



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2025 – 08:50 AM EDT

PDB ID : 9DSX / pdb_00009dsx
Title : Crystal structure of the complex of M. tuberculosis PheRS with cognate precursor tRNA and fragment DDD00107555
Authors : Chang, C.; Michalska, K.; Forte, B.; Baragana, B.; Gilbert, I.H.; Wower, J.; Joachimiak, A.
Deposited on : 2024-09-30
Resolution : 2.05 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 Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

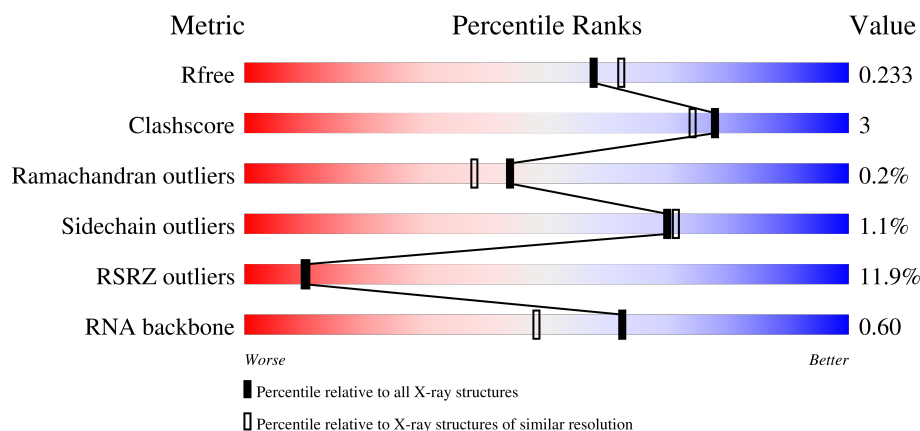
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)
RNA backbone	3690	1036 (2.40-1.68)

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	342	<div> <div>21%</div> <div>87%</div> <div>8%</div> <div>.</div> </div>
1	D	342	<div> <div>13%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
2	B	835	<div> <div>2%</div> <div>95%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	835	<div><div></div><div>14%</div><div>88%</div><div>8%</div><div></div><div></div></div>
3	C	77	<div><div></div><div>16%</div><div>86%</div><div>9%</div><div>5%</div><div></div></div>
3	F	77	<div><div></div><div>42%</div><div>70%</div><div>17%</div><div>8%</div><div>5%</div><div></div></div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 22325 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	328	Total	C	N	O	S	0	4	0
			2545	1606	458	472	9			
1	D	339	Total	C	N	O	S	0	8	0
			2680	1691	483	497	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP P9WUFU3
D	0	ALA	-	expression tag	UNP P9WUFU3

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	834	Total	C	N	O	S	0	11	0
			6321	3971	1146	1182	22			
2	E	804	Total	C	N	O	S	0	10	0
			6088	3824	1109	1135	20			

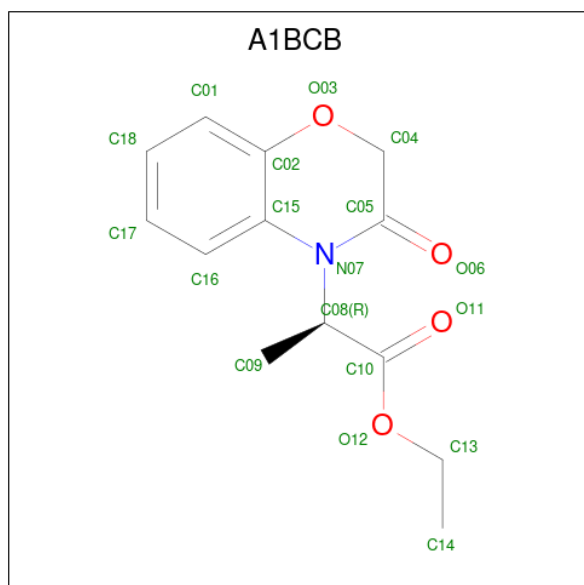
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLN	-	expression tag	UNP P9WUFU1
B	-2	SER	-	expression tag	UNP P9WUFU1
B	-1	ASN	-	expression tag	UNP P9WUFU1
B	0	ALA	-	expression tag	UNP P9WUFU1
E	-3	GLN	-	expression tag	UNP P9WUFU1
E	-2	SER	-	expression tag	UNP P9WUFU1
E	-1	ASN	-	expression tag	UNP P9WUFU1
E	0	ALA	-	expression tag	UNP P9WUFU1

- Molecule 3 is a RNA chain called tRNA(Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	73	Total	C	N	O	P	0	0	0
			1563	695	283	512	73			
3	F	73	Total	C	N	O	P	0	0	0
			1563	695	283	512	73			

- Molecule 4 is ethyl (2R)-2-(3-oxo-2,3-dihydro-4H-1,4-benzoxazin-4-yl)propanoate (CCD ID: A1BCB) (formula: C₁₃H₁₅NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			18	13	1	4		
4	D	1	Total	C	N	O	0	0
			18	13	1	4		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	3	Total	Mg	0	0
			3	3		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

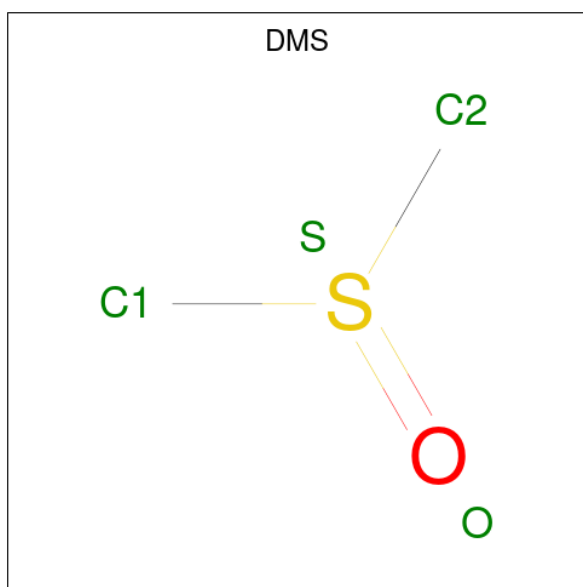
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0
7	E	1	Total Na 1 1	0	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



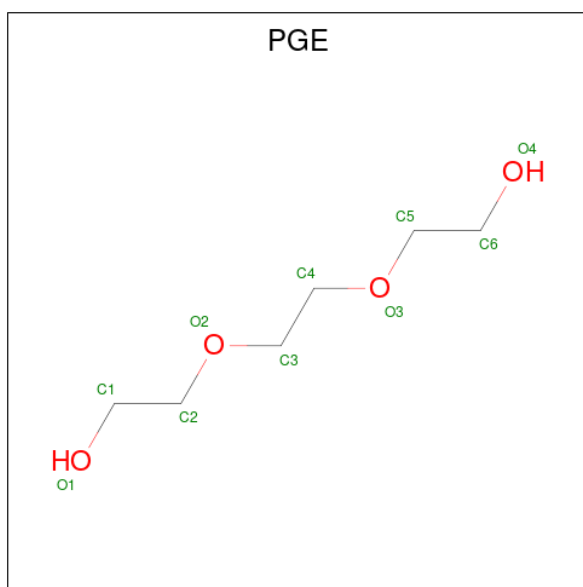
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	E	1	Total	C	O	0	0
			6	3	3		
8	E	1	Total	C	O	0	0
			6	3	3		
8	E	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

- Molecule 10 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



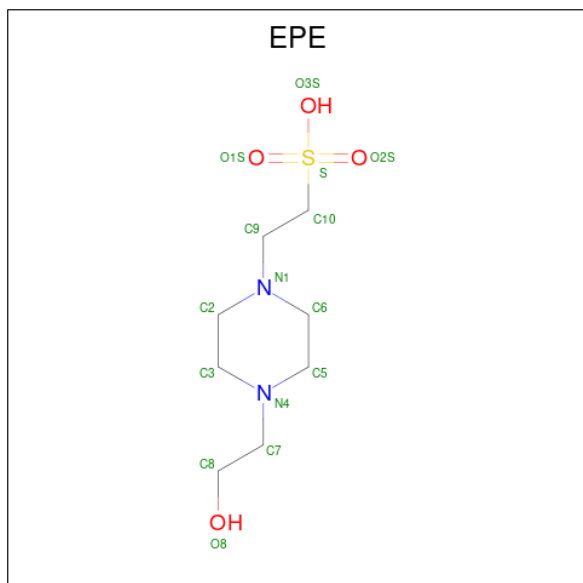
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			10	6	4		
10	E	1	Total	C	O	0	0
			10	6	4		

- Molecule 11 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
11	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	101	Total	O	0	0
			101	101		
12	B	633	Total	O	0	0
			633	633		
12	C	115	Total	O	0	0
			115	115		
12	D	114	Total	O	0	0
			114	114		
12	E	359	Total	O	0	0
			359	359		

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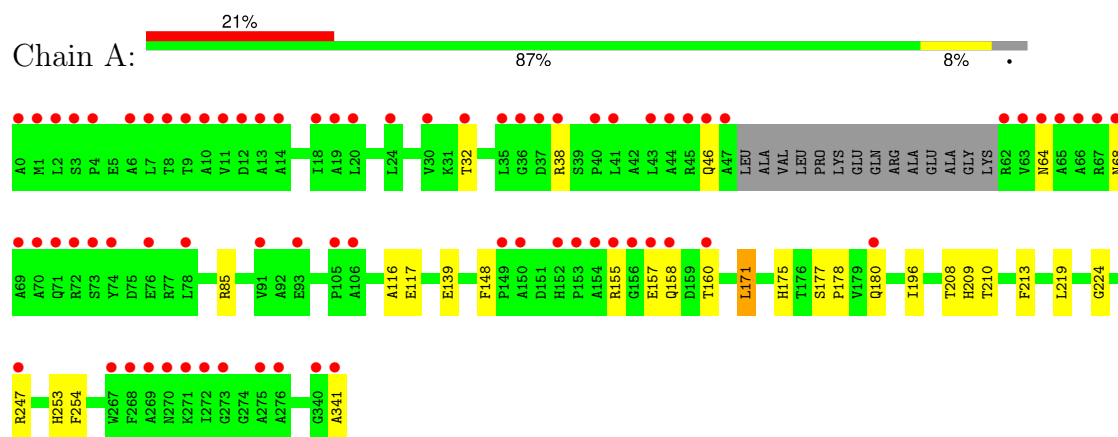
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	F	34	Total	O	0	0
			34	34		

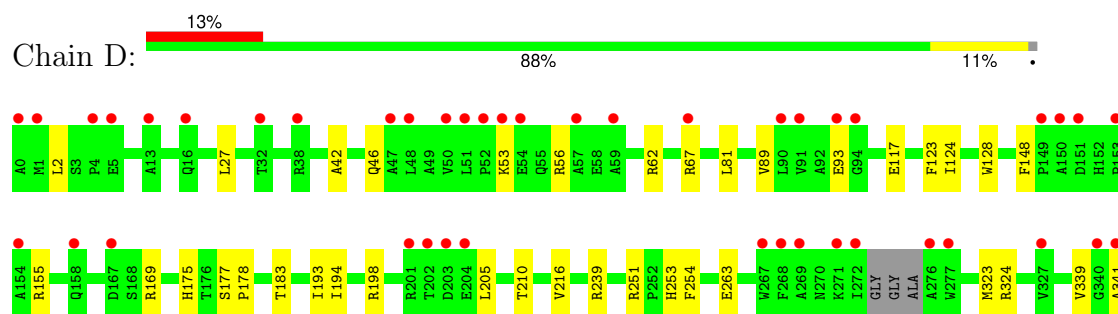
3 Residue-property plots [i](#)

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.

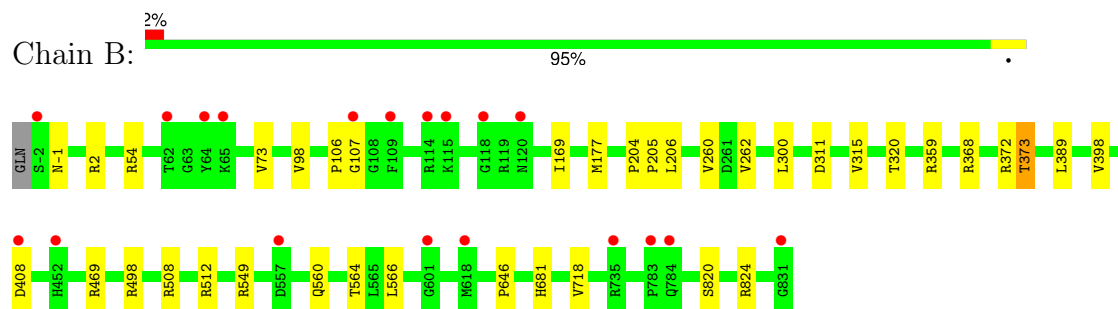
- Molecule 1: Phenylalanine-tRNA ligase alpha subunit



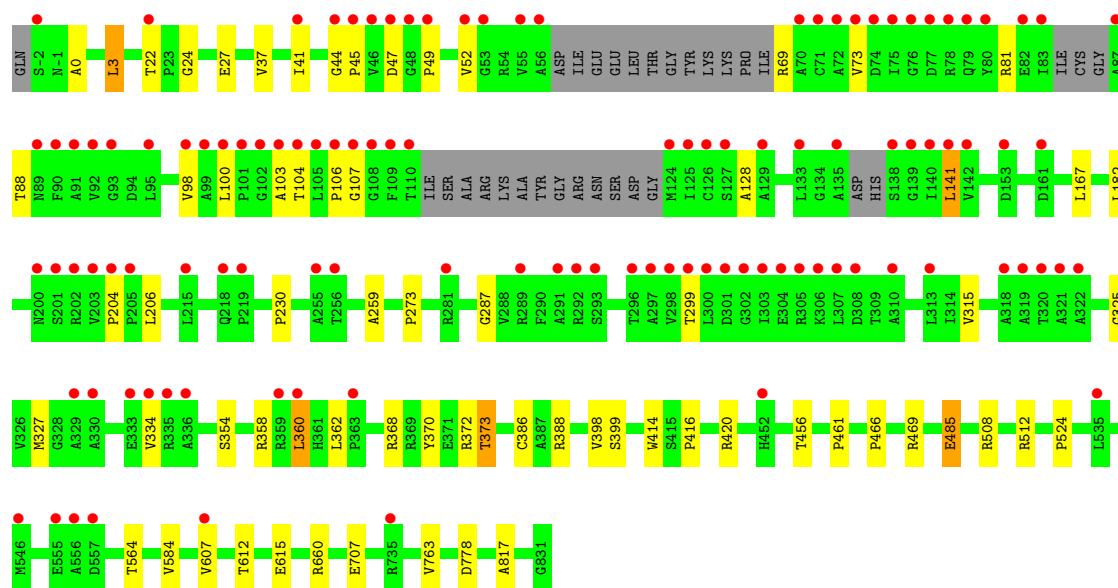
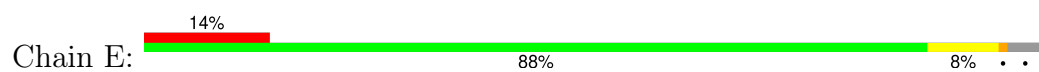
- Molecule 1: Phenylalanine-tRNA ligase alpha subunit



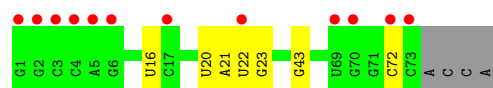
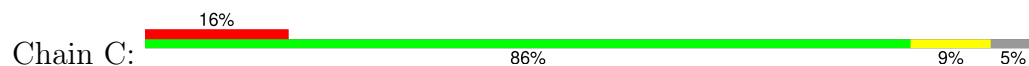
- Molecule 2: Phenylalanine-tRNA ligase beta subunit



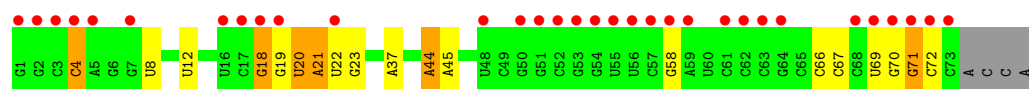
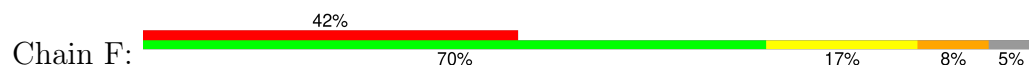
- Molecule 2: Phenylalanine-tRNA ligase beta subunit



• Molecule 3: tRNA(Phe)



• Molecule 3: tRNA(Phe)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	147.36Å 65.03Å 189.49Å 90.00° 110.86° 90.00°	Depositor
Resolution (Å)	48.86 – 2.05 48.86 – 2.05	Depositor EDS
% Data completeness (in resolution range)	94.3 (48.86-2.05) 94.3 (48.86-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.199 , 0.233 0.199 , 0.233	Depositor DCC
R_{free} test set	10518 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22325	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: DMS, PGE, MG, ACT, A1BCB, GOL, EPE, NA

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	0.10	0/2604	0.28	0/3546
1	D	0.10	0/2739	0.27	0/3726
2	B	0.11	0/6458	0.28	0/8842
2	E	0.09	0/6218	0.26	0/8513
3	C	0.09	0/1746	0.22	0/2720
3	F	0.07	0/1746	0.18	0/2720
All	All	0.10	0/21511	0.26	0/30067

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	2545	0	2484	21	0
1	D	2680	0	2641	22	0
2	B	6321	0	6344	24	0
2	E	6088	0	6118	40	0
3	C	1563	0	792	1	0
3	F	1563	0	792	10	0
4	A	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	18	0	0	0	0
5	A	1	0	0	0	0
5	C	3	0	0	0	0
5	D	1	0	0	0	0
6	A	4	0	3	1	0
6	B	12	0	9	0	0
6	E	12	0	9	2	0
7	A	1	0	0	0	0
7	E	1	0	0	0	0
8	B	30	0	40	3	0
8	C	6	0	8	0	0
8	D	6	0	8	2	0
8	E	18	0	24	0	0
8	F	6	0	8	0	0
9	B	8	0	12	0	0
9	D	4	0	6	1	0
10	B	20	0	28	3	0
10	E	10	0	14	3	0
11	B	30	0	36	0	0
12	A	101	0	0	1	0
12	B	633	0	0	6	0
12	C	115	0	0	0	0
12	D	114	0	0	1	0
12	E	359	0	0	3	0
12	F	34	0	0	1	0
All	All	22325	0	19376	108	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 (108) 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)
3:F:4:C:H42	3:F:70:G:H1	1.11	0.96
3:C:20:U:H5''	1:D:46:GLN:HG2	1.71	0.71
2:E:49:PRO:HB2	2:E:100:LEU:HB2	1.72	0.70
1:D:2:LEU:O	1:D:62:ARG:NH1	2.23	0.69
2:E:27:GLU:HG3	2:E:37:VAL:HG21	1.78	0.66
1:A:85:ARG:NH2	2:E:707:GLU:OE1	2.30	0.65
2:B:206:LEU:HD13	2:B:398:VAL:HG11	1.79	0.63
1:D:93[A]:GLU:HB3	9:D:402:DMS:H22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:22:THR:HG22	2:E:24:GLY:H	1.63	0.63
2:E:204[A]:PRO:O	2:E:388:ARG:NH2	2.28	0.63
1:D:210:THR:HG22	1:D:323:MET:HE3	1.81	0.62
1:A:341:ALA:HA	2:B:512:ARG:HG2	1.79	0.62
1:A:148:PHE:HB3	1:A:155:ARG:HD2	1.83	0.61
1:A:180:GLN:HB3	1:A:219:LEU:HD22	1.84	0.59
2:E:414:TRP:H	6:E:904:ACT:H1	1.69	0.58
2:E:273:PRO:HG2	2:E:370:TYR:CZ	2.39	0.58
1:A:224:GLY:HA2	8:B:913:GOL:H2	1.84	0.57
2:E:128:ALA:HB2	2:E:141:LEU:HD23	1.85	0.57
3:F:18:G:O2'	3:F:58:G:N2	2.33	0.56
2:B:54:ARG:NH2	12:B:1018:HOH:O	2.39	0.56
1:A:247:ARG:NH2	12:A:501:HOH:O	2.38	0.55
3:F:70:G:H2'	3:F:71:G:C8	2.41	0.55
2:E:3:LEU:HD21	2:E:182:LEU:HD12	1.89	0.54
2:E:612:THR:HG23	2:E:615:GLU:H	1.72	0.54
2:E:420:ARG:HH21	2:E:456:THR:HG21	1.72	0.54
1:A:64:ASN:O	1:A:68:ASN:ND2	2.30	0.54
1:D:183:THR:HG21	1:D:193:ILE:HG21	1.91	0.53
1:D:205:LEU:HG	1:D:324:ARG:HG2	1.90	0.53
2:B:646:PRO:O	12:B:1001:HOH:O	2.19	0.52
1:A:46:GLN:HG2	3:F:20:U:H5''	1.91	0.52
2:E:230:PRO:HG2	2:E:399:SER:HB3	1.91	0.52
2:B:311:ASP:OD2	2:B:359[A]:ARG:NH2	2.42	0.52
2:E:373[B]:THR:HG21	2:E:466:PRO:HG3	1.92	0.52
1:D:251:ARG:NH2	1:D:263:GLU:OE1	2.42	0.51
1:A:139:GLU:OE2	1:A:155:ARG:NH2	2.38	0.50
1:D:253:HIS:CG	1:D:254:PHE:H	2.29	0.50
2:E:508:ARG:HH21	10:E:901:PGE:H2	1.77	0.50
1:D:341:ALA:C	2:E:512:ARG:HE	2.19	0.50
3:F:12:U:OP1	12:F:201:HOH:O	2.20	0.49
10:B:914:PGE:H2	2:E:778:ASP:HA	1.95	0.49
1:D:148:PHE:O	1:D:155:ARG:NH2	2.44	0.49
2:B:106:PRO:HA	2:B:107:GLY:HA2	1.47	0.49
2:E:206:LEU:HD13	2:E:398:VAL:HG11	1.94	0.49
2:E:299:THR:HB	2:E:327:MET:HE3	1.94	0.49
2:E:485:GLU:H	2:E:485:GLU:CD	2.20	0.49
2:B:372:ARG:O	2:B:373:THR:OG1	2.28	0.48
2:B:177:MET:HE1	2:B:368:ARG:HG3	1.95	0.48
2:E:508:ARG:HE	10:E:901:PGE:H12	1.78	0.48
1:A:117:GLU:HG3	2:B:508:ARG:CZ	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:LYS:HG2	1:D:56:ARG:HH12	1.79	0.48
2:B:549:ARG:HG2	2:B:560:GLN:HG2	1.95	0.47
2:E:49:PRO:HD2	2:E:103:ALA:HA	1.95	0.47
2:E:47:ASP:OD1	2:E:104:THR:OG1	2.31	0.47
2:E:372:ARG:NH1	12:E:1010:HOH:O	2.38	0.47
1:A:157:GLU:OE2	2:B:372:ARG:NH2	2.47	0.47
1:D:123:PHE:HB2	1:D:194[A]:ILE:HD13	1.97	0.46
1:D:239:ARG:HH21	8:D:401:GOL:H31	1.81	0.46
2:E:73:VAL:HG11	2:E:98:VAL:HG11	1.96	0.46
1:D:198:ARG:NH1	2:E:524:PRO:O	2.48	0.46
2:B:315:VAL:HG12	2:B:320:THR:HA	1.97	0.46
3:F:66:C:H2'	3:F:67:C:C6	2.50	0.46
2:E:416:PRO:HG2	2:E:461:PRO:HD2	1.98	0.46
2:E:354:SER:OG	2:E:358:ARG:NH1	2.49	0.45
1:D:169:ARG:NH1	12:D:506:HOH:O	2.49	0.45
2:E:287:GLY:N	2:E:315:VAL:O	2.47	0.45
3:F:8:U:O2'	3:F:21:A:N1	2.46	0.45
1:A:253:HIS:CG	1:A:254:PHE:H	2.34	0.45
1:D:53:LYS:HG2	1:D:56:ARG:NH1	2.32	0.45
10:B:906:PGE:H2	12:B:1012:HOH:O	2.16	0.44
1:A:116:ALA:HB1	1:A:196:ILE:HG21	1.99	0.44
2:B:2:ARG:NH1	12:B:1030:HOH:O	2.48	0.44
2:E:259:ALA:HB3	2:E:334:VAL:HG11	1.99	0.44
2:B:260:VAL:HG11	8:B:903:GOL:H32	1.99	0.44
1:D:117:GLU:HG3	2:E:508:ARG:CZ	2.47	0.44
2:E:660[A]:ARG:NH1	12:E:1030:HOH:O	2.50	0.44
2:B:681:HIS:CE1	1:D:89[B]:VAL:HG13	2.53	0.44
2:B:73:VAL:HG11	2:B:98:VAL:HG21	2.00	0.44
2:B:-1:ASN:HB2	2:B:169:ILE:O	2.18	0.43
1:D:27:LEU:HD22	1:D:81:LEU:HD12	2.00	0.43
1:A:32:THR:HG21	3:F:45:A:H5''	2.01	0.43
1:A:208:THR:HG23	1:A:209:HIS:CE1	2.54	0.43
2:E:763:VAL:HG13	2:E:817:ALA:HB1	2.01	0.43
2:E:106:PRO:HA	2:E:107:GLY:HA2	1.47	0.43
1:A:253:HIS:CE1	6:A:403:ACT:H1	2.54	0.43
1:A:160:THR:HG21	1:A:171:LEU:HD22	2.00	0.43
10:B:906:PGE:H4	12:B:1391:HOH:O	2.19	0.43
1:A:210:THR:HG23	1:A:213:PHE:HB3	2.00	0.43
2:E:37:VAL:HG12	2:E:167:LEU:HD22	2.01	0.43
2:E:469:ARG:NH1	12:E:1032:HOH:O	2.52	0.43
2:E:325:GLY:H	6:E:906:ACT:H2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:498:ARG:HG2	8:D:401:GOL:H32	2.00	0.42
2:B:262:VAL:HG13	2:B:389:LEU:HD23	2.01	0.42
2:E:0:ALA:O	2:E:368:ARG:NH2	2.53	0.42
3:F:4:C:N4	3:F:70:G:H1	1.96	0.42
1:D:177:SER:N	1:D:178:PRO:HD2	2.35	0.41
1:A:177:SER:N	1:A:178:PRO:HD2	2.35	0.41
2:B:820:SER:O	2:B:824:ARG:HG3	2.19	0.41
1:D:124:ILE:HD13	1:D:128:TRP:O	2.20	0.41
2:E:44:GLY:HA3	2:E:45:PRO:HA	1.74	0.41
2:E:360:LEU:HD13	2:E:362:LEU:HD12	2.02	0.41
2:B:469:ARG:NH1	12:B:1039:HOH:O	2.52	0.41
1:A:38:ARG:HH22	3:F:44:A:H5'	1.85	0.41
2:E:508:ARG:HE	10:E:901:PGE:C1	2.34	0.41
2:B:204:PRO:HA	2:B:205:PRO:HD3	1.90	0.41
2:B:300:LEU:HD13	8:B:903:GOL:H2	2.02	0.41
2:B:566:LEU:HD23	2:B:566:LEU:HA	1.93	0.41
1:A:247:ARG:HA	1:A:247:ARG:HD2	1.88	0.40
1:D:42:ALA:HA	1:D:67:ARG:HH12	1.87	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	328/342 (96%)	316 (96%)	11 (3%)	1 (0%)	37	30
1	D	343/342 (100%)	335 (98%)	8 (2%)	0	100	100
2	B	843/835 (101%)	824 (98%)	18 (2%)	1 (0%)	48	44
2	E	804/835 (96%)	779 (97%)	22 (3%)	3 (0%)	30	23
All	All	2318/2354 (98%)	2254 (97%)	59 (2%)	5 (0%)	44	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	GLN
2	B	373	THR
2	E	88	THR
2	E	373[A]	THR
2	E	373[B]	THR

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	257/268 (96%)	255 (99%)	2 (1%)	79	80
1	D	273/268 (102%)	270 (99%)	3 (1%)	70	71
2	B	661/652 (101%)	658 (100%)	3 (0%)	86	88
2	E	636/652 (98%)	624 (98%)	12 (2%)	52	50
All	All	1827/1840 (99%)	1807 (99%)	20 (1%)	70	71

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	LEU
1	A	175	HIS
2	B	408	ASP
2	B	564	THR
2	B	718	VAL
1	D	175	HIS
1	D	216	VAL
1	D	339	VAL
2	E	3	LEU
2	E	41	ILE
2	E	52	VAL
2	E	69	ARG
2	E	81	ARG
2	E	141	LEU
2	E	360	LEU
2	E	386	CYS
2	E	485	GLU

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Mol	Chain	Res	Type
2	E	564	THR
2	E	584	VAL
2	E	607	VAL

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

Mol	Chain	Res	Type
1	A	170	GLN
1	A	215	GLN
1	D	170	GLN
2	E	132	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	72/77 (93%)	6 (8%)	0
3	F	72/77 (93%)	12 (16%)	0
All	All	144/154 (93%)	18 (12%)	0

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	16	U
3	C	21	A
3	C	22	U
3	C	23	G
3	C	43	G
3	C	72	C
3	F	4	C
3	F	18	G
3	F	19	G
3	F	20	U
3	F	21	A
3	F	22	U
3	F	23	G
3	F	37	A
3	F	44	A
3	F	69	U
3	F	71	G
3	F	72	C

There are no RNA pucker outliers to report.

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 35 ligands modelled in this entry, 7 are monoatomic - leaving 28 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	$\# Z > 2$
10	PGE	B	914	-	9,9,9	0.33	0	8,8,8	0.54	0
6	ACT	B	912	-	3,3,3	1.14	0	3,3,3	1.20	0
8	GOL	E	908	-	5,5,5	0.35	0	5,5,5	0.42	0
8	GOL	E	902	-	5,5,5	0.32	0	5,5,5	0.33	0
9	DMS	B	905	-	3,3,3	0.58	0	3,3,3	0.13	0
4	A1BCB	D	403	-	18,19,19	2.36	5 (27%)	23,26,26	1.56	5 (21%)
6	ACT	E	905	-	3,3,3	1.14	0	3,3,3	1.21	0
8	GOL	F	101	-	5,5,5	0.33	0	5,5,5	0.39	0
6	ACT	B	911	-	3,3,3	1.13	0	3,3,3	1.17	0
8	GOL	E	903	-	5,5,5	0.34	0	5,5,5	0.41	0
6	ACT	A	403	-	3,3,3	1.12	0	3,3,3	1.26	0
8	GOL	B	903	-	5,5,5	0.35	0	5,5,5	0.40	0
8	GOL	C	104	-	5,5,5	0.34	0	5,5,5	0.43	0
8	GOL	B	904	-	5,5,5	0.34	0	5,5,5	0.42	0
6	ACT	E	906	-	3,3,3	1.12	0	3,3,3	1.22	0
8	GOL	B	913	-	5,5,5	0.34	0	5,5,5	0.42	0
9	DMS	D	402	-	3,3,3	0.57	0	3,3,3	0.24	0
6	ACT	B	910	-	3,3,3	1.13	0	3,3,3	1.17	0
8	GOL	B	902	-	5,5,5	0.33	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	EPE	B	909	-	15,15,15	0.84	1 (6%)	19,20,20	0.53	0
4	A1BCB	A	401	-	18,19,19	2.34	4 (22%)	23,26,26	1.48	4 (17%)
8	GOL	D	401	-	5,5,5	0.32	0	5,5,5	0.39	0
10	PGE	E	901	-	9,9,9	0.32	0	8,8,8	0.52	0
10	PGE	B	906	-	9,9,9	0.32	0	8,8,8	0.45	0
11	EPE	B	908	-	15,15,15	0.80	1 (6%)	19,20,20	0.68	0
9	DMS	B	907	-	3,3,3	0.58	0	3,3,3	0.14	0
8	GOL	B	901	-	5,5,5	0.32	0	5,5,5	0.54	0
6	ACT	E	904	-	3,3,3	1.13	0	3,3,3	1.20	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
11	EPE	B	908	-	-	3/9/19/19	0/1/1/1
8	GOL	B	902	-	-	2/4/4/4	-
11	EPE	B	909	-	-	3/9/19/19	0/1/1/1
8	GOL	E	902	-	-	4/4/4/4	-
8	GOL	B	913	-	-	0/4/4/4	-
8	GOL	E	903	-	-	2/4/4/4	-
8	GOL	B	903	-	-	2/4/4/4	-
4	A1BCB	D	403	-	-	5/11/24/24	0/2/2/2
8	GOL	C	104	-	-	2/4/4/4	-
10	PGE	B	914	-	-	4/7/7/7	-
4	A1BCB	A	401	-	-	5/11/24/24	0/2/2/2
8	GOL	D	401	-	-	0/4/4/4	-
8	GOL	F	101	-	-	0/4/4/4	-
10	PGE	B	906	-	-	5/7/7/7	-
8	GOL	B	904	-	-	0/4/4/4	-
8	GOL	E	908	-	-	0/4/4/4	-
8	GOL	B	901	-	-	2/4/4/4	-
10	PGE	E	901	-	-	4/7/7/7	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	403	A1BCB	O03-C02	7.44	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	A1BCB	O03-C02	7.37	1.45	1.37
4	D	403	A1BCB	O12-C10	3.43	1.40	1.33
4	A	401	A1BCB	O12-C10	3.41	1.40	1.33
4	D	403	A1BCB	C05-N07	2.98	1.42	1.36
4	A	401	A1BCB	C05-N07	2.91	1.42	1.36
11	B	909	EPE	C10-S	2.48	1.81	1.77
11	B	908	EPE	C10-S	2.19	1.80	1.77
4	D	403	A1BCB	C15-N07	2.13	1.45	1.42
4	A	401	A1BCB	C15-N07	2.12	1.45	1.42
4	D	403	A1BCB	O12-C13	-2.00	1.40	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	403	A1BCB	O12-C10-C08	4.44	121.44	111.14
4	A	401	A1BCB	O12-C10-C08	4.39	121.32	111.14
4	A	401	A1BCB	O12-C10-O11	-2.57	119.43	124.14
4	D	403	A1BCB	C08-N07-C05	2.55	121.50	117.43
4	D	403	A1BCB	O12-C10-O11	-2.46	119.64	124.14
4	A	401	A1BCB	C02-C15-N07	2.18	119.86	118.24
4	A	401	A1BCB	C08-N07-C05	2.15	120.86	117.43
4	D	403	A1BCB	O03-C02-C01	2.10	120.23	116.89
4	D	403	A1BCB	C02-C15-N07	2.08	119.79	118.24

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	A1BCB	N07-C08-C10-O11
4	A	401	A1BCB	N07-C08-C10-O12
4	D	403	A1BCB	N07-C08-C10-O11
4	D	403	A1BCB	N07-C08-C10-O12
8	B	901	GOL	O1-C1-C2-C3
8	C	104	GOL	C1-C2-C3-O3
8	E	902	GOL	C1-C2-C3-O3
11	B	908	EPE	C10-C9-N1-C2
10	E	901	PGE	O2-C3-C4-O3
8	E	902	GOL	O1-C1-C2-O2
8	B	902	GOL	C1-C2-C3-O3
8	B	903	GOL	O1-C1-C2-C3
8	E	902	GOL	O1-C1-C2-C3
8	C	104	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
8	E	902	GOL	O2-C2-C3-O3
10	B	914	PGE	O2-C3-C4-O3
10	E	901	PGE	O1-C1-C2-O2
4	D	403	A1BCB	O11-C10-O12-C13
8	B	901	GOL	O1-C1-C2-O2
4	A	401	A1BCB	O11-C10-O12-C13
11	B	908	EPE	C10-C9-N1-C6
8	E	903	GOL	O1-C1-C2-O2
4	D	403	A1BCB	C08-C10-O12-C13
4	A	401	A1BCB	C08-C10-O12-C13
11	B	909	EPE	N4-C7-C8-O8
10	B	906	PGE	O3-C5-C6-O4
8	E	903	GOL	O2-C2-C3-O3
10	B	906	PGE	C4-C3-O2-C2
10	B	914	PGE	C3-C4-O3-C5
10	B	906	PGE	C3-C4-O3-C5
11	B	908	EPE	N4-C7-C8-O8
10	E	901	PGE	C3-C4-O3-C5
8	B	903	GOL	O1-C1-C2-O2
11	B	909	EPE	C10-C9-N1-C2
11	B	909	EPE	C10-C9-N1-C6
10	B	914	PGE	C6-C5-O3-C4
10	B	906	PGE	C1-C2-O2-C3
10	B	906	PGE	O2-C3-C4-O3
10	E	901	PGE	C4-C3-O2-C2
8	B	902	GOL	O2-C2-C3-O3
10	B	914	PGE	O1-C1-C2-O2
4	A	401	A1BCB	C14-C13-O12-C10
4	D	403	A1BCB	C14-C13-O12-C10

There are no ring outliers.

10 monomers are involved in 15 short contacts:

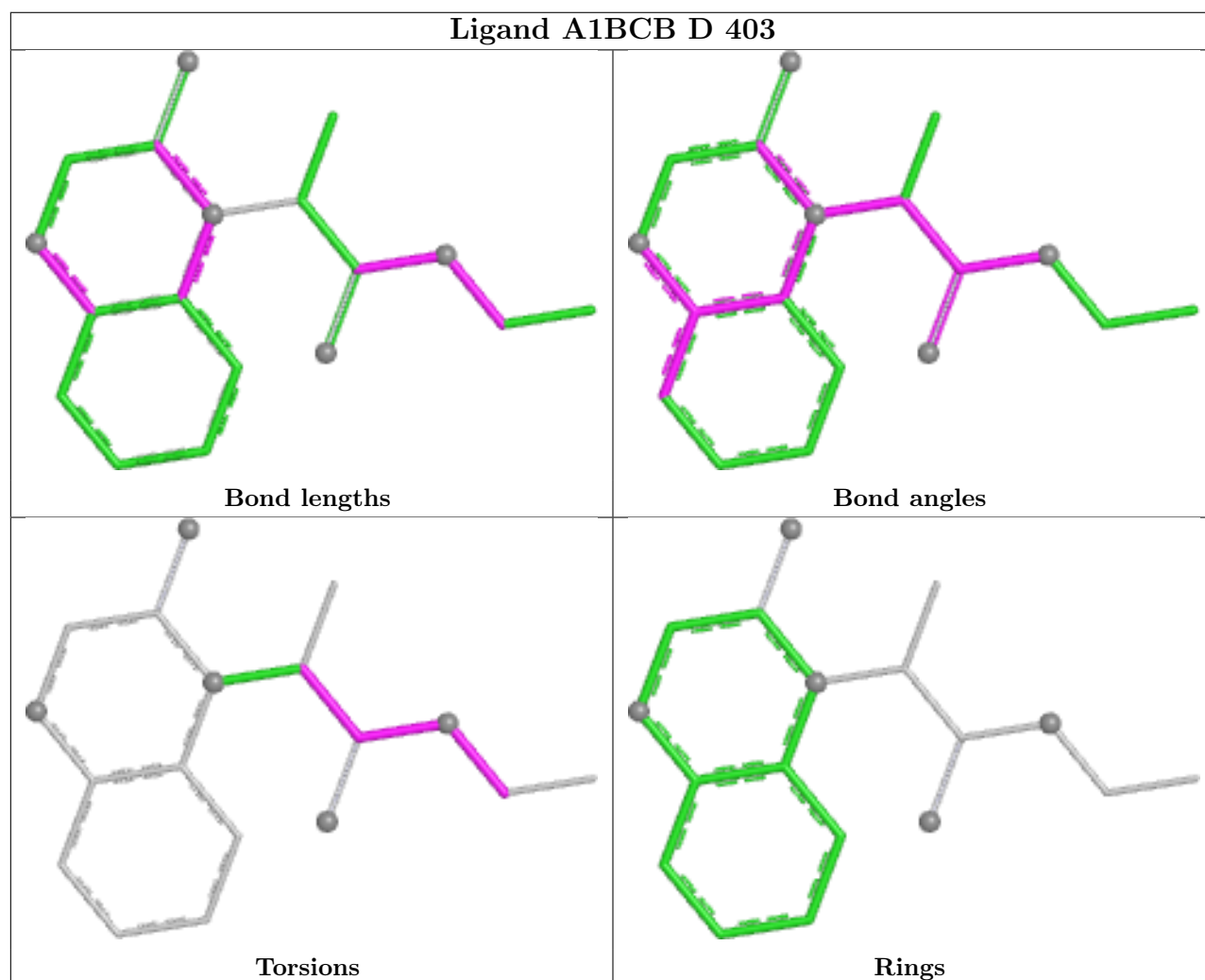
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	914	PGE	1	0
6	A	403	ACT	1	0
8	B	903	GOL	2	0
6	E	906	ACT	1	0
8	B	913	GOL	1	0
9	D	402	DMS	1	0
8	D	401	GOL	2	0
10	E	901	PGE	3	0

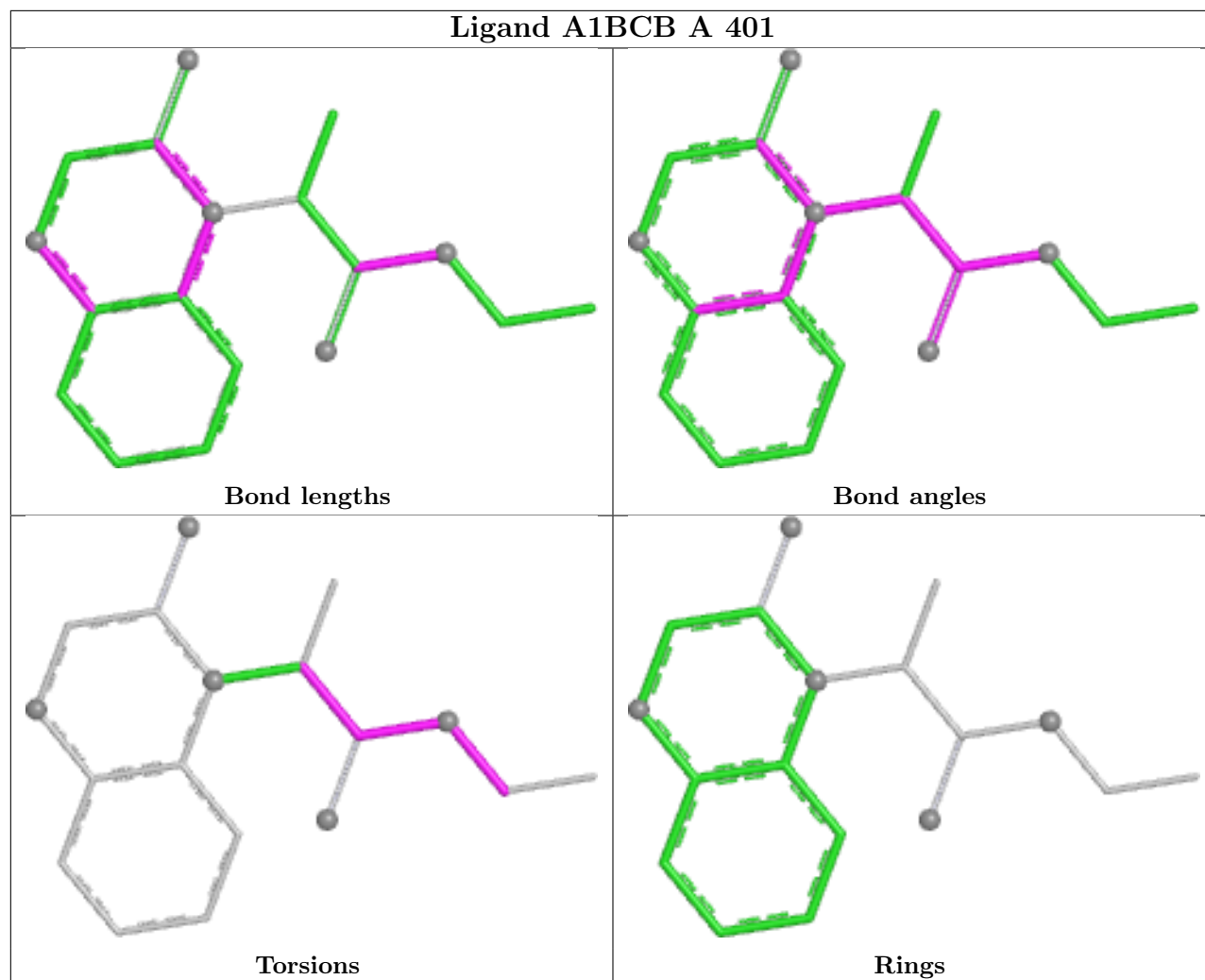
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	906	PGE	2	0
6	E	904	ACT	1	0

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	328/342 (95%)	0.90	73 (22%) 3 2	10, 33, 100, 140	4 (1%)
1	D	339/342 (99%)	0.65	43 (12%) 9 9	12, 35, 71, 99	8 (2%)
2	B	834/835 (99%)	-0.24	19 (2%) 61 63	6, 22, 47, 80	11 (1%)
2	E	804/835 (96%)	0.54	113 (14%) 7 7	10, 33, 87, 126	10 (1%)
3	C	73/77 (94%)	0.12	12 (16%) 5 5	16, 40, 156, 201	0
3	F	73/77 (94%)	1.46	32 (43%) 1 0	28, 63, 205, 235	0
All	All	2451/2508 (97%)	0.35	292 (11%) 10 10	6, 29, 87, 235	33 (1%)

All (292) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	90[A]	LEU	10.2
1	D	91[A]	VAL	8.5
1	A	106[A]	ALA	7.1
1	A	105[A]	PRO	7.0
1	D	341	ALA	6.7
2	B	-2	SER	6.6
1	A	47	ALA	6.5
2	E	203[A]	VAL	6.3
2	E	83	ILE	6.2
1	A	341	ALA	6.2
2	E	72	ALA	5.7
1	D	272	ILE	5.7
1	A	66	ALA	5.6
1	A	63	VAL	5.5
1	A	65	ALA	5.4
1	A	43	LEU	5.3
1	A	154	ALA	5.3
1	A	44	ALA	5.1
1	A	12	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	156	GLY	4.8
1	A	69	ALA	4.7
1	A	70	ALA	4.7
2	E	87	ALA	4.7
2	E	135	ALA	4.7
2	E	336	ALA	4.7
1	D	93[A]	GLU	4.6
1	D	1	MET	4.5
1	A	340	GLY	4.5
3	F	19	G	4.4
2	E	303	ILE	4.2
1	D	268	PHE	4.2
2	E	202[A]	ARG	4.2
1	D	0	ALA	4.1
2	E	318	ALA	4.1
1	A	2	LEU	4.1
1	A	158	GLN	4.0
2	E	107	GLY	4.0
1	A	153	PRO	4.0
1	A	152	HIS	4.0
1	A	150	ALA	3.9
2	E	110	THR	3.9
1	A	41	LEU	3.9
1	A	157	GLU	3.9
2	E	89	ASN	3.8
1	A	62	ARG	3.8
1	D	276	ALA	3.8
1	A	272	ILE	3.8
2	E	102	GLY	3.7
2	E	91	ALA	3.7
1	A	35	LEU	3.7
3	F	3	C	3.7
2	E	100	LEU	3.6
2	E	56	ALA	3.6
2	B	783	PRO	3.6
2	E	45	PRO	3.6
3	F	17	C	3.6
1	A	7	LEU	3.6
1	A	0	ALA	3.5
3	F	57	C	3.5
1	D	269	ALA	3.5
2	E	-2	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	267	TRP	3.5
1	A	276	ALA	3.5
2	E	109	PHE	3.5
2	E	301	ASP	3.5
2	E	300	LEU	3.5
2	E	360	LEU	3.5
2	E	79	GLN	3.4
2	E	48	GLY	3.4
3	F	48	U	3.4
1	A	269	ALA	3.4
2	E	92	VAL	3.4
2	E	302	GLY	3.4
2	E	98	VAL	3.4
2	E	296	THR	3.4
2	E	329	ALA	3.4
2	E	330	ALA	3.4
2	E	139	GLY	3.3
2	E	46	VAL	3.3
1	D	153	PRO	3.3
1	A	268	PHE	3.3
3	C	5	A	3.3
2	E	90	PHE	3.3
2	E	359	ARG	3.3
2	E	219	PRO	3.2
3	C	4	C	3.2
1	A	149	PRO	3.2
1	D	158	GLN	3.2
1	A	30	VAL	3.2
1	D	50	VAL	3.2
1	A	73	SER	3.2
1	A	10	ALA	3.2
2	E	291	ALA	3.2
1	A	46	GLN	3.2
2	E	101	PRO	3.2
2	E	70	ALA	3.2
1	A	72	ARG	3.1
3	F	53	G	3.1
2	E	76	GLY	3.1
1	A	19	ALA	3.1
2	E	201[A]	SER	3.1
2	E	307	LEU	3.1
3	F	71	G	3.1

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Mol	Chain	Res	Type	RSRZ
2	E	47	ASP	3.1
2	E	78	ARG	3.1
2	E	306	LYS	3.0
2	E	308	ASP	3.0
1	A	1	MET	3.0
1	A	91	VAL	3.0
1	A	74	TYR	2.9
3	F	1	G	2.9
1	D	52	PRO	2.9
2	E	106	PRO	2.9
1	A	6	ALA	2.9
2	E	319	ALA	2.9
1	A	64	ASN	2.9
3	F	61	C	2.9
1	A	4	PRO	2.9
2	E	105	LEU	2.9
2	B	109[A]	PHE	2.9
3	F	5	A	2.9
2	E	138	SER	2.9
2	E	82	GLU	2.9
2	E	73	VAL	2.9
2	E	99	ALA	2.9
3	F	56	U	2.9
3	C	3	C	2.9
1	A	20	LEU	2.8
2	E	297	ALA	2.8
2	E	310	ALA	2.8
3	F	59	A	2.8
2	E	41	ILE	2.8
3	F	4	C	2.8
2	B	831	GLY	2.8
3	F	7	G	2.8
2	E	142	VAL	2.8
2	E	334	VAL	2.8
2	E	452	HIS	2.8
1	D	150	ALA	2.8
2	E	140	ILE	2.8
3	F	72	C	2.8
1	A	36	GLY	2.8
2	E	53	GLY	2.8
3	F	55	U	2.8
1	D	4	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
3	F	58	G	2.8
1	D	203	ASP	2.8
1	D	13	ALA	2.8
3	F	22	U	2.8
1	A	13	ALA	2.7
1	D	57	ALA	2.7
1	A	9	THR	2.7
2	B	452	HIS	2.7
1	A	45	ARG	2.7
2	E	161	ASP	2.7
2	E	557	ASP	2.7
1	A	38	ARG	2.7
1	D	53	LYS	2.7
3	C	1	G	2.7
2	E	52	VAL	2.7
2	E	124	MET	2.7
1	A	273	GLY	2.7
1	A	67	ARG	2.7
1	A	11	VAL	2.7
1	D	47	ALA	2.7
2	E	305	ARG	2.7
2	E	95	LEU	2.6
2	E	129	ALA	2.6
2	B	62	THR	2.6
2	E	126	CYS	2.6
3	F	2	G	2.6
2	E	103	ALA	2.6
1	D	5	GLU	2.6
1	D	38	ARG	2.6
2	E	218	GLN	2.6
2	E	289	ARG	2.6
3	F	18	G	2.6
3	F	51	G	2.6
1	A	76	GLU	2.6
1	D	154	ALA	2.6
2	E	321	ALA	2.6
2	E	104	THR	2.6
1	D	149	PRO	2.6
2	E	75	ILE	2.6
2	E	125	ILE	2.6
1	A	93	GLU	2.6
3	F	52	C	2.6

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Mol	Chain	Res	Type	RSRZ
3	F	54	G	2.5
2	E	256	THR	2.5
1	A	155	ARG	2.5
1	D	201	ARG	2.5
2	B	114	ARG	2.5
2	E	363	PRO	2.5
3	F	62	C	2.5
3	F	73	C	2.5
2	E	80	TYR	2.5
2	E	93	GLY	2.5
3	C	22	U	2.5
2	E	204[A]	PRO	2.5
2	E	304	GLU	2.5
2	E	71	CYS	2.5
3	F	69	U	2.5
1	A	3	SER	2.4
2	E	293	SER	2.4
1	A	18	ILE	2.4
3	C	17	C	2.4
3	C	72	C	2.4
2	E	215	LEU	2.4
1	A	275	ALA	2.4
2	E	556	ALA	2.4
3	F	70	G	2.4
1	A	68	ASN	2.4
2	E	22	THR	2.4
3	F	68	C	2.4
1	D	94[A]	GLY	2.4
2	E	108	GLY	2.4
1	D	151	ASP	2.4
1	A	8	THR	2.4
2	E	298	VAL	2.4
2	B	735	ARG	2.4
1	A	71	GLN	2.4
2	E	141	LEU	2.4
2	E	333	GLU	2.4
1	A	14	ALA	2.4
1	A	160	THR	2.4
2	B	65	LYS	2.4
2	E	607	VAL	2.4
2	E	49	PRO	2.4
1	D	271	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	59	ALA	2.3
2	B	618	MET	2.3
1	A	271	LYS	2.3
3	C	6	G	2.3
3	C	73	C	2.3
3	F	63	C	2.3
2	B	408	ASP	2.3
2	E	77	ASP	2.3
1	D	54	GLU	2.3
1	A	24	LEU	2.3
2	E	133	LEU	2.3
2	E	313	LEU	2.3
2	E	281	ARG	2.3
2	E	292	ARG	2.3
2	E	335	ARG	2.3
2	E	255	ALA	2.3
1	D	340	GLY	2.3
2	E	735	ARG	2.3
1	D	51	LEU	2.3
2	E	535	LEU	2.3
1	A	37	ASP	2.2
2	E	74	ASP	2.2
1	D	267	TRP	2.2
1	A	78	LEU	2.2
2	E	299	THR	2.2
1	A	270	ASN	2.2
1	D	16	GLN	2.2
1	D	48	LEU	2.2
1	A	32	THR	2.2
1	D	202	THR	2.2
3	C	2	G	2.2
2	B	120	ASN	2.2
2	E	555	GLU	2.2
2	B	557	ASP	2.2
3	C	69	U	2.2
1	D	167	ASP	2.1
1	D	277	TRP	2.1
2	B	115	LYS	2.1
2	E	153	ASP	2.1
2	E	322	ALA	2.1
2	B	107	GLY	2.1
2	B	784	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	127	SER	2.1
2	B	64	TYR	2.1
2	E	200	ASN	2.1
1	D	204	GLU	2.1
3	F	50	G	2.1
3	F	64	G	2.1
3	F	16	U	2.1
1	D	327	VAL	2.1
2	E	55	VAL	2.1
1	A	247	ARG	2.1
2	E	320	THR	2.1
1	A	180	GLN	2.1
2	B	118	GLY	2.0
2	B	601	GLY	2.0
2	E	205[A]	PRO	2.0
1	D	32	THR	2.0
2	E	546	MET	2.0
2	E	44	GLY	2.0
1	A	40	PRO	2.0
1	D	67	ARG	2.0
3	C	70	G	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(\AA^2)	Q<0.9
8	GOL	B	902	6/6	0.70	0.19	27,43,52,53	0
8	GOL	B	903	6/6	0.71	0.18	48,49,58,62	0

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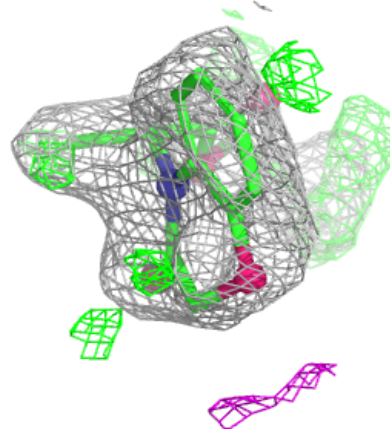
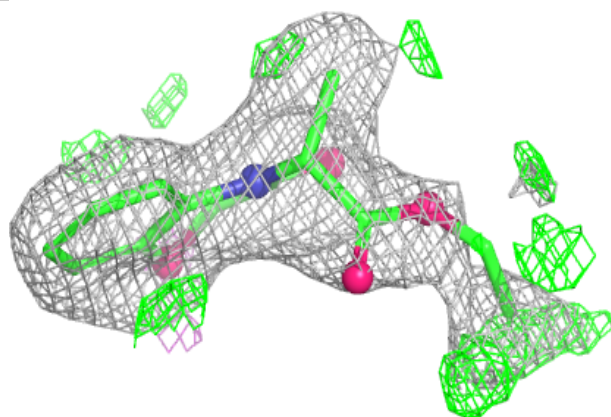
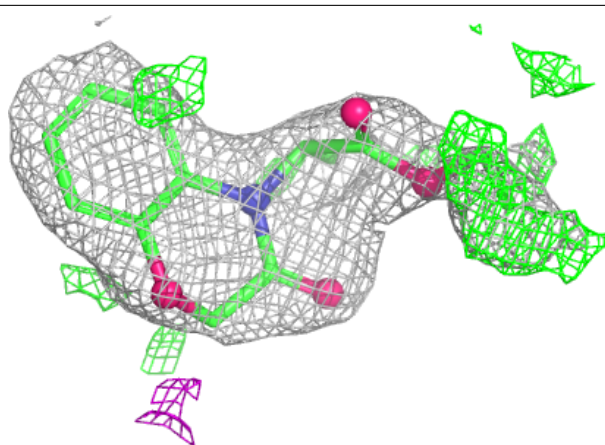
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	PGE	B	914	10/10	0.72	0.20	27,37,49,57	0
8	GOL	E	902	6/6	0.73	0.17	36,46,54,55	0
8	GOL	B	913	6/6	0.74	0.14	42,47,50,66	0
4	A1BCB	A	401	18/18	0.74	0.17	29,40,60,64	0
4	A1BCB	D	403	18/18	0.74	0.17	31,45,68,69	0
6	ACT	B	912	4/4	0.76	0.17	44,46,49,50	0
8	GOL	F	101	6/6	0.78	0.23	39,43,44,45	0
10	PGE	B	906	10/10	0.79	0.17	15,32,38,42	10
6	ACT	A	403	4/4	0.79	0.21	36,42,55,62	0
10	PGE	E	901	10/10	0.80	0.16	33,46,52,56	0
8	GOL	E	908	6/6	0.82	0.15	49,52,59,61	0
6	ACT	E	906	4/4	0.86	0.13	36,51,54,55	0
8	GOL	D	401	6/6	0.86	0.13	38,42,44,44	0
9	DMS	D	402	4/4	0.87	0.19	42,50,53,68	0
8	GOL	C	104	6/6	0.87	0.27	25,35,49,50	0
6	ACT	E	905	4/4	0.88	0.14	36,40,44,44	0
8	GOL	E	903	6/6	0.88	0.10	41,43,45,57	0
11	EPE	B	908	15/15	0.88	0.14	32,41,54,55	0
6	ACT	E	904	4/4	0.89	0.12	33,37,44,45	0
8	GOL	B	901	6/6	0.89	0.12	22,25,31,35	0
8	GOL	B	904	6/6	0.89	0.10	41,48,51,58	0
11	EPE	B	909	15/15	0.89	0.12	37,44,55,60	0
6	ACT	B	911	4/4	0.92	0.10	23,24,37,38	0
7	NA	E	907	1/1	0.93	0.21	37,37,37,37	0
9	DMS	B	905	4/4	0.93	0.15	28,34,47,58	0
9	DMS	B	907	4/4	0.93	0.12	33,45,52,54	0
6	ACT	B	910	4/4	0.94	0.09	17,27,28,33	0
5	MG	C	101	1/1	0.95	0.07	43,43,43,43	0
5	MG	C	103	1/1	0.96	0.08	33,33,33,33	0
7	NA	A	404	1/1	0.98	0.04	28,28,28,28	0
5	MG	D	404	1/1	0.98	0.03	21,21,21,21	0
5	MG	A	402	1/1	0.98	0.03	16,16,16,16	0
5	MG	C	102	1/1	0.99	0.03	34,34,34,34	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.

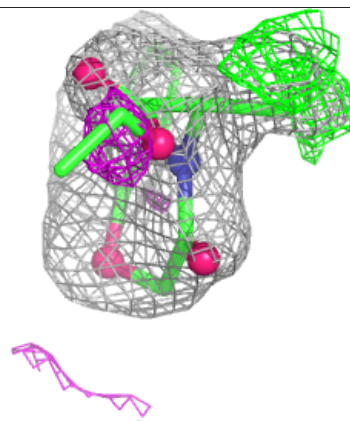
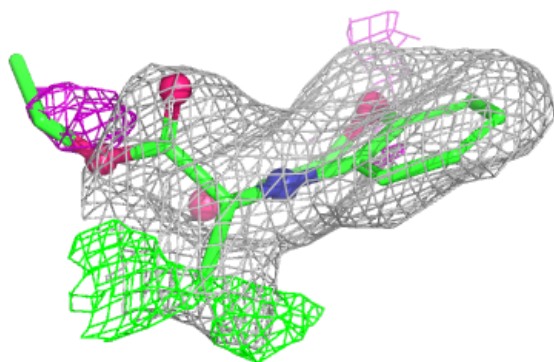
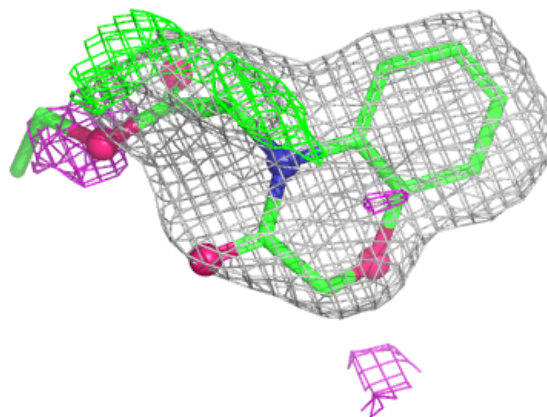
Electron density around A1BCB A 401:

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



Electron density around A1BCB D 403:

$2mF_o-DF_c$ (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.