



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2020 – 10:54 AM EST

PDB ID : 6OZ5
Title : Escherichia coli tRNA synthetase in complex with compound 3
Authors : Kahne, D.; Baidin, V.; Owens, T.W.
Deposited on : 2019-05-15
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

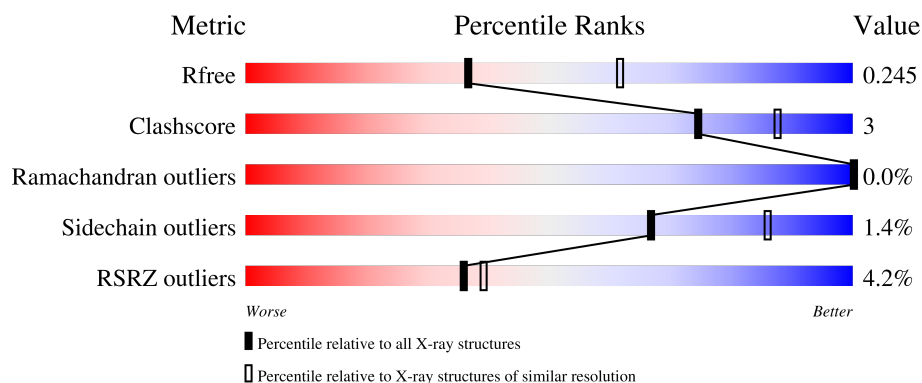
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	332	<div> <div>2%</div> <div>66%</div> <div>7%</div> <div>27%</div> </div>
1	C	332	<div> <div>12%</div> <div>86%</div> <div>11%</div> <div>.</div> </div>
2	B	795	<div> <div>4%</div> <div>91%</div> <div>9%</div> </div>
2	D	795	<div> <div>%</div> <div>90%</div> <div>10%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16932 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 Phenylalanine-tRNA ligase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1929	1228	338	354	9			
1	C	322	Total	C	N	O	S	0	0	0
			2454	1551	437	456	10			

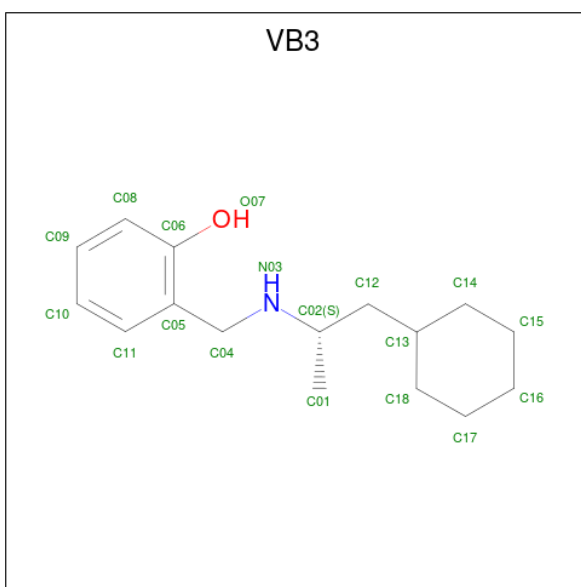
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP A0A387D3L6
A	-3	SER	-	expression tag	UNP A0A387D3L6
A	-2	HIS	-	expression tag	UNP A0A387D3L6
A	-1	MET	-	expression tag	UNP A0A387D3L6
A	0	ALA	-	expression tag	UNP A0A387D3L6
A	1	SER	-	expression tag	UNP A0A387D3L6
C	-4	GLY	-	expression tag	UNP A0A387D3L6
C	-3	SER	-	expression tag	UNP A0A387D3L6
C	-2	HIS	-	expression tag	UNP A0A387D3L6
C	-1	MET	-	expression tag	UNP A0A387D3L6
C	0	ALA	-	expression tag	UNP A0A387D3L6
C	1	SER	-	expression tag	UNP A0A387D3L6

- Molecule 2 is a protein called Phenylalanine-tRNA ligase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	793	Total	C	N	O	S	0	0	0
			6065	3813	1068	1157	27			
2	D	794	Total	C	N	O	S	0	0	0
			6096	3834	1077	1158	27			

- Molecule 3 is 2-([(2S)-1-cyclohexylpropan-2-yl]amino)methylphenol (three-letter code: VB3) (formula: C₁₆H₂₅NO) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	16	1	1		
3	C	1	Total	C	N	O	0	0
			18	16	1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

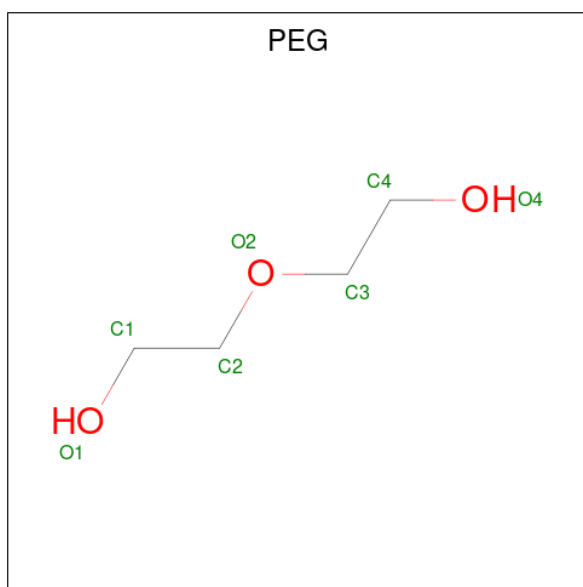
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



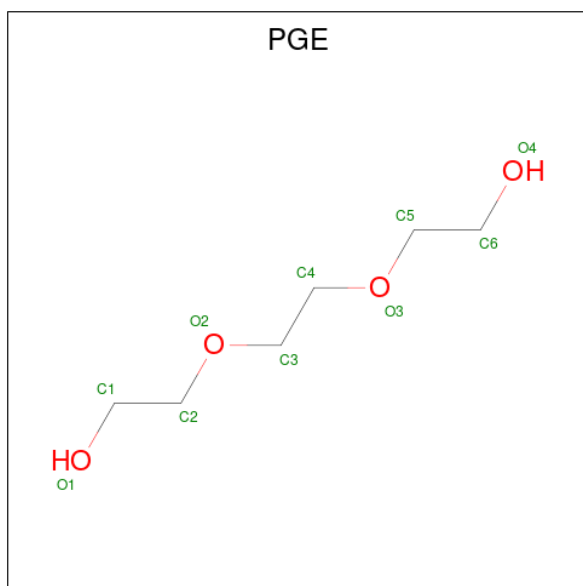
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			10	6	4		

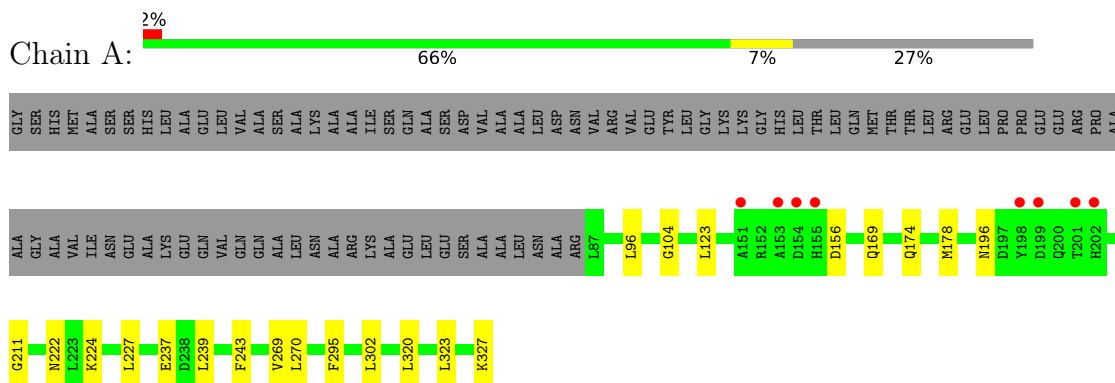
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	33	Total 33	O 33	0	0
8	B	83	Total 83	O 83	0	0
8	C	36	Total 36	O 36	0	0
8	D	149	Total 149	O 149	0	0

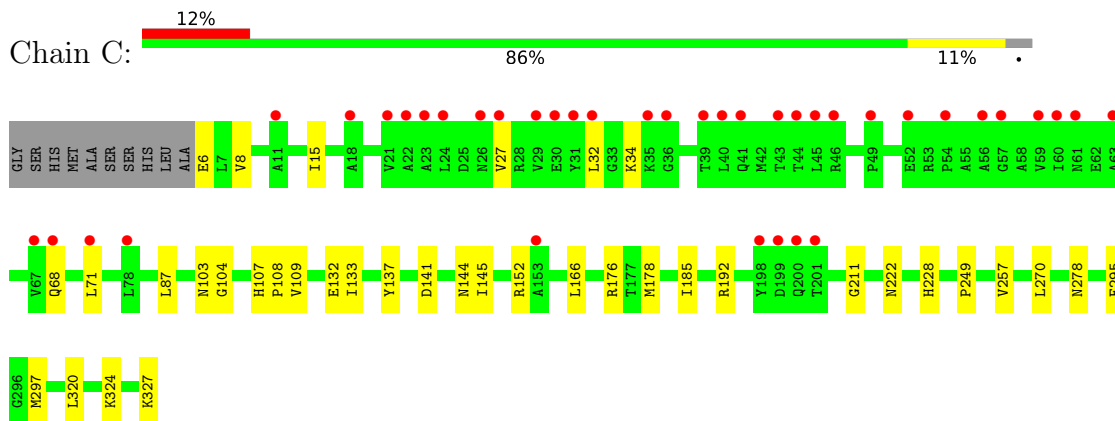
3 Residue-property plots [i](#)

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.

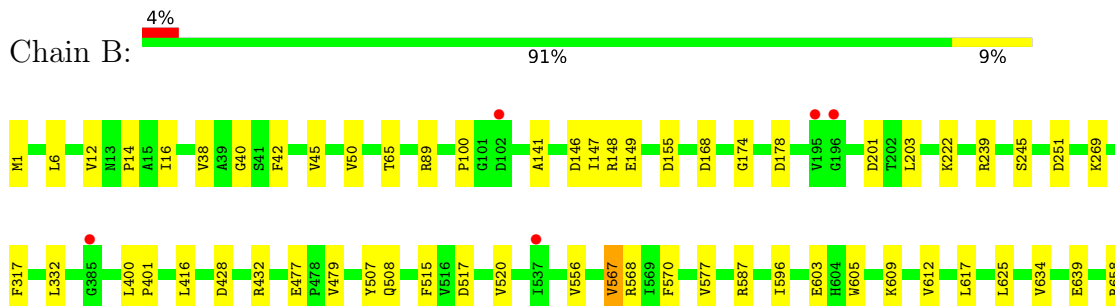
• Molecule 1: Phenylalanine-tRNA ligase alpha subunit

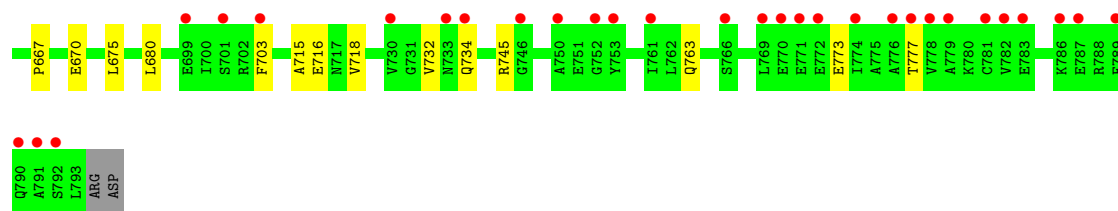


• Molecule 1: Phenylalanine-tRNA ligase alpha subunit

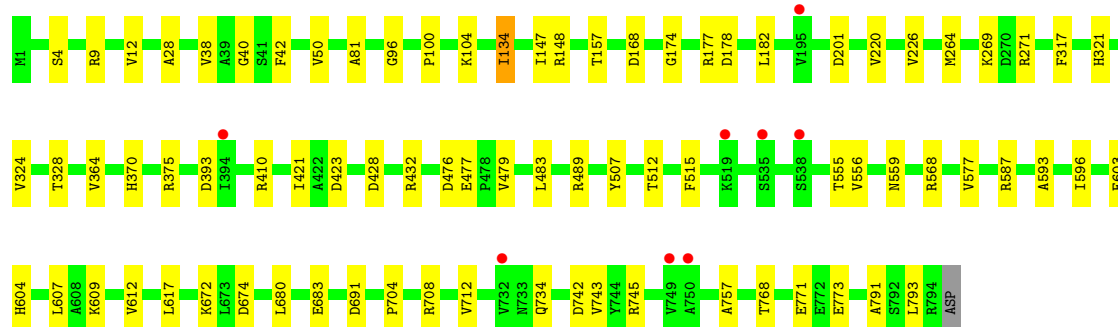
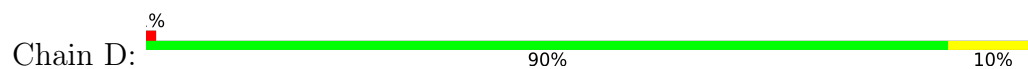


• Molecule 2: Phenylalanine-tRNA ligase beta subunit





● Molecule 2: Phenylalanine-tRNA ligase beta subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.77Å 174.51Å 252.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.23 – 2.50 58.23 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (58.23-2.50) 100.0 (58.23-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.206 , 0.245 0.207 , 0.245	Depositor DCC
R_{free} test set	2000 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16932	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.58% 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: VB3, MG, PGE, PEG, EDO

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	0/1981	0.43	0/2687
1	C	0.25	0/2511	0.42	0/3413
2	B	0.24	0/6167	0.43	0/8381
2	D	0.25	0/6198	0.45	0/8418
All	All	0.25	0/16857	0.44	0/22899

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1929	0	1833	14	0
1	C	2454	0	2296	24	0
2	B	6065	0	6061	40	0
2	D	6096	0	6125	42	0
3	A	18	0	0	0	0
3	C	18	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	B	12	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	20	0	30	1	0
6	B	7	0	10	0	0
7	D	10	0	14	0	0
8	A	33	0	0	0	0
8	B	83	0	0	0	0
8	C	36	0	0	1	0
8	D	149	0	0	2	0
All	All	16932	0	16387	107	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 3.

All (107) 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)
2:D:28:ALA:HB2	2:D:182:LEU:HD11	1.67	0.75
2:D:226:VAL:HG11	2:D:328:THR:HG23	1.76	0.68
2:B:716:GLU:OE2	2:B:745:ARG:NH1	2.28	0.67
2:B:568:ARG:HB3	2:B:596:ILE:HG22	1.76	0.67
2:B:639:GLU:OE2	2:B:658:ARG:NH2	2.28	0.67
2:D:489:ARG:NH2	2:D:691:ASP:OD2	2.29	0.66
2:B:40:GLY:O	2:B:148:ARG:NH2	2.30	0.64
2:D:96:GLY:HA2	2:D:104:LYS:HE2	1.82	0.62
2:B:45:VAL:HB	2:B:147:ILE:HD11	1.83	0.61
1:C:137:TYR:HA	1:C:141:ASP:HB2	1.81	0.60
1:C:178:MET:HG2	1:C:185:ILE:HD13	1.82	0.60
1:C:176:ARG:NH1	8:C:502:HOH:O	2.34	0.59
2:B:203:LEU:HD21	2:B:332:LEU:HD22	1.85	0.59
1:C:257:VAL:HB	1:C:270:LEU:HB2	1.86	0.57
1:A:227:LEU:HD13	1:A:270:LEU:HD11	1.85	0.57
2:B:42:PHE:HB3	2:B:100:PRO:HD3	1.87	0.56
1:C:103:ASN:O	1:C:327:LYS:NZ	2.30	0.56
2:D:38:VAL:HG12	2:D:157:THR:HG23	1.88	0.56
1:A:222:ASN:HB3	2:B:479:VAL:HG22	1.88	0.56
2:B:596:ILE:HD11	2:B:617:LEU:HB2	1.88	0.55
1:A:327:LYS:OXT	5:D:805:EDO:O1	2.23	0.55
2:B:38:VAL:HG13	2:B:239:ARG:HH22	1.72	0.55
2:D:577:VAL:HG23	2:D:587:ARG:HB3	1.90	0.53
1:C:228:HIS:ND1	2:D:476:ASP:OD2	2.35	0.53
2:D:734:GLN:NE2	2:D:773:GLU:OE2	2.42	0.53
2:D:168:ASP:O	2:D:174:GLY:HA3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:VAL:HG13	2:B:65:THR:HG23	1.91	0.53
1:C:222:ASN:HB3	2:D:479:VAL:HG22	1.92	0.52
2:D:596:ILE:HD12	2:D:612:VAL:HG21	1.91	0.51
2:B:703:PHE:O	2:B:763:GLN:NE2	2.41	0.51
1:C:192:ARG:NH2	2:D:512:THR:O	2.43	0.51
2:D:40:GLY:O	2:D:148:ARG:NH2	2.44	0.51
2:D:708:ARG:NH2	2:D:771:GLU:OE2	2.43	0.51
2:D:410:ARG:NH2	2:D:421:ILE:O	2.35	0.51
1:A:123:LEU:HG	2:D:483:LEU:HB3	1.91	0.51
2:D:596:ILE:HD11	2:D:617:LEU:HB2	1.92	0.50
2:B:168:ASP:O	2:B:174:GLY:HA3	2.11	0.50
2:B:612:VAL:HG12	2:B:680:LEU:HD13	1.94	0.50
2:B:715:ALA:HB3	2:B:718:VAL:HG23	1.94	0.49
1:C:211:GLY:HA3	1:C:295:PHE:CZ	2.47	0.49
2:B:12:VAL:HG22	2:B:14:PRO:HD3	1.95	0.49
1:C:270:LEU:HD23	1:C:297:MET:HB3	1.94	0.49
2:D:712:VAL:HG13	2:D:791:ALA:HB1	1.94	0.48
1:C:144:ASN:HD21	1:C:278:ASN:HB2	1.78	0.48
2:B:6:LEU:HD22	2:B:155:ASP:HB2	1.96	0.47
1:C:320:LEU:O	1:C:324:LYS:HG2	2.14	0.47
2:B:625:LEU:HD13	2:B:634:VAL:HG11	1.97	0.47
1:A:269:VAL:HG13	1:A:302:LEU:HD21	1.97	0.47
2:D:42:PHE:HB3	2:D:100:PRO:HD3	1.97	0.47
2:D:201:ASP:HB2	2:D:220:VAL:HG11	1.97	0.47
1:A:211:GLY:HA3	1:A:295:PHE:CZ	2.50	0.46
2:B:577:VAL:HG23	2:B:587:ARG:HB3	1.97	0.46
2:D:324:VAL:HG13	2:D:328:THR:HG21	1.98	0.46
2:B:146:ASP:HB3	2:B:149:GLU:HG2	1.96	0.46
2:D:410:ARG:NH1	2:D:423:ASP:OD1	2.47	0.46
2:D:428:ASP:O	2:D:432:ARG:HG3	2.16	0.46
2:B:245:SER:OG	2:B:251:ASP:OD2	2.25	0.46
2:D:271:ARG:HD2	2:D:321:HIS:O	2.16	0.46
2:D:604:HIS:HB3	2:D:607:LEU:HB2	1.98	0.46
1:A:174:GLN:O	1:A:178:MET:HG3	2.16	0.45
1:A:224:LYS:HA	1:A:243:PHE:CZ	2.52	0.45
2:B:734:GLN:NE2	2:B:773:GLU:OE2	2.49	0.45
2:B:89:ARG:NH2	2:B:141:ALA:O	2.50	0.45
2:D:603:GLU:HG2	2:D:609:LYS:HE2	1.98	0.44
2:D:672:LYS:C	2:D:674:ASP:H	2.21	0.44
1:A:237:GLU:HG3	1:A:239:LEU:HB3	1.99	0.44
2:B:428:ASP:O	2:B:432:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:HIS:CG	1:C:108:PRO:HD2	2.52	0.44
2:D:220:VAL:HG23	2:D:269:LYS:HD2	2.00	0.44
1:C:222:ASN:HA	2:D:477:GLU:O	2.17	0.44
1:C:15:ILE:HA	1:C:34:LYS:HE3	1.99	0.43
2:B:517:ASP:HB3	2:B:520:VAL:HG13	1.99	0.43
1:A:323:LEU:HB3	2:B:508:GLN:NE2	2.34	0.43
2:D:9:ARG:HA	2:D:12:VAL:O	2.18	0.43
2:B:416:LEU:HA	2:B:416:LEU:HD23	1.85	0.43
2:D:593:ALA:HB2	2:D:683:GLU:HG3	2.01	0.43
1:C:133:ILE:HG12	1:C:166:LEU:HD23	2.01	0.43
1:C:132:GLU:OE2	1:C:192:ARG:HD3	2.19	0.43
2:B:605:TRP:HB2	2:D:743:VAL:HG12	2.00	0.43
1:C:141:ASP:OD1	1:C:152:ARG:NH2	2.52	0.42
1:C:144:ASN:ND2	1:C:278:ASN:HB2	2.34	0.42
2:B:667:PRO:HG3	1:C:87:LEU:HD21	2.01	0.42
2:B:400:LEU:HD12	2:B:401:PRO:HD2	2.01	0.42
1:C:6:GLU:O	1:C:8:VAL:N	2.44	0.42
2:D:147:ILE:HG13	2:D:147:ILE:H	1.56	0.42
1:A:222:ASN:HA	2:B:477:GLU:O	2.19	0.42
2:D:617:LEU:HD22	2:D:680:LEU:HB3	2.01	0.42
2:D:742:ASP:HB2	2:D:757:ALA:HB3	2.01	0.42
2:B:222:LYS:HE2	2:B:269:LYS:NZ	2.34	0.42
2:D:370:HIS:NE2	2:D:393:ASP:OD1	2.52	0.42
2:B:16:ILE:HD12	2:B:16:ILE:HA	1.88	0.41
2:D:81:ALA:HB2	2:D:134:ILE:HD13	2.02	0.41
1:C:104:GLY:HA3	2:D:507:TYR:O	2.21	0.41
2:B:603:GLU:HG2	2:B:609:LYS:HE3	2.02	0.41
2:D:555:THR:O	2:D:559:ASN:ND2	2.47	0.41
1:A:156:ASP:HB3	1:A:196:ASN:H	1.85	0.41
2:B:147:ILE:HG13	2:B:147:ILE:H	1.60	0.41
2:D:704:PRO:HD2	2:D:768:THR:HG22	2.03	0.41
2:B:507:TYR:HB3	2:B:570:PHE:HD2	1.86	0.41
2:B:42:PHE:H	2:B:148:ARG:HH21	1.69	0.40
1:C:27:VAL:HG13	1:C:71:LEU:HD22	2.02	0.40
2:D:568:ARG:NH2	8:D:912:HOH:O	2.54	0.40
1:A:320:LEU:HD11	2:B:567:VAL:HB	2.03	0.40
2:B:670:GLU:HG3	2:B:675:LEU:HB2	2.02	0.40
2:D:177:ARG:NH1	8:D:913:HOH:O	2.54	0.40
1:A:104:GLY:HA3	2:B:507:TYR:O	2.22	0.40
1:C:145:ILE:HG12	1:C:249:PRO:HG2	2.04	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	239/332 (72%)	227 (95%)	12 (5%)	0	100	100
1	C	320/332 (96%)	299 (93%)	21 (7%)	0	100	100
2	B	791/795 (100%)	770 (97%)	20 (2%)	1 (0%)	51	73
2	D	792/795 (100%)	774 (98%)	18 (2%)	0	100	100
All	All	2142/2254 (95%)	2070 (97%)	71 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	732	VAL

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	204/279 (73%)	202 (99%)	2 (1%)	76	90
1	C	241/279 (86%)	238 (99%)	3 (1%)	71	88
2	B	647/663 (98%)	639 (99%)	8 (1%)	71	88
2	D	653/663 (98%)	641 (98%)	12 (2%)	59	81
All	All	1745/1884 (93%)	1720 (99%)	25 (1%)	67	86

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LEU
1	A	169	GLN
2	B	1	MET
2	B	178	ASP
2	B	201	ASP
2	B	317	PHE
2	B	515	PHE
2	B	556	VAL
2	B	567	VAL
2	B	777	THR
1	C	32	LEU
1	C	68	GLN
1	C	109	VAL
2	D	4	SER
2	D	50	VAL
2	D	134	ILE
2	D	178	ASP
2	D	264	MET
2	D	317	PHE
2	D	364	VAL
2	D	375	ARG
2	D	515	PHE
2	D	556	VAL
2	D	745	ARG
2	D	793	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	HIS
2	B	480	GLN
2	B	739	ASN
1	C	84	ASN

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	VB3	A	401	-	19,19,19	2.21	7 (36%)	22,24,24	2.30	6 (27%)
5	EDO	D	804	-	3,3,3	0.47	0	2,2,2	0.26	0
3	VB3	C	401	-	19,19,19	2.37	7 (36%)	22,24,24	2.17	7 (31%)
7	PGE	D	806	-	9,9,9	0.33	0	8,8,8	0.24	0
5	EDO	D	803	-	3,3,3	0.48	0	2,2,2	0.24	0
6	PEG	B	803	-	6,6,6	0.71	0	5,5,5	0.51	0
5	EDO	D	802	-	3,3,3	0.43	0	2,2,2	0.47	0
5	EDO	B	802	-	3,3,3	0.44	0	2,2,2	0.45	0
5	EDO	D	805	-	3,3,3	0.47	0	2,2,2	0.40	0
5	EDO	B	801	-	3,3,3	0.48	0	2,2,2	0.27	0
5	EDO	D	801	-	3,3,3	0.43	0	2,2,2	0.54	0
5	EDO	B	804	-	3,3,3	0.49	0	2,2,2	0.13	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	VB3	A	401	-	-	2/9/17/17	0/2/2/2
5	EDO	D	804	-	-	0/1/1/1	-
3	VB3	C	401	-	-	3/9/17/17	0/2/2/2
7	PGE	D	806	-	-	5/7/7/7	-
5	EDO	D	803	-	-	0/1/1/1	-
6	PEG	B	803	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	802	-	-	0/1/1/1	-
5	EDO	B	802	-	-	0/1/1/1	-
5	EDO	D	805	-	-	0/1/1/1	-
5	EDO	B	801	-	-	0/1/1/1	-
5	EDO	D	801	-	-	0/1/1/1	-
5	EDO	B	804	-	-	0/1/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	VB3	O07-C06	4.89	1.46	1.36
3	A	401	VB3	O07-C06	4.88	1.46	1.36
3	C	401	VB3	C02-N03	4.48	1.54	1.48
3	A	401	VB3	C12-C02	4.02	1.59	1.53
3	C	401	VB3	C12-C02	3.84	1.59	1.53
3	C	401	VB3	C12-C13	3.41	1.58	1.53
3	A	401	VB3	C12-C13	3.39	1.58	1.53
3	A	401	VB3	C02-N03	3.10	1.52	1.48
3	C	401	VB3	C18-C13	2.56	1.59	1.52
3	A	401	VB3	C14-C13	2.31	1.59	1.52
3	A	401	VB3	C10-C11	2.30	1.43	1.38
3	C	401	VB3	C10-C11	2.28	1.43	1.38
3	C	401	VB3	C14-C13	2.25	1.58	1.52
3	A	401	VB3	C18-C13	2.04	1.58	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	VB3	C08-C06-C05	6.06	127.74	120.41
3	A	401	VB3	C08-C06-C05	6.04	127.72	120.41
3	A	401	VB3	C04-C05-C06	4.94	126.55	120.00
3	C	401	VB3	C04-C05-C06	4.50	125.97	120.00
3	A	401	VB3	C15-C14-C13	3.76	119.27	112.15
3	A	401	VB3	C11-C05-C06	-3.16	114.79	118.16
3	C	401	VB3	C11-C05-C06	-2.99	114.97	118.16
3	C	401	VB3	C17-C18-C13	2.91	117.65	112.15
3	C	401	VB3	C09-C08-C06	-2.74	116.59	120.05
3	A	401	VB3	C09-C08-C06	-2.59	116.77	120.05
3	C	401	VB3	C15-C14-C13	2.59	117.05	112.15
3	C	401	VB3	C18-C13-C14	2.51	115.46	109.33
3	A	401	VB3	C18-C13-C14	2.47	115.38	109.33

There are no chirality outliers.

All (12) torsion outliers are listed below:

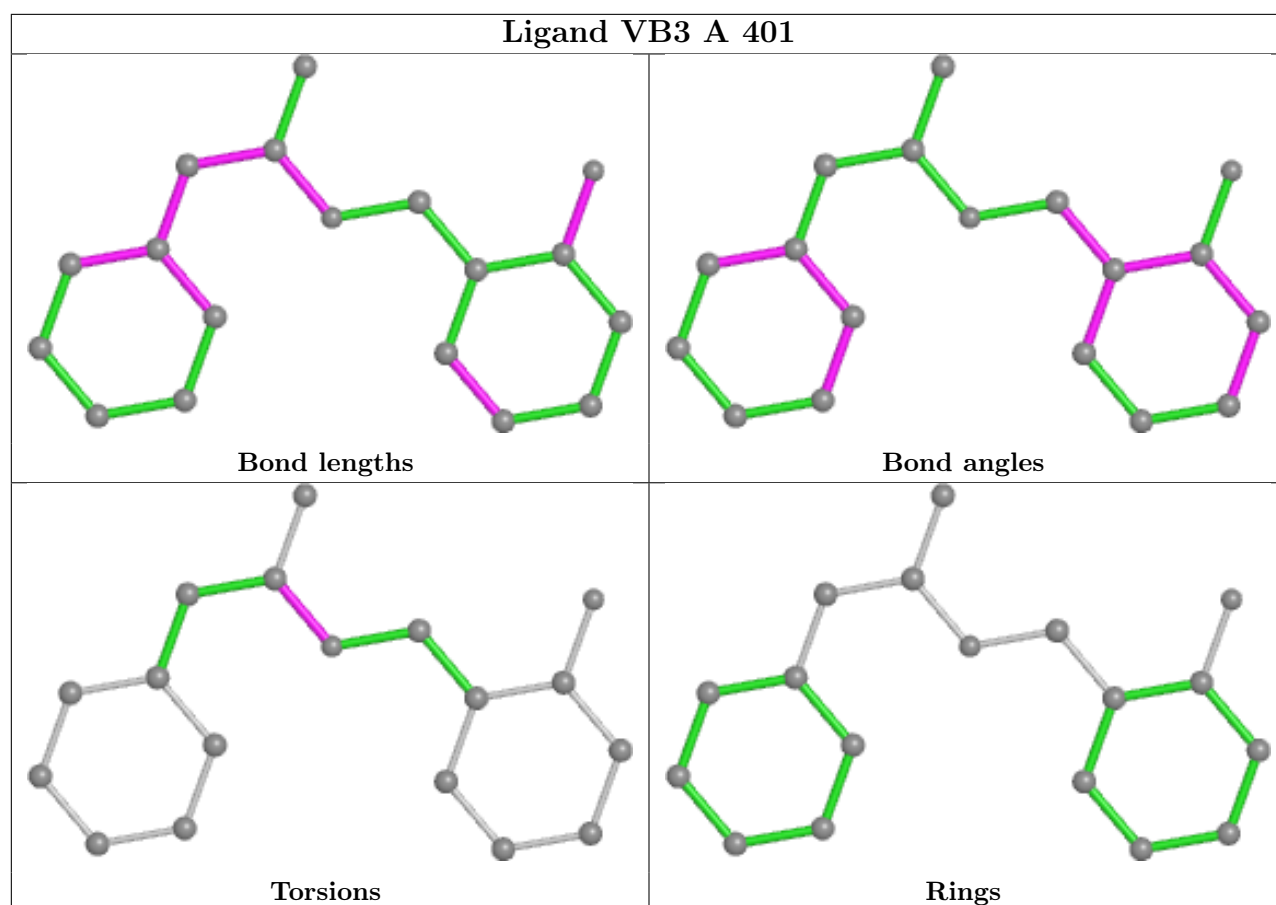
Mol	Chain	Res	Type	Atoms
3	A	401	VB3	C01-C02-N03-C04
3	A	401	VB3	C12-C02-N03-C04
3	C	401	VB3	N03-C02-C12-C13
7	D	806	PGE	O3-C5-C6-O4
7	D	806	PGE	O1-C1-C2-O2
6	B	803	PEG	O1-C1-C2-O2
3	C	401	VB3	N03-C04-C05-C06
3	C	401	VB3	N03-C04-C05-C11
7	D	806	PGE	O2-C3-C4-O3
7	D	806	PGE	C6-C5-O3-C4
6	B	803	PEG	C4-C3-O2-C2
7	D	806	PGE	C3-C4-O3-C5

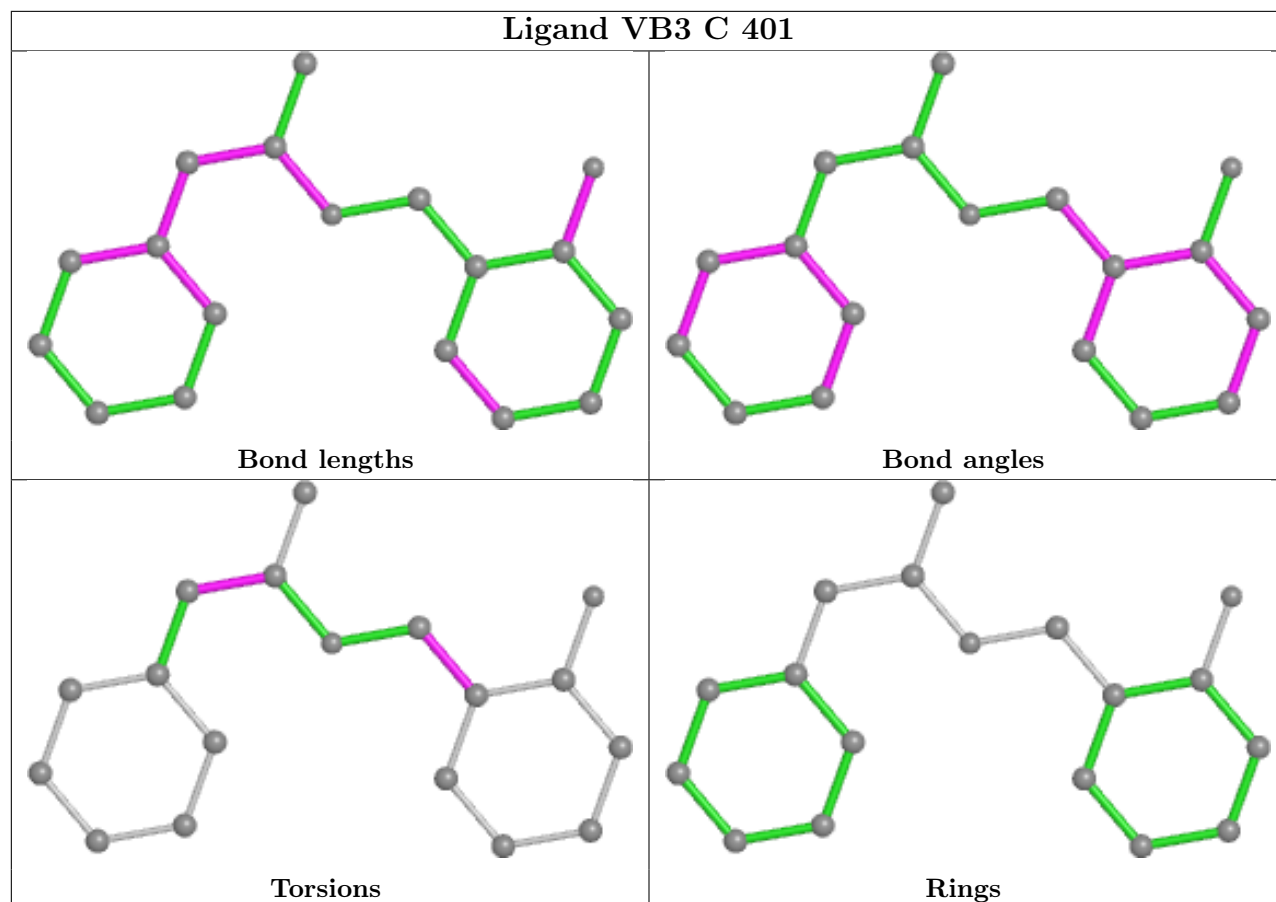
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	805	EDO	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	A	241/332 (72%)	0.10	8 (3%) 46 50	39, 51, 87, 114	0
1	C	322/332 (96%)	0.50	39 (12%) 4 4	40, 57, 118, 134	0
2	B	793/795 (99%)	0.22	35 (4%) 34 37	39, 58, 97, 125	0
2	D	794/795 (99%)	0.08	8 (1%) 82 84	35, 54, 76, 92	0
All	All	2150/2254 (95%)	0.20	90 (4%) 36 39	35, 55, 98, 134	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	791	ALA	6.3
1	C	198	TYR	5.3
1	A	153	ALA	5.0
2	B	787	GLU	5.0
1	C	39	THR	4.9
1	C	36	GLY	4.8
2	D	535	SER	4.7
2	B	792	SER	4.5
1	C	41	GLN	4.3
1	C	46	ARG	4.3
1	C	43	THR	4.2
1	C	27	VAL	4.2
2	B	746	GLY	4.1
1	C	29	VAL	4.1
1	C	40	LEU	4.0
2	B	703	PHE	3.9
2	B	769	LEU	3.8
2	B	778	VAL	3.8
2	B	783	GLU	3.8
1	C	31	TYR	3.7
1	C	32	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	68	GLN	3.6
1	C	199	ASP	3.5
1	C	57	GLY	3.5
1	A	151	ALA	3.5
1	C	200	GLN	3.4
2	B	776	ALA	3.3
2	D	732	VAL	3.3
1	C	52	GLU	3.2
2	B	779	ALA	3.2
1	C	26	ASN	3.2
1	C	201	THR	3.1
1	C	67	VAL	3.1
1	A	154	ASP	3.1
1	A	199	ASP	3.1
1	C	18	ALA	3.1
2	B	774	ILE	3.0
1	A	155	HIS	3.0
1	A	201	THR	2.9
1	A	198	TYR	2.9
2	B	777	THR	2.9
1	C	21	VAL	2.9
2	B	734	GLN	2.9
1	C	54	PRO	2.8
1	C	59	VAL	2.8
1	C	23	ALA	2.7
2	B	766	SER	2.7
2	B	782	VAL	2.7
2	B	385	GLY	2.6
2	D	749	VAL	2.6
1	C	44	THR	2.6
1	C	78	LEU	2.6
2	B	771	GLU	2.6
2	B	750	ALA	2.6
1	C	35	LYS	2.5
2	B	770	GLU	2.5
1	C	22	ALA	2.5
1	C	24	LEU	2.4
2	B	730	VAL	2.4
2	B	753	TYR	2.4
2	D	538	SER	2.4
2	B	752	GLY	2.4
1	C	60	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	11	ALA	2.4
2	B	196	GLY	2.4
1	C	30	GLU	2.3
1	A	202	HIS	2.3
2	D	195	VAL	2.3
2	B	537	ILE	2.3
1	C	56	ALA	2.2
2	B	733	ASN	2.2
2	B	772	GLU	2.2
2	B	195	VAL	2.1
2	B	781	CYS	2.1
2	D	750	ALA	2.1
2	D	394	ILE	2.1
1	C	153	ALA	2.1
1	C	61	ASN	2.1
2	B	786	LYS	2.1
2	B	789	PHE	2.1
2	B	790	GLN	2.1
1	C	49	PRO	2.1
2	B	761	ILE	2.1
2	B	701	SER	2.0
1	C	45	LEU	2.0
2	B	102	ASP	2.0
1	C	63	ALA	2.0
2	D	519	LYS	2.0
2	B	699	GLU	2.0
1	C	71	LEU	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,

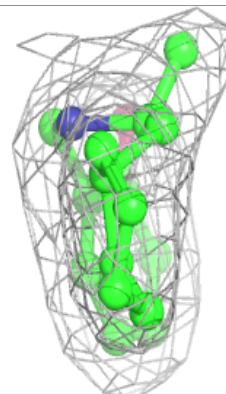
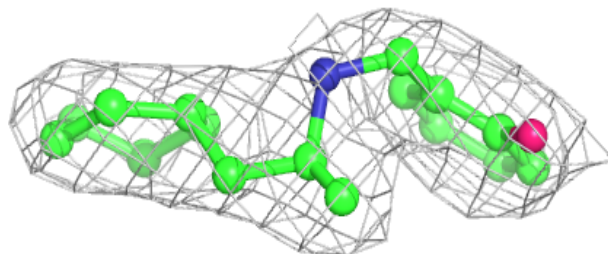
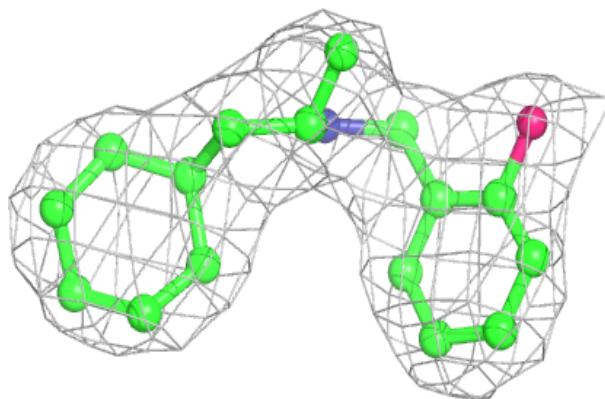
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	PGE	D	806	10/10	0.71	0.23	48,67,71,81	0
5	EDO	D	805	4/4	0.79	0.40	57,61,73,81	0
6	PEG	B	803	7/7	0.84	0.20	57,57,69,75	0
5	EDO	B	804	4/4	0.90	0.21	52,57,57,61	0
5	EDO	D	802	4/4	0.93	0.24	46,48,54,82	0
4	MG	C	402	1/1	0.94	0.10	44,44,44,44	0
5	EDO	D	801	4/4	0.94	0.20	48,57,57,69	0
5	EDO	D	803	4/4	0.94	0.17	42,49,49,52	0
3	VB3	C	401	18/18	0.95	0.19	38,46,55,57	0
5	EDO	D	804	4/4	0.95	0.21	44,50,56,58	0
5	EDO	B	801	4/4	0.95	0.34	64,67,71,73	0
3	VB3	A	401	18/18	0.96	0.24	40,47,58,65	0
4	MG	A	402	1/1	0.96	0.10	45,45,45,45	0
5	EDO	B	802	4/4	0.96	0.25	48,61,65,77	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.

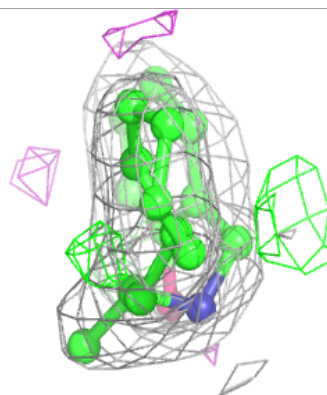
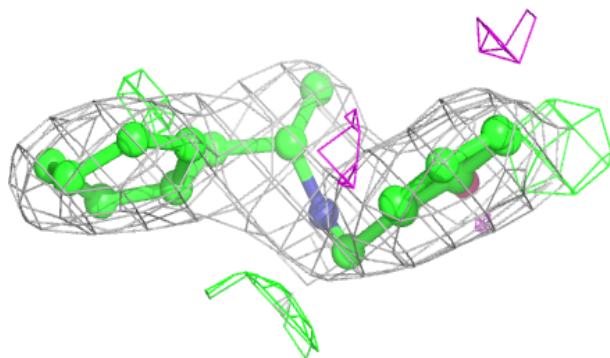
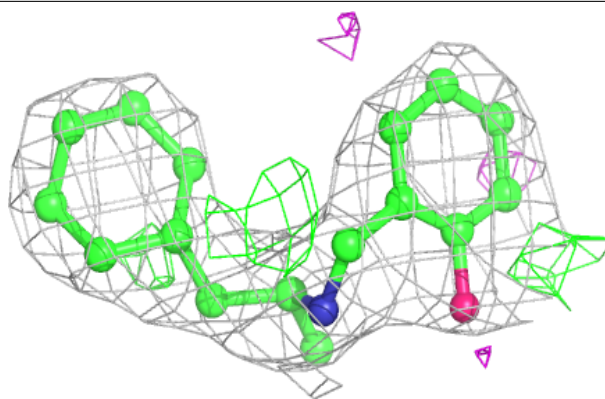
Electron density around VB3 C 401:

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 VB3 A 401:

$2mF_o-DF_c$ (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.