Full wwPDB X-ray Structure Validation Report (i)

Oct 13, 2021 – 12:12 pm BST

PDB ID	:	6ZGS
Title	:	Crystal structure of a MFS transporter with bound 3-phenylpropanoic acid at 2.39 Angstroem resolution
Authors	:	Kalbermatter, D.; Bosshart, P.; Bonetti, S.; Fotiadis, D.
Deposited on	:	2020-06-19
Resolution	:	2.15 Å(reported)

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

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

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

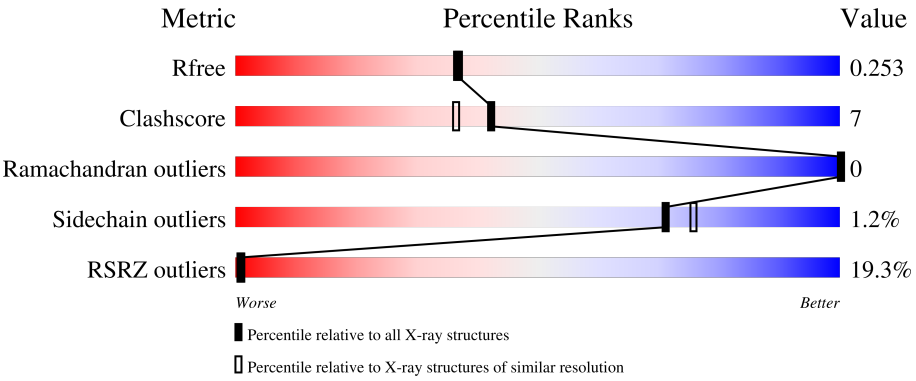
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	420	15% 83% 13% .
1	B	420	20% 69% 17% 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5819 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.

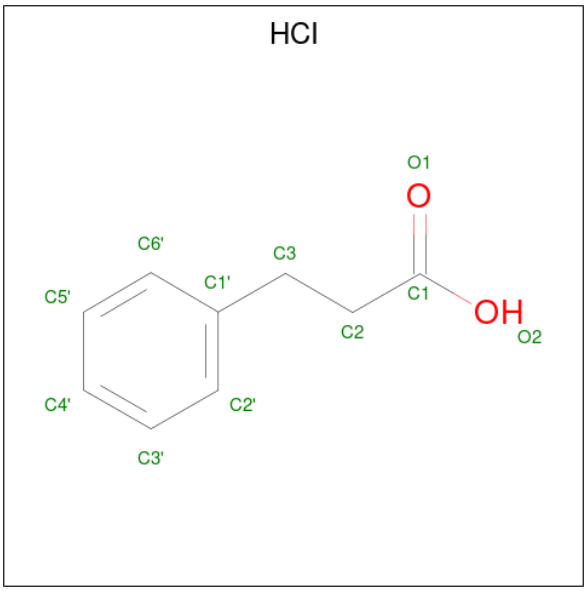
- Molecule 1 is a protein called L-lactate transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3055	2044	481	505	25			
1	B	364	Total	C	N	O	S	0	0	0
			2735	1832	428	452	23			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	413	LEU	-	expression tag	UNP A0LNN5
A	414	GLU	-	expression tag	UNP A0LNN5
A	415	LEU	-	expression tag	UNP A0LNN5
A	416	GLU	-	expression tag	UNP A0LNN5
A	417	VAL	-	expression tag	UNP A0LNN5
A	418	LEU	-	expression tag	UNP A0LNN5
A	419	PHE	-	expression tag	UNP A0LNN5
A	420	GLN	-	expression tag	UNP A0LNN5
B	413	LEU	-	expression tag	UNP A0LNN5
B	414	GLU	-	expression tag	UNP A0LNN5
B	415	LEU	-	expression tag	UNP A0LNN5
B	416	GLU	-	expression tag	UNP A0LNN5
B	417	VAL	-	expression tag	UNP A0LNN5
B	418	LEU	-	expression tag	UNP A0LNN5
B	419	PHE	-	expression tag	UNP A0LNN5
B	420	GLN	-	expression tag	UNP A0LNN5

- Molecule 2 is HYDROCINNAMIC ACID (three-letter code: HCI) (formula: $C_9H_{10}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 11 9 2	0	0
2	B	1	Total C O 11 9 2	0	0

- Molecule 3 is water.

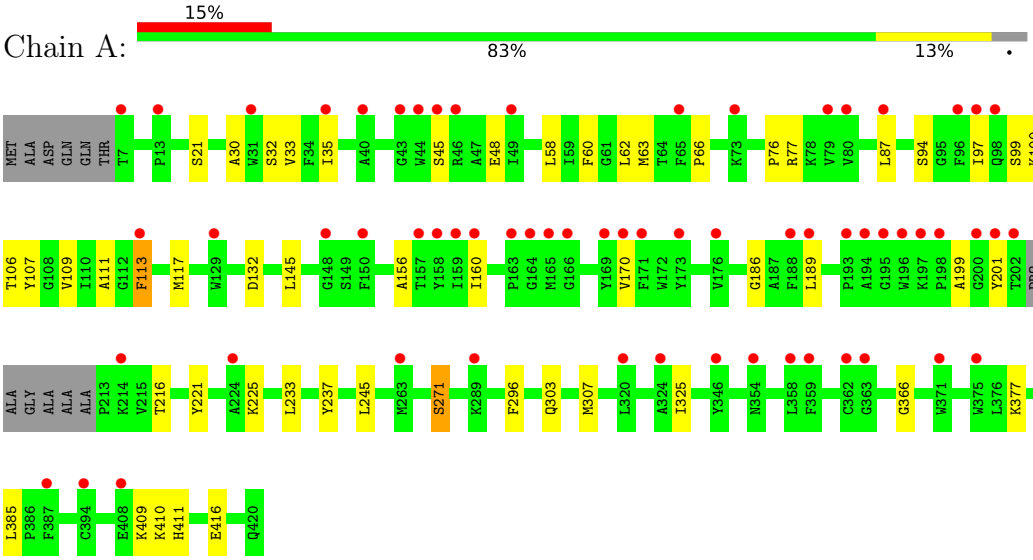
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total O 6 6	0	0
3	B	1	Total O 1 1	0	0

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.

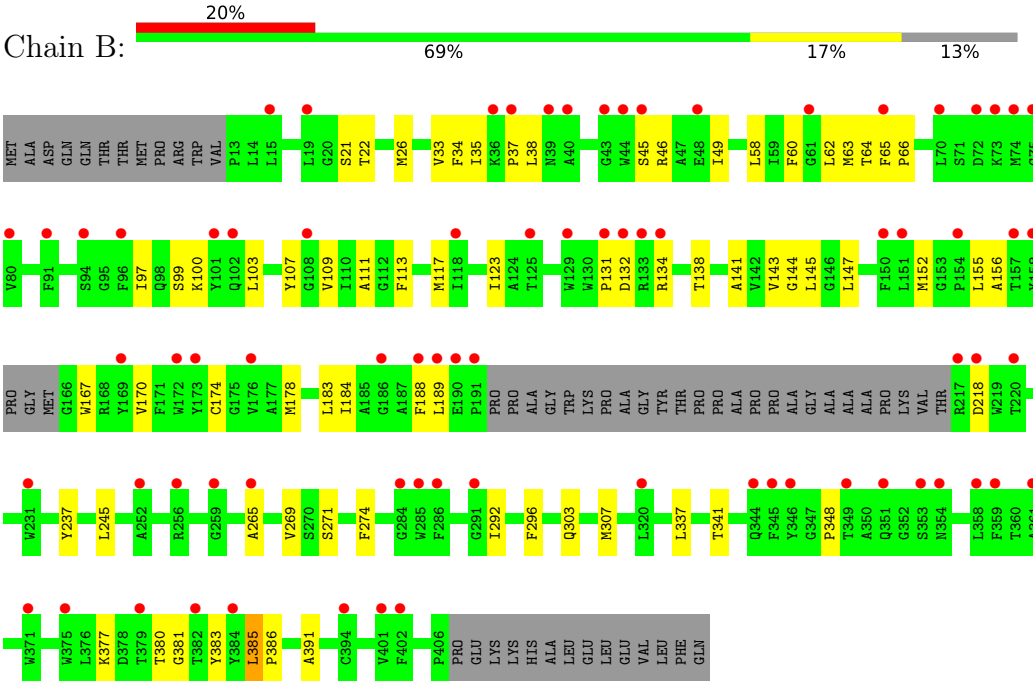
• Molecule 1: L-lactate transporter

Chain A:



• Molecule 1: L-lactate transporter

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	102.15Å 199.68Å 61.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.97 – 2.15 14.97 – 2.15	Depositor EDS
% Data completeness (in resolution range)	59.1 (14.97-2.15) 59.1 (14.97-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.14_3228	Depositor
R, R_{free}	0.216 , 0.252 0.216 , 0.253	Depositor DCC
R_{free} test set	1988 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	65.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	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	0.95	EDS
Total number of atoms	5819	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: HCI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.49	0/3152	0.66	0/4290
1	B	0.41	0/2817	0.61	0/3830
All	All	0.46	0/5969	0.64	0/8120

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

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	3055	0	3094	36	0
1	B	2735	0	2766	45	0
2	A	11	0	9	2	0
2	B	11	0	9	2	0
3	A	6	0	0	0	0
3	B	1	0	0	0	0
All	All	5819	0	5878	81	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 7.

All (81) 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:380:THR:HG21	1:B:385:LEU:HG	1.72	0.71
1:A:60:PHE:CD1	2:A:501:HCI:H3'	2.31	0.66
1:B:159:ILE:HB	1:B:170:VAL:HG22	1.77	0.66
1:A:145:LEU:HD22	2:A:501:HCI:H22	1.80	0.62
1:B:131:PRO:HA	1:B:134:ARG:HE	1.66	0.60
1:B:76:PRO:HB2	1:B:189:LEU:HD23	1.83	0.60
1:A:221:TYR:O	1:A:225:LYS:HB3	2.03	0.59
1:A:94:SER:O	1:A:97:ILE:HG12	2.04	0.57
1:B:35:ILE:HA	1:B:49:ILE:HD13	1.87	0.57
1:A:33:VAL:HG11	1:A:156:ALA:HB1	1.88	0.56
1:A:199:ALA:HB1	1:A:201:TYR:O	2.06	0.55
1:B:58:LEU:O	1:B:62:LEU:HG	2.07	0.55
1:A:45:SER:HB3	1:A:48:GLU:HG3	1.90	0.54
1:B:97:ILE:HD13	1:B:103:LEU:HB2	1.90	0.54
1:B:99:SER:OG	1:B:100:LYS:N	2.42	0.52
1:A:94:SER:HA	1:A:97:ILE:HG23	1.90	0.52
1:A:30:ALA:O	1:A:33:VAL:HB	2.11	0.51
1:B:271:SER:HA	1:B:274:PHE:HD2	1.76	0.51
1:A:303:GLN:O	1:A:307:MET:HG2	2.11	0.51
1:B:33:VAL:HG11	1:B:156:ALA:HB1	1.93	0.50
1:B:307:MET:HB2	1:B:391:ALA:HB2	1.94	0.50
1:B:63:MET:HG3	1:B:113:PHE:HA	1.93	0.50
1:B:145:LEU:HD22	2:B:501:HCI:C1	2.41	0.50
1:B:132:ASP:OD1	1:B:132:ASP:N	2.41	0.50
1:B:292:ILE:HG21	1:B:341:THR:OG1	2.12	0.49
1:A:77:ARG:HG3	1:A:186:GLY:O	2.13	0.49
1:B:26:MET:HG2	1:B:152:MET:HB2	1.95	0.48
1:A:411:HIS:CE1	1:A:416:GLU:OE2	2.67	0.47
1:B:383:TYR:O	1:B:386:PRO:HD2	2.14	0.47
1:B:131:PRO:HB3	1:B:134:ARG:HH21	1.79	0.47
1:B:26:MET:HB3	1:B:178:MET:HE2	1.96	0.47
1:B:37:PRO:HG2	1:B:160:ILE:HD13	1.97	0.46
1:B:65:PHE:HB3	1:B:66:PRO:HD3	1.97	0.46
1:B:34:PHE:HB3	1:B:38:LEU:HG	1.98	0.46
1:A:377:LYS:O	1:A:381:GLY:N	2.45	0.46
1:B:109:VAL:O	1:B:113:PHE:HB2	2.16	0.46
1:A:102:GLN:O	1:A:106:THR:HG23	2.17	0.45
1:A:99:SER:OG	1:A:100:LYS:N	2.50	0.45
1:B:245:LEU:HD13	1:B:366:GLY:HA2	1.97	0.45
1:B:160:ILE:HG13	1:B:170:VAL:HG21	1.98	0.45
1:A:409:LYS:HA	1:A:409:LYS:HD2	1.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:SER:HB2	1:A:325:ILE:CG1	2.47	0.45
1:B:21:SER:HB3	1:B:141:ALA:O	2.17	0.45
1:A:113:PHE:O	1:A:117:MET:HG3	2.17	0.45
1:A:76:PRO:HB2	1:A:189:LEU:HD23	2.00	0.44
1:A:87:LEU:HA	1:A:111:ALA:HA	1.99	0.44
1:A:63:MET:C	1:A:66:PRO:HD2	2.37	0.44
1:A:377:LYS:HE2	1:A:383:TYR:CZ	2.52	0.44
1:A:63:MET:O	1:A:66:PRO:HD2	2.18	0.44
1:A:160:ILE:HG13	1:A:170:VAL:HG21	1.99	0.44
1:A:216:THR:HA	1:A:410:LYS:O	2.18	0.43
1:B:174:CYS:HB3	1:B:178:MET:HE3	2.01	0.43
1:A:63:MET:SD	1:A:66:PRO:HG2	2.59	0.43
1:B:60:PHE:O	1:B:64:THR:HG23	2.18	0.43
1:B:107:TYR:O	1:B:111:ALA:HB3	2.19	0.43
1:A:32:SER:HA	1:A:35:ILE:HG13	2.00	0.43
1:B:45:SER:OG	1:B:46:ARG:N	2.51	0.43
1:A:107:TYR:O	1:A:111:ALA:HB3	2.18	0.43
1:A:245:LEU:HD13	1:A:366:GLY:HA2	2.01	0.43
1:B:143:VAL:O	1:B:147:LEU:HG	2.19	0.43
1:B:184:ILE:O	1:B:188:PHE:HD2	2.02	0.43
1:B:22:THR:N	1:B:144:GLY:HA3	2.34	0.42
1:B:60:PHE:CD1	2:B:501:HCI:H3'	2.54	0.42
1:A:132:ASP:OD1	1:A:132:ASP:N	2.45	0.42
1:B:377:LYS:O	1:B:381:GLY:N	2.50	0.42
1:A:21:SER:HB2	1:A:145:LEU:HD12	2.01	0.42
1:A:385:LEU:HD12	1:A:385:LEU:HA	1.64	0.42
1:A:109:VAL:O	1:A:113:PHE:HB2	2.20	0.42
1:A:58:LEU:O	1:A:62:LEU:HG	2.19	0.42
1:B:155:LEU:O	1:B:159:ILE:HG13	2.20	0.42
1:B:218:ASP:OD2	1:B:348:PRO:HD2	2.20	0.41
1:B:113:PHE:O	1:B:117:MET:HG3	2.21	0.41
1:B:123:ILE:HG23	1:B:138:THR:HG23	2.02	0.41
1:B:271:SER:HA	1:B:274:PHE:CD2	2.56	0.41
1:B:167:TRP:O	1:B:170:VAL:HB	2.22	0.40
1:B:337:LEU:HD23	1:B:337:LEU:HA	1.85	0.40
1:A:233:LEU:HD23	1:A:233:LEU:HA	1.69	0.40
1:B:183:LEU:HD23	1:B:183:LEU:HA	1.91	0.40
1:A:48:GLU:OE1	1:A:100:LYS:HD3	2.22	0.40
1:B:265:ALA:O	1:B:269:VAL:HG23	2.21	0.40
1:B:303:GLN:O	1:B:307:MET:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	400/420 (95%)	393 (98%)	7 (2%)	0	100	100
1	B	358/420 (85%)	354 (99%)	4 (1%)	0	100	100
All	All	758/840 (90%)	747 (98%)	11 (2%)	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	298/307 (97%)	294 (99%)	4 (1%)	69	74
1	B	264/307 (86%)	261 (99%)	3 (1%)	73	78
All	All	562/614 (92%)	555 (99%)	7 (1%)	71	76

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	PHE
1	A	237	TYR
1	A	271	SER
1	A	296	PHE
1	B	237	TYR
1	B	296	PHE
1	B	385	LEU

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

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

2 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	$\#\|Z\| > 2$
2	HCI	B	501	-	8,11,11	0.29	0	10,13,13	0.88	1 (10%)
2	HCI	A	501	-	8,11,11	0.39	0	10,13,13	0.78	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
2	HCI	B	501	-	-	0/3/5/5	0/1/1/1
2	HCI	A	501	-	-	2/3/5/5	0/1/1/1

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	B	501	HCI	C3-C2-C1	-2.17	109.02	112.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

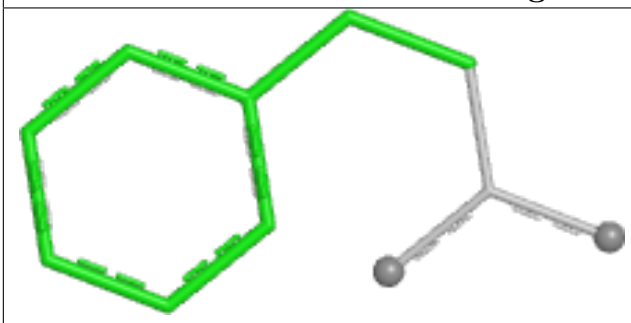
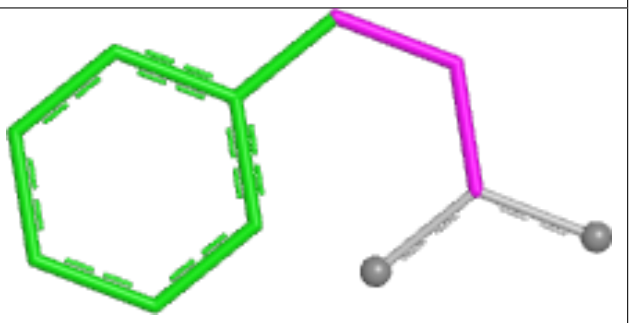
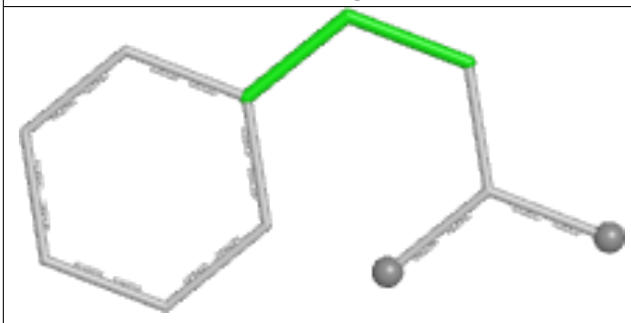
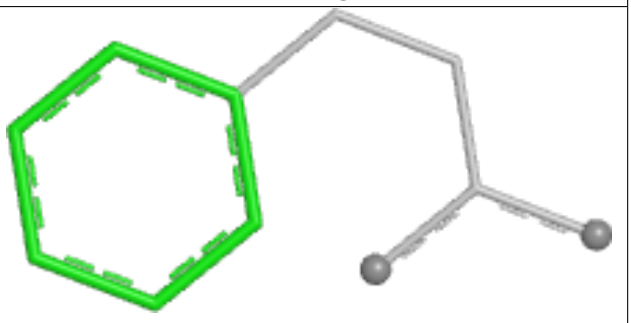
Mol	Chain	Res	Type	Atoms
2	A	501	HCI	C2'-C1'-C3-C2
2	A	501	HCI	C6'-C1'-C3-C2

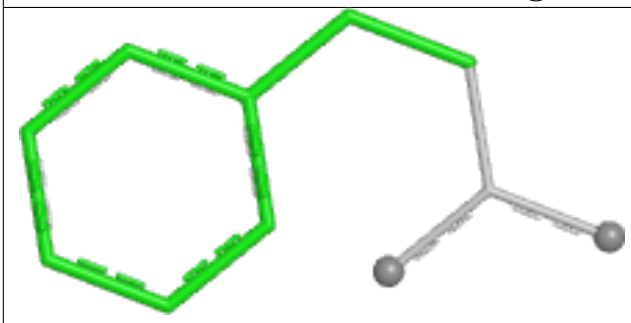
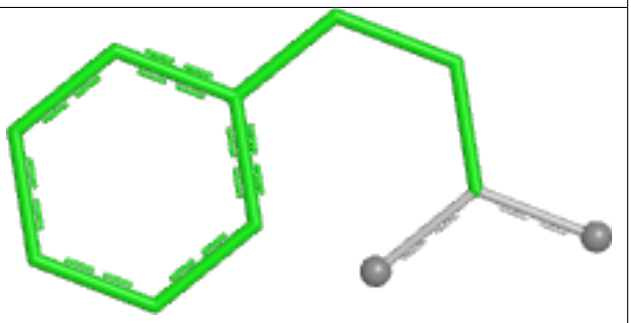
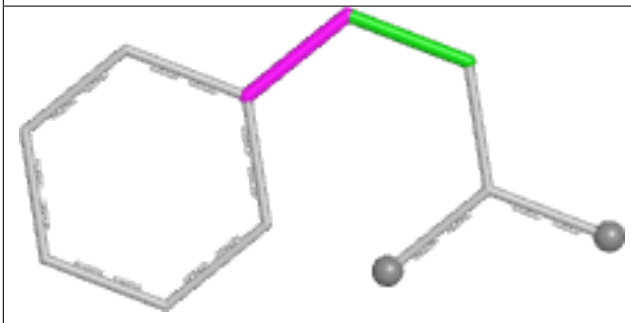
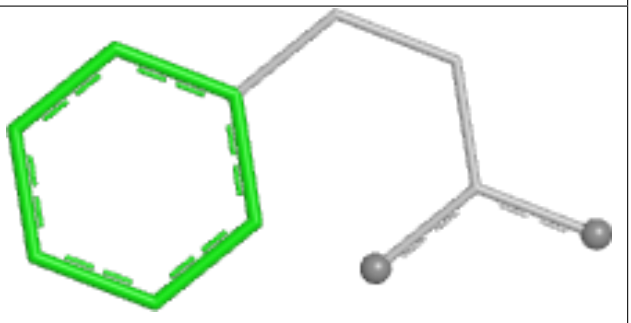
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HCI	2	0
2	A	501	HCI	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 HCI B 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HCI A 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

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	404/420 (96%)	0.94	65 (16%)	1	2	39, 75, 132, 171	0
1	B	364/420 (86%)	1.15	83 (22%)	0	0	49, 95, 144, 172	0
All	All	768/840 (91%)	1.04	148 (19%)	1	1	39, 84, 140, 172	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	TYR	11.3
1	B	158	TYR	10.4
1	A	158	TYR	10.2
1	A	196	TRP	9.7
1	A	169	TYR	8.8
1	B	96	PHE	8.0
1	B	188	PHE	7.9
1	B	43	GLY	7.9
1	A	214	LYS	7.9
1	B	217	ARG	7.7
1	A	194	ALA	7.4
1	A	159	ILE	6.9
1	B	169	TYR	6.8
1	B	349	THR	6.8
1	B	70	LEU	6.8
1	A	164	GLY	6.8
1	B	189	LEU	6.5
1	B	74	MET	6.3
1	B	129	TRP	6.1
1	A	43	GLY	6.0
1	B	40	ALA	5.9
1	B	150	PHE	5.7
1	A	173	TYR	5.7
1	A	163	PRO	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	15	LEU	5.3
1	B	172	TRP	5.2
1	B	173	TYR	5.1
1	A	166	GLY	4.8
1	A	346	TYR	4.8
1	A	7	THR	4.8
1	B	19	LEU	4.7
1	B	73	LYS	4.7
1	B	101	TYR	4.7
1	A	198	PRO	4.7
1	A	202	THR	4.7
1	B	190	GLU	4.6
1	B	354	ASN	4.3
1	A	165	MET	4.1
1	B	371	TRP	4.0
1	B	125	THR	4.0
1	A	200	GLY	4.0
1	B	320	LEU	4.0
1	B	154	PRO	4.0
1	A	188	PHE	3.9
1	B	36	LYS	3.9
1	B	259	GLY	3.9
1	B	44	TRP	3.8
1	B	384	TYR	3.8
1	A	193	PRO	3.8
1	B	45	SER	3.6
1	B	131	PRO	3.6
1	A	170	VAL	3.5
1	B	186	GLY	3.5
1	B	358	LEU	3.4
1	A	98	GLN	3.4
1	A	408	GLU	3.4
1	A	101	TYR	3.4
1	B	151	LEU	3.4
1	B	176	VAL	3.3
1	A	40	ALA	3.3
1	B	226	GLY	3.2
1	A	44	TRP	3.2
1	A	387	PHE	3.2
1	B	91	PHE	3.2
1	B	286	PHE	3.2
1	B	94	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	371	TRP	3.1
1	B	285	TRP	3.1
1	B	134	ARG	3.1
1	B	256	ARG	3.1
1	B	346	TYR	3.1
1	A	324	ALA	3.0
1	A	79	VAL	3.0
1	A	394	CYS	3.0
1	A	65	PHE	3.0
1	B	362	CYS	3.0
1	B	379	THR	3.0
1	A	189	LEU	3.0
1	A	197	LYS	2.9
1	B	225	LYS	2.9
1	B	402	PHE	2.9
1	B	132	ASP	2.9
1	A	31	TRP	2.9
1	B	102	GLN	2.8
1	B	265	ALA	2.8
1	B	218	ASP	2.8
1	A	176	VAL	2.8
1	A	35	ILE	2.7
1	A	97	ILE	2.7
1	B	375	TRP	2.7
1	B	72	ASP	2.7
1	A	195	GLY	2.7
1	A	363	GLY	2.7
1	A	358	LEU	2.7
1	A	73	LYS	2.6
1	B	344	GLN	2.6
1	B	39	ASN	2.6
1	A	362	CYS	2.5
1	A	289	LYS	2.5
1	B	133	ARG	2.5
1	A	80	VAL	2.5
1	B	228	THR	2.5
1	A	13	PRO	2.5
1	B	382	THR	2.5
1	B	363	GLY	2.5
1	A	320	LEU	2.4
1	B	291	GLY	2.4
1	A	354	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	359	PHE	2.4
1	B	345	PHE	2.4
1	B	359	PHE	2.4
1	A	49	ILE	2.4
1	A	157	THR	2.4
1	A	129	TRP	2.4
1	B	65	PHE	2.3
1	A	45	SER	2.3
1	B	108	GLY	2.3
1	A	46	ARG	2.3
1	A	113	PHE	2.3
1	B	351	GLN	2.3
1	B	220	THR	2.3
1	A	375	TRP	2.3
1	B	353	SER	2.3
1	B	37	PRO	2.3
1	A	87	LEU	2.3
1	B	157	THR	2.3
1	A	103	LEU	2.3
1	B	78	LYS	2.2
1	B	361	ALA	2.2
1	A	96	PHE	2.2
1	A	148	GLY	2.2
1	A	171	PHE	2.2
1	B	76	PRO	2.2
1	A	150	PHE	2.2
1	B	401	VAL	2.2
1	B	118	ILE	2.2
1	B	284	GLY	2.2
1	A	224	ALA	2.2
1	B	48	GLU	2.1
1	B	61	GLY	2.1
1	B	75	GLY	2.1
1	A	263	MET	2.1
1	B	252	ALA	2.1
1	B	231	TRP	2.1
1	B	80	VAL	2.0
1	A	160	ILE	2.0
1	B	394	CYS	2.0
1	B	191	PRO	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)

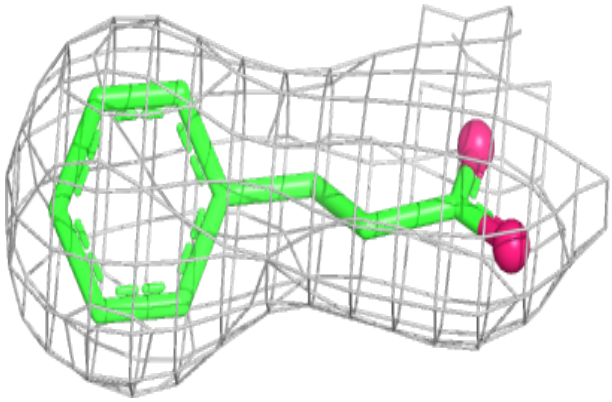
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

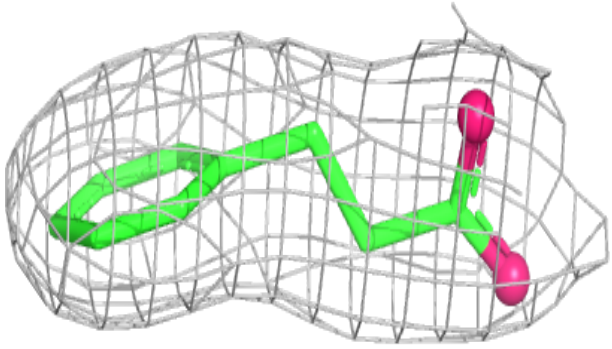
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HCI	B	501	11/11	0.92	0.16	61,67,77,92	0
2	HCI	A	501	11/11	0.94	0.14	46,53,68,70	0

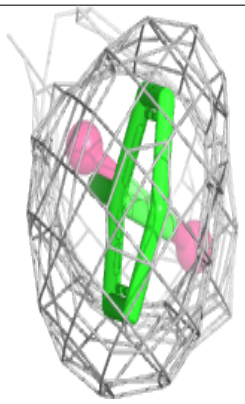
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HCI B 501:

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

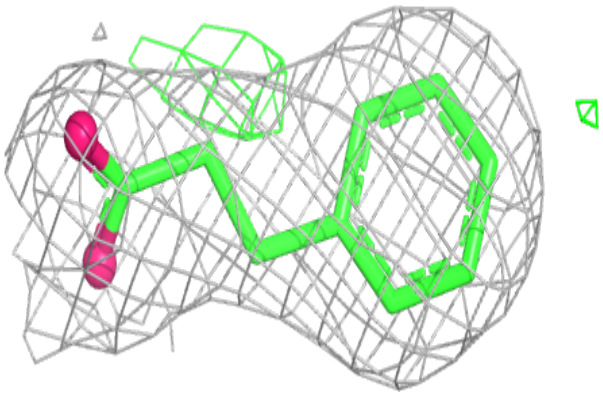


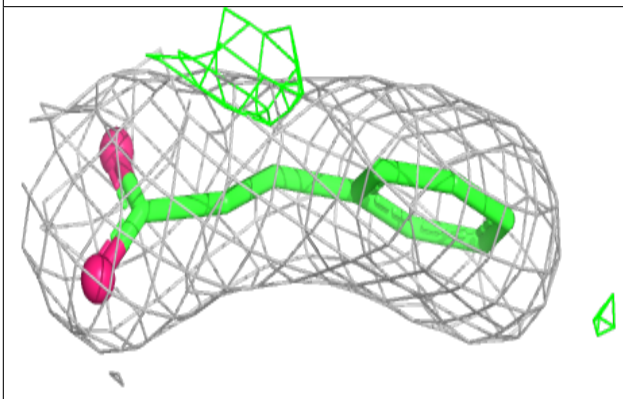


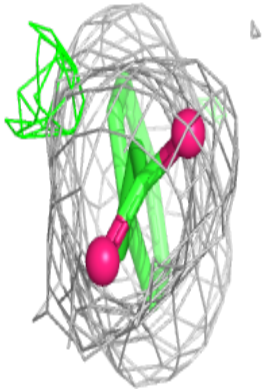


Electron density around HCI A 501:

$2mF_o$-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.