



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 07:45 AM UTC

PDB ID : 8AY0 / pdb_00008ay0
Title : Crystal Structure of the peptide binding protein DppE from *Bacillus subtilis* in complex with murein tripeptide
Authors : Hughes, A.M.; Dodson, E.J.; Wilkinson, A.J.
Deposited on : 2022-09-01
Resolution : 1.51 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

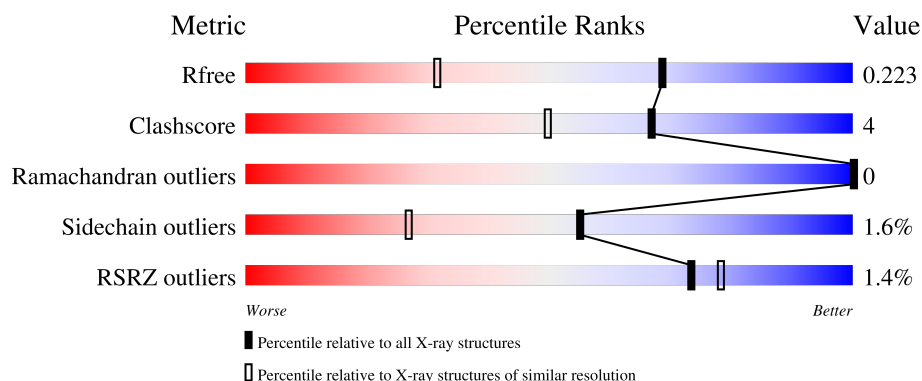
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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}	180053	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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	A	521	87% 8% 5%
1	B	521	88% 7% 5%
1	C	521	85% 7% 7%

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
4	EDO	A	612	-	-	X	-
4	EDO	A	614	-	-	X	-
4	EDO	B	609	-	-	X	-

2 Entry composition [i](#)

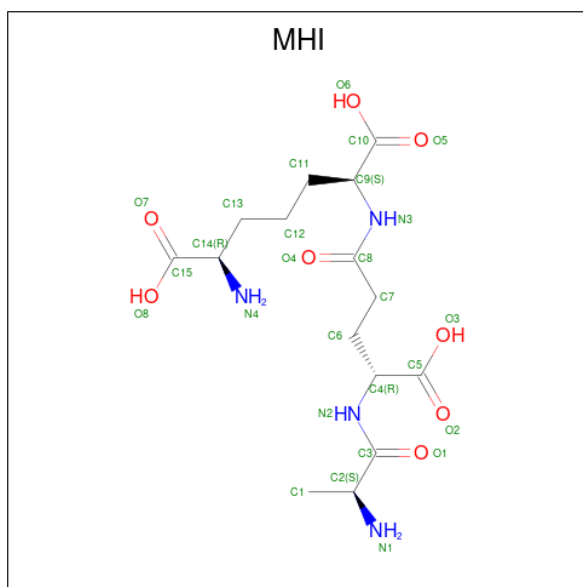
There are 5 unique types of molecules in this entry. The entry contains 24992 atoms, of which 11699 are hydrogens and 0 are deuteriums.

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 Dipeptide-binding protein DppE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	494	Total	C	H	N	O	S	228	4	0
			7886	2559	3879	661	775	12			
1	B	496	Total	C	H	N	O	S	233	1	0
			7870	2552	3865	663	778	12			
1	C	484	Total	C	H	N	O	S	227	1	0
			7640	2488	3742	641	757	12			

- Molecule 2 is L-ALA-GAMMA-D-GLU-MESO-DIAMINOPIMELIC ACID (CCD ID: MHI) (formula: $C_{15}H_{26}N_4O_8$) (labeled as "Ligand of Interest" by depositor).

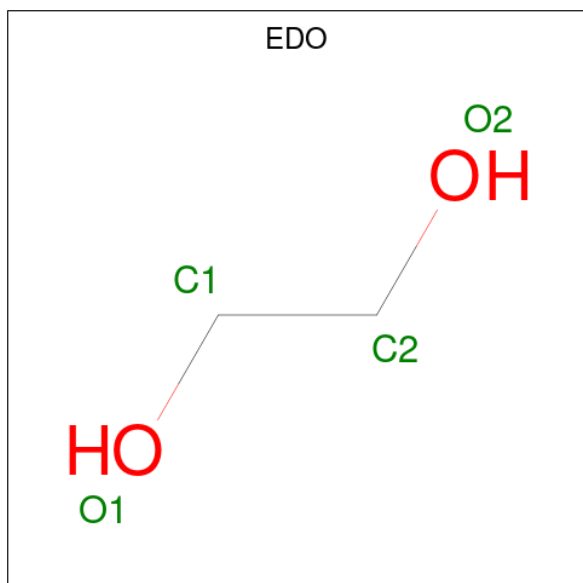


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			52	15	25	4	8		
2	B	1	Total	C	H	N	O	0	0
			52	15	25	4	8		
2	C	1	Total	C	H	N	O	0	0
			52	15	25	4	8		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

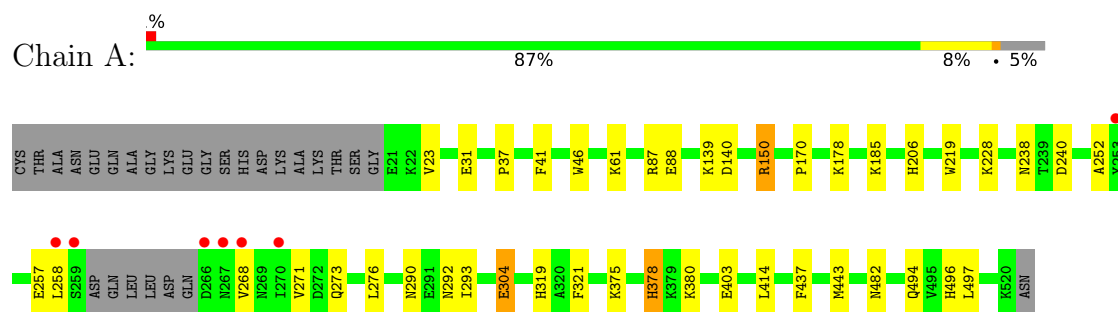
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	447	Total 447	O 447	0	0
5	B	439	Total 439	O 439	0	0
5	C	320	Total 320	O 320	0	0

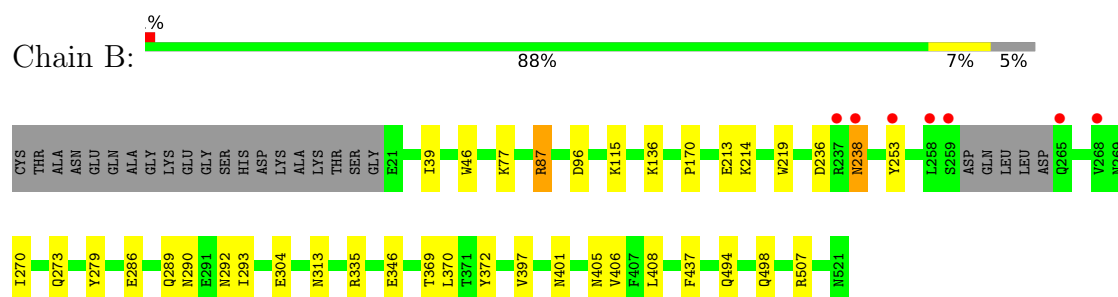
3 Residue-property plots [i](#)

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.

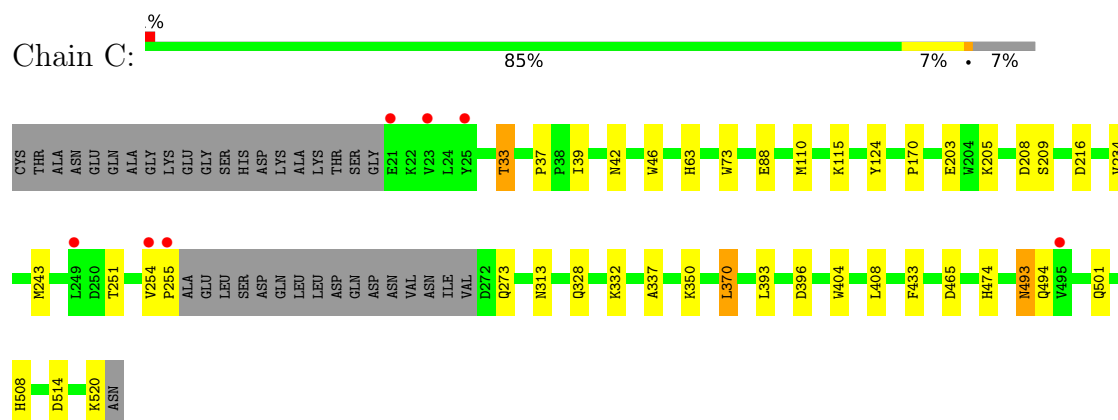
• Molecule 1: Dipeptide-binding protein DppE



• Molecule 1: Dipeptide-binding protein DppE



• Molecule 1: Dipeptide-binding protein DppE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.85Å 61.31Å 124.07Å 78.09° 82.67° 61.60°	Depositor
Resolution (Å)	60.74 – 1.51 60.74 – 1.51	Depositor EDS
% Data completeness (in resolution range)	96.3 (60.74-1.51) 85.4 (60.74-1.51)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.51Å)	Xtriage
Refinement program	REFMAC 5.8.0352, REFMAC 5.8.0352	Depositor
R, R_{free}	0.184 , 0.221 0.186 , 0.223	Depositor DCC
R_{free} test set	11490 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for h-k,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	24992	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EDO, MHI

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	0.62	2/4119 (0.0%)	0.99	3/5577 (0.1%)
1	B	0.61	0/4108	0.99	3/5562 (0.1%)
1	C	0.56	0/4001	0.99	2/5422 (0.0%)
All	All	0.60	2/12228 (0.0%)	0.99	8/16561 (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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	ASP	CG-OD1	5.31	1.35	1.25
1	A	304	GLU	CD-OE1	5.21	1.35	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	PRO	N-CA-C	5.90	117.89	110.70
1	B	437	PHE	CA-CB-CG	-5.83	107.97	113.80
1	B	313	ASN	CA-CB-CG	5.45	118.05	112.60
1	A	437	PHE	CA-CB-CG	-5.45	108.35	113.80
1	C	37	PRO	N-CA-C	5.42	117.31	110.70
1	B	96	ASP	CA-CB-CG	5.40	118.00	112.60
1	C	433	PHE	CA-CB-CG	5.15	118.95	113.80
1	A	378	HIS	CA-CB-CG	-5.14	108.66	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	87	ARG	Sidechain

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	4007	3879	3862	26	0
1	B	4005	3865	3847	25	0
1	C	3898	3742	3714	31	0
2	A	27	25	23	0	0
2	B	27	25	23	2	0
2	C	27	25	23	0	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
4	A	52	78	78	9	0
4	B	20	30	30	6	0
4	C	20	30	30	3	0
5	A	447	0	0	3	0
5	B	439	0	0	7	0
5	C	320	0	0	6	0
All	All	13293	11699	11630	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:B:304:GLU:OE2	5:B:701:HOH:O	1.69	1.10
1:C:33:THR:HG21	1:C:42:ASN:HD21	1.24	1.03
1:C:88:GLU:OE1	5:C:701:HOH:O	2.02	0.76
1:C:33:THR:CG2	1:C:42:ASN:HD21	1.98	0.76
1:B:253:TYR:CE2	5:B:705:HOH:O	2.39	0.75
1:A:482:ASN:HD22	4:A:612:EDO:C2	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:ASN:OD1	1:B:406:VAL:HG23	1.89	0.73
1:C:33:THR:HG21	1:C:42:ASN:ND2	2.03	0.73
1:B:290:ASN:HD22	1:B:293:ILE:H	1.38	0.71
1:C:493:ASN:HD22	1:C:493:ASN:C	2.00	0.70
1:C:254:VAL:HG23	1:C:313:ASN:OD1	1.92	0.69
1:C:33:THR:HG22	5:C:968:HOH:O	1.95	0.67
1:B:346:GLU:OE2	5:B:702:HOH:O	2.13	0.66
1:C:328:GLN:OE1	1:C:474:HIS:HE1	1.78	0.66
1:B:253:TYR:CZ	5:B:705:HOH:O	2.49	0.66
1:A:290:ASN:HD22	1:A:293:ILE:H	1.45	0.64
1:C:474:HIS:HD2	5:C:761:HOH:O	1.80	0.64
1:A:482:ASN:HD22	4:A:612:EDO:C1	2.12	0.63
1:C:465:ASP:OD2	5:C:702:HOH:O	2.16	0.63
1:C:254:VAL:CG2	1:C:313:ASN:OD1	2.46	0.63
1:A:31:GLU:OE2	1:A:206:HIS:HD2	1.82	0.62
1:C:370:LEU:C	1:C:370:LEU:HD23	2.24	0.61
1:A:482:ASN:HD22	4:A:612:EDO:H12	1.69	0.57
1:B:253:TYR:CD1	4:B:609:EDO:H12	2.40	0.56
1:C:332:LYS:HE3	1:C:337:ALA:HB2	1.88	0.55
1:A:273:GLN:HB2	1:A:494:GLN:HG3	1.90	0.54
1:C:63:HIS:ND1	1:C:508:HIS:HD2	2.06	0.53
1:A:276:LEU:HD21	1:A:321:PHE:CE1	2.43	0.53
1:B:290:ASN:HD21	1:B:292:ASN:HB2	1.74	0.52
1:C:404:TRP:CH2	1:C:408:LEU:HD21	2.44	0.52
1:A:240:ASP:OD1	1:A:252:ALA:HB1	2.10	0.51
1:C:273:GLN:HB2	1:C:494:GLN:HG3	1.92	0.51
1:B:405:ASN:ND2	5:B:708:HOH:O	2.43	0.51
1:A:87:ARG:HD3	1:A:219:TRP:CE3	2.46	0.51
1:A:88:GLU:HG3	1:A:150[B]:ARG:CZ	2.42	0.50
1:A:304:GLU:OE2	1:A:319:HIS:NE2	2.43	0.50
1:C:350:LYS:HD3	1:C:393:LEU:HA	1.93	0.50
1:B:253:TYR:CE1	4:B:609:EDO:H12	2.47	0.49
4:C:602:EDO:H12	5:C:934:HOH:O	2.12	0.49
1:B:270:ILE:HD12	1:B:270:ILE:O	2.12	0.49
1:C:493:ASN:C	1:C:493:ASN:ND2	2.68	0.49
1:C:508:HIS:HE1	1:C:514:ASP:OD2	1.95	0.49
1:C:39:ILE:HD11	1:C:115:LYS:HE3	1.93	0.48
2:B:601:MHI:H42N	4:B:609:EDO:H21	1.78	0.48
1:C:501:GLN:O	1:C:520:LYS:HA	2.13	0.48
1:A:273:GLN:HB2	1:A:494:GLN:CG	2.44	0.48
1:A:378:HIS:CD2	4:A:614:EDO:H22	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:GLU:C	1:A:258:LEU:HD23	2.38	0.47
1:C:370:LEU:C	1:C:370:LEU:CD2	2.87	0.47
1:A:375:LYS:HB2	4:A:614:EDO:H11	1.96	0.47
1:B:498:GLN:HE22	1:B:507:ARG:HH12	1.62	0.47
1:A:31:GLU:OE2	1:A:206:HIS:CD2	2.65	0.47
1:A:46:TRP:CE2	1:A:170:PRO:HB2	2.50	0.46
4:A:614:EDO:C1	5:A:702:HOH:O	2.63	0.46
4:B:609:EDO:H11	5:B:722:HOH:O	2.16	0.46
1:C:234:VAL:HG21	1:C:243:MET:SD	2.56	0.46
1:B:87:ARG:HD3	1:B:219:TRP:CE3	2.51	0.45
2:B:601:MHI:H42N	4:B:609:EDO:C2	2.29	0.45
1:A:268:VAL:HG22	1:A:497:LEU:CD2	2.46	0.45
1:A:290:ASN:HD21	1:A:292:ASN:HB2	1.82	0.45
1:B:273:GLN:HB2	1:B:494:GLN:CG	2.47	0.44
1:C:203:GLU:HG3	5:C:822:HOH:O	2.18	0.44
1:B:46:TRP:CE2	1:B:170:PRO:HB2	2.54	0.43
1:B:236:ASP:C	1:B:238:ASN:N	2.77	0.43
1:A:23:VAL:HG22	1:A:228:LYS:HB2	2.01	0.42
1:A:61[B]:LYS:HG3	4:A:615:EDO:H21	2.01	0.42
1:A:139:LYS:HE2	5:A:710:HOH:O	2.18	0.42
1:B:253:TYR:HD1	4:B:609:EDO:H12	1.83	0.42
1:C:73:TRP:CE2	4:C:604:EDO:H22	2.55	0.42
1:C:273:GLN:HB2	1:C:494:GLN:HE21	1.85	0.42
1:C:493:ASN:HD22	1:C:494:GLN:N	2.16	0.42
1:B:39:ILE:HD11	1:B:115:LYS:HE3	2.01	0.42
1:B:286:GLU:HA	1:B:289:GLN:OE1	2.20	0.42
1:A:496:HIS:CE1	5:A:742:HOH:O	2.73	0.41
1:A:41:PHE:HE2	1:A:443:MET:SD	2.44	0.41
4:A:606:EDO:H22	4:A:614:EDO:O1	2.20	0.41
1:C:205:LYS:HB2	1:C:208:ASP:HB3	2.01	0.41
1:A:482:ASN:HD22	4:A:612:EDO:H22	1.84	0.41
1:B:238:ASN:ND2	1:B:238:ASN:C	2.77	0.41
1:C:46:TRP:CE2	1:C:170:PRO:HB2	2.55	0.41
1:C:254:VAL:HA	1:C:255:PRO:HD3	1.91	0.41
1:B:213:GLU:O	1:B:214:LYS:C	2.64	0.41
1:B:279:TYR:CE1	1:B:370:LEU:HD11	2.55	0.40
1:C:124:TYR:HB2	4:C:606:EDO:H22	2.04	0.40
1:B:77:LYS:NZ	5:B:703:HOH:O	2.18	0.40
1:B:372:TYR:O	1:B:401:ASN:HA	2.21	0.40
1:B:335:ARG:CZ	1:B:335:ARG:HA	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	494/521 (95%)	481 (97%)	13 (3%)	0	100	100
1	B	493/521 (95%)	480 (97%)	13 (3%)	0	100	100
1	C	481/521 (92%)	471 (98%)	10 (2%)	0	100	100
All	All	1468/1563 (94%)	1432 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	431/454 (95%)	423 (98%)	8 (2%)	50	21
1	B	431/454 (95%)	426 (99%)	5 (1%)	63	37
1	C	415/454 (91%)	407 (98%)	8 (2%)	50	21
All	All	1277/1362 (94%)	1256 (98%)	21 (2%)	55	27

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150[A]	ARG
1	A	150[B]	ARG
1	A	178	LYS
1	A	185	LYS
1	A	238	ASN

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Mol	Chain	Res	Type
1	A	271	VAL
1	A	403	GLU
1	A	414	LEU
1	B	136	LYS
1	B	238	ASN
1	B	369	THR
1	B	397	VAL
1	B	408	LEU
1	C	33	THR
1	C	110	MET
1	C	209	SER
1	C	216	ASP
1	C	251	THR
1	C	370	LEU
1	C	396	ASP
1	C	493	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	133	ASN
1	A	206	HIS
1	A	290	ASN
1	A	292	ASN
1	A	363	ASN
1	A	462	ASN
1	A	482	ASN
1	A	498	GLN
1	B	43	ASN
1	B	238	ASN
1	B	245	GLN
1	B	290	ASN
1	B	387	GLN
1	B	475	GLN
1	B	498	GLN
1	B	521	ASN
1	C	42	ASN
1	C	133	ASN
1	C	238	ASN
1	C	245	GLN
1	C	401	ASN

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Mol	Chain	Res	Type
1	C	438	GLN
1	C	459	GLN
1	C	462	ASN
1	C	474	HIS
1	C	493	ASN
1	C	494	GLN
1	C	498	GLN
1	C	508	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 4 are monoatomic - leaving 26 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	B	609	-	3,3,3	0.27	0	2,2,2	0.04	0
4	EDO	A	606	-	3,3,3	0.24	0	2,2,2	0.31	0
4	EDO	C	604	-	3,3,3	0.10	0	2,2,2	0.24	0
4	EDO	B	607	-	3,3,3	0.04	0	2,2,2	0.04	0
2	MHI	B	601	-	24,26,26	0.85	2 (8%)	30,34,34	0.91	1 (3%)
4	EDO	A	611	-	3,3,3	0.12	0	2,2,2	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	615	-	3,3,3	0.18	0	2,2,2	0.41	0
4	EDO	B	608	-	3,3,3	0.21	0	2,2,2	0.22	0
4	EDO	A	605	-	3,3,3	0.40	0	2,2,2	0.58	0
4	EDO	A	609	-	3,3,3	0.30	0	2,2,2	0.24	0
4	EDO	C	603	-	3,3,3	0.10	0	2,2,2	0.09	0
4	EDO	A	613	-	3,3,3	0.14	0	2,2,2	0.10	0
4	EDO	A	614	-	3,3,3	0.14	0	2,2,2	0.12	0
2	MHI	C	601	-	24,26,26	0.85	1 (4%)	30,34,34	0.83	0
4	EDO	A	607	-	3,3,3	0.06	0	2,2,2	0.16	0
4	EDO	C	602	-	3,3,3	0.21	0	2,2,2	0.23	0
4	EDO	A	603	-	3,3,3	0.12	0	2,2,2	0.29	0
4	EDO	C	606	-	3,3,3	0.13	0	2,2,2	0.44	0
4	EDO	A	610	-	3,3,3	0.14	0	2,2,2	0.04	0
4	EDO	A	608	-	3,3,3	0.14	0	2,2,2	0.24	0
4	EDO	A	604	-	3,3,3	0.15	0	2,2,2	0.19	0
4	EDO	C	605	-	3,3,3	0.13	0	2,2,2	0.10	0
4	EDO	B	606	-	3,3,3	0.55	0	2,2,2	0.68	0
4	EDO	A	612	-	3,3,3	0.18	0	2,2,2	0.47	0
2	MHI	A	601	-	24,26,26	0.74	1 (4%)	30,34,34	0.87	2 (6%)
4	EDO	B	605	-	3,3,3	0.05	0	2,2,2	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	609	-	-	1/1/1/1	-
4	EDO	A	606	-	-	1/1/1/1	-
4	EDO	C	604	-	-	0/1/1/1	-
4	EDO	B	607	-	-	1/1/1/1	-
2	MHI	B	601	-	-	1/35/35/35	-
4	EDO	A	611	-	-	0/1/1/1	-
4	EDO	A	615	-	-	1/1/1/1	-
4	EDO	B	608	-	-	0/1/1/1	-
4	EDO	A	605	-	-	0/1/1/1	-
4	EDO	A	609	-	-	0/1/1/1	-
4	EDO	C	603	-	-	1/1/1/1	-
4	EDO	A	613	-	-	0/1/1/1	-
4	EDO	A	614	-	-	1/1/1/1	-
2	MHI	C	601	-	-	0/35/35/35	-
4	EDO	A	607	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	602	-	-	0/1/1/1	-
4	EDO	A	603	-	-	1/1/1/1	-
4	EDO	C	606	-	-	1/1/1/1	-
4	EDO	A	610	-	-	0/1/1/1	-
4	EDO	A	608	-	-	0/1/1/1	-
4	EDO	A	604	-	-	0/1/1/1	-
4	EDO	C	605	-	-	1/1/1/1	-
4	EDO	B	606	-	-	1/1/1/1	-
4	EDO	A	612	-	-	1/1/1/1	-
2	MHI	A	601	-	-	2/35/35/35	-
4	EDO	B	605	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	MHI	O8-C15	-2.41	1.23	1.30
2	C	601	MHI	O8-C15	-2.32	1.23	1.30
2	A	601	MHI	O6-C10	-2.10	1.24	1.30
2	B	601	MHI	O6-C10	-2.07	1.24	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	MHI	C9-N3-C8	2.24	127.29	121.68
2	B	601	MHI	O5-C10-C9	-2.13	115.39	122.26
2	A	601	MHI	O2-C5-C4	-2.12	115.41	122.26

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	614	EDO	O1-C1-C2-O2
4	A	603	EDO	O1-C1-C2-O2
4	A	606	EDO	O1-C1-C2-O2
4	B	606	EDO	O1-C1-C2-O2
4	B	609	EDO	O1-C1-C2-O2
4	C	605	EDO	O1-C1-C2-O2
4	A	612	EDO	O1-C1-C2-O2
4	A	615	EDO	O1-C1-C2-O2
4	B	607	EDO	O1-C1-C2-O2
4	C	603	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	601	MHI	N4-C14-C15-O8
4	A	607	EDO	O1-C1-C2-O2
4	C	606	EDO	O1-C1-C2-O2
2	B	601	MHI	N4-C14-C15-O8
2	A	601	MHI	N4-C14-C15-O7

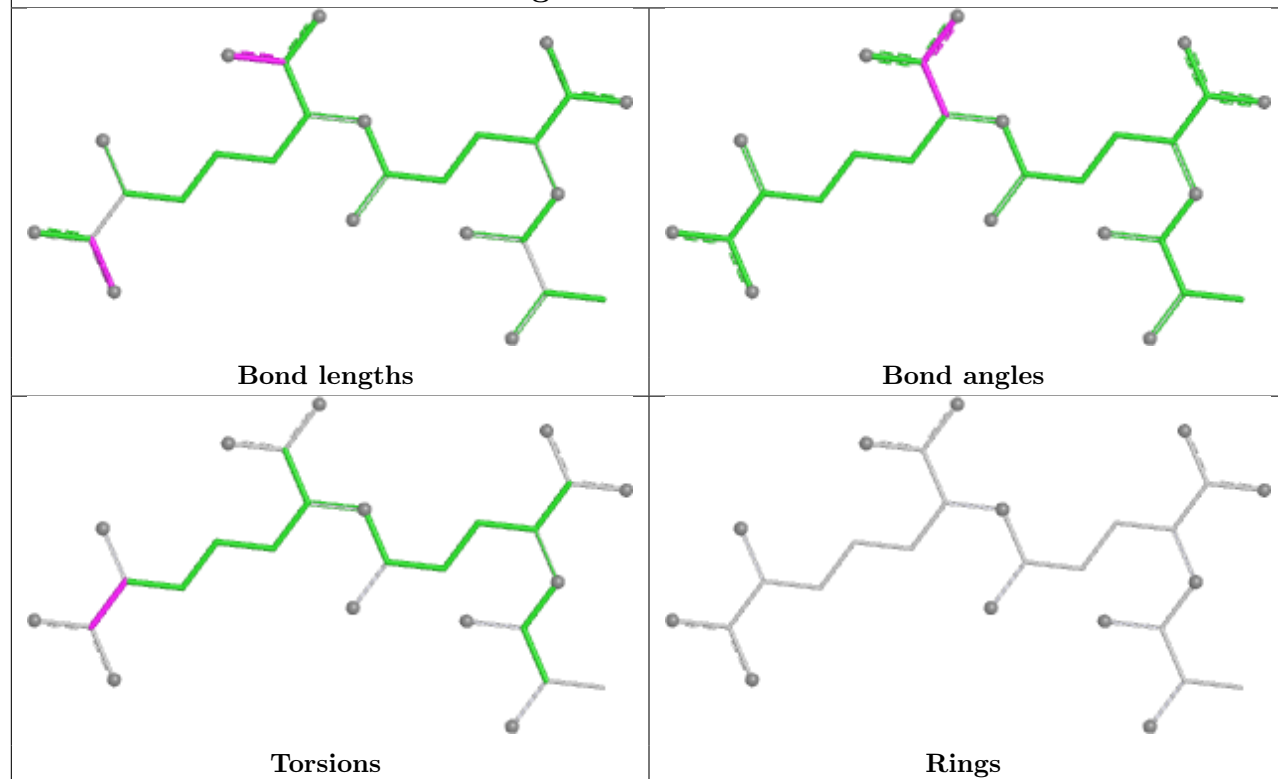
There are no ring outliers.

9 monomers are involved in 18 short contacts:

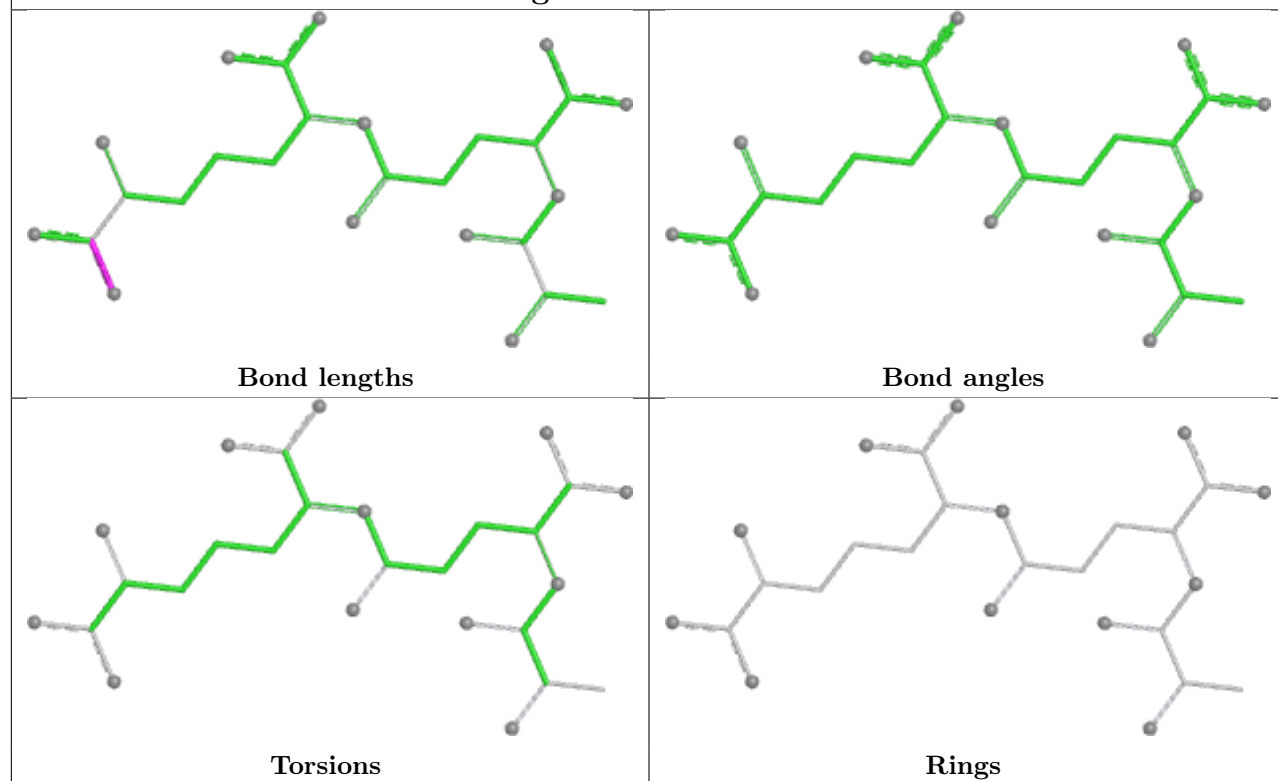
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	609	EDO	6	0
4	A	606	EDO	1	0
4	C	604	EDO	1	0
2	B	601	MHI	2	0
4	A	615	EDO	1	0
4	A	614	EDO	4	0
4	C	602	EDO	1	0
4	C	606	EDO	1	0
4	A	612	EDO	4	0

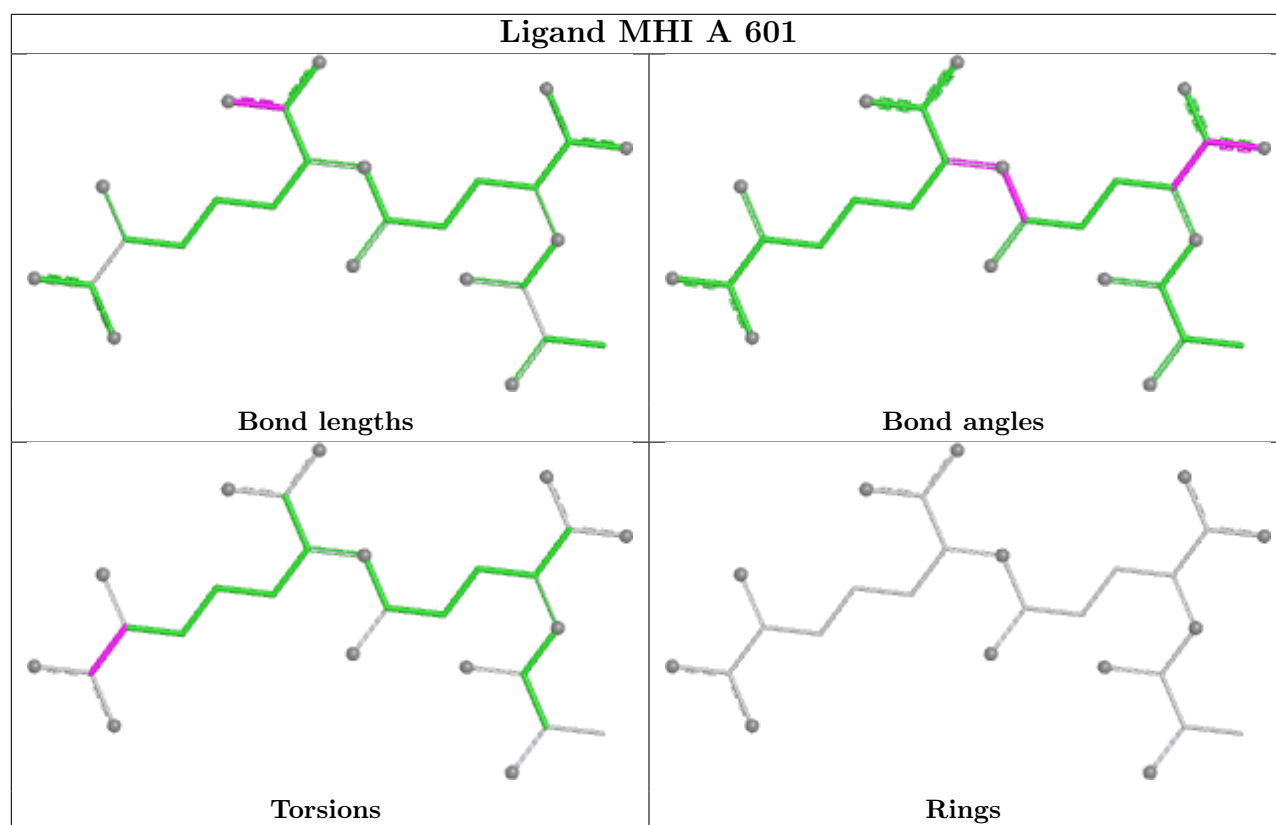
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand MHI B 601



Ligand MHI C 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	494/521 (94%)	-0.18	7 (1%) 73 78	11, 21, 39, 81	4 (0%)
1	B	496/521 (95%)	-0.15	7 (1%) 73 78	12, 22, 41, 65	1 (0%)
1	C	484/521 (92%)	0.25	7 (1%) 73 78	16, 29, 49, 63	1 (0%)
All	All	1474/1563 (94%)	-0.03	21 (1%) 73 78	11, 25, 45, 81	6 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	SER	6.0
1	B	253	TYR	4.5
1	C	495	VAL	4.2
1	B	237	ARG	4.0
1	B	259	SER	3.8
1	A	270	ILE	3.8
1	C	255	PRO	3.5
1	A	253	TYR	2.8
1	C	21	GLU	2.8
1	B	265	GLN	2.7
1	C	23	VAL	2.7
1	B	268	VAL	2.5
1	A	266	ASP	2.4
1	C	254	VAL	2.3
1	B	238	ASN	2.3
1	C	25	TYR	2.3
1	C	249	LEU	2.3
1	B	258	LEU	2.2
1	A	268	VAL	2.2
1	A	258	LEU	2.1
1	A	267	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

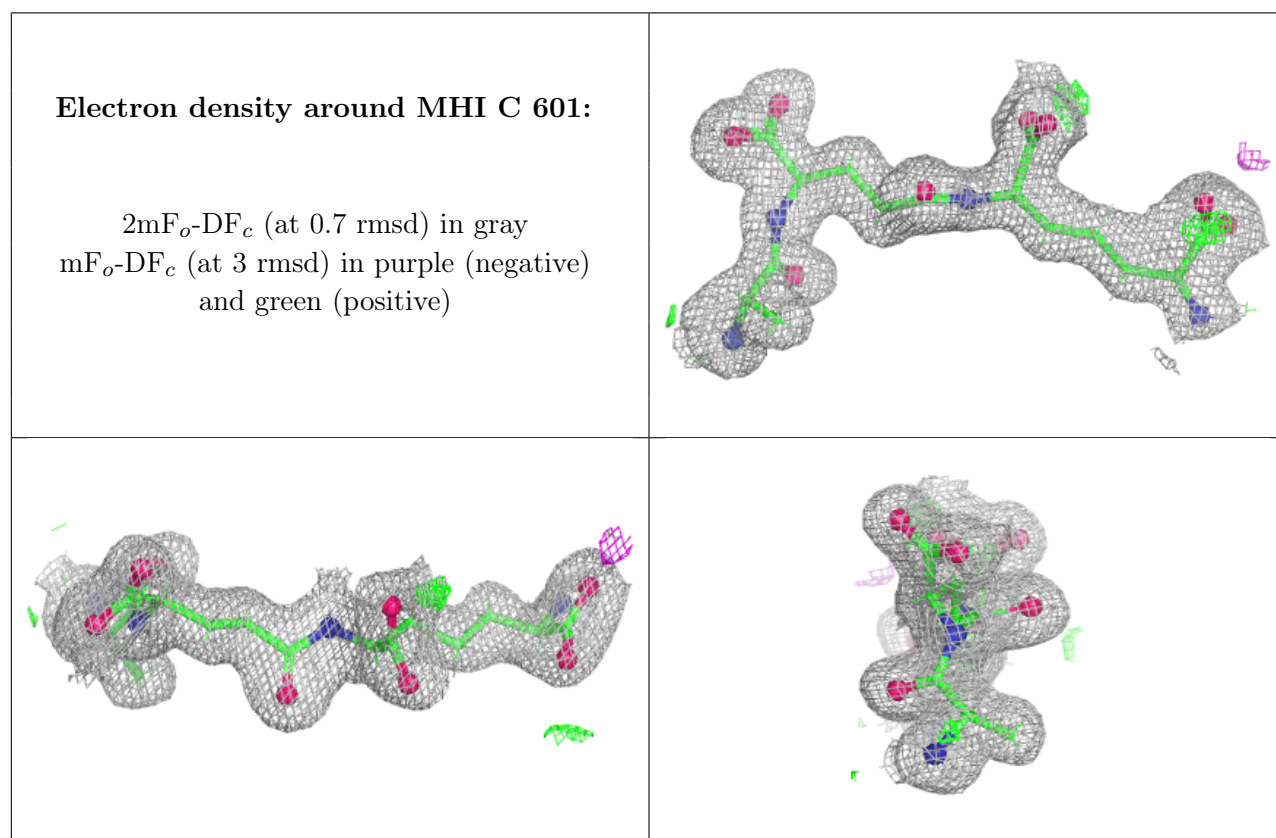
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	C	605	4/4	0.76	0.16	62,68,69,69	1
4	EDO	A	607	4/4	0.83	0.18	73,77,82,84	1
4	EDO	A	613	4/4	0.83	0.13	49,50,50,51	1
4	EDO	A	606	4/4	0.83	0.15	38,40,51,51	1
4	EDO	B	606	4/4	0.84	0.14	41,45,47,47	1
4	EDO	A	614	4/4	0.84	0.15	55,56,60,62	1
4	EDO	C	606	4/4	0.86	0.12	36,42,44,44	1
4	EDO	A	603	4/4	0.88	0.11	32,39,48,48	1
4	EDO	C	604	4/4	0.88	0.11	40,44,49,49	1
4	EDO	C	603	4/4	0.89	0.12	54,56,56,57	1
4	EDO	A	611	4/4	0.89	0.10	48,50,57,58	1
4	EDO	A	608	4/4	0.89	0.10	33,39,40,40	1
4	EDO	B	607	4/4	0.89	0.11	51,54,55,56	1
4	EDO	A	610	4/4	0.90	0.09	40,46,52,54	1
4	EDO	A	612	4/4	0.90	0.07	43,44,47,47	1
4	EDO	B	609	4/4	0.90	0.12	32,40,43,44	1
4	EDO	C	602	4/4	0.90	0.11	37,37,39,40	1
4	EDO	A	615	4/4	0.91	0.10	34,37,48,48	1
4	EDO	A	605	4/4	0.92	0.11	27,30,32,34	1
4	EDO	A	604	4/4	0.92	0.08	38,39,39,40	1
3	MG	A	602	1/1	0.94	0.07	39,39,39,39	0
3	MG	B	603	1/1	0.95	0.08	42,42,42,42	0
4	EDO	A	609	4/4	0.95	0.07	25,26,28,29	1
4	EDO	B	605	4/4	0.96	0.07	30,33,37,38	1
3	MG	B	602	1/1	0.97	0.08	30,30,30,30	0
2	MHI	C	601	27/27	0.97	0.06	18,21,35,38	0
2	MHI	A	601	27/27	0.97	0.05	15,18,25,31	0

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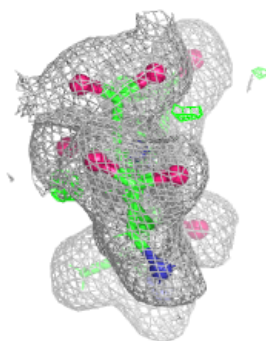
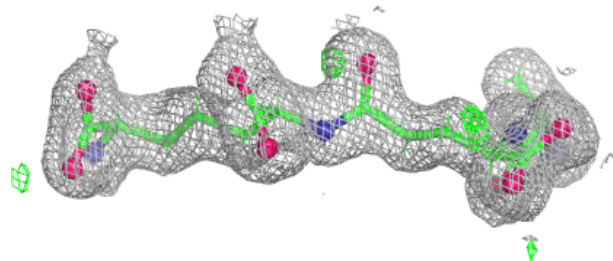
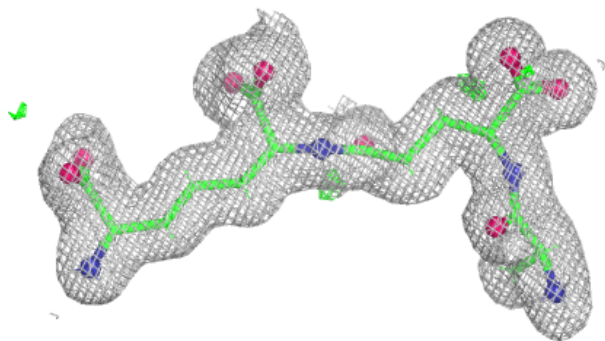
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MHI	B	601	27/27	0.98	0.04	15,18,24,29	0
3	MG	B	604	1/1	0.98	0.07	21,21,21,21	0
4	EDO	B	608	4/4	0.98	0.05	21,21,22,22	1

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.

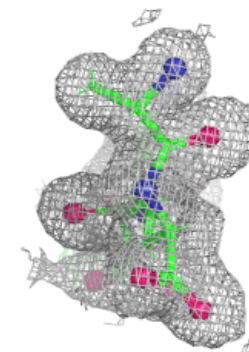
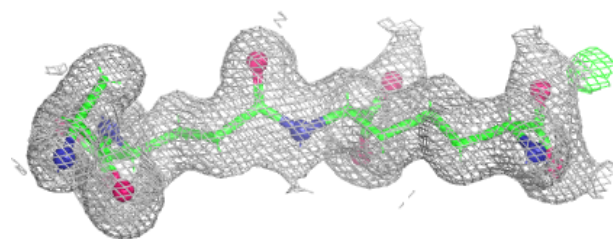
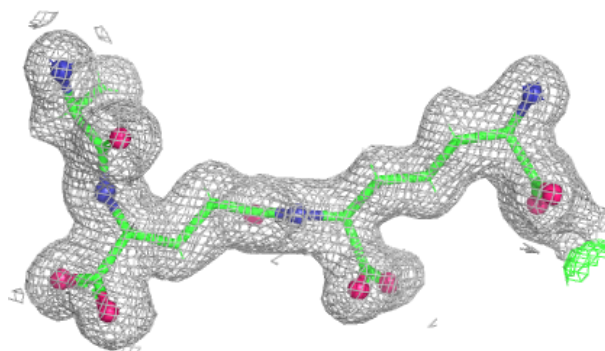


Electron density around MHI A 601:

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

**Electron density around MHI B 601:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.