Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2025 – 06:13 PM EDT

PDB ID	:	9MY7
Title	:	Structure of the BasE mutant V336G, an NRPS adenylation domain in the acinetobactin biosynthetic pathway bound to 4-amino salicylic acid
Authors	:	Ahmed, S.F.; Gulick, A.M.
Deposited on	:	2025-01-21
Resolution	:	2.53 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:

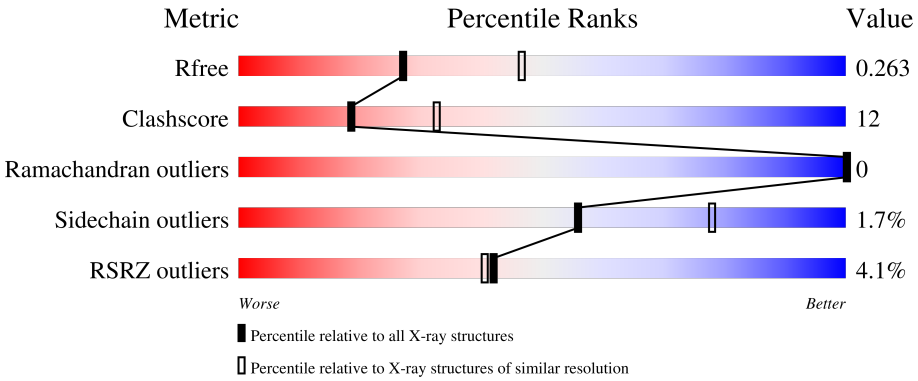
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.53 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}	164625	6935 (2.54-2.50)
Clashscore	180529	7778 (2.54-2.50)
Ramachandran outliers	177936	7674 (2.54-2.50)
Sidechain outliers	177891	7676 (2.54-2.50)
RSRZ outliers	164620	6935 (2.54-2.50)

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 <=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	562	3% 59% 19% 23%
1	B	562	3% 59% 18% 23%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6872 atoms, of which 30 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 (2,3-dihydroxybenzoyl)adenylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	435	Total	C	N	O	S	0	2	0
			3314	2123	567	609	15			
1	A	435	Total	C	N	O	S	0	2	0
			3332	2127	571	619	15			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP A0A505MWF2
B	-18	GLY	-	expression tag	UNP A0A505MWF2
B	-17	SER	-	expression tag	UNP A0A505MWF2
B	-16	SER	-	expression tag	UNP A0A505MWF2
B	-15	HIS	-	expression tag	UNP A0A505MWF2
B	-14	HIS	-	expression tag	UNP A0A505MWF2
B	-13	HIS	-	expression tag	UNP A0A505MWF2
B	-12	HIS	-	expression tag	UNP A0A505MWF2
B	-11	HIS	-	expression tag	UNP A0A505MWF2
B	-10	SER	-	expression tag	UNP A0A505MWF2
B	-9	SER	-	expression tag	UNP A0A505MWF2
B	-8	GLY	-	expression tag	UNP A0A505MWF2
B	-7	GLU	-	expression tag	UNP A0A505MWF2
B	-6	ASN	-	expression tag	UNP A0A505MWF2
B	-5	LEU	-	expression tag	UNP A0A505MWF2
B	-4	TYR	-	expression tag	UNP A0A505MWF2
B	-3	PHE	-	expression tag	UNP A0A505MWF2
B	-2	GLN	-	expression tag	UNP A0A505MWF2
B	-1	GLY	-	expression tag	UNP A0A505MWF2
B	0	HIS	-	expression tag	UNP A0A505MWF2
B	45	LEU	PRO	engineered mutation	UNP A0A505MWF2
B	68	THR	SER	conflict	UNP A0A505MWF2
B	149	ASP	GLU	conflict	UNP A0A505MWF2
B	336	GLY	VAL	engineered mutation	UNP A0A505MWF2
B	378	ARG	LYS	conflict	UNP A0A505MWF2

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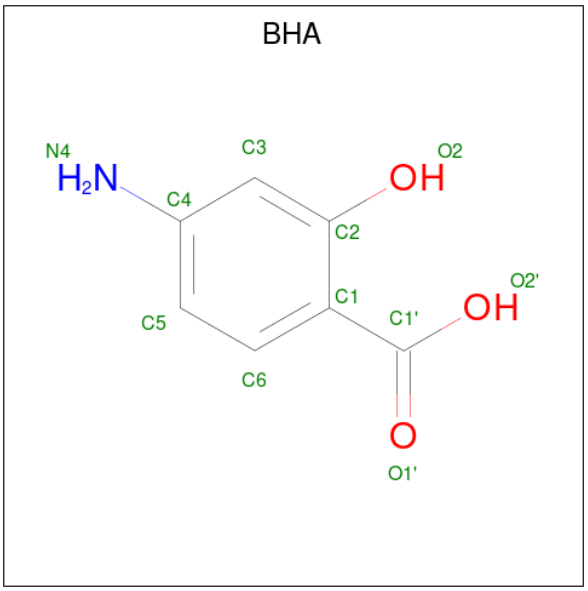
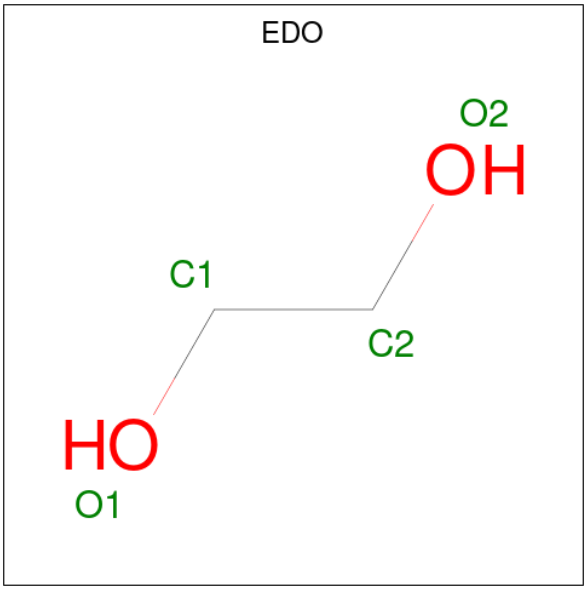
Chain	Residue	Modelled	Actual	Comment	Reference
B	385	ILE	VAL	conflict	UNP A0A505MWF2
A	-19	MET	-	initiating methionine	UNP A0A505MWF2
A	-18	GLY	-	expression tag	UNP A0A505MWF2
A	-17	SER	-	expression tag	UNP A0A505MWF2
A	-16	SER	-	expression tag	UNP A0A505MWF2
A	-15	HIS	-	expression tag	UNP A0A505MWF2
A	-14	HIS	-	expression tag	UNP A0A505MWF2
A	-13	HIS	-	expression tag	UNP A0A505MWF2
A	-12	HIS	-	expression tag	UNP A0A505MWF2
A	-11	HIS	-	expression tag	UNP A0A505MWF2
A	-10	SER	-	expression tag	UNP A0A505MWF2
A	-9	SER	-	expression tag	UNP A0A505MWF2
A	-8	GLY	-	expression tag	UNP A0A505MWF2
A	-7	GLU	-	expression tag	UNP A0A505MWF2
A	-6	ASN	-	expression tag	UNP A0A505MWF2
A	-5	LEU	-	expression tag	UNP A0A505MWF2
A	-4	TYR	-	expression tag	UNP A0A505MWF2
A	-3	PHE	-	expression tag	UNP A0A505MWF2
A	-2	GLN	-	expression tag	UNP A0A505MWF2
A	-1	GLY	-	expression tag	UNP A0A505MWF2
A	0	HIS	-	expression tag	UNP A0A505MWF2
A	45	LEU	PRO	engineered mutation	UNP A0A505MWF2
A	68	THR	SER	conflict	UNP A0A505MWF2
A	149	ASP	GLU	conflict	UNP A0A505MWF2
A	336	GLY	VAL	engineered mutation	UNP A0A505MWF2
A	378	ARG	LYS	conflict	UNP A0A505MWF2
A	385	ILE	VAL	conflict	UNP A0A505MWF2

- Molecule 2 is 2-HYDROXY-4-AMINOBENZOIC ACID (three-letter code: BHA) (formula: $C_7H_7NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	0	0
			17	7	6	1	3		
2	A	1	Total	C	H	N	O	0	0
			17	7	6	1	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	5	Total Ca 5 5	0	0
4	A	4	Total Ca 4 4	0	0

- Molecule 5 is water.

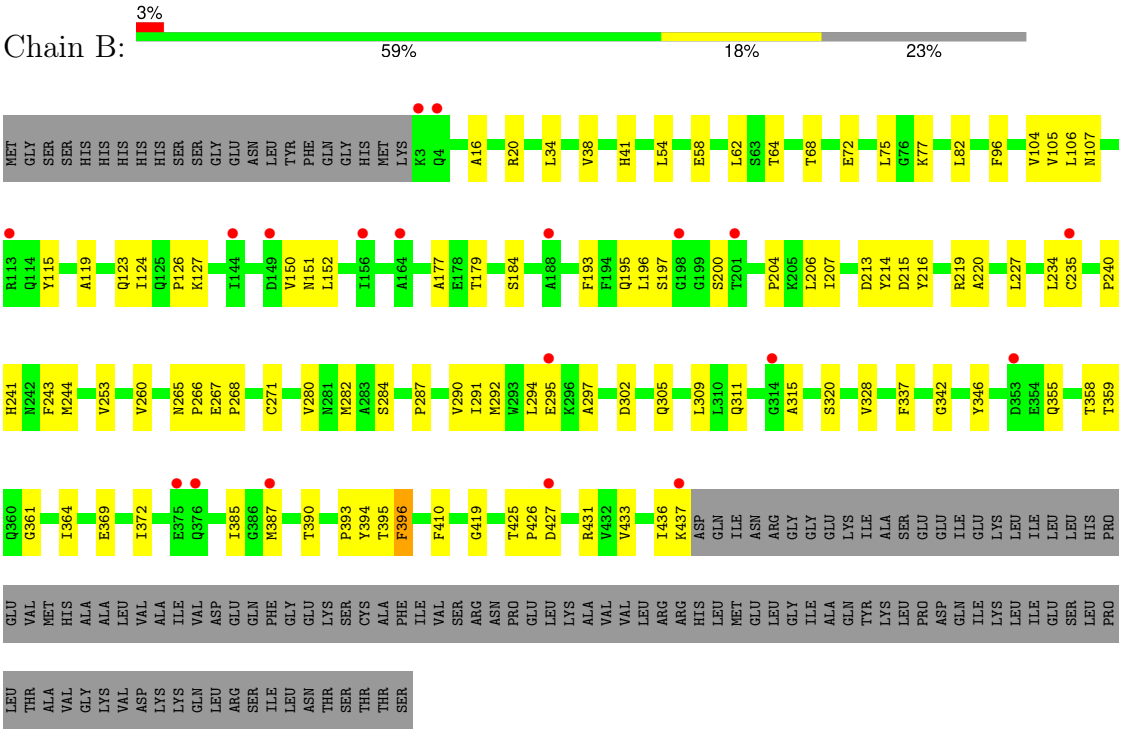
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	91	Total O 91 91	0	0
5	A	62	Total O 62 62	0	0

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.

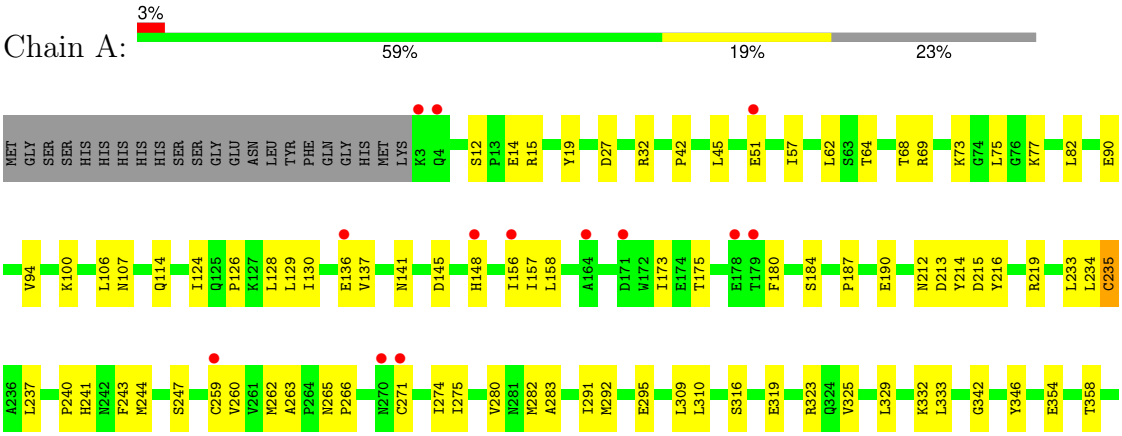
• Molecule 1: (2,3-dihydroxybenzoyl)adenylate synthase

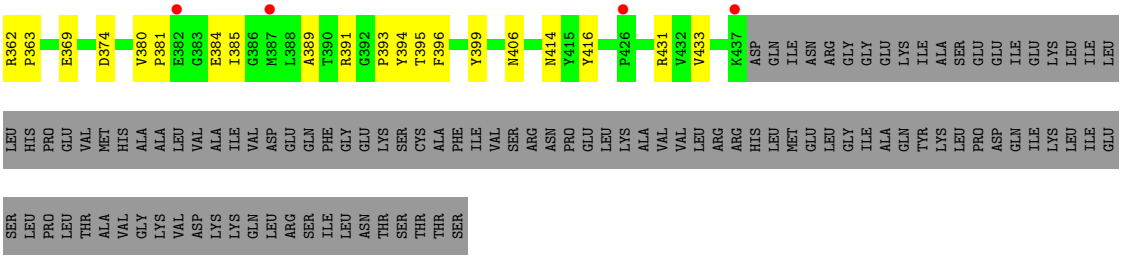
Chain B:



• Molecule 1: (2,3-dihydroxybenzoyl)adenylate synthase

Chain A:




R362 P363 E369 D374 V380 P381 E382 G383 E384 I385 G386 M387 L388 A389 T390 R391 G392 P393 Y394 T395 F396 Y399 N406 N414 Y415 Y416 P426 R431 V432 V433 K437
ASP GLN ILE ASN ARG GLY GLY GLU LYS ILE ALA SER GLU GLU ILE GLU LYS LEU ILE LEU
LEU HIS PRO GLU VAL MET HIS ALA ALA LEU VAL ALA ILE VAL ASP GLU GLN PHE GLY GLU LYS SER CYS ALA PHE ILE VAL SER ARG ASN PRO GLU LEU LYS ALA VAL VAL LEU ARG ARG HIS LEU MET GLU LEU GLY ILE ALA GLN TYR LYS LEU PRO ASP GLN ILE LYS LEU ILE GLU
SER LEU PRO LEU THR ALA VAL GLY LYS VAL ASP LYS LYS GLN LEU ARG SER ILE LEU ASN THR SER THR THR SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.29Å 143.35Å 149.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.17 – 2.53 66.17 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.0 (66.17-2.53) 99.0 (66.17-2.53)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.213 , 0.263 0.213 , 0.263	Depositor DCC
R_{free} test set	45520 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.801	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6872	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: BHA, EDO, CA

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	0.25	0/3417	0.46	0/4660
1	B	0.25	0/3398	0.45	0/4635
All	All	0.25	0/6815	0.46	0/9295

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	3332	0	3199	85	0
1	B	3314	0	3202	72	0
2	A	11	6	5	0	0
2	B	11	6	5	0	0
3	A	8	12	12	3	0
3	B	4	6	6	1	0
4	A	4	0	0	0	0
4	B	5	0	0	0	0
5	A	62	0	0	1	0
5	B	91	0	0	5	0
All	All	6842	30	6429	155	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 12.

All (155) 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:235[A]:CYS:HA	1:B:244:MET:HE2	1.19	1.09
1:A:385:ILE:HD13	1:A:433:VAL:HG21	1.33	1.09
1:B:235[B]:CYS:HA	1:B:244:MET:HE2	1.19	1.08
1:A:332:LYS:HD2	1:A:333:LEU:H	1.21	1.02
1:A:75:LEU:HD11	1:A:156:ILE:HD12	1.39	1.02
1:A:51:GLU:OE1	1:A:51:GLU:N	2.01	0.93
1:A:90:GLU:N	1:A:90:GLU:OE2	2.04	0.90
1:A:384:GLU:OE2	1:A:384:GLU:N	2.08	0.87
1:B:196:LEU:HD22	1:B:204:PRO:HB2	1.54	0.86
1:A:14:GLU:OE1	1:A:14:GLU:N	2.08	0.85
1:A:233:LEU:HD12	1:A:282:MET:HG2	1.61	0.82
1:A:62:LEU:HD22	1:A:173:ILE:HG22	1.63	0.81
1:A:332:LYS:HD2	1:A:333:LEU:N	1.94	0.81
1:A:399:TYR:H	1:A:406:ASN:HD21	1.30	0.80
1:B:206:LEU:HA	5:B:712:HOH:O	1.82	0.79
1:A:325:VAL:HG13	1:A:329:LEU:HD12	1.64	0.78
1:B:54:LEU:HD23	1:B:58:GLU:HB3	1.64	0.77
1:A:282:MET:CE	1:A:309:LEU:HD23	2.17	0.74
1:B:196:LEU:HD23	5:B:712:HOH:O	1.88	0.73
1:A:64:THR:O	1:A:68:THR:HG23	1.90	0.71
1:B:34:LEU:O	1:B:38:VAL:HG23	1.91	0.71
1:B:241:HIS:HD2	1:B:243:PHE:H	1.38	0.71
1:A:233:LEU:CD1	1:A:282:MET:HG2	2.21	0.70
1:A:385:ILE:CD1	1:A:433:VAL:HG21	2.18	0.69
1:A:136:GLU:OE1	1:A:136:GLU:N	2.20	0.69
1:B:115:TYR:OH	1:A:295:GLU:HG3	1.93	0.68
1:B:235[B]:CYS:CA	1:B:244:MET:HE2	2.11	0.68
1:B:282:MET:HE1	1:B:311:GLN:HE22	1.59	0.66
1:A:260:VAL:HG12	1:A:262:MET:HE3	1.78	0.66
1:A:15:ARG:HH11	3:A:603:EDO:H22	1.61	0.65
1:A:213:ASP:HB2	1:A:394:TYR:HA	1.79	0.64
1:B:282:MET:CE	1:B:311:GLN:HE22	2.10	0.64
1:A:12:SER:HB3	3:A:603:EDO:H21	1.79	0.64
1:A:107:ASN:HB3	1:A:240:PRO:HB3	1.79	0.63
1:B:34:LEU:HD23	1:B:96:PHE:CE1	2.34	0.63
1:B:385:ILE:HD12	1:B:385:ILE:H	1.64	0.63
1:A:266:PRO:HA	1:A:271:CYS:SG	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:THR:O	1:B:431:ARG:NH1	2.29	0.61
1:B:197:SER:HB2	5:B:708:HOH:O	2.01	0.61
1:A:215:ASP:O	1:A:219:ARG:HG3	2.01	0.60
1:A:399:TYR:H	1:A:406:ASN:ND2	1.99	0.60
1:B:227:LEU:HD13	1:B:253:VAL:HG22	1.84	0.60
1:A:291:ILE:O	1:A:295:GLU:HG2	2.02	0.59
1:B:64:THR:O	1:B:68:THR:HG23	2.03	0.59
1:A:145:ASP:HA	1:A:148[A]:HIS:HD2	1.67	0.59
1:B:82:LEU:CD1	1:B:106:LEU:HD22	2.33	0.59
1:B:213:ASP:HB2	1:B:394:TYR:HA	1.84	0.58
1:A:73:LYS:NZ	5:A:701:HOH:O	2.35	0.58
1:A:51:GLU:H	1:A:51:GLU:CD	2.04	0.58
1:A:15:ARG:HD3	3:A:603:EDO:H22	1.86	0.58
1:A:32:ARG:HG2	1:A:32:ARG:HH11	1.69	0.58
1:B:305:GLN:HA	1:B:305:GLN:OE1	2.01	0.58
1:A:136:GLU:H	1:A:136:GLU:CD	2.07	0.57
1:B:119:ALA:O	1:B:123:GLN:HG3	2.05	0.57
1:B:235[B]:CYS:SG	1:B:260:VAL:HG13	2.45	0.56
1:A:156:ILE:HG22	1:A:158:LEU:CD1	2.35	0.56
1:A:235[B]:CYS:SG	1:A:260:VAL:HG13	2.46	0.56
1:B:265:ASN:HB2	1:B:266:PRO:CD	2.35	0.56
1:B:385:ILE:HD12	1:B:385:ILE:N	2.20	0.56
1:A:42:PRO:O	1:A:57:ILE:HG22	2.05	0.56
1:A:235[B]:CYS:HB2	1:A:262:MET:HE2	1.88	0.56
1:A:282:MET:HE2	1:A:309:LEU:HD23	1.85	0.56
1:B:124:ILE:HG13	1:B:126:PRO:HD3	1.88	0.56
1:A:389:ALA:HA	1:A:416:TYR:O	2.07	0.55
1:A:241:HIS:CD2	1:A:243:PHE:H	2.24	0.55
1:A:237:LEU:HD12	1:A:244:MET:HE3	1.90	0.54
1:A:75:LEU:HD11	1:A:156:ILE:CD1	2.24	0.54
1:A:77:LYS:NZ	1:A:184:SER:O	2.41	0.53
1:B:195:GLN:HG3	5:B:726:HOH:O	2.08	0.53
1:B:436:ILE:HG13	1:B:437:LYS:H	1.73	0.52
1:B:82:LEU:HD12	1:B:106:LEU:HD22	1.89	0.52
1:B:268:PRO:HD3	1:B:292:MET:HE2	1.91	0.52
1:B:425:THR:HB	1:B:426:PRO:HD2	1.92	0.52
1:B:34:LEU:HD23	1:B:96:PHE:CZ	2.45	0.51
1:A:247:SER:O	1:A:346:TYR:OH	2.24	0.51
1:B:436:ILE:HG13	1:B:437:LYS:N	2.25	0.51
1:A:237:LEU:HD12	1:A:244:MET:CE	2.40	0.51
1:B:266:PRO:HA	1:B:271:CYS:SG	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ILE:HG23	1:A:280:VAL:HB	1.91	0.51
1:A:124:ILE:HG13	1:A:126:PRO:HD3	1.93	0.51
1:B:77:LYS:NZ	1:B:184:SER:OG	2.39	0.51
1:B:105:VAL:O	1:B:193:PHE:HB2	2.11	0.51
1:B:54:LEU:HD21	1:B:62:LEU:HD12	1.92	0.51
1:A:216:TYR:HE2	1:A:393:PRO:HG2	1.75	0.51
1:A:332:LYS:CD	1:A:333:LEU:H	2.09	0.50
1:B:234:LEU:HB2	1:B:280:VAL:HG11	1.94	0.50
1:B:265:ASN:HB2	1:B:266:PRO:HD2	1.93	0.50
1:B:213:ASP:OD2	1:B:214:TYR:N	2.45	0.50
1:B:268:PRO:HD3	1:B:292:MET:CE	2.42	0.49
1:B:220:ALA:HB1	1:B:364:ILE:HG23	1.95	0.49
1:B:410:PHE:O	3:B:602:EDO:H11	2.13	0.48
1:B:150:VAL:O	1:B:152:LEU:HG	2.12	0.48
1:A:69:ARG:NE	1:A:175:THR:O	2.41	0.48
1:B:419:GLY:O	1:B:436:ILE:HG22	2.14	0.48
1:A:32:ARG:HG2	1:A:32:ARG:NH1	2.29	0.48
1:B:433:VAL:HG22	1:B:433:VAL:O	2.14	0.48
1:B:265:ASN:OD1	1:B:267:GLU:HB2	2.13	0.48
1:A:362:ARG:HB2	1:A:363:PRO:CD	2.43	0.48
1:A:187:PRO:HB2	1:A:190:GLU:HG2	1.96	0.47
1:A:234:LEU:HD11	1:A:263:ALA:HB2	1.96	0.47
1:B:297:ALA:HB3	1:B:328:VAL:HG12	1.97	0.47
1:A:323:ARG:HH11	1:A:323:ARG:HG2	1.79	0.47
1:A:358:THR:O	1:A:431:ARG:HD3	2.14	0.47
1:A:90:GLU:O	1:A:94:VAL:HG23	2.14	0.47
1:B:207:ILE:HG23	1:B:396:PHE:CD2	2.49	0.47
1:A:213:ASP:OD1	1:A:214:TYR:N	2.48	0.47
1:A:271:CYS:O	1:A:275:ILE:HG13	2.15	0.46
1:A:374:ASP:HB3	1:A:380:VAL:HG12	1.98	0.46
1:B:302:ASP:HA	1:B:305:GLN:HG2	1.98	0.46
1:A:19:TYR:CE2	1:A:393:PRO:HA	2.50	0.46
1:B:115:TYR:OH	1:A:292:MET:HA	2.16	0.46
1:B:291:ILE:O	1:B:295:GLU:HG2	2.17	0.45
1:A:319:GLU:OE2	1:A:323:ARG:NH2	2.43	0.45
1:A:106:LEU:C	1:A:106:LEU:HD23	2.36	0.45
1:A:128:LEU:HD21	1:A:130:ILE:HD11	1.99	0.45
1:A:260:VAL:HG12	1:A:262:MET:CE	2.44	0.44
1:B:106:LEU:C	1:B:106:LEU:HD23	2.38	0.44
1:B:284:SER:OG	1:B:311:GLN:HB2	2.17	0.44
1:B:287:PRO:HG2	1:B:315:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:THR:OG1	1:A:100:LYS:NZ	2.45	0.44
1:A:244:MET:HE2	1:A:244:MET:HA	1.98	0.44
1:B:72:GLU:CD	1:B:177:ALA:HB1	2.38	0.44
1:A:82:LEU:CD1	1:A:106:LEU:HD22	2.47	0.44
1:B:75:LEU:HD21	1:B:127:LYS:HB3	2.00	0.43
1:B:282:MET:HE3	1:B:309:LEU:HD23	1.99	0.43
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.87	0.43
1:B:355:GLN:HE21	1:B:427:ASP:CB	2.31	0.43
1:B:369:GLU:O	1:B:390:THR:HA	2.18	0.43
1:A:114:GLN:CD	1:A:137:VAL:HG22	2.39	0.43
1:A:323:ARG:HG2	1:A:323:ARG:NH1	2.33	0.43
1:A:380:VAL:HG23	1:A:381:PRO:O	2.17	0.43
1:A:381:PRO:HB2	1:A:384:GLU:OE1	2.18	0.43
1:B:359:THR:HG22	1:B:431:ARG:NH1	2.33	0.43
1:B:215:ASP:O	1:B:219:ARG:HG3	2.19	0.43
1:B:216:TYR:HE2	1:B:393:PRO:HG2	1.84	0.43
1:A:129:LEU:HD22	1:A:157:ILE:HD13	2.00	0.42
1:B:107:ASN:HB3	1:B:240:PRO:HB3	2.00	0.42
1:B:290:VAL:O	1:B:294:LEU:HG	2.20	0.42
1:A:241:HIS:CD2	1:A:243:PHE:HB3	2.55	0.42
1:B:16:ALA:O	1:B:20:ARG:HG3	2.20	0.42
1:B:104:VAL:HG13	1:B:193:PHE:HA	2.01	0.42
1:A:265:ASN:HB2	1:A:266:PRO:HD2	2.02	0.42
1:A:342:GLY:HA3	1:A:395:THR:HA	2.01	0.42
1:A:180:PHE:CD2	1:A:180:PHE:C	2.94	0.41
1:A:235[A]:CYS:HB3	1:A:262:MET:HE2	2.00	0.41
1:B:346:TYR:C	1:B:361:GLY:HA3	2.41	0.41
1:A:141:ASN:HB3	1:A:145:ASP:OD1	2.21	0.41
1:A:369:GLU:OE2	1:A:391:ARG:NH1	2.54	0.41
1:B:41:HIS:HE1	5:B:781:HOH:O	2.03	0.41
1:B:342:GLY:HA3	1:B:395:THR:HA	2.02	0.41
1:B:150:VAL:O	1:B:151:ASN:OD1	2.39	0.40
1:A:319:GLU:CG	1:A:323:ARG:HE	2.33	0.40
1:A:27:ASP:HA	1:A:212:ASN:OD1	2.20	0.40
1:B:372:ILE:HA	1:B:387:MET:O	2.21	0.40
1:A:283:ALA:O	1:A:310:LEU:HD12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/562 (77%)	416 (96%)	19 (4%)	0	100	100
1	B	435/562 (77%)	424 (98%)	11 (2%)	0	100	100
All	All	870/1124 (77%)	840 (97%)	30 (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	349/487 (72%)	341 (98%)	8 (2%)	45	70
1	B	345/487 (71%)	340 (99%)	5 (1%)	62	82
All	All	694/974 (71%)	681 (98%)	13 (2%)	56	75

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	179	THR
1	B	200	SER
1	B	320	SER
1	B	337	PHE
1	B	396	PHE
1	A	235[A]	CYS
1	A	235[B]	CYS
1	A	259	CYS

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Mol	Chain	Res	Type
1	A	274	ILE
1	A	316	SER
1	A	354	GLU
1	A	396	PHE
1	A	414	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	18	HIS
1	B	241	HIS
1	B	311	GLN
1	A	241	HIS
1	A	406	ASN

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 14 ligands modelled in this entry, 9 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	$\#\|Z\|>2$
3	EDO	A	602	-	3,3,3	0.43	0	2,2,2	0.37	0
2	BHA	A	601	-	11,11,11	0.58	0	15,15,15	0.62	0
3	EDO	B	602	-	3,3,3	0.42	0	2,2,2	0.43	0
2	BHA	B	601	-	11,11,11	0.59	0	15,15,15	0.60	0
3	EDO	A	603	-	3,3,3	0.42	0	2,2,2	0.42	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
3	EDO	A	602	-	-	0/1/1/1	-
2	BHA	A	601	-	-	0/4/4/4	0/1/1/1
3	EDO	B	602	-	-	0/1/1/1	-
2	BHA	B	601	-	-	2/4/4/4	0/1/1/1
3	EDO	A	603	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	EDO	O1-C1-C2-O2
2	B	601	BHA	C2-C1-C1'-O1'
2	B	601	BHA	C2-C1-C1'-O2'

There are no ring outliers.

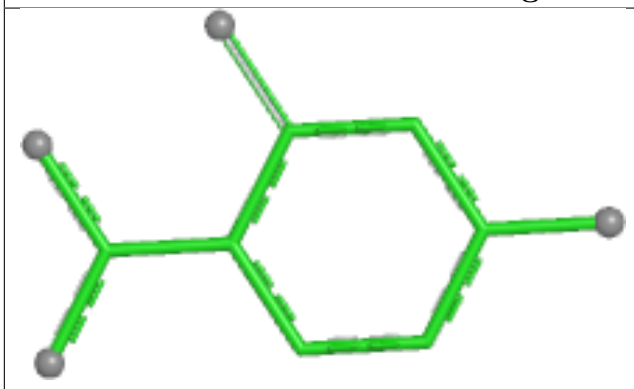
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	EDO	1	0
3	A	603	EDO	3	0

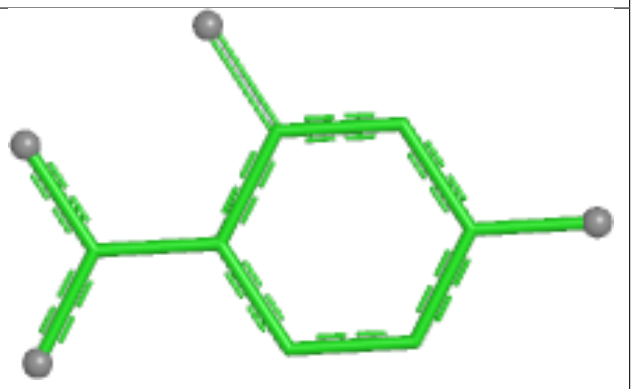
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

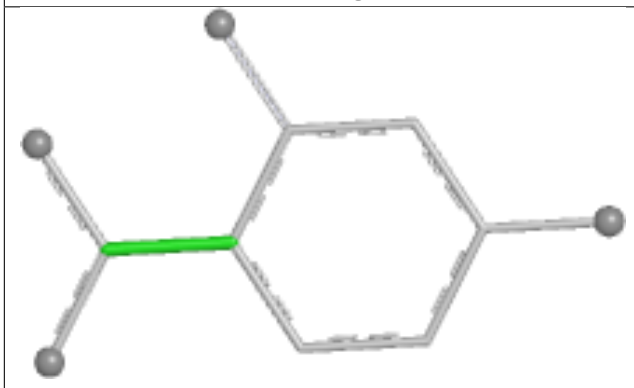
Ligand BHA A 601



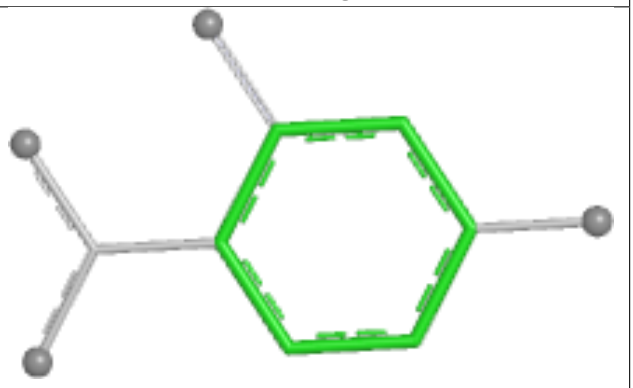
Bond lengths



Bond angles

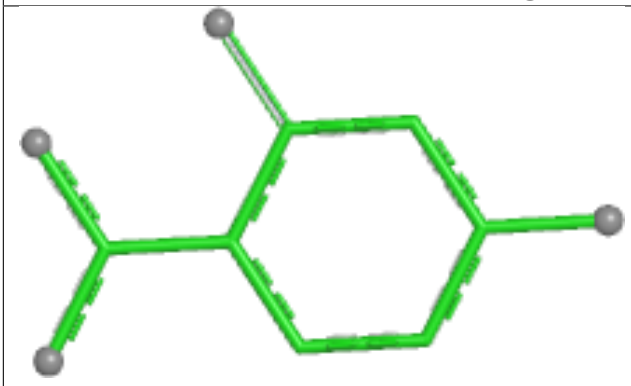


Torsions

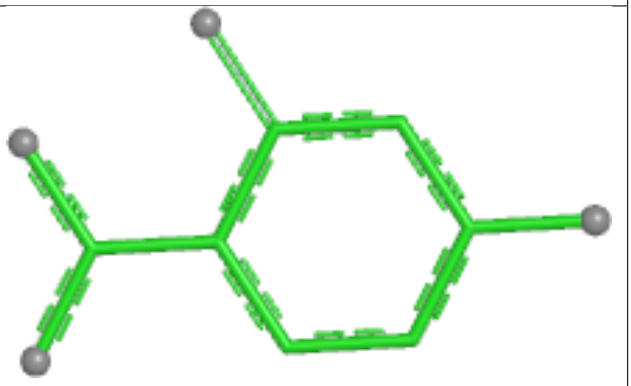


Rings

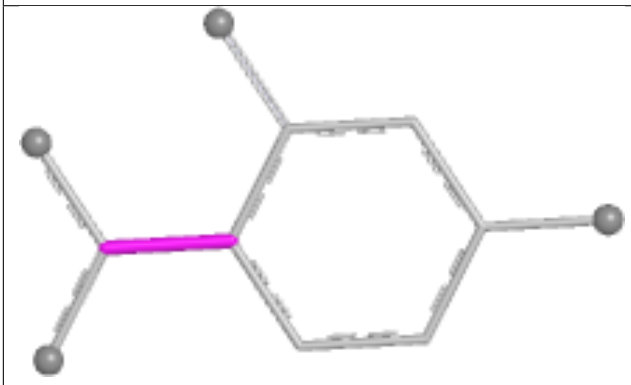
Ligand BHA B 601



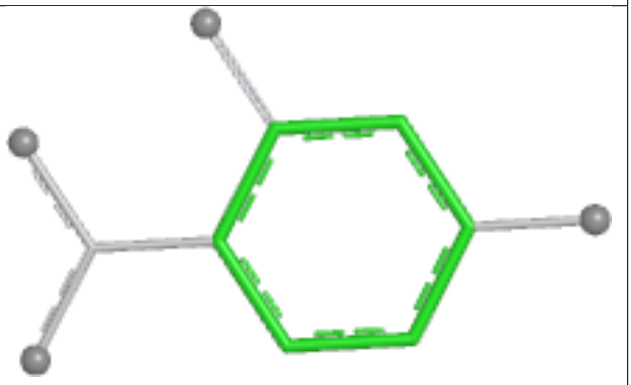
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	435/562 (77%)	0.45	17 (3%)	44	42	46, 72, 96, 117	2 (0%)
1	B	435/562 (77%)	0.42	19 (4%)	39	38	40, 64, 90, 99	2 (0%)
All	All	870/1124 (77%)	0.43	36 (4%)	42	40	40, 68, 94, 117	4 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	ASP	5.2
1	B	149	ASP	4.1
1	A	270	ASN	4.0
1	A	148[A]	HIS	3.8
1	B	375	GLU	3.6
1	A	271	CYS	3.6
1	A	178	GLU	3.3
1	B	314	GLY	3.0
1	A	426	PRO	2.9
1	B	3	LYS	2.9
1	A	51	GLU	2.9
1	A	437	LYS	2.8
1	A	382	GLU	2.7
1	B	427	ASP	2.5
1	B	295	GLU	2.5
1	B	188	ALA	2.5
1	A	179	THR	2.5
1	A	136	GLU	2.4
1	B	113	ARG	2.4
1	B	353	ASP	2.3
1	B	235[A]	CYS	2.3
1	B	144	ILE	2.3
1	B	156	ILE	2.3
1	A	156	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	201	THR	2.3
1	B	376	GLN	2.3
1	B	164	ALA	2.3
1	B	198	GLY	2.2
1	B	387	MET	2.2
1	A	4	GLN	2.2
1	A	164	ALA	2.2
1	B	4	GLN	2.1
1	A	259	CYS	2.1
1	B	437	LYS	2.1
1	A	3	LYS	2.1
1	A	387	MET	2.1

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
4	CA	B	605	1/1	0.47	0.28	102,102,102,102	0
3	EDO	A	602	4/4	0.56	0.15	94,113,123,123	0
3	EDO	B	602	4/4	0.72	0.15	74,90,99,101	0
4	CA	A	607	1/1	0.77	0.12	112,112,112,112	0
3	EDO	A	603	4/4	0.85	0.22	62,75,88,88	0
4	CA	B	606	1/1	0.88	0.22	82,82,82,82	0
2	BHA	A	601	11/11	0.89	0.16	58,66,88,88	17
4	CA	A	605	1/1	0.91	0.08	103,103,103,103	0
4	CA	B	607	1/1	0.92	0.09	90,90,90,90	0
2	BHA	B	601	11/11	0.92	0.14	57,61,78,78	17
4	CA	B	603	1/1	0.92	0.11	86,86,86,86	0

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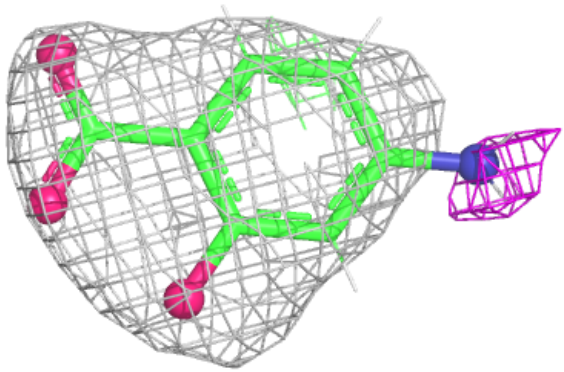
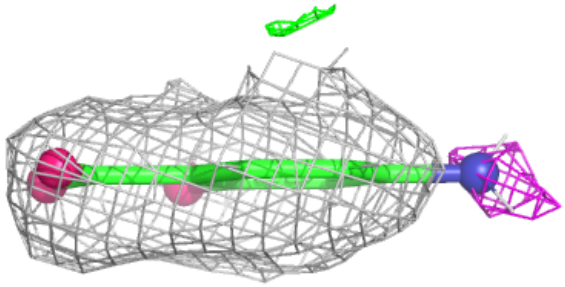
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	A	604	1/1	0.96	0.07	77,77,77,77	0
4	CA	A	606	1/1	0.97	0.05	74,74,74,74	0
4	CA	B	604	1/1	0.99	0.06	64,64,64,64	0

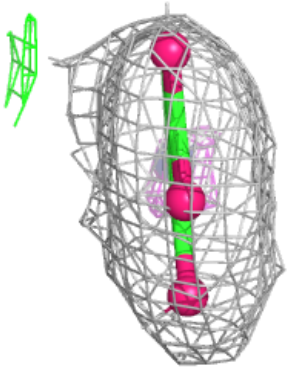
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BHA 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)

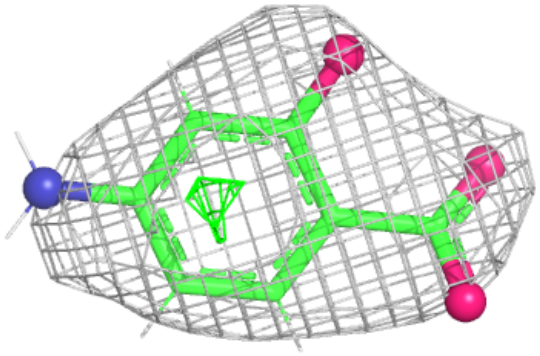


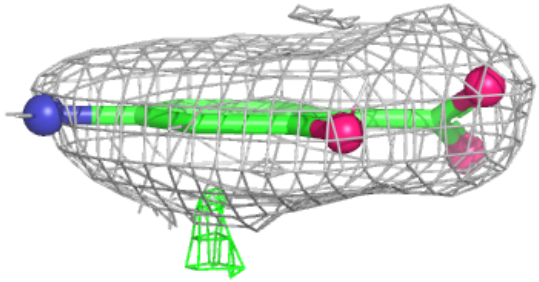


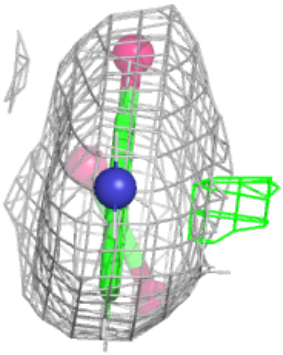


Electron density around BHA B 601:

$2mF_o$-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

There are no such residues in this entry.