



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 19, 2022 – 06:16 am GMT

PDB ID : 7NR2
Title : The structure of the SBP TarP_Sse in complex with coumarate
Authors : Bisson, C.; Salmon, R.C.; West, L.; Rafferty, J.B.; Hitchcock, A.; Thomas, G.H.; Kelly, D.J.
Deposited on : 2021-03-02
Resolution : 2.13 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.24
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.24

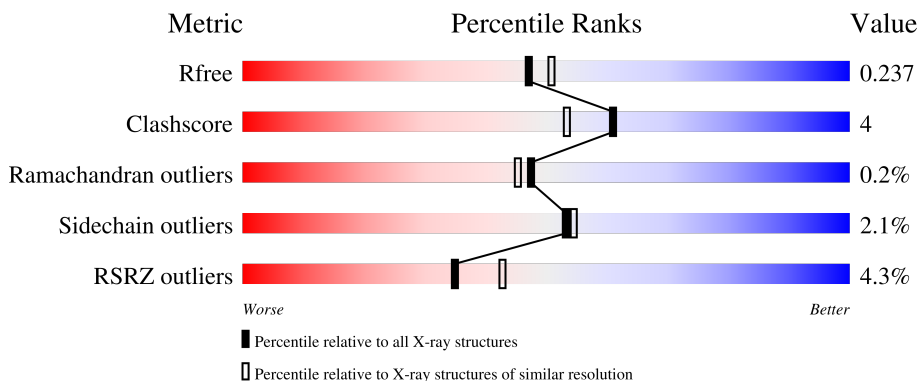
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


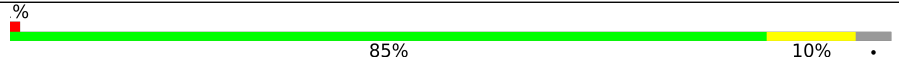
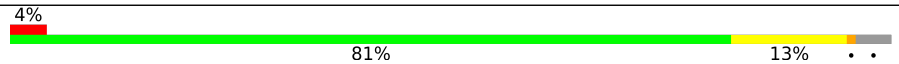

The reported resolution of this entry is 2.13 Å.

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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	337	
1	BBB	337	
1	CCC	337	
1	EEE	337	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	BBB	405	-	-	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 20041 atoms, of which 9603 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 TRAP dicarboxylate transporter, DctP subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	Se			
1	AAA	322	4861	1570	2386	399	494	12	55	0	0
1	BBB	324	4903	1582	2410	402	496	13	55	1	0
1	CCC	322	4876	1575	2392	400	497	12	55	1	0
1	EEE	321	4846	1565	2380	398	491	12	55	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	0	MSE	-	initiating methionine	UNP A3K0X1
AAA	326	ALA	-	expression tag	UNP A3K0X1
AAA	327	ALA	-	expression tag	UNP A3K0X1
AAA	328	ALA	-	expression tag	UNP A3K0X1
AAA	329	LEU	-	expression tag	UNP A3K0X1
AAA	330	GLU	-	expression tag	UNP A3K0X1
AAA	331	HIS	-	expression tag	UNP A3K0X1
AAA	332	HIS	-	expression tag	UNP A3K0X1
AAA	333	HIS	-	expression tag	UNP A3K0X1
AAA	334	HIS	-	expression tag	UNP A3K0X1
AAA	335	HIS	-	expression tag	UNP A3K0X1
AAA	336	HIS	-	expression tag	UNP A3K0X1
BBB	0	MSE	-	initiating methionine	UNP A3K0X1
BBB	326	ALA	-	expression tag	UNP A3K0X1
BBB	327	ALA	-	expression tag	UNP A3K0X1
BBB	328	ALA	-	expression tag	UNP A3K0X1
BBB	329	LEU	-	expression tag	UNP A3K0X1
BBB	330	GLU	-	expression tag	UNP A3K0X1
BBB	331	HIS	-	expression tag	UNP A3K0X1
BBB	332	HIS	-	expression tag	UNP A3K0X1
BBB	333	HIS	-	expression tag	UNP A3K0X1

Continued on next page...

Continued from previous page...

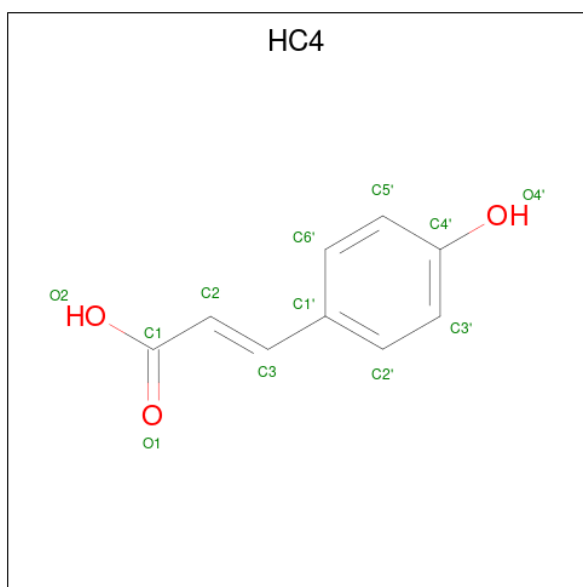
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	334	HIS	-	expression tag	UNP A3K0X1
BBB	335	HIS	-	expression tag	UNP A3K0X1
BBB	336	HIS	-	expression tag	UNP A3K0X1
CCC	0	MSE	-	initiating methionine	UNP A3K0X1
CCC	326	ALA	-	expression tag	UNP A3K0X1
CCC	327	ALA	-	expression tag	UNP A3K0X1
CCC	328	ALA	-	expression tag	UNP A3K0X1
CCC	329	LEU	-	expression tag	UNP A3K0X1
CCC	330	GLU	-	expression tag	UNP A3K0X1
CCC	331	HIS	-	expression tag	UNP A3K0X1
CCC	332	HIS	-	expression tag	UNP A3K0X1
CCC	333	HIS	-	expression tag	UNP A3K0X1
CCC	334	HIS	-	expression tag	UNP A3K0X1
CCC	335	HIS	-	expression tag	UNP A3K0X1
CCC	336	HIS	-	expression tag	UNP A3K0X1
EEE	0	MSE	-	initiating methionine	UNP A3K0X1
EEE	326	ALA	-	expression tag	UNP A3K0X1
EEE	327	ALA	-	expression tag	UNP A3K0X1
EEE	328	ALA	-	expression tag	UNP A3K0X1
EEE	329	LEU	-	expression tag	UNP A3K0X1
EEE	330	GLU	-	expression tag	UNP A3K0X1
EEE	331	HIS	-	expression tag	UNP A3K0X1
EEE	332	HIS	-	expression tag	UNP A3K0X1
EEE	333	HIS	-	expression tag	UNP A3K0X1
EEE	334	HIS	-	expression tag	UNP A3K0X1
EEE	335	HIS	-	expression tag	UNP A3K0X1
EEE	336	HIS	-	expression tag	UNP A3K0X1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	O	S	0	0
			5	4	1		
2	BBB	1	Total	O	S	0	0
			5	4	1		
2	BBB	1	Total	O	S	0	0
			5	4	1		
2	BBB	1	Total	O	S	0	0
			5	4	1		
2	BBB	1	Total	O	S	0	0
			5	4	1		
2	EEE	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 4'-HYDROXYCINNAMIC ACID (three-letter code: HC4) (formula: C₉H₈O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	1	0
			19	9	7	3		
3	BBB	1	Total	C	H	O	1	0
			19	9	7	3		
3	CCC	1	Total	C	H	O	1	0
			19	9	7	3		
3	CCC	1	Total	C	H	O	1	0
			19	9	7	3		
3	EEE	1	Total	C	H	O	1	0
			19	9	7	3		

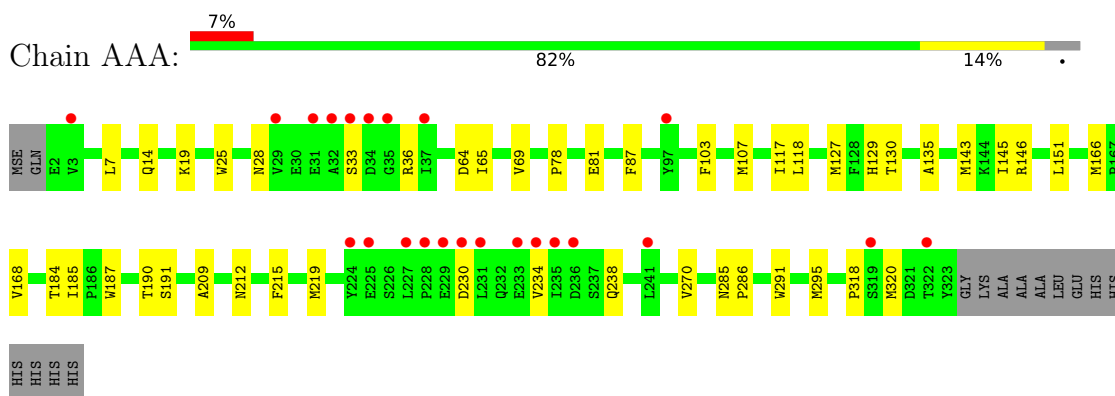
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	120	Total	O	0	0
			120	120		
4	BBB	98	Total	O	0	0
			98	98		
4	CCC	131	Total	O	0	0
			131	131		
4	EEE	76	Total	O	0	0
			76	76		

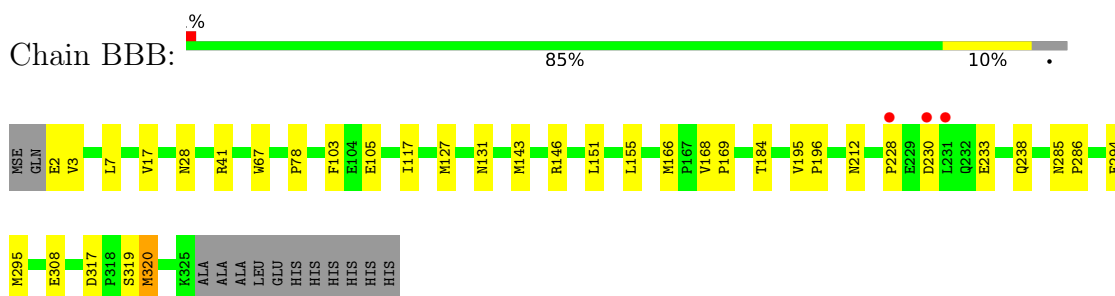
3 Residue-property plots [i](#)

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.

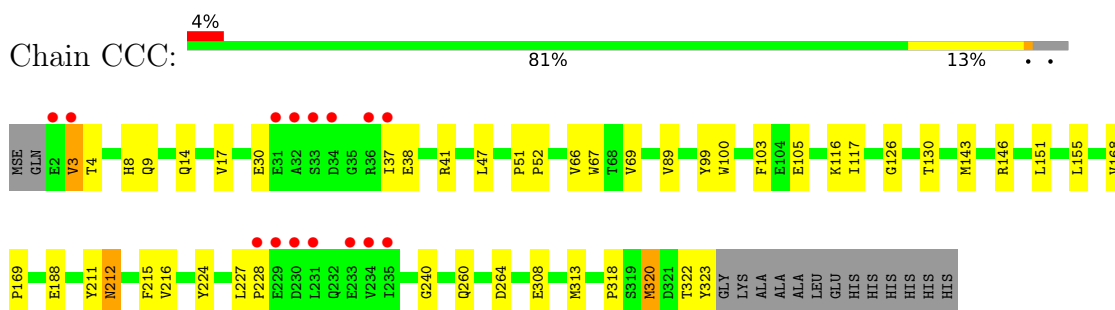
- Molecule 1: TRAP dicarboxylate transporter, DctP subunit



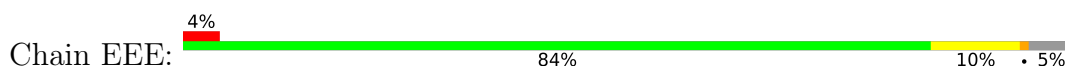
- Molecule 1: TRAP dicarboxylate transporter, DctP subunit

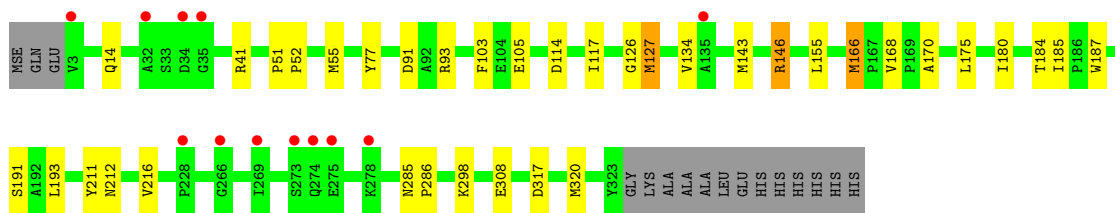


- Molecule 1: TRAP dicarboxylate transporter, DctP subunit



- Molecule 1: TRAP dicarboxylate transporter, DctP subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.84Å 88.08Å 96.58Å 90.00° 92.28° 90.00°	Depositor
Resolution (Å)	50.50 – 2.13 50.50 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.50-2.13) 99.7 (50.50-2.13)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.12Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.180 , 0.236 0.179 , 0.237	Depositor DCC
R_{free} test set	3698 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtrriage
Anisotropy	0.304	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20041	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HC4, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AAA	0.77	0/2522	0.93	2/3422 (0.1%)
1	BBB	0.76	0/2543	0.92	1/3448 (0.0%)
1	CCC	0.77	0/2530	0.91	4/3431 (0.1%)
1	EEE	0.76	0/2513	0.94	4/3410 (0.1%)
All	All	0.76	0/10108	0.93	11/13711 (0.1%)

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	CCC	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EEE	320	MSE	CG-SE-CE	11.31	123.78	98.90
1	AAA	320	MSE	CG-SE-CE	8.27	117.09	98.90
1	AAA	107	MSE	CG-SE-CE	8.17	116.88	98.90
1	CCC	313	MSE	CG-SE-CE	7.35	115.08	98.90
1	EEE	166	MSE	CG-SE-CE	7.09	114.50	98.90
1	CCC	320	MSE	CG-SE-CE	6.70	113.63	98.90
1	CCC	99	TYR	CB-CG-CD1	5.75	124.45	121.00
1	EEE	127	MSE	CG-SE-CE	-5.36	87.10	98.90
1	CCC	99	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	EEE	143	MSE	CG-SE-CE	5.16	110.25	98.90
1	BBB	166	MSE	CG-SE-CE	5.03	109.97	98.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	CCC	216	VAL	Peptide
1	CCC	9	GLN	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	AAA	2475	2386	2380	24	0
1	BBB	2493	2410	2405	19	0
1	CCC	2484	2392	2385	27	0
1	EEE	2466	2380	2374	20	0
2	AAA	5	0	0	0	0
2	BBB	25	0	0	0	0
2	EEE	5	0	0	0	0
3	AAA	12	7	6	0	0
3	BBB	12	7	6	0	0
3	CCC	24	14	12	1	0
3	EEE	12	7	6	0	0
4	AAA	120	0	0	1	0
4	BBB	98	0	0	1	0
4	CCC	131	0	0	0	0
4	EEE	76	0	0	0	0
All	All	10438	9603	9574	88	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 4.

All (88) 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:AAA:143:MSE:HE2	1:AAA:145:ILE:HD11	1.53	0.89
1:EEE:184:THR:O	1:EEE:185:ILE:HG23	1.92	0.69
1:CCC:105:GLU:OE1	1:CCC:308:GLU:OE2	2.12	0.67
1:AAA:130:THR:HB	1:AAA:143:MSE:HE1	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:291:TRP:CZ2	1:AAA:295:MSE:HE2	2.34	0.62
1:AAA:285:ASN:N	1:AAA:286:PRO:CD	2.67	0.58
1:BBB:105:GLU:OE1	1:BBB:308:GLU:OE2	2.22	0.57
1:AAA:230:ASP:O	1:AAA:234:VAL:HG23	2.05	0.56
1:BBB:2:GLU:HG2	1:BBB:3:VAL:HG23	1.87	0.55
1:CCC:8:HIS:CE1	1:CCC:47:LEU:HB2	2.43	0.53
1:AAA:127:MSE:HE2	1:AAA:129:HIS:CE1	2.44	0.53
1:AAA:135:ALA:HA	1:AAA:270:VAL:HG11	1.91	0.52
1:AAA:14:GLN:HE22	1:AAA:19:LYS:HE3	1.75	0.52
1:BBB:228:PRO:HB2	1:BBB:230:ASP:OD1	2.10	0.52
1:BBB:285:ASN:N	1:BBB:286:PRO:CD	2.72	0.52
1:CCC:130:THR:HB	1:CCC:143:MSE:HE1	1.93	0.52
1:AAA:28:ASN:HB3	1:AAA:238:GLN:OE1	2.10	0.51
1:EEE:175:LEU:HD23	1:EEE:180:ILE:HG13	1.91	0.51
4:BBB:556:HOH:O	1:EEE:298:LYS:HE2	2.10	0.51
1:EEE:126:GLY:HA3	1:EEE:211:TYR:CE1	2.46	0.51
1:AAA:33:SER:O	1:AAA:36:ARG:HD3	2.12	0.50
1:AAA:78:PRO:HB2	1:AAA:295:MSE:HE1	1.94	0.50
1:EEE:105:GLU:OE2	1:EEE:308:GLU:OE2	2.29	0.50
1:BBB:317:ASP:OD2	1:BBB:319:SER:OG	2.19	0.49
1:CCC:116:LYS:HE2	1:CCC:224:TYR:CZ	2.47	0.49
1:EEE:55:MSE:HE1	1:EEE:216:VAL:HG21	1.95	0.48
1:BBB:28:ASN:HB3	1:BBB:238:GLN:OE1	2.13	0.48
1:EEE:155:LEU:HD23	1:EEE:155:LEU:O	2.14	0.48
1:EEE:103:PHE:CZ	1:EEE:117:ILE:HB	2.48	0.48
1:BBB:78:PRO:HB2	1:BBB:295:MSE:HE1	1.96	0.48
1:CCC:126:GLY:HA3	1:CCC:211:TYR:CE1	2.49	0.47
1:AAA:130:THR:CG2	1:AAA:143:MSE:HE1	2.44	0.47
1:CCC:100:TRP:CH2	1:CCC:240:GLY:HA2	2.49	0.47
1:AAA:285:ASN:N	1:AAA:286:PRO:HD3	2.29	0.47
1:CCC:4:THR:HG22	1:CCC:38:GLU:HB3	1.95	0.47
1:BBB:168:VAL:HG12	1:BBB:169:PRO:HD3	1.96	0.47
1:AAA:187:TRP:O	1:AAA:190:THR:OG1	2.24	0.47
1:CCC:155:LEU:C	1:CCC:155:LEU:HD23	2.34	0.47
1:EEE:155:LEU:HD23	1:EEE:155:LEU:C	2.35	0.47
1:EEE:168:VAL:HG22	1:EEE:193:LEU:HD11	1.95	0.47
1:BBB:103:PHE:CZ	1:BBB:117:ILE:HB	2.50	0.47
1:BBB:127:MSE:O	1:BBB:184:THR:HA	2.15	0.46
1:CCC:100:TRP:CZ2	1:CCC:240:GLY:HA2	2.50	0.46
1:AAA:87:PHE:HA	1:AAA:209:ALA:O	2.15	0.46
1:EEE:91:ASP:OD1	1:EEE:93:ARG:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:17:VAL:HG11	1:BBB:67:TRP:CZ2	2.50	0.46
1:CCC:14:GLN:HG3	1:EEE:14:GLN:CG	2.46	0.46
1:BBB:155:LEU:C	1:BBB:155:LEU:HD23	2.36	0.46
1:CCC:322:THR:O	1:CCC:323:TYR:C	2.54	0.46
1:AAA:69:VAL:HG22	1:AAA:215:PHE:CE2	2.51	0.46
1:CCC:30:GLU:HG2	1:CCC:37:ILE:O	2.16	0.45
1:CCC:14:GLN:HG3	1:EEE:14:GLN:HG2	1.98	0.45
1:AAA:64:ASP:O	1:AAA:219:MSE:HA	2.16	0.45
1:AAA:143:MSE:HE3	4:AAA:591:HOH:O	2.16	0.45
1:CCC:69:VAL:HG22	1:CCC:215:PHE:CE1	2.52	0.45
1:AAA:81:GLU:HB3	1:AAA:151:LEU:HD11	1.99	0.45
1:AAA:184:THR:O	1:AAA:185:ILE:HG12	2.17	0.45
1:BBB:195:VAL:N	1:BBB:196:PRO:CD	2.79	0.45
1:EEE:166:MSE:HE3	1:EEE:170:ALA:HB3	1.98	0.45
1:BBB:7:LEU:C	1:BBB:7:LEU:HD23	2.38	0.44
1:EEE:55:MSE:HG2	1:EEE:77:TYR:OH	2.18	0.44
1:CCC:227:LEU:O	1:CCC:228:PRO:C	2.56	0.44
1:BBB:151:LEU:HD23	1:BBB:151:LEU:HA	1.91	0.43
1:CCC:3:VAL:HG11	1:CCC:227:LEU:HD21	2.00	0.43
1:CCC:8:HIS:O	1:CCC:66:VAL:HA	2.18	0.43
1:CCC:168:VAL:HG12	1:CCC:169:PRO:HD3	2.00	0.43
1:EEE:51:PRO:HB2	1:EEE:52:PRO:HD3	2.00	0.43
1:EEE:55:MSE:HE1	1:EEE:216:VAL:CG2	2.48	0.43
1:CCC:17:VAL:HG11	1:CCC:67:TRP:CZ2	2.54	0.43
1:BBB:168:VAL:N	1:BBB:169:PRO:CD	2.82	0.43
1:CCC:151:LEU:HD23	1:CCC:151:LEU:HA	1.93	0.42
1:AAA:103:PHE:CZ	1:AAA:117:ILE:HB	2.54	0.42
1:BBB:285:ASN:N	1:BBB:286:PRO:HD3	2.35	0.42
1:AAA:130:THR:CB	1:AAA:143:MSE:HE1	2.46	0.42
1:BBB:320:MSE:HE2	1:BBB:320:MSE:HB2	2.01	0.42
1:EEE:127:MSE:SE	1:EEE:187:TRP:CD1	3.22	0.42
1:EEE:285:ASN:N	1:EEE:286:PRO:CD	2.82	0.42
1:AAA:7:LEU:HA	1:AAA:65:ILE:O	2.20	0.41
1:CCC:51:PRO:N	1:CCC:52:PRO:CD	2.83	0.41
1:CCC:103:PHE:CZ	1:CCC:117:ILE:HB	2.55	0.41
1:CCC:188:GLU:OE2	3:CCC:401:HC4:H5'	2.20	0.41
1:AAA:25:TRP:CZ2	1:AAA:118:LEU:HD13	2.55	0.41
1:BBB:131:ASN:OD1	1:BBB:143[B]:MSE:HE3	2.21	0.41
1:CCC:224:TYR:O	1:CCC:227:LEU:HB2	2.21	0.41
1:EEE:146:ARG:HG3	1:EEE:166:MSE:HE2	2.02	0.41
1:CCC:168:VAL:N	1:CCC:169:PRO:CD	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:260:GLN:NE2	1:CCC:264:ASP:OD1	2.49	0.41
1:CCC:89:VAL:HG21	1:CCC:212:ASN:HD21	1.84	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	AAA	320/337 (95%)	304 (95%)	15 (5%)	1 (0%)	41	36
1	BBB	323/337 (96%)	318 (98%)	5 (2%)	0	100	100
1	CCC	321/337 (95%)	313 (98%)	7 (2%)	1 (0%)	41	36
1	EEE	319/337 (95%)	312 (98%)	6 (2%)	1 (0%)	41	36
All	All	1283/1348 (95%)	1247 (97%)	33 (3%)	3 (0%)	47	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	318	PRO
1	CCC	318	PRO
1	EEE	134	VAL

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	AAA	265/263 (101%)	260 (98%)	5 (2%)	57	59
1	BBB	267/263 (102%)	261 (98%)	6 (2%)	52	53
1	CCC	266/263 (101%)	261 (98%)	5 (2%)	57	59
1	EEE	264/263 (100%)	258 (98%)	6 (2%)	50	51
All	All	1062/1052 (101%)	1040 (98%)	22 (2%)	53	54

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

Mol	Chain	Res	Type
1	AAA	146	ARG
1	AAA	166	MSE
1	AAA	168	VAL
1	AAA	191	SER
1	AAA	212	ASN
1	BBB	41	ARG
1	BBB	146	ARG
1	BBB	212	ASN
1	BBB	233	GLU
1	BBB	294	GLU
1	BBB	320	MSE
1	CCC	3	VAL
1	CCC	41	ARG
1	CCC	146	ARG
1	CCC	212	ASN
1	CCC	320	MSE
1	EEE	41	ARG
1	EEE	114	ASP
1	EEE	146	ARG
1	EEE	191	SER
1	EEE	212	ASN
1	EEE	317	ASP

Sometimes 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 [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](#)

12 ligands 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	$\# Z > 2$
3	HC4	AAA	402	-	9,12,12	0.38	0	12,15,15	0.37	0
3	HC4	BBB	406	-	9,12,12	0.43	0	12,15,15	0.47	0
2	SO4	BBB	401	-	4,4,4	0.27	0	6,6,6	0.20	0
3	HC4	CCC	401	-	9,12,12	0.39	0	12,15,15	0.51	0
2	SO4	BBB	403	-	4,4,4	0.31	0	6,6,6	0.16	0
3	HC4	EEE	401	-	9,12,12	0.50	0	12,15,15	0.46	0
2	SO4	BBB	402	-	4,4,4	0.29	0	6,6,6	0.15	0
2	SO4	AAA	401	-	4,4,4	0.29	0	6,6,6	0.11	0
2	SO4	BBB	405	-	4,4,4	0.29	0	6,6,6	0.09	0
2	SO4	BBB	404	-	4,4,4	0.31	0	6,6,6	0.07	0
2	SO4	EEE	402	-	4,4,4	0.28	0	6,6,6	0.11	0
3	HC4	CCC	402	-	9,12,12	0.20	0	12,15,15	0.47	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HC4	AAA	402	-	-	1/3/5/5	0/1/1/1
3	HC4	BBB	406	-	-	3/3/5/5	0/1/1/1
3	HC4	CCC	401	-	-	1/3/5/5	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HC4	EEE	401	-	-	1/3/5/5	0/1/1/1
3	HC4	CCC	402	-	-	0/3/5/5	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

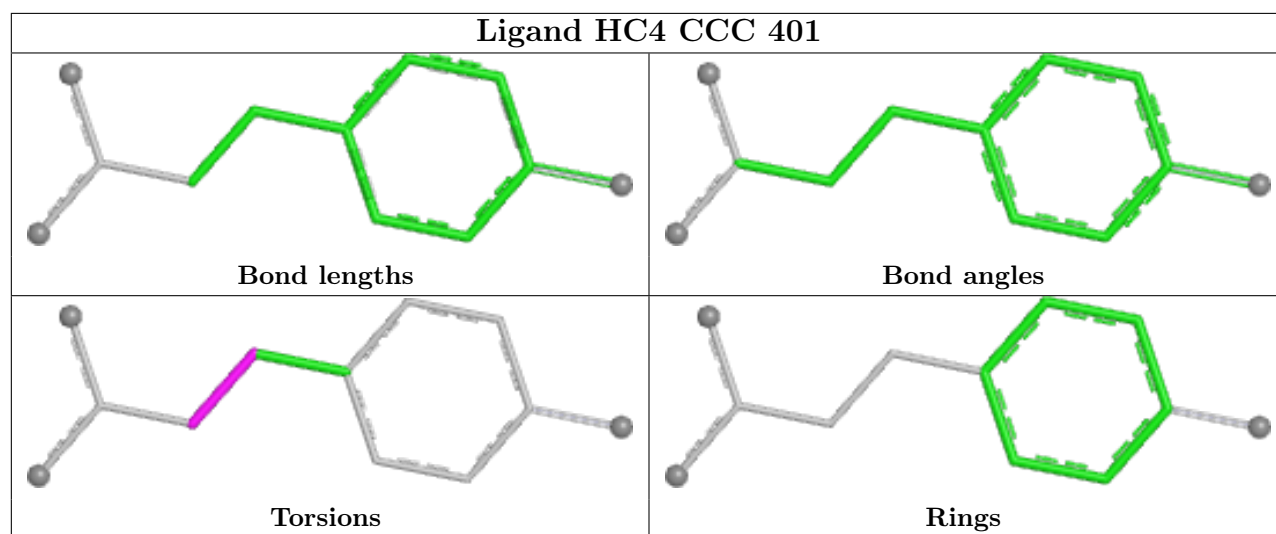
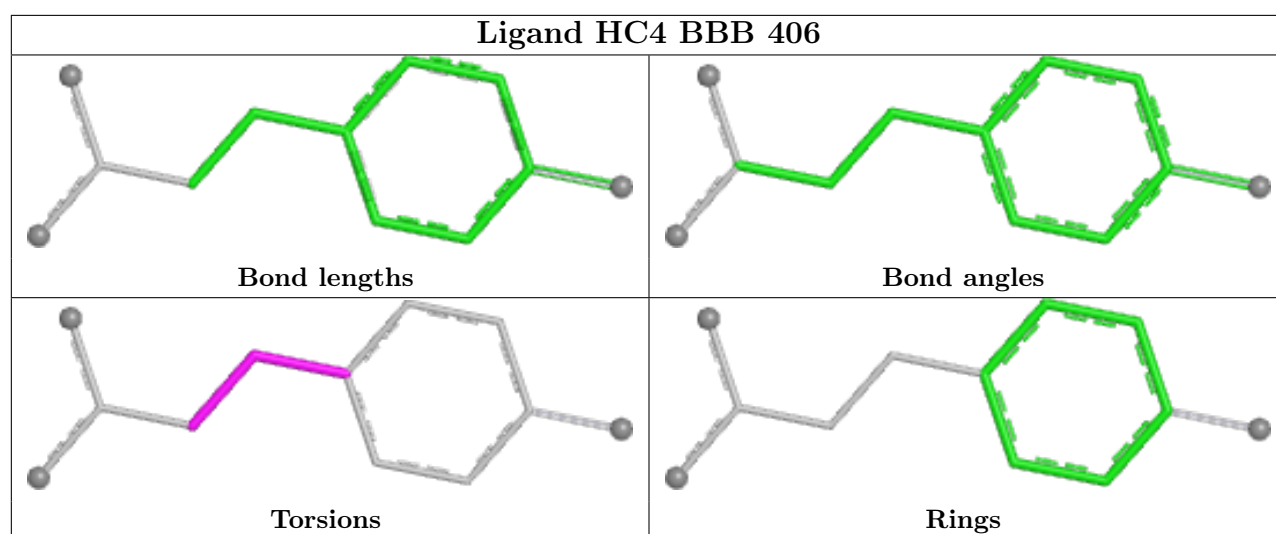
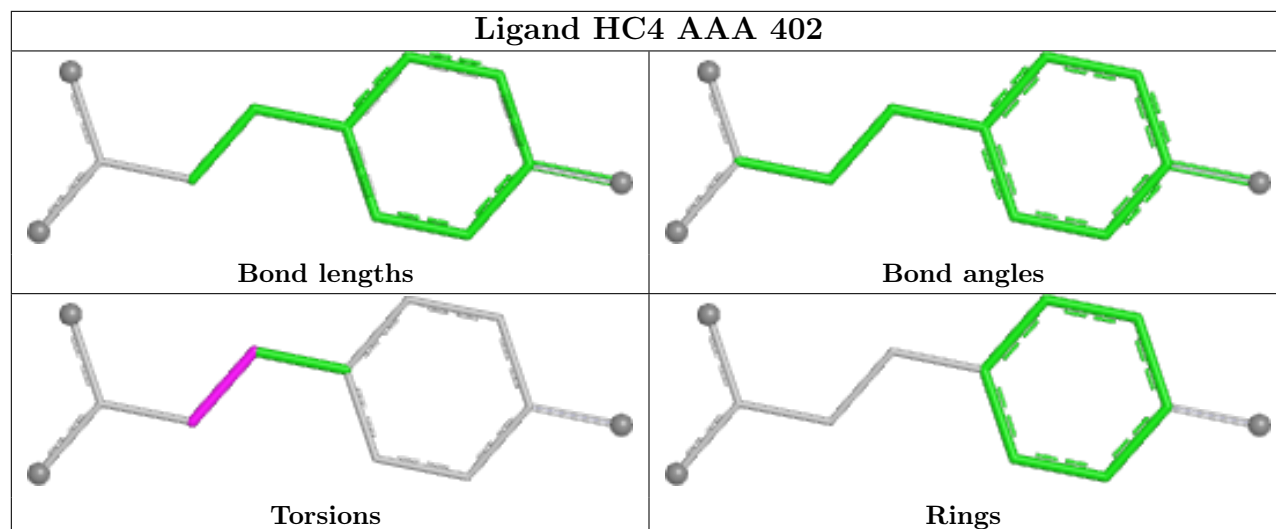
Mol	Chain	Res	Type	Atoms
3	BBB	406	HC4	C1-C2-C3-C1'
3	EEE	401	HC4	C1-C2-C3-C1'
3	AAA	402	HC4	C1-C2-C3-C1'
3	CCC	401	HC4	C1-C2-C3-C1'
3	BBB	406	HC4	C6'-C1'-C3-C2
3	BBB	406	HC4	C2'-C1'-C3-C2

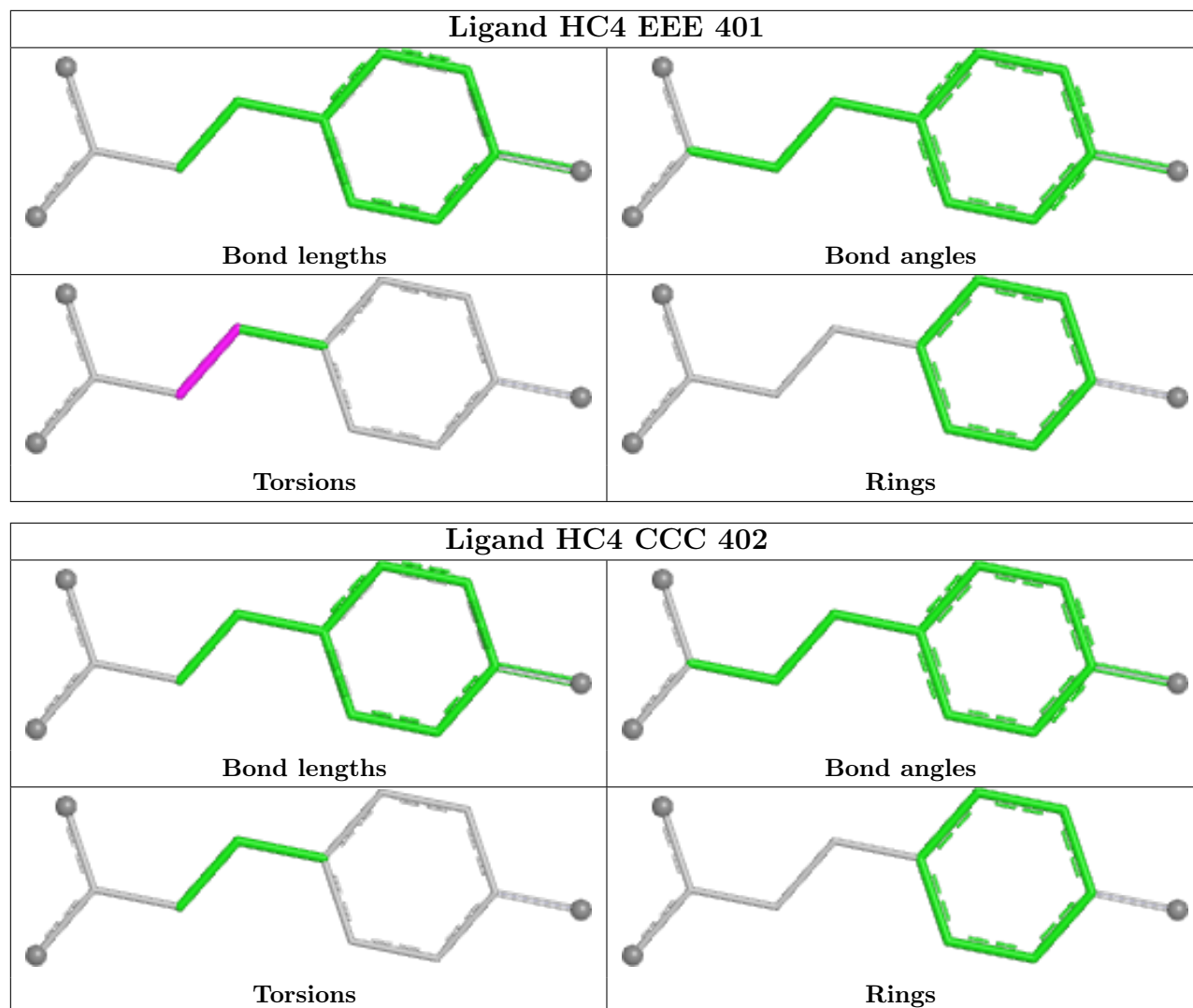
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	CCC	401	HC4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	310/337 (91%)	0.36	23 (7%) 14 18	23, 37, 64, 93	0
1	BBB	312/337 (92%)	0.08	3 (0%) 82 86	20, 32, 52, 68	0
1	CCC	310/337 (91%)	0.36	15 (4%) 30 37	22, 33, 57, 106	0
1	EEE	309/337 (91%)	0.30	12 (3%) 39 47	20, 37, 62, 94	0
All	All	1241/1348 (92%)	0.28	53 (4%) 35 43	20, 35, 60, 106	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	228	PRO	4.8
1	CCC	3	VAL	4.6
1	AAA	229	GLU	4.4
1	CCC	229	GLU	4.4
1	AAA	233	GLU	4.2
1	CCC	228	PRO	4.2
1	BBB	231	LEU	3.9
1	AAA	33	SER	3.7
1	AAA	34	ASP	3.4
1	AAA	29	VAL	3.4
1	CCC	234	VAL	3.4
1	BBB	228	PRO	3.3
1	AAA	3	VAL	3.3
1	CCC	235	ILE	3.3
1	AAA	231	LEU	3.2
1	CCC	2	GLU	3.1
1	AAA	230	ASP	3.1
1	EEE	34	ASP	3.0
1	CCC	37	ILE	3.0
1	EEE	274	GLN	3.0
1	CCC	34	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	AAA	241	LEU	3.0
1	EEE	135	ALA	3.0
1	CCC	231	LEU	2.9
1	EEE	35	GLY	2.9
1	AAA	319	SER	2.9
1	AAA	37	ILE	2.8
1	EEE	228	PRO	2.8
1	CCC	31	GLU	2.7
1	CCC	230	ASP	2.7
1	AAA	227	LEU	2.7
1	EEE	3	VAL	2.7
1	EEE	278	LYS	2.6
1	EEE	266	GLY	2.6
1	AAA	322	THR	2.5
1	CCC	32	ALA	2.5
1	BBB	230	ASP	2.5
1	EEE	269	ILE	2.5
1	EEE	275	GLU	2.5
1	AAA	235	ILE	2.4
1	AAA	224	TYR	2.4
1	AAA	234	VAL	2.4
1	AAA	236	ASP	2.4
1	AAA	31	GLU	2.3
1	AAA	225	GLU	2.3
1	AAA	35	GLY	2.3
1	EEE	273	SER	2.3
1	EEE	32	ALA	2.3
1	CCC	33	SER	2.2
1	AAA	97	TYR	2.1
1	CCC	36	ARG	2.1
1	CCC	233	GLU	2.1
1	AAA	32	ALA	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](#)

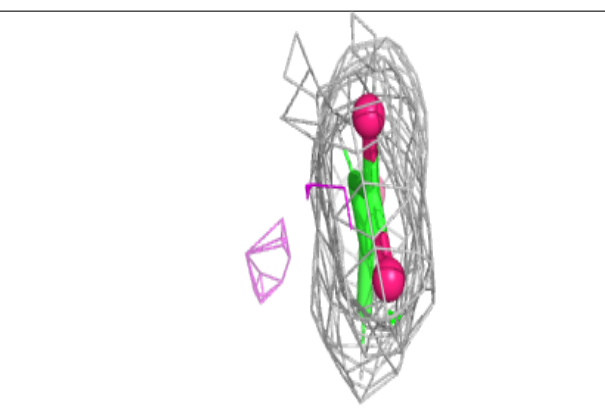
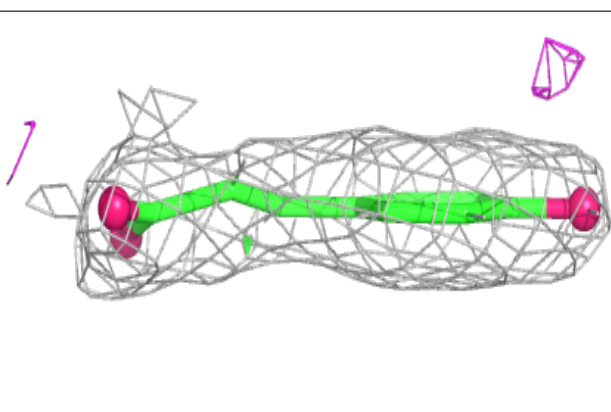
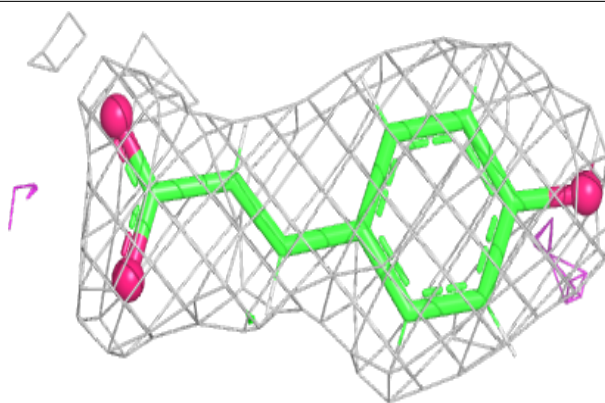
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	BBB	405	5/5	0.60	0.46	71,95,101,106	0
2	SO4	BBB	402	5/5	0.84	0.28	66,68,80,84	0
2	SO4	BBB	404	5/5	0.85	0.16	85,94,105,110	0
2	SO4	AAA	401	5/5	0.85	0.34	81,88,95,110	0
2	SO4	BBB	403	5/5	0.87	0.38	84,91,99,109	0
2	SO4	BBB	401	5/5	0.90	0.27	45,54,64,74	0
2	SO4	EEE	402	5/5	0.92	0.27	61,70,86,86	0
3	HC4	CCC	402	12/12	0.92	0.18	29,33,43,45	1
3	HC4	CCC	401	12/12	0.95	0.20	22,23,26,28	1
3	HC4	AAA	402	12/12	0.95	0.13	25,28,32,35	1
3	HC4	BBB	406	12/12	0.97	0.15	23,26,30,30	1
3	HC4	EEE	401	12/12	0.97	0.17	20,24,34,42	1

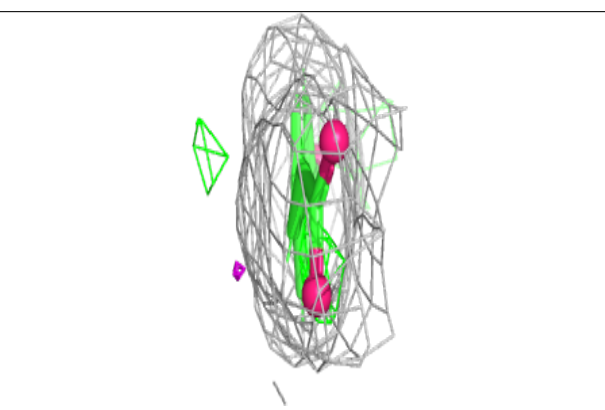
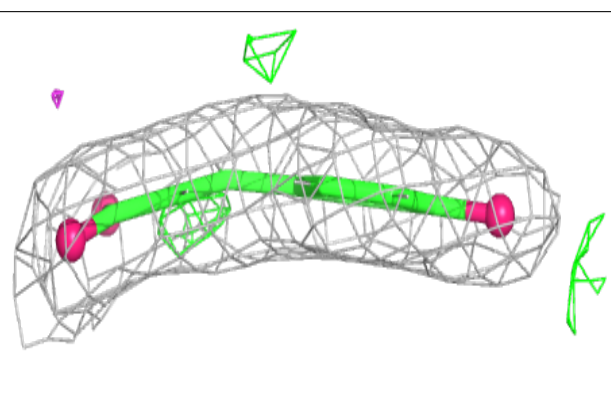
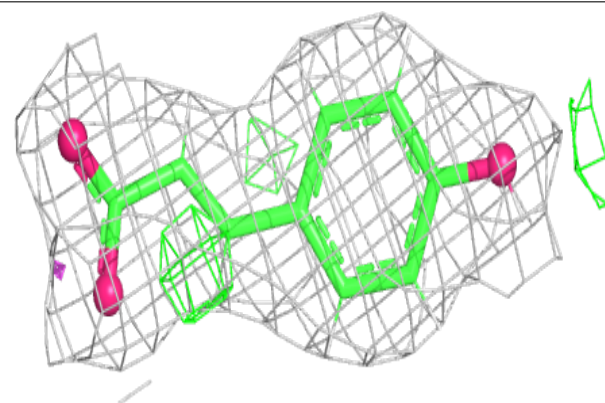
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HC4 CCC 402:

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

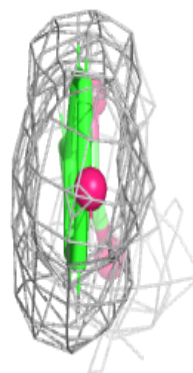
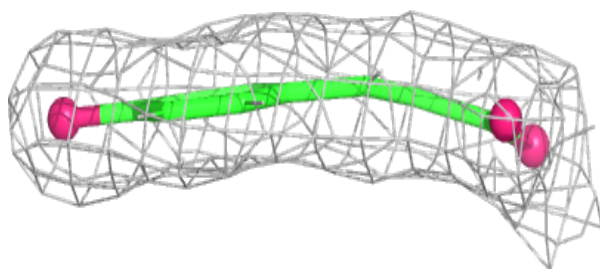
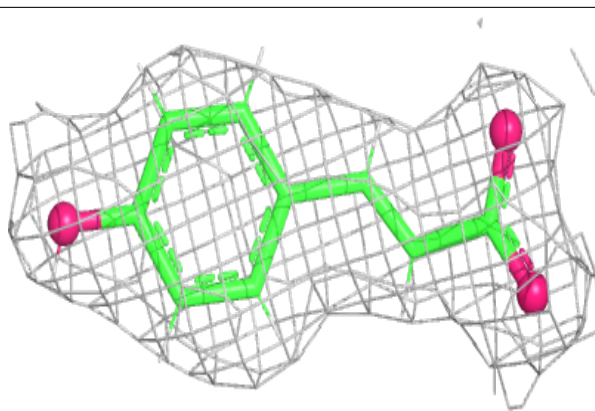
**Electron density around HC4 CCC 401:**

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

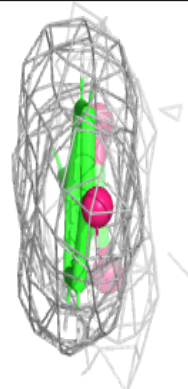
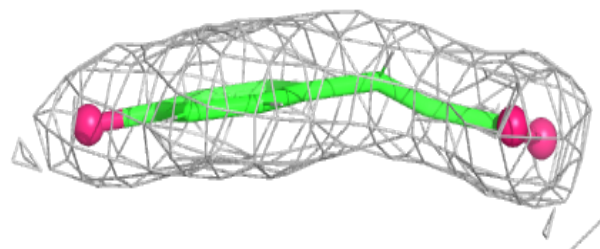
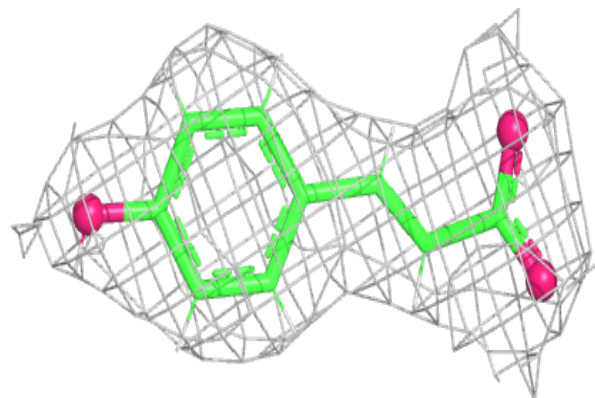


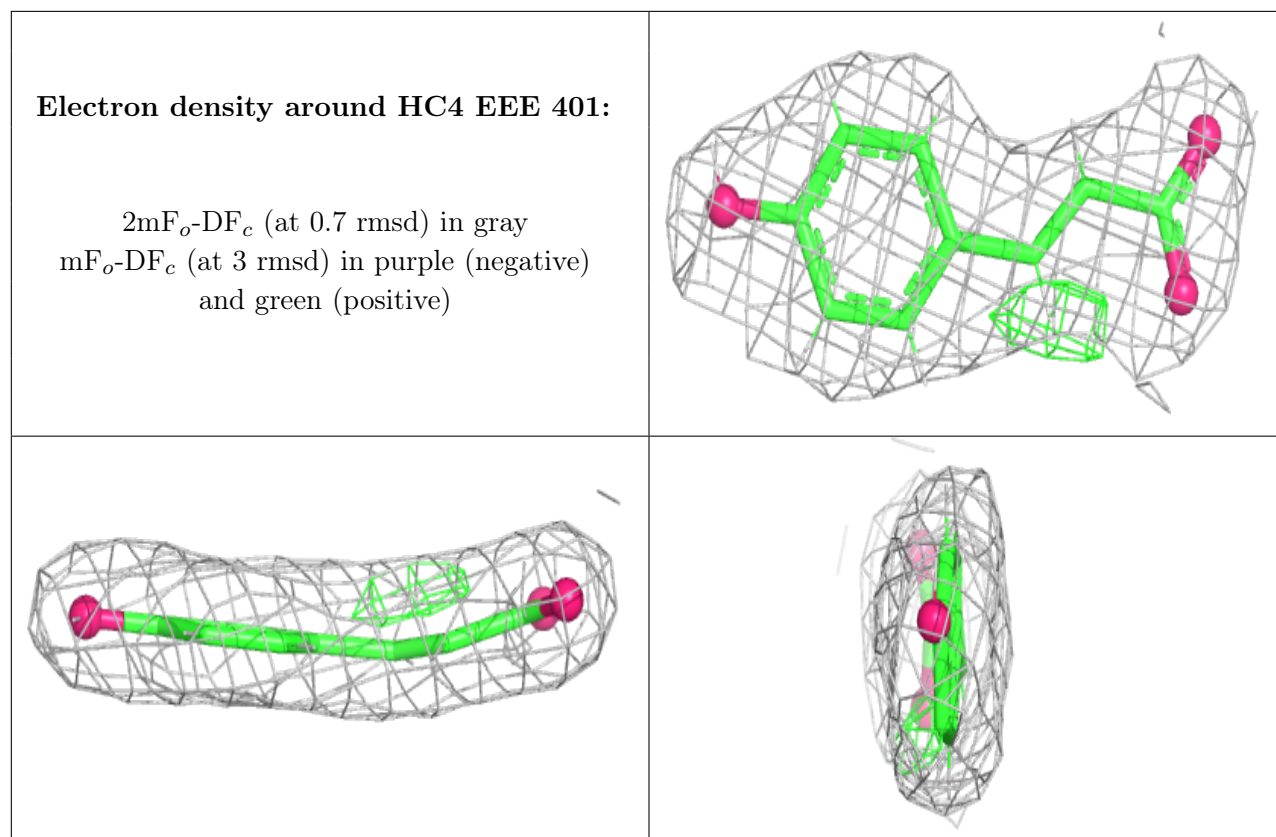
Electron density around HC4 AAA 402:

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

**Electron density around HC4 BBB 406:**

$2mF_o-DF_c$ (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.