Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2025 – 08:49 AM EDT

PDB ID	:	9DTF / pdb_00009dtf
Title	:	Crystal structure of the complex of M. tuberculosis PheRS with cognate precursor tRNA and fragment DDD01008876
Authors	:	Chang, C.; Michalska, K.; Forte, B.; Baragana, B.; Gilbert, I.H.; Wower, J.; Joachimiak, A.
Deposited on	:	2024-09-30
Resolution	:	2.45 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:

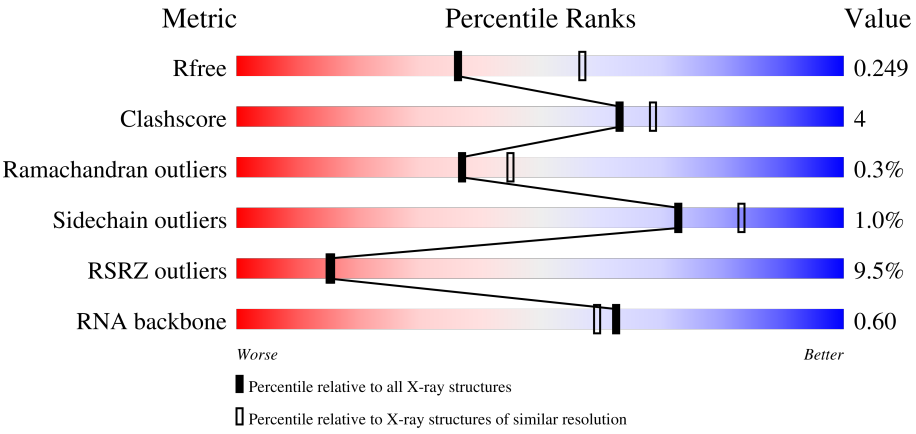
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1096 (2.46-2.46)
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (2.46-2.46)
RNA backbone	3690	1040 (2.76-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	342	15% 80% 17%
1	D	342	9% 86% 13%
2	B	835	% 91% 9%

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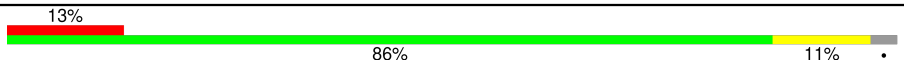
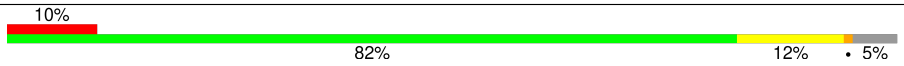
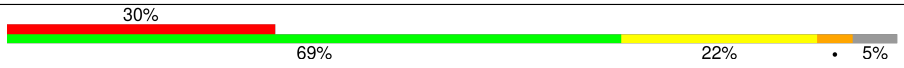
Mol	Chain	Length	Quality of chain
2	E	835	
3	C	77	
3	F	77	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 21921 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	335	Total	C	N	O	S	0	0	0
			2535	1603	452	471	9			
1	D	338	Total	C	N	O	S	0	8	0
			2662	1679	480	495	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP P9WFU3
D	0	ALA	-	expression tag	UNP P9WFU3

- 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	12	0
			6329	3976	1150	1181	22			
2	E	806	Total	C	N	O	S	0	10	0
			6083	3821	1108	1135	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLN	-	expression tag	UNP P9WFU1
B	-2	SER	-	expression tag	UNP P9WFU1
B	-1	ASN	-	expression tag	UNP P9WFU1
B	0	ALA	-	expression tag	UNP P9WFU1
E	-3	GLN	-	expression tag	UNP P9WFU1
E	-2	SER	-	expression tag	UNP P9WFU1
E	-1	ASN	-	expression tag	UNP P9WFU1
E	0	ALA	-	expression tag	UNP P9WFU1

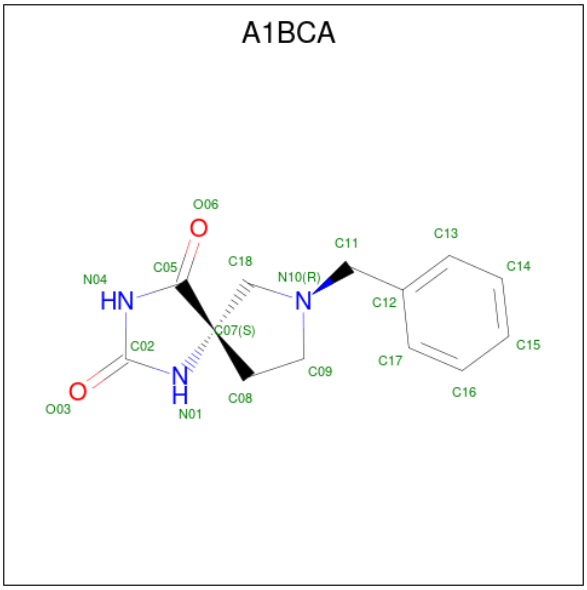
- Molecule 3 is a RNA chain called tRNA(Phe).

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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

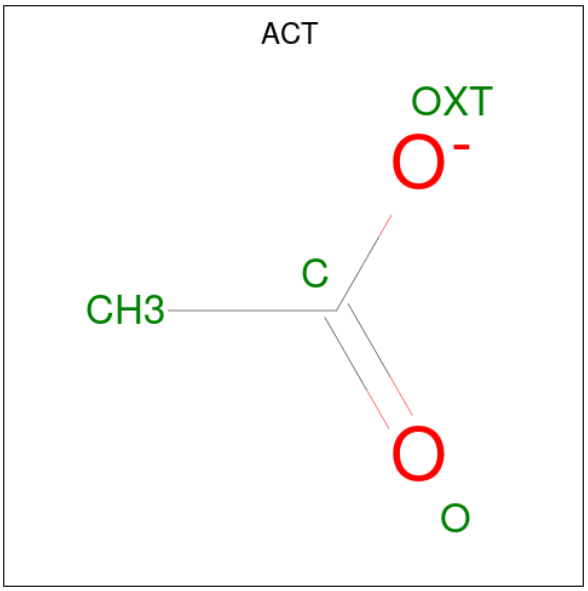
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	2	Total	Mg	0	0
			2	2		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is (5S)-7-benzyl-1,3,7-triazaspiro[4.4]nonane-2,4-dione (CCD ID: A1BCA) (formula: $C_{13}H_{15}N_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			18	13	3	2		
5	D	1	Total	C	N	O	0	0
			18	13	3	2		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).

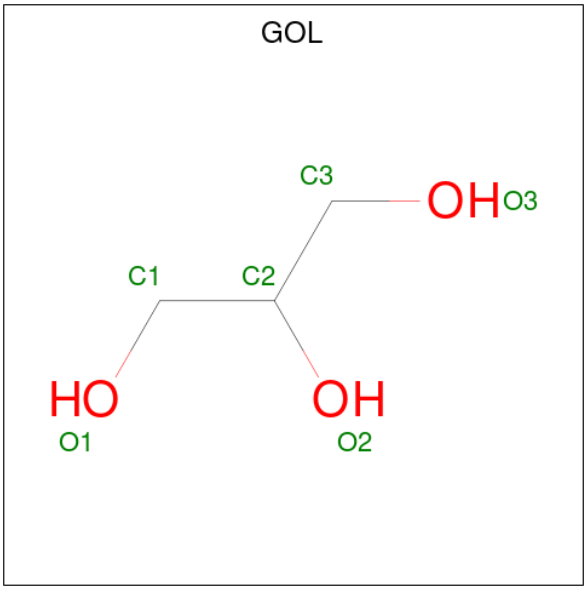


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0
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: $C_3H_8O_3$).



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

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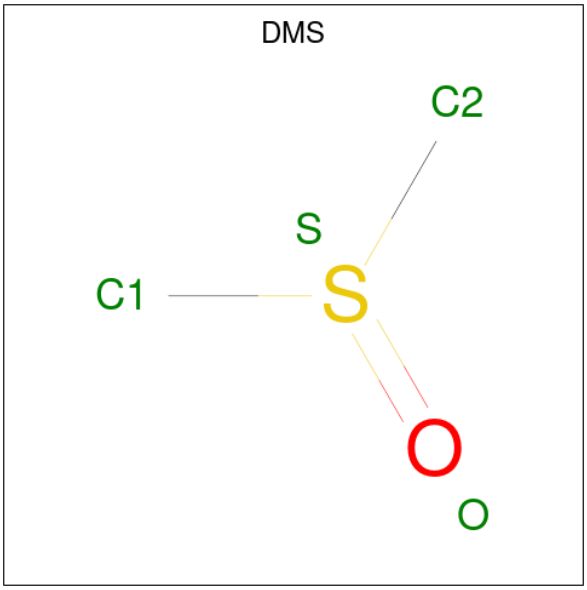
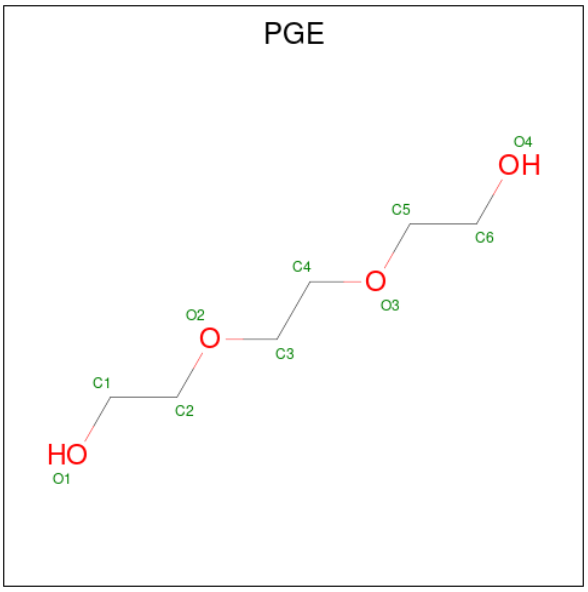
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	1	Total C O 6 3 3	0	0

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



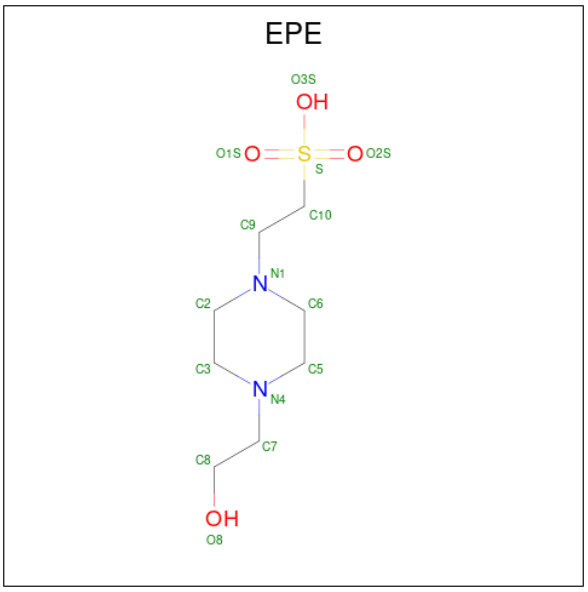
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O S 4 2 1 1	0	0
9	B	1	Total C O S 4 2 1 1	0	0
9	D	1	Total C O S 4 2 1 1	0	0
9	E	1	Total C O S 4 2 1 1	0	0

- Molecule 10 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 11 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

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

- Molecule 12 is water.

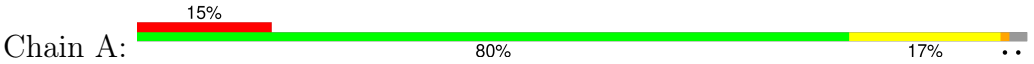
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	78	Total	O	0	0
			78	78		
12	B	433	Total	O	0	0
			433	433		
12	C	86	Total	O	0	0
			86	86		
12	D	71	Total	O	0	0
			71	71		
12	E	262	Total	O	0	0
			262	262		
12	F	34	Total	O	0	0
			34	34		

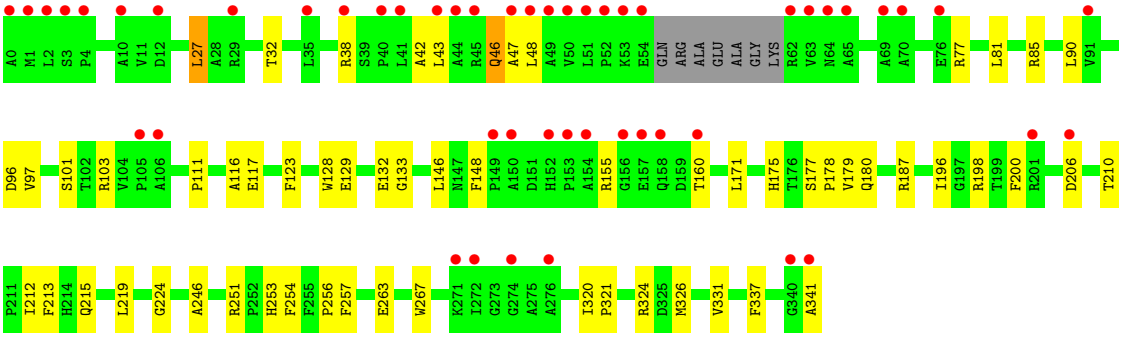
3 Residue-property plots (i)

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

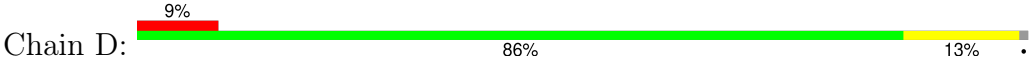
Chain A:

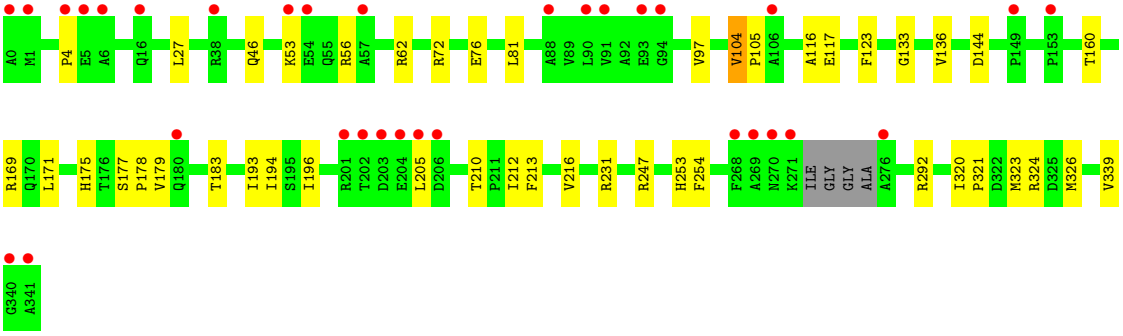




• Molecule 1: Phenylalanine–tRNA ligase alpha subunit

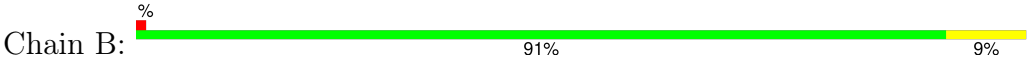
Chain D:

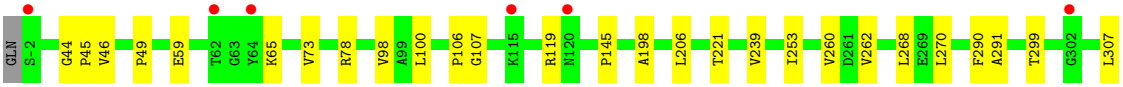


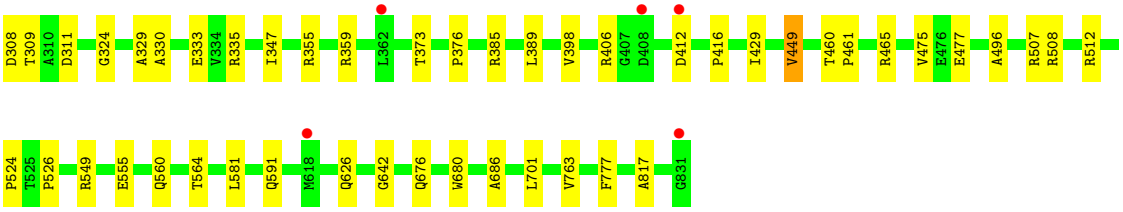


• Molecule 2: Phenylalanine–tRNA ligase beta subunit

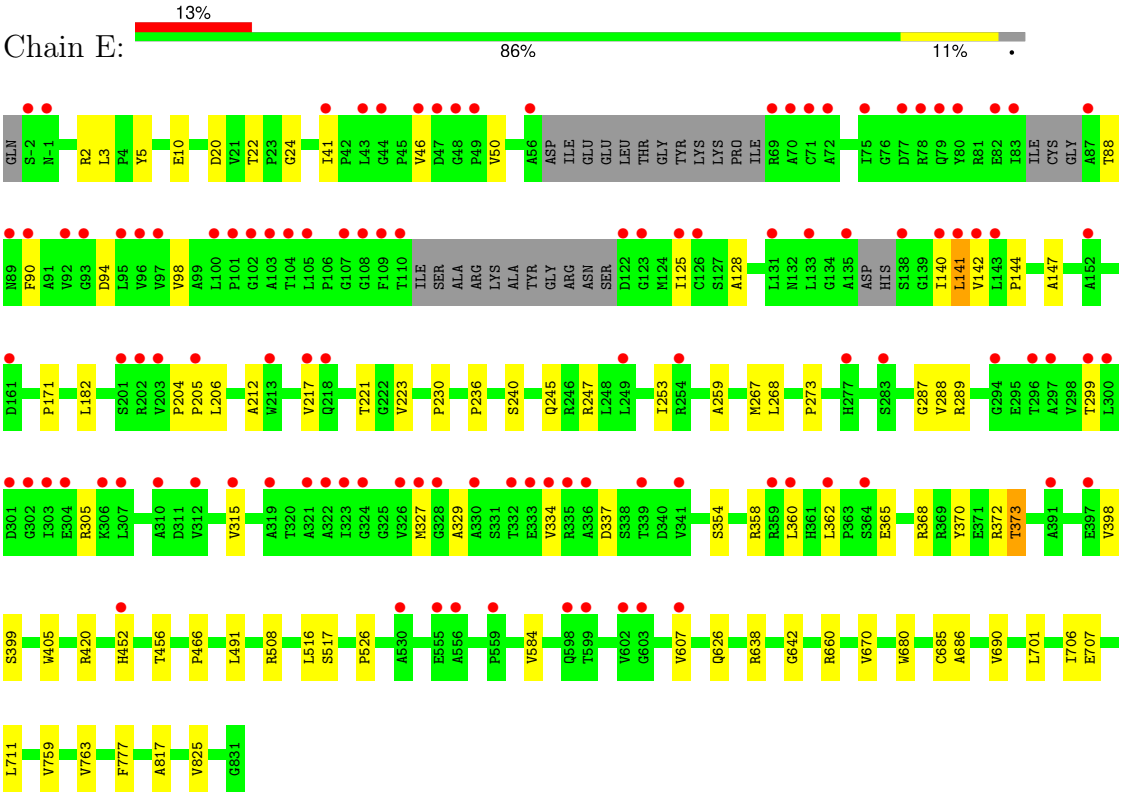
Chain B:



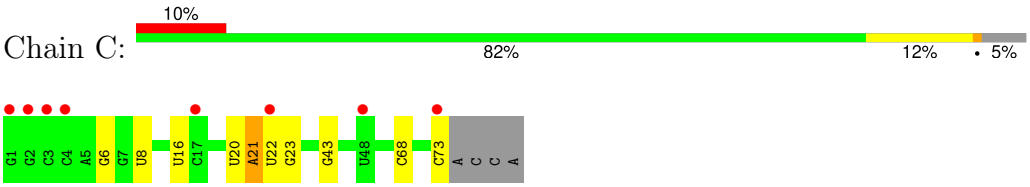




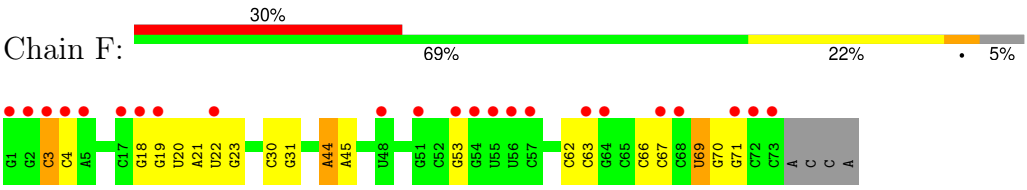
• Molecule 2: Phenylalanine–tRNA ligase beta subunit



• Molecule 3: tRNA(Phe)



• Molecule 3: tRNA(Phe)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	146.69Å 64.06Å 187.92Å 90.00° 110.86° 90.00°	Depositor
Resolution (Å)	48.64 – 2.45 48.64 – 2.45	Depositor EDS
% Data completeness (in resolution range)	90.0 (48.64-2.45) 90.1 (48.64-2.45)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.203 , 0.249 0.204 , 0.249	Depositor DCC
R_{free} test set	6125 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	21921	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: ACT, DMS, NA, A1BCA, MG, PGE, GOL, EPE

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	0.07	0/2594	0.23	0/3538
1	D	0.07	0/2721	0.21	0/3704
2	B	0.07	0/6466	0.22	0/8852
2	E	0.08	0/6213	0.22	0/8508
3	C	0.06	0/1746	0.13	0/2720
3	F	0.06	0/1746	0.14	0/2720
All	All	0.07	0/21486	0.21	0/30042

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	2535	0	2449	37	0
1	D	2662	0	2608	27	0
2	B	6329	0	6354	46	0
2	E	6083	0	6096	53	0
3	C	1563	0	792	3	0
3	F	1563	0	792	9	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	2	0	0	0	0
4	D	1	0	0	0	0
5	A	18	0	0	1	0
5	D	18	0	0	0	0
6	A	4	0	3	0	0
6	B	28	0	21	1	0
6	E	16	0	12	0	0
7	A	1	0	0	0	0
7	E	1	0	0	0	0
8	B	42	0	56	2	0
8	E	18	0	24	2	0
8	F	6	0	8	0	0
9	B	8	0	12	2	0
9	D	4	0	6	0	0
9	E	4	0	6	1	0
10	B	10	0	14	1	0
10	D	10	0	14	0	0
11	B	30	0	34	1	0
12	A	78	0	0	1	0
12	B	433	0	0	2	0
12	C	86	0	0	0	0
12	D	71	0	0	1	0
12	E	262	0	0	0	0
12	F	34	0	0	0	0
All	All	21921	0	19301	153	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (153) 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:C:20:U:H5"	1:D:46:GLN:HG2	1.69	0.74
1:A:341:ALA:HA	2:B:512:ARG:HG2	1.76	0.68
3:F:69:U:H2'	3:F:70:G:C8	2.29	0.67
1:A:180:GLN:HB3	1:A:219:LEU:HD22	1.78	0.65
1:D:231:ARG:HE	1:D:247:ARG:HH12	1.44	0.65
2:E:3:LEU:HD21	2:E:182:LEU:HD12	1.78	0.64
1:A:27:LEU:HD12	1:A:81:LEU:HD12	1.81	0.63
2:B:206:LEU:HD13	2:B:398:VAL:HG11	1.81	0.62
2:E:236:PRO:HB3	2:E:337:ASP:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:217:VAL:HG12	2:E:288:VAL:HB	1.82	0.59
1:A:85:ARG:NH2	2:E:707:GLU:OE1	2.35	0.59
2:B:311:ASP:OD2	2:B:359[A]:ARG:NH2	2.37	0.57
1:A:132:GLU:OE2	2:B:507:ARG:NH2	2.37	0.57
1:A:32:THR:HG21	3:F:45:A:H5"	1.87	0.56
1:A:101:SER:OG	2:E:660[B]:ARG:NH1	2.39	0.56
1:A:42:ALA:O	1:A:46:GLN:N	2.39	0.55
1:A:43:LEU:HA	1:A:46:GLN:HB2	1.88	0.55
2:B:59:GLU:OE1	2:B:119:ARG:NH2	2.38	0.55
3:F:69:U:H2'	3:F:70:G:H8	1.71	0.55
2:B:73:VAL:HG11	2:B:98:VAL:HG21	1.88	0.54
1:D:212:ILE:HD13	2:E:526:PRO:HD2	1.89	0.54
2:E:354:SER:OG	2:E:358:ARG:NH2	2.41	0.54
2:E:763:VAL:HG13	2:E:817:ALA:HB1	1.89	0.54
2:E:420:ARG:HH21	2:E:456:THR:HG21	1.72	0.54
9:B:908:DMS:H22	2:E:517:SER:HA	1.88	0.54
1:A:148:PHE:HB3	1:A:155:ARG:HD2	1.89	0.54
3:F:3:C:H42	3:F:71:G:H22	1.56	0.53
2:B:262:VAL:HG13	2:B:389:LEU:HD23	1.91	0.53
2:E:128:ALA:HB2	2:E:141:LEU:HD23	1.89	0.53
2:E:373[B]:THR:HG21	2:E:466:PRO:HG3	1.89	0.53
1:A:210:THR:HG23	1:A:213:PHE:HB3	1.90	0.53
2:B:429:ILE:HD12	2:B:475:VAL:HG21	1.91	0.53
1:D:253:HIS:CG	1:D:254:PHE:H	2.27	0.53
1:D:27:LEU:HD22	1:D:81:LEU:HD12	1.91	0.53
3:F:66:C:H2'	3:F:67:C:C6	2.43	0.53
9:B:908:DMS:H21	1:D:104:VAL:HG21	1.91	0.52
1:D:210:THR:HG22	1:D:323:MET:HE3	1.91	0.52
1:D:53:LYS:HG2	1:D:56:ARG:HH22	1.74	0.52
2:E:22:THR:HG22	2:E:24:GLY:H	1.74	0.52
2:B:308:ASP:OD1	2:B:309:THR:N	2.41	0.52
2:B:78:ARG:HH12	6:B:911:ACT:H3	1.73	0.52
2:E:206:LEU:HD13	2:E:398:VAL:HG11	1.92	0.52
3:F:53:G:H1	3:F:63:C:H42	1.56	0.51
2:B:198:ALA:HB2	2:B:270:LEU:HD22	1.92	0.51
1:D:205:LEU:HG	1:D:324:ARG:HG2	1.91	0.51
2:E:223:VAL:HG21	2:E:288:VAL:HG11	1.91	0.51
2:E:289:ARG:HH21	2:E:315:VAL:HG21	1.75	0.51
2:E:171:PRO:HA	2:E:372:ARG:HE	1.76	0.51
1:D:4:PRO:HG3	1:D:62:ARG:HD2	1.91	0.50
1:A:251:ARG:NH1	1:A:263:GLU:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:98:VAL:HG12	2:E:125:ILE:HA	1.94	0.50
2:E:240:SER:O	2:E:245:GLN:NE2	2.45	0.50
2:B:686:ALA:HB2	1:D:97:VAL:HB	1.94	0.49
1:A:38:ARG:HH12	3:F:44:A:H5'	1.77	0.49
2:E:638:ARG:NH1	8:E:901:GOL:H11	2.26	0.49
1:D:320:ILE:HD12	1:D:326:MET:HE2	1.94	0.49
1:D:123:PHE:HB2	1:D:194[A]:ILE:HD13	1.95	0.49
2:B:496:ALA:HB3	2:E:491:LEU:HD13	1.94	0.49
2:B:260:VAL:HG11	8:B:903:GOL:H32	1.95	0.48
2:E:680:TRP:HA	2:E:701:LEU:HA	1.94	0.48
1:A:253:HIS:CG	1:A:254:PHE:H	2.31	0.48
2:B:49:PRO:HB2	2:B:100:LEU:HB2	1.95	0.48
2:B:777:PHE:HA	2:E:642:GLY:HA2	1.96	0.48
2:E:10:GLU:OE1	2:E:247:ARG:NH1	2.33	0.48
2:E:90:PHE:HB3	2:E:140:ILE:HD11	1.95	0.48
2:E:230:PRO:HG2	2:E:399:SER:HB3	1.95	0.48
1:A:133:GLY:HA3	1:A:179:VAL:HG22	1.96	0.48
2:B:406:ARG:NH2	2:B:412:ASP:OD1	2.46	0.48
1:D:160:THR:HG21	1:D:171:LEU:HD22	1.95	0.48
1:A:198:ARG:NH1	2:B:524:PRO:O	2.47	0.47
3:C:8:U:O2'	3:C:21:A:N1	2.39	0.47
2:E:759:VAL:HG22	2:E:825:VAL:HG21	1.96	0.47
2:E:2:ARG:HH12	2:E:41:ILE:HD11	1.78	0.47
2:B:307:LEU:HA	2:B:359[A]:ARG:HH22	1.79	0.47
1:D:105:PRO:HG2	8:E:901:GOL:H2	1.96	0.47
2:E:273:PRO:HG2	2:E:370:TYR:CZ	2.49	0.47
2:B:253:ILE:HD12	2:B:268:LEU:HD11	1.97	0.47
1:D:117:GLU:HG3	2:E:508:ARG:CZ	2.45	0.47
2:E:5:TYR:OH	2:E:20:ASP:OD1	2.31	0.47
1:A:96:ASP:HA	9:E:908:DMS:H13	1.96	0.47
2:B:676:GLN:NE2	12:B:1021:HOH:O	2.39	0.47
1:A:200:PHE:HE2	2:B:526:PRO:HG2	1.80	0.46
2:E:365:GLU:OE1	2:E:368:ARG:NH1	2.48	0.46
2:B:106:PRO:HA	2:B:107:GLY:HA2	1.53	0.46
1:D:183:THR:HG21	1:D:193:ILE:HG21	1.98	0.46
2:B:299:THR:HA	2:B:329:ALA:HA	1.96	0.46
2:E:212:ALA:HB1	2:E:230:PRO:HD3	1.97	0.46
1:A:117:GLU:HG3	2:B:508:ARG:CZ	2.45	0.46
2:B:347:ILE:HG13	2:B:376:PRO:HA	1.96	0.46
2:B:145:PRO:HD2	2:B:239:VAL:HG21	1.98	0.46
2:E:144:PRO:HG2	2:E:147:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLU:OE1	1:A:187:ARG:NH1	2.49	0.45
1:A:97:VAL:HB	2:E:686:ALA:HB2	1.98	0.45
1:A:320:ILE:HD12	1:A:326:MET:HE2	1.98	0.45
2:E:259:ALA:HB3	2:E:334:VAL:HG11	1.99	0.45
1:A:177:SER:N	1:A:178:PRO:HD2	2.31	0.45
1:A:215:GLN:NE2	5:A:402:A1BCA:O06	2.50	0.45
2:B:355:ARG:NH2	12:B:1036:HOH:O	2.47	0.45
2:E:287:GLY:N	2:E:315:VAL:O	2.50	0.45
2:B:763:VAL:HG13	2:B:817:ALA:HB1	1.99	0.45
2:E:670:VAL:HG12	2:E:690:VAL:HG22	1.98	0.45
2:B:385:ARG:NE	10:B:906:PGE:H4	2.32	0.45
1:D:53:LYS:HG2	1:D:56:ARG:NH2	2.32	0.45
2:B:549:ARG:HG2	2:B:560:GLN:HG2	1.99	0.44
1:D:133:GLY:HA3	1:D:179:VAL:HG22	1.97	0.44
1:D:339:VAL:HG11	2:E:516:LEU:HD23	1.99	0.44
2:E:299:THR:HA	2:E:329:ALA:HA	1.99	0.44
1:D:144:ASP:OD2	1:D:169:ARG:NH2	2.48	0.44
2:B:221:THR:HA	2:B:290:PHE:CZ	2.52	0.44
2:E:217:VAL:HG21	2:E:405:TRP:CE2	2.52	0.44
2:B:555:GLU:HG2	3:C:68:C:H5”	1.99	0.44
2:B:642:GLY:HA2	2:E:777:PHE:HA	2.00	0.44
1:D:116:ALA:HB1	1:D:196:ILE:HG21	2.00	0.44
2:E:267:MET:HB2	2:E:273:PRO:HA	2.00	0.44
2:B:44:GLY:HA3	2:B:45:PRO:HA	1.88	0.43
2:B:291:ALA:O	2:B:309:THR:HA	2.18	0.43
2:B:680:TRP:HA	2:B:701:LEU:HA	2.00	0.43
1:A:160:THR:HG21	1:A:171:LEU:HD22	2.00	0.43
1:A:253:HIS:CD2	1:A:254:PHE:H	2.36	0.43
2:E:204[A]:PRO:HA	2:E:205[A]:PRO:HD3	1.93	0.43
1:A:331:VAL:HG22	2:B:581:LEU:HD13	2.01	0.43
2:E:46:VAL:HG21	2:E:50:VAL:HG11	2.00	0.43
1:A:116:ALA:HB1	1:A:196:ILE:HG21	1.99	0.43
1:A:224:GLY:HA2	8:B:914:GOL:H2	1.99	0.43
1:A:148:PHE:CE2	1:A:256:PRO:HG2	2.54	0.43
2:B:449:VAL:HG13	2:B:460:THR:HB	1.99	0.43
1:A:206:ASP:HA	1:A:324:ARG:NH1	2.34	0.42
2:E:680:TRP:HB3	2:E:685:CYS:HB2	2.02	0.42
2:E:253:ILE:HD12	2:E:268:LEU:HD11	2.02	0.42
3:F:30:C:H2’	3:F:31:G:H8	1.85	0.42
1:D:210:THR:HG23	1:D:213:PHE:HB3	2.02	0.42
1:D:177:SER:N	1:D:178:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:465:ARG:HH12	2:B:477:GLU:CD	2.28	0.42
1:A:123:PHE:HB3	1:A:128:TRP:HB2	2.02	0.42
2:B:591:GLN:NE2	2:B:626:GLN:OE1	2.46	0.42
2:E:221:THR:HG23	2:E:223:VAL:HG23	2.02	0.41
2:E:299:THR:HB	2:E:327:MET:HE3	2.01	0.41
2:E:94:ASP:HB3	2:E:142:VAL:HG13	2.02	0.41
2:E:706:ILE:HG23	2:E:711:LEU:HB2	2.03	0.41
1:A:111:PRO:HG3	1:A:337:PHE:CG	2.56	0.41
1:A:212:ILE:HD13	2:B:526:PRO:HD2	2.03	0.41
1:A:103:ARG:NH2	12:A:508:HOH:O	2.50	0.41
1:A:146:LEU:HB3	1:A:257:PHE:HB3	2.02	0.41
2:B:416:PRO:HB2	2:B:461:PRO:HG2	2.03	0.41
2:B:333:GLU:O	2:B:335:ARG:NH1	2.54	0.40
1:D:72:ARG:O	1:D:76:GLU:HG2	2.21	0.40
2:B:46:VAL:O	11:B:909:EPE:H101	2.21	0.40
2:B:330:ALA:O	2:B:335:ARG:NH2	2.44	0.40
1:D:292:ARG:NE	12:D:503:HOH:O	2.40	0.40
2:E:305:ARG:NH2	2:E:362:LEU:HD21	2.37	0.40
3:F:70:G:H2'	3:F:71:G:O4'	2.20	0.40
1:A:246:ALA:HA	1:A:267:TRP:O	2.21	0.40
1:D:136:VAL:HB	2:E:626:GLN:NE2	2.36	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	331/342 (97%)	312 (94%)	16 (5%)	3 (1%)	14 18
1	D	342/342 (100%)	332 (97%)	9 (3%)	1 (0%)	37 45
2	B	844/835 (101%)	823 (98%)	19 (2%)	2 (0%)	44 54
2	E	806/835 (96%)	772 (96%)	32 (4%)	2 (0%)	44 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2323/2354 (99%)	2239 (96%)	76 (3%)	8 (0%)	37 45

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
2	B	373	THR
2	E	373[A]	THR
2	E	373[B]	THR
1	A	47	ALA
1	A	321	PRO
1	D	321	PRO
2	B	324	GLY

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	252/268 (94%)	247 (98%)	5 (2%)	50 65
1	D	269/268 (100%)	266 (99%)	3 (1%)	70 81
2	B	661/652 (101%)	658 (100%)	3 (0%)	86 92
2	E	632/652 (97%)	626 (99%)	6 (1%)	75 86
All	All	1814/1840 (99%)	1797 (99%)	17 (1%)	73 86

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	46	GLN
1	A	77	ARG
1	A	90	LEU
1	A	175	HIS
2	B	65	LYS
2	B	449	VAL

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Mol	Chain	Res	Type
2	B	564	THR
1	D	104	VAL
1	D	175	HIS
1	D	216	VAL
2	E	88	THR
2	E	141	LEU
2	E	360	LEU
2	E	452	HIS
2	E	584	VAL
2	E	607	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	170	GLN
2	B	35	HIS
2	B	628	GLN
2	B	687	GLN
1	D	215	GLN
2	E	132	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	72/77 (93%)	7 (9%)	0
3	F	72/77 (93%)	11 (15%)	0
All	All	144/154 (93%)	18 (12%)	0

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	6	G
3	C	16	U
3	C	21	A
3	C	22	U
3	C	23	G
3	C	43	G
3	C	73	C
3	F	3	C

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Mol	Chain	Res	Type
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	44	A
3	F	62	C
3	F	69	U

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 39 ligands modelled in this entry, 6 are monoatomic - leaving 33 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	$\#\|Z\| > 2$
6	ACT	B	911	-	3,3,3	1.34	0	3,3,3	1.36	0
8	GOL	B	919	-	5,5,5	0.94	0	5,5,5	1.05	0
10	PGE	B	906	-	9,9,9	0.31	0	8,8,8	0.30	0
6	ACT	B	913	-	3,3,3	1.39	0	3,3,3	1.36	0
6	ACT	E	905	-	3,3,3	1.37	0	3,3,3	1.36	0
8	GOL	E	907	-	5,5,5	0.94	0	5,5,5	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	EPE	B	910	-	15,15,15	0.82	1 (6%)	19,20,20	1.69	3 (15%)
6	ACT	B	915	-	3,3,3	1.41	1 (33%)	3,3,3	1.37	0
9	DMS	B	908	-	3,3,3	0.67	0	3,3,3	0.51	0
9	DMS	E	908	-	3,3,3	0.67	0	3,3,3	0.59	0
10	PGE	D	402	-	9,9,9	0.31	0	8,8,8	0.29	0
8	GOL	B	901	-	5,5,5	0.92	0	5,5,5	1.09	0
8	GOL	B	902	-	5,5,5	0.94	0	5,5,5	1.06	0
8	GOL	E	901	-	5,5,5	0.93	0	5,5,5	1.03	0
6	ACT	B	916	-	3,3,3	1.36	0	3,3,3	1.37	0
8	GOL	B	907	-	5,5,5	0.93	0	5,5,5	1.06	0
9	DMS	D	401	-	3,3,3	0.67	0	3,3,3	0.52	0
6	ACT	B	917	-	3,3,3	1.40	1 (33%)	3,3,3	1.37	0
6	ACT	E	909	-	3,3,3	1.40	1 (33%)	3,3,3	1.37	0
8	GOL	B	904	-	5,5,5	0.93	0	5,5,5	1.07	0
5	A1BCA	A	402	-	20,20,20	7.18	12 (60%)	24,29,29	2.44	5 (20%)
6	ACT	A	403	-	3,3,3	1.36	0	3,3,3	1.37	0
6	ACT	B	912	-	3,3,3	1.37	0	3,3,3	1.36	0
6	ACT	E	903	-	3,3,3	1.39	0	3,3,3	1.35	0
8	GOL	E	902	-	5,5,5	0.95	0	5,5,5	1.08	0
8	GOL	B	903	-	5,5,5	0.95	0	5,5,5	1.05	0
8	GOL	B	914	-	5,5,5	0.95	0	5,5,5	1.09	0
9	DMS	B	905	-	3,3,3	0.67	0	3,3,3	0.53	0
6	ACT	E	904	-	3,3,3	1.37	0	3,3,3	1.37	0
8	GOL	F	101	-	5,5,5	0.94	0	5,5,5	1.06	0
6	ACT	B	918	-	3,3,3	1.35	0	3,3,3	1.38	0
11	EPE	B	909	-	15,15,15	0.79	1 (6%)	19,20,20	1.77	3 (15%)
5	A1BCA	D	403	-	20,20,20	7.23	12 (60%)	24,29,29	2.51	4 (16%)

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
8	GOL	B	914	-	-	0/4/4/4	-
8	GOL	B	904	-	-	0/4/4/4	-
5	A1BCA	A	402	-	-	0/4/30/30	0/3/3/3
10	PGE	D	402	-	-	4/7/7/7	-
11	EPE	B	910	-	-	4/9/19/19	0/1/1/1
8	GOL	F	101	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	B	901	-	-	2/4/4/4	-
8	GOL	B	919	-	-	0/4/4/4	-
8	GOL	B	902	-	-	0/4/4/4	-
10	PGE	B	906	-	-	3/7/7/7	-
11	EPE	B	909	-	-	2/9/19/19	0/1/1/1
8	GOL	E	901	-	-	3/4/4/4	-
5	A1BCA	D	403	-	-	0/4/30/30	0/3/3/3
8	GOL	B	907	-	-	0/4/4/4	-
8	GOL	E	907	-	-	0/4/4/4	-
8	GOL	E	902	-	-	1/4/4/4	-
8	GOL	B	903	-	-	0/4/4/4	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	403	A1BCA	C18-C07	-17.84	1.31	1.53
5	A	402	A1BCA	C18-C07	-17.64	1.31	1.53
5	D	403	A1BCA	C11-N10	-15.81	1.17	1.47
5	A	402	A1BCA	C11-N10	-15.74	1.17	1.47
5	D	403	A1BCA	C18-N10	14.92	1.60	1.46
5	A	402	A1BCA	C18-N10	14.75	1.60	1.46
5	A	402	A1BCA	C09-N10	-10.59	1.26	1.47
5	D	403	A1BCA	C09-N10	-10.51	1.26	1.47
5	D	403	A1BCA	C02-N01	6.61	1.47	1.35
5	A	402	A1BCA	C02-N01	6.57	1.46	1.35
5	D	403	A1BCA	C05-N04	4.71	1.44	1.37
5	A	402	A1BCA	C05-N04	4.70	1.44	1.37
5	D	403	A1BCA	C08-C07	-4.12	1.48	1.54
5	A	402	A1BCA	C08-C07	-4.06	1.48	1.54
5	D	403	A1BCA	C02-N04	3.91	1.47	1.38
5	A	402	A1BCA	C02-N04	3.91	1.47	1.38
5	A	402	A1BCA	O03-C02	-3.89	1.15	1.23
5	D	403	A1BCA	O03-C02	-3.88	1.15	1.23
5	D	403	A1BCA	O06-C05	-2.92	1.17	1.22
5	A	402	A1BCA	O06-C05	-2.89	1.17	1.22
11	B	910	EPE	C10-S	2.81	1.81	1.77
11	B	909	EPE	C10-S	2.68	1.81	1.77
5	A	402	A1BCA	C11-C12	2.48	1.55	1.51
5	D	403	A1BCA	C11-C12	2.36	1.55	1.51
5	D	403	A1BCA	C07-C05	-2.26	1.49	1.53
5	A	402	A1BCA	C07-C05	-2.20	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	917	ACT	CH3-C	2.03	1.57	1.49
6	B	915	ACT	CH3-C	2.02	1.57	1.49
6	E	909	ACT	CH3-C	2.02	1.57	1.49

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	403	A1BCA	C05-C07-N01	9.51	108.13	100.35
5	A	402	A1BCA	C05-C07-N01	9.36	108.00	100.35
11	B	909	EPE	C5-N4-C3	5.21	120.07	108.84
5	D	403	A1BCA	C07-N01-C02	-5.02	107.95	112.90
5	A	402	A1BCA	C07-N01-C02	-4.91	108.05	112.90
11	B	910	EPE	C5-N4-C3	4.62	118.78	108.84
5	D	403	A1BCA	C05-N04-C02	-3.71	107.90	111.69
5	A	402	A1BCA	C05-N04-C02	-3.66	107.96	111.69
5	D	403	A1BCA	C11-N10-C18	-3.46	108.32	112.89
11	B	910	EPE	C7-N4-C5	3.03	119.32	111.24
5	A	402	A1BCA	C08-C07-N01	-2.82	110.78	113.19
11	B	910	EPE	C7-N4-C3	2.72	118.49	111.24
11	B	909	EPE	C7-N4-C5	2.62	118.21	111.24
11	B	909	EPE	C7-N4-C3	2.54	118.01	111.24
5	A	402	A1BCA	C11-N10-C18	-2.49	109.60	112.89

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	901	GOL	O1-C1-C2-O2
8	B	901	GOL	O1-C1-C2-C3
11	B	910	EPE	C8-C7-N4-C5
8	E	901	GOL	O1-C1-C2-C3
8	E	901	GOL	O1-C1-C2-O2
10	B	906	PGE	O1-C1-C2-O2
10	D	402	PGE	O1-C1-C2-O2
10	D	402	PGE	O3-C5-C6-O4
11	B	909	EPE	C10-C9-N1-C2
11	B	909	EPE	C10-C9-N1-C6
11	B	910	EPE	C10-C9-N1-C2
11	B	910	EPE	C10-C9-N1-C6
10	B	906	PGE	C1-C2-O2-C3
10	B	906	PGE	C4-C3-O2-C2
10	D	402	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
11	B	910	EPE	N4-C7-C8-O8
8	E	902	GOL	O2-C2-C3-O3
8	E	901	GOL	O2-C2-C3-O3
10	D	402	PGE	C4-C3-O2-C2

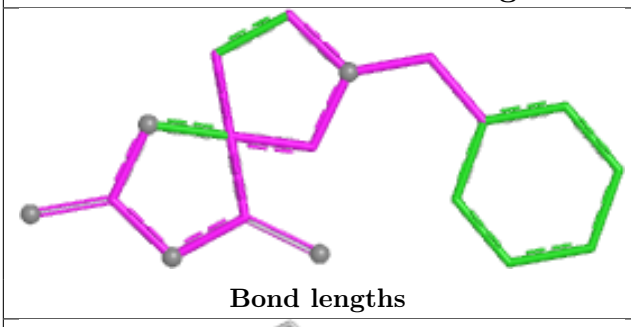
There are no ring outliers.

9 monomers are involved in 11 short contacts:

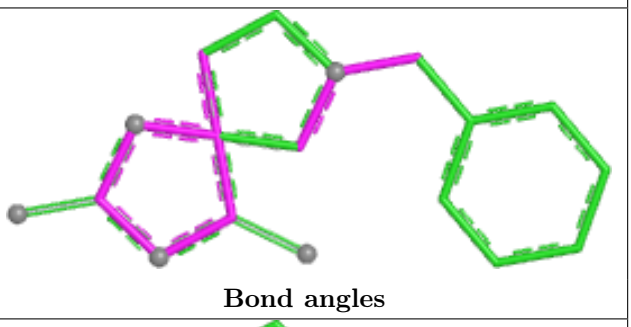
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	911	ACT	1	0
10	B	906	PGE	1	0
9	B	908	DMS	2	0
9	E	908	DMS	1	0
8	E	901	GOL	2	0
5	A	402	A1BCA	1	0
8	B	903	GOL	1	0
8	B	914	GOL	1	0
11	B	909	EPE	1	0

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 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.

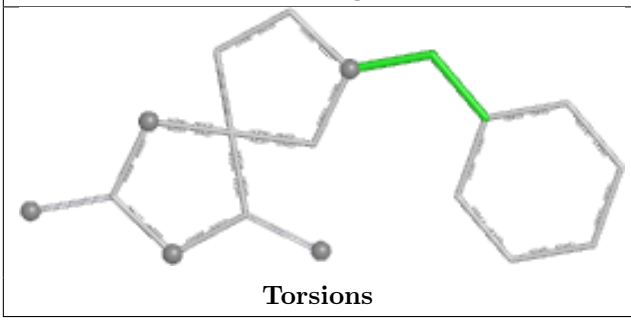
Ligand A1BCA A 402



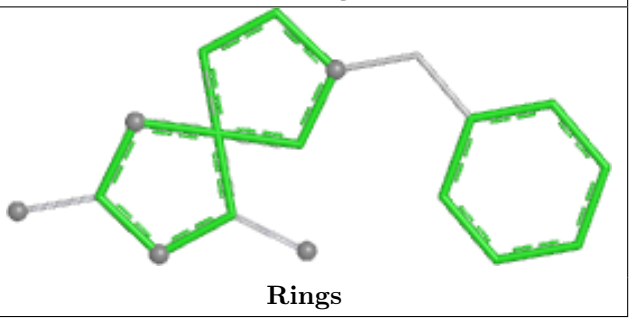
Bond lengths



Bond angles

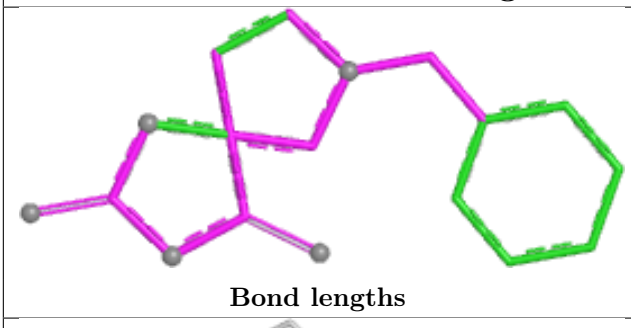


Torsions

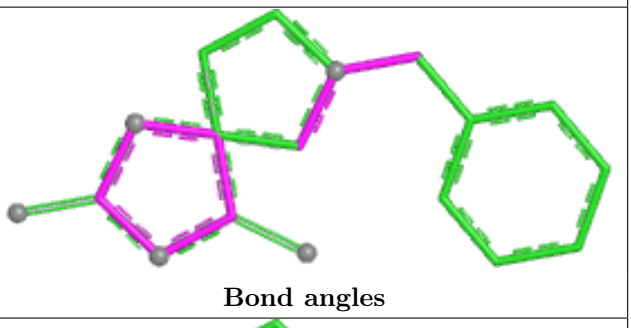


Rings

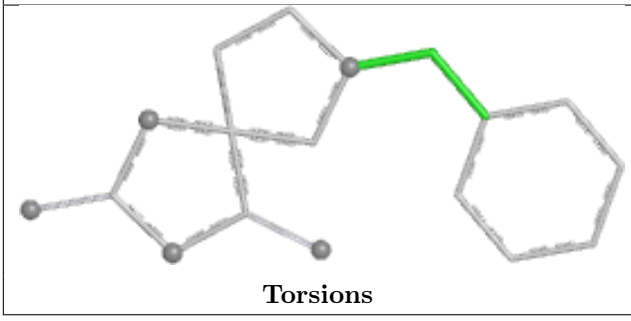
Ligand A1BCA D 403



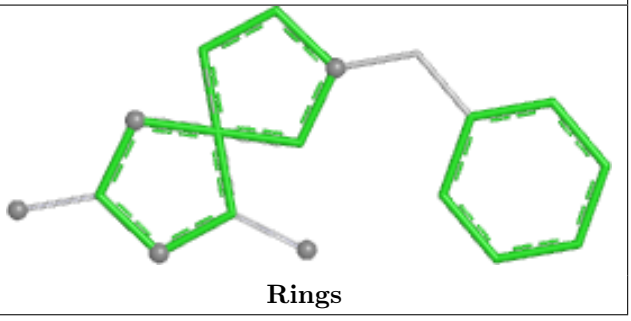
Bond lengths



Bond angles



Torsions



Rings

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, 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	335/342 (97%)	0.72	50 (14%) 7 6	19, 47, 122, 214	0
1	D	338/342 (98%)	0.55	32 (9%) 15 15	16, 47, 90, 115	8 (2%)
2	B	834/835 (99%)	-0.12	11 (1%) 74 76	10, 30, 65, 105	12 (1%)
2	E	806/835 (96%)	0.53	110 (13%) 8 7	12, 47, 118, 170	10 (1%)
3	C	73/77 (94%)	0.07	8 (10%) 12 11	25, 50, 176, 226	0
3	F	73/77 (94%)	1.18	23 (31%) 1 1	35, 87, 188, 230	0
All	All	2459/2508 (98%)	0.34	234 (9%) 15 15	10, 39, 112, 230	30 (1%)

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	90[A]	LEU	8.8
2	E	364[A]	SER	8.3
1	D	91[A]	VAL	8.3
2	E	203[A]	VAL	6.9
1	D	0	ALA	6.2
1	A	50	VAL	5.9
1	A	65	ALA	5.7
1	A	51	LEU	5.6
1	D	93[A]	GLU	5.6
2	E	90	PHE	5.1
1	A	54	GLU	5.1
1	A	44	ALA	5.0
1	D	341	ALA	5.0
1	A	341	ALA	4.9
2	E	56	ALA	4.8
1	A	48	LEU	4.8
3	F	17	C	4.6
1	A	47	ALA	4.6
1	D	1	MET	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	62	ARG	4.4
1	A	43	LEU	4.3
1	A	49	ALA	4.3
2	E	72	ALA	4.2
1	A	2	LEU	4.2
2	E	-2	SER	4.2
2	E	300	LEU	4.1
1	A	0	ALA	4.0
2	E	135	ALA	4.0
2	E	319	ALA	3.9
2	E	341	VAL	3.9
2	E	330	ALA	3.9
2	E	321	ALA	3.8
2	E	69	ARG	3.8
2	E	107	GLY	3.8
2	E	71	CYS	3.7
1	A	154	ALA	3.6
1	D	153	PRO	3.6
2	E	87	ALA	3.6
1	A	272	ILE	3.6
1	D	180	GLN	3.6
1	A	52	PRO	3.5
3	F	22	U	3.5
2	B	831	GLY	3.5
1	A	41	LEU	3.4
2	E	46	VAL	3.4
1	A	152	HIS	3.4
2	B	62	THR	3.4
1	A	1	MET	3.4
2	E	142	VAL	3.3
2	E	102	GLY	3.3
2	E	315	VAL	3.3
1	D	201	ARG	3.3
1	D	202	THR	3.3
2	E	133	LEU	3.3
1	A	153	PRO	3.3
2	E	110	THR	3.3
2	E	100	LEU	3.2
2	E	334	VAL	3.2
2	E	70	ALA	3.2
2	E	126	CYS	3.2
1	A	45	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
2	E	202[A]	ARG	3.2
2	E	306	LYS	3.2
3	F	3	C	3.2
1	A	4	PRO	3.2
2	E	83	ILE	3.1
2	B	120	ASN	3.1
3	F	4	C	3.1
2	E	333	GLU	3.1
2	B	-2	SER	3.1
2	E	141	LEU	3.1
1	A	40	PRO	3.1
2	E	310	ALA	3.1
1	A	91	VAL	3.1
2	E	97	VAL	3.1
3	F	5	A	3.1
2	E	131	LEU	3.0
1	A	53	LYS	3.0
2	E	103	ALA	3.0
2	E	95	LEU	3.0
1	A	12	ASP	3.0
1	A	276	ALA	3.0
2	E	559	PRO	2.9
1	A	206	ASP	2.9
2	E	328	GLY	2.9
1	A	10	ALA	2.9
3	C	17	C	2.9
1	D	271	LYS	2.9
2	E	48	GLY	2.9
2	E	47	ASP	2.9
2	E	336	ALA	2.9
3	F	19	G	2.9
2	E	335	ARG	2.8
1	A	160	THR	2.8
1	A	156	GLY	2.8
1	A	157	GLU	2.8
3	C	22	U	2.8
2	E	92	VAL	2.8
2	B	408	ASP	2.8
2	E	104	THR	2.8
1	D	4	PRO	2.8
2	E	205[A]	PRO	2.8
2	E	301	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	38	ARG	2.7
2	E	78	ARG	2.7
3	C	4	C	2.7
2	E	41	ILE	2.7
1	A	340	GLY	2.7
2	E	304	GLU	2.7
2	E	125	ILE	2.7
3	F	68	C	2.7
2	E	303	ILE	2.7
2	E	323	ILE	2.7
2	E	79	GLN	2.7
2	E	143	LEU	2.7
3	F	48	U	2.7
2	E	294	GLY	2.7
2	E	296	THR	2.6
1	D	340	GLY	2.6
2	E	138	SER	2.6
2	E	332	THR	2.6
2	E	96	VAL	2.6
1	D	5	GLU	2.6
2	E	82	GLU	2.6
2	B	618	MET	2.6
2	E	201[A]	SER	2.6
1	D	6	ALA	2.6
2	E	89	ASN	2.6
2	E	140	ILE	2.5
2	E	44	GLY	2.5
3	F	55	U	2.5
1	D	203	ASP	2.5
1	A	64	ASN	2.5
1	D	268	PHE	2.5
2	E	607	VAL	2.5
2	E	327	MET	2.5
3	C	73	C	2.5
2	E	213	TRP	2.5
1	A	3	SER	2.5
2	E	218	GLN	2.5
2	E	598	GLN	2.5
1	D	53	LYS	2.5
1	A	63	VAL	2.4
3	F	2	G	2.4
2	E	80	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	452	HIS	2.4
1	D	269	ALA	2.4
3	C	3	C	2.4
1	A	35	LEU	2.4
2	E	249	LEU	2.4
2	B	64	TYR	2.4
1	D	204	GLU	2.4
2	E	75	ILE	2.4
3	F	57	C	2.4
3	F	63	C	2.4
2	E	360	LEU	2.4
2	E	312	VAL	2.4
1	D	54	GLU	2.4
2	E	109	PHE	2.3
1	A	69	ALA	2.3
1	D	106	ALA	2.3
1	D	276	ALA	2.3
2	E	93	GLY	2.3
1	D	206	ASP	2.3
3	F	54	G	2.3
2	E	152	ALA	2.3
2	E	108	GLY	2.3
2	E	302	GLY	2.3
2	E	43	LEU	2.3
2	E	77	ASP	2.3
2	E	161	ASP	2.3
3	F	72	C	2.3
1	D	88[A]	ALA	2.3
3	F	51	G	2.3
2	E	599	THR	2.3
2	E	391	ALA	2.3
2	B	302	GLY	2.2
2	B	362	LEU	2.2
2	E	359	ARG	2.2
2	E	49	PRO	2.2
2	E	217	VAL	2.2
2	E	122	ASP	2.2
1	D	270	ASN	2.2
2	E	555	GLU	2.2
1	D	57	ALA	2.2
2	E	556	ALA	2.2
1	D	205	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	123	GLY	2.2
1	A	201	ARG	2.2
3	C	1	G	2.2
3	F	1	G	2.2
2	E	602	VAL	2.2
2	E	307	LEU	2.2
2	E	603	GLY	2.2
1	A	29	ARG	2.2
2	E	339	THR	2.2
1	D	149	PRO	2.2
2	E	101	PRO	2.2
3	C	48	U	2.2
1	A	106	ALA	2.2
2	E	297	ALA	2.2
3	F	53	G	2.2
3	F	71	G	2.2
2	E	324	GLY	2.1
3	F	73	C	2.1
1	A	271	LYS	2.1
1	A	150	ALA	2.1
2	E	362	LEU	2.1
2	E	254	ARG	2.1
2	E	299	THR	2.1
1	A	158	GLN	2.1
1	D	16	GLN	2.1
2	B	115	LYS	2.1
2	B	412	ASP	2.1
2	E	530	ALA	2.1
3	F	56	U	2.1
3	F	64	G	2.1
2	E	105	LEU	2.1
2	E	322	ALA	2.1
1	D	94[A]	GLY	2.1
1	A	105	PRO	2.1
1	A	76	GLU	2.1
3	C	2	G	2.1
2	E	-1	ASN	2.1
2	E	326	VAL	2.0
1	D	38	ARG	2.0
1	A	70	ALA	2.0
2	E	283	SER	2.0
2	E	277	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
3	F	18	G	2.0
1	A	274	GLY	2.0
1	A	149	PRO	2.0
3	F	67	C	2.0
2	E	397	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	GOL	E	901	6/6	0.67	0.22	55,58,62,65	0
10	PGE	B	906	10/10	0.74	0.17	31,44,52,58	0
6	ACT	B	915	4/4	0.75	0.18	35,36,41,49	0
7	NA	E	906	1/1	0.75	0.20	43,43,43,43	0
8	GOL	B	903	6/6	0.76	0.20	54,59,61,63	0
5	A1BCA	D	403	18/18	0.78	0.17	31,61,93,95	0
10	PGE	D	402	10/10	0.78	0.17	41,46,54,56	0
6	ACT	A	403	4/4	0.79	0.20	51,52,57,59	0
5	A1BCA	A	402	18/18	0.80	0.16	33,52,75,82	0
6	ACT	E	903	4/4	0.81	0.18	49,53,55,56	0
9	DMS	E	908	4/4	0.81	0.22	26,33,61,64	0
11	EPE	B	909	15/15	0.81	0.17	49,58,71,76	0
8	GOL	E	907	6/6	0.82	0.16	61,65,75,78	0
9	DMS	D	401	4/4	0.82	0.23	46,61,62,74	0
6	ACT	E	905	4/4	0.82	0.22	55,62,65,66	0
8	GOL	B	914	6/6	0.83	0.12	44,52,57,62	0
8	GOL	B	902	6/6	0.84	0.16	45,55,65,70	0
6	ACT	B	918	4/4	0.84	0.13	27,31,40,47	0

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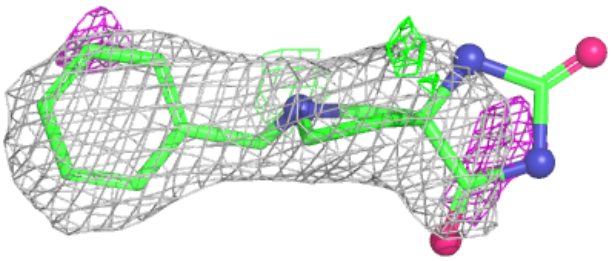
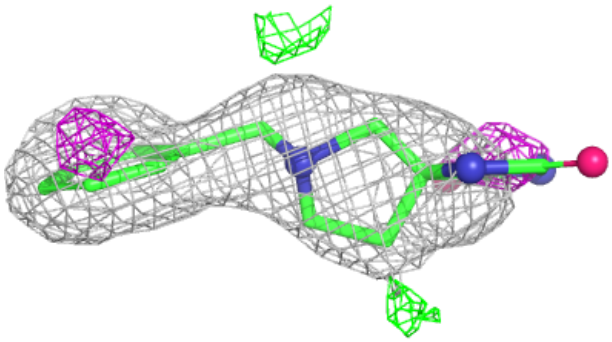
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ACT	B	916	4/4	0.85	0.14	38,48,50,50	0
8	GOL	B	907	6/6	0.85	0.14	44,46,48,51	0
6	ACT	B	917	4/4	0.86	0.23	33,35,43,46	0
6	ACT	B	913	4/4	0.86	0.13	43,46,48,49	0
8	GOL	B	904	6/6	0.87	0.12	47,53,58,59	0
11	EPE	B	910	15/15	0.87	0.15	44,59,70,71	0
6	ACT	E	909	4/4	0.88	0.12	51,53,55,57	0
8	GOL	E	902	6/6	0.88	0.11	40,41,45,48	0
8	GOL	B	919	6/6	0.88	0.27	30,40,46,53	0
6	ACT	B	912	4/4	0.89	0.11	35,44,50,51	0
8	GOL	F	101	6/6	0.89	0.19	44,47,50,52	0
9	DMS	B	908	4/4	0.91	0.12	31,45,51,54	0
9	DMS	B	905	4/4	0.92	0.19	34,42,47,58	0
8	GOL	B	901	6/6	0.92	0.10	25,30,37,37	0
6	ACT	B	911	4/4	0.93	0.11	30,31,32,35	0
6	ACT	E	904	4/4	0.93	0.09	35,41,42,45	0
7	NA	A	404	1/1	0.96	0.05	33,33,33,33	0
4	MG	C	101	1/1	0.97	0.07	35,35,35,35	0
4	MG	D	404	1/1	0.99	0.02	34,34,34,34	0
4	MG	A	401	1/1	0.99	0.02	26,26,26,26	0
4	MG	C	102	1/1	0.99	0.03	37,37,37,37	0

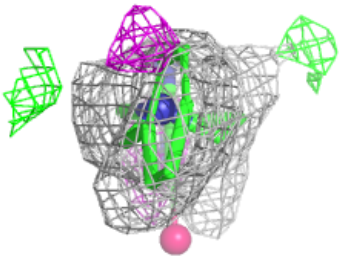
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1BCA 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)

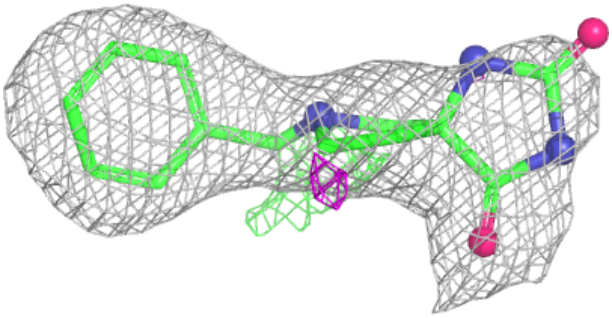


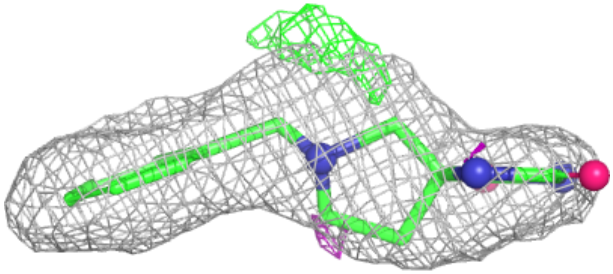


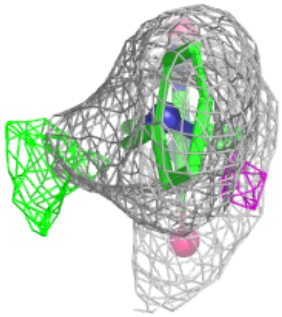


Electron density around A1BCA A 402:

$2mF_o$-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.