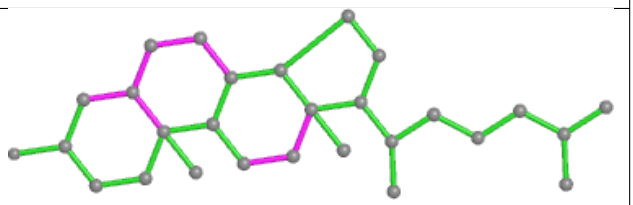


Rings

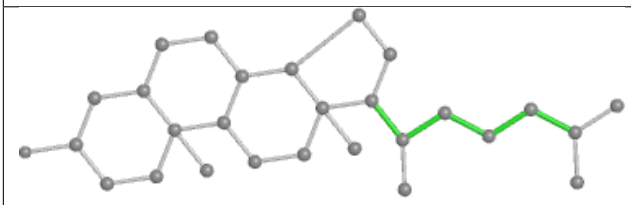
Ligand CLR A 705



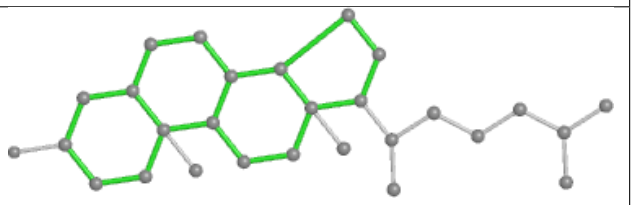
Bond lengths



Bond angles

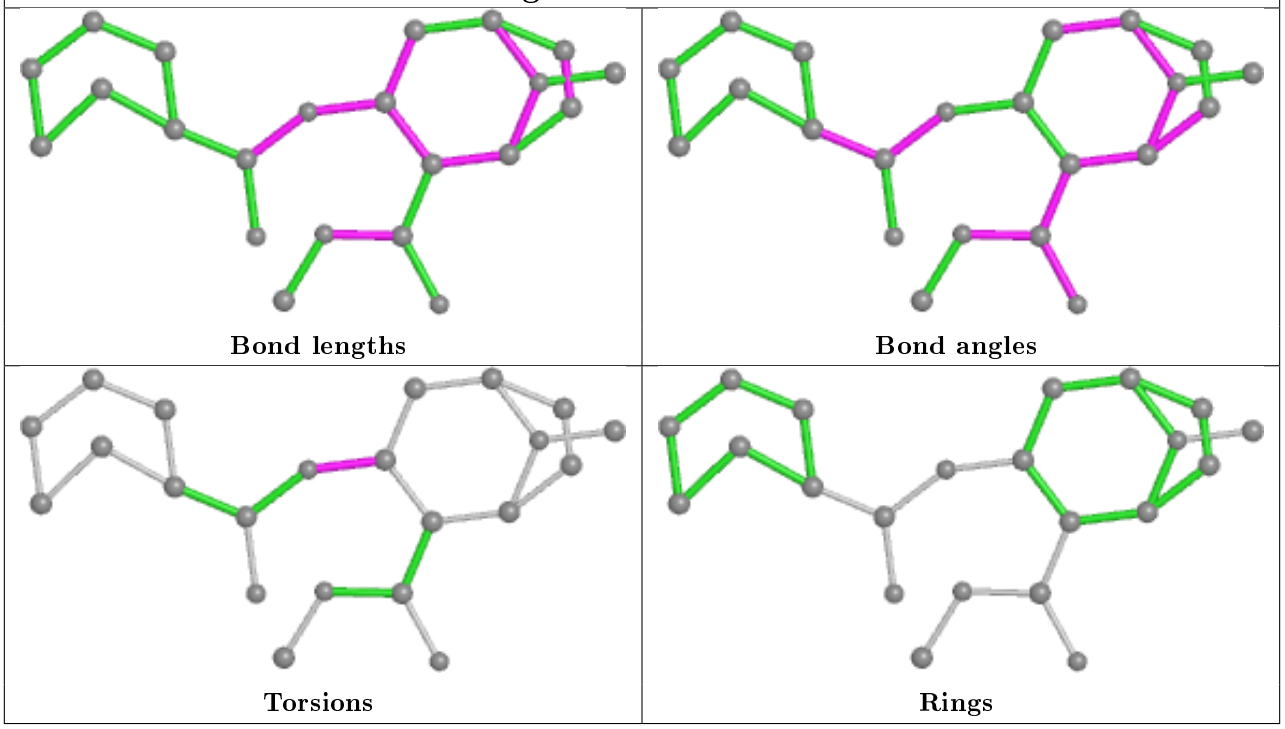


Torsions



Rings

Ligand COC A 706



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	534/545 (97%)	-0.07	4 (0%)	87 84	55, 70, 92, 122	0
2	L	214/237 (90%)	-0.05	6 (2%)	53 43	51, 67, 99, 122	0
3	H	219/240 (91%)	-0.04	6 (2%)	54 44	53, 68, 104, 140	0
All	All	967/1022 (94%)	-0.06	16 (1%)	70 63	51, 69, 98, 140	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	138	THR	3.4
1	A	136	PHE	2.9
2	L	123	SER	2.9
3	H	216	ILE	2.8
3	H	162	SER	2.8
1	A	290	PHE	2.7
2	L	130	GLY	2.7
1	A	586	LEU	2.6
2	L	191	ASN	2.5
3	H	163	GLY	2.5
3	H	139	GLY	2.5
2	L	154	SER	2.4
2	L	127	THR	2.3
2	L	56	ALA	2.2
3	H	133	VAL	2.2
1	A	480	GLY	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 (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^{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	GLC	B	1	12/12	0.82	0.22	94,110,126,133	0
4	GLC	B	2	11/12	0.84	0.16	90,106,127,127	0

6.4 Ligands (i)

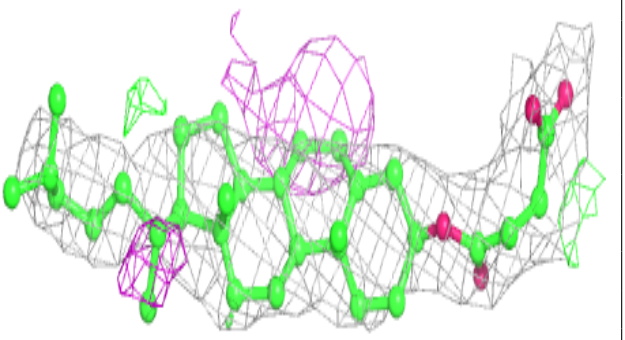
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

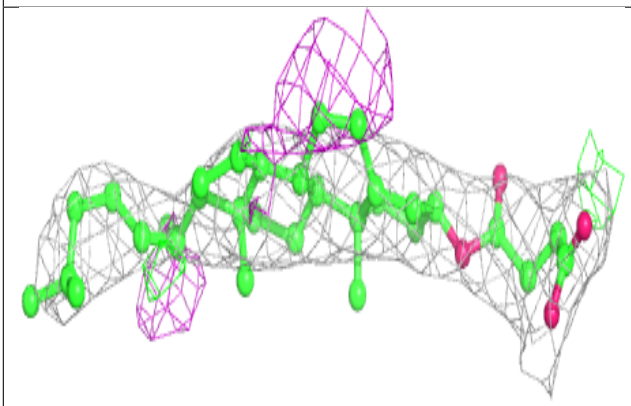
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	P4G	A	702	11/11	0.57	0.41	89,108,119,126	0
6	P4G	A	703	11/11	0.58	0.28	96,121,130,132	0
5	Y01	A	701	35/35	0.85	0.35	67,85,102,108	0
9	NA	A	708	1/1	0.89	0.19	56,56,56,56	0
10	CL	A	709	1/1	0.90	0.16	79,79,79,79	0
9	NA	A	707	1/1	0.93	0.40	62,62,62,62	0
7	CLR	A	705	28/28	0.95	0.21	57,71,77,79	0
8	COC	A	706	22/22	0.97	0.22	56,65,70,72	0

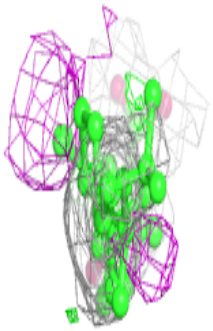
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around Y01 A 701:

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

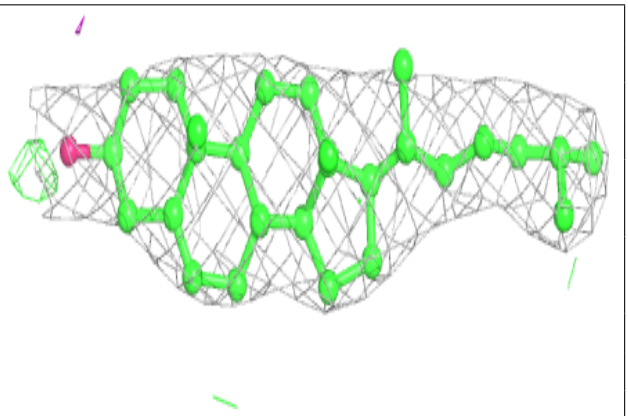


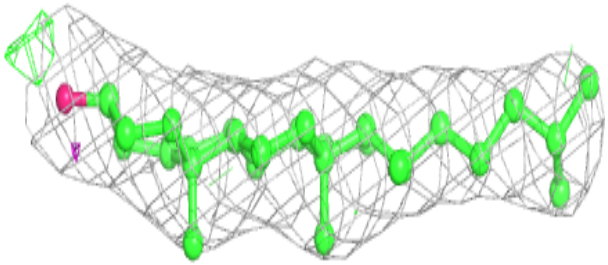


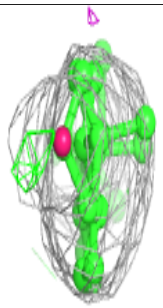


Electron density around CLR A 705:

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

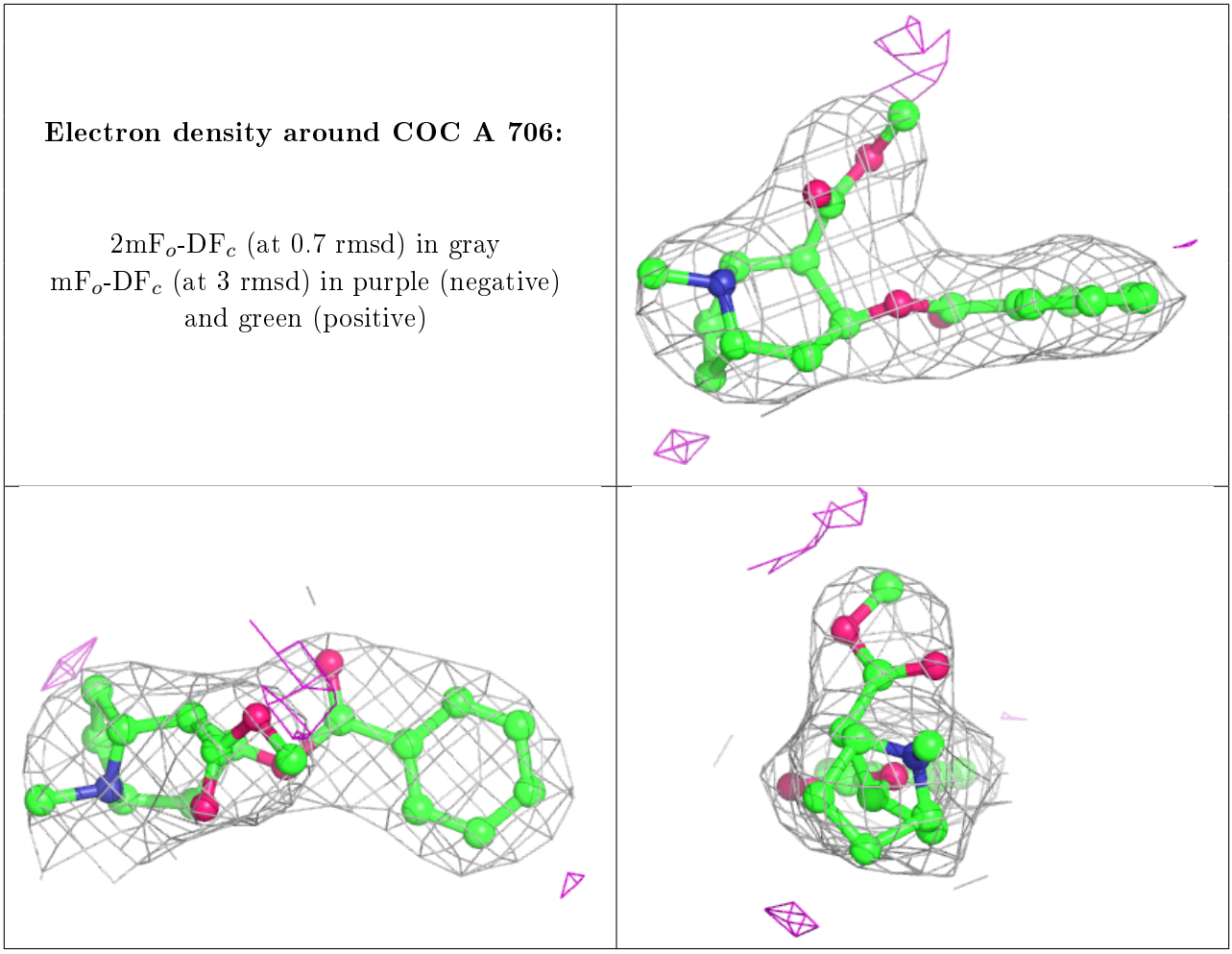






Electron density around COC A 706:

$2mF_o$-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.