



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 01:26 PM GMT

PDB ID : 1D8T
Title : CRYSTAL STRUCTURE OF ELONGATION FACTOR, TU (EF-TU-MGGDP) COMPLEXED WITH GE2270A, A THIAZOLYL PEPTIDE ANTIBIOTIC
Authors : Heffron, S.E.; Journak, F.
Deposited on : 1999-10-25
Resolution : 2.35 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

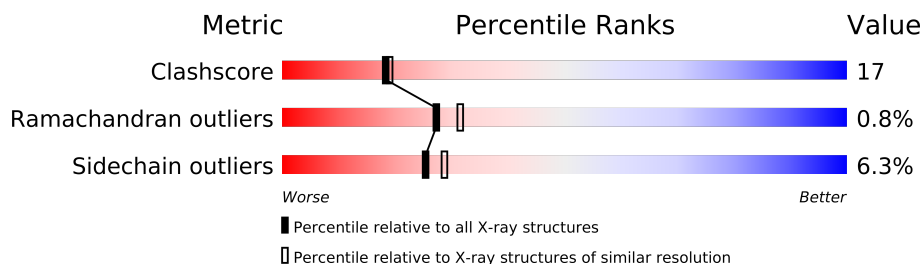
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.35 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))
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	393	
1	B	393	
2	C	15	
2	D	15	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6718 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	1	0
			3024	1911	520	580	13			
1	B	385	Total	C	N	O	S	0	0	0
			2963	1873	510	567	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	393	GLY	SER	CONFLICT	UNP P0A6N1
B	393	GLY	SER	CONFLICT	UNP P0A6N1

- Molecule 2 is a protein called THIOCILLIN GE2270.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	S	0	0	1
			87	56	15	10	6			
2	D	15	Total	C	N	O	S	0	0	1
			87	56	15	10	6			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

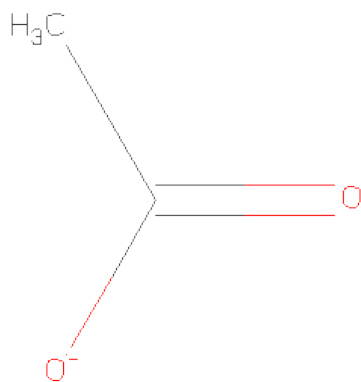
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
4	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	227	Total O 227 227	0	0
6	B	146	Total O 146 146	0	0
6	C	4	Total O 4 4	0	0
6	D	2	Total O 2 2	0	0

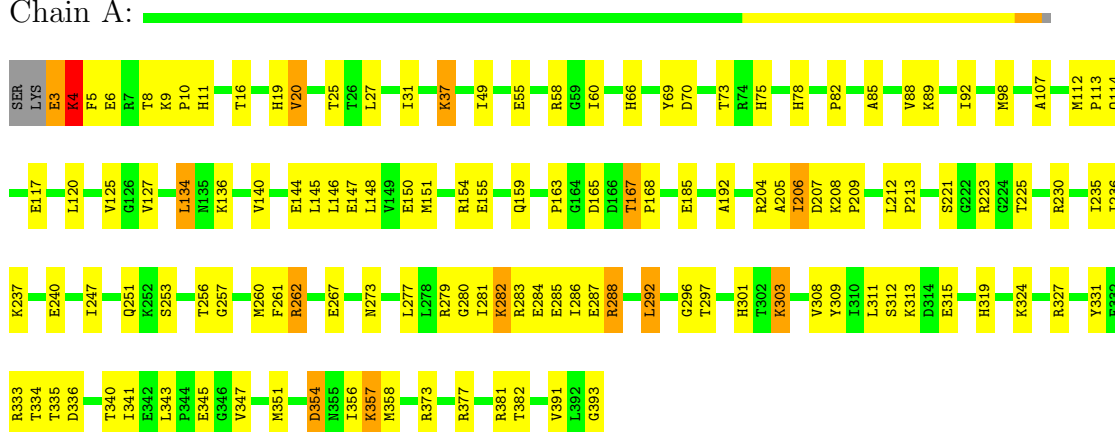
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

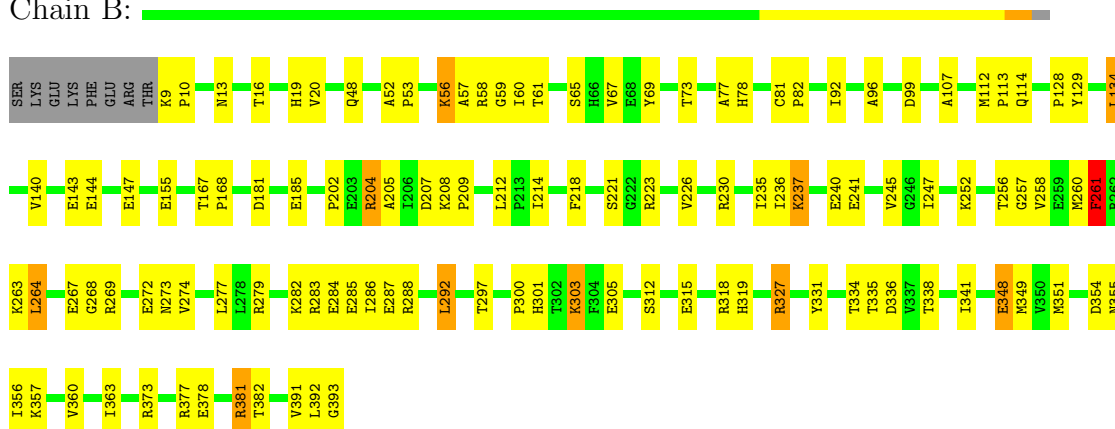
• Molecule 1: ELONGATION FACTOR TU

Chain A:



• Molecule 1: ELONGATION FACTOR TU

Chain B:



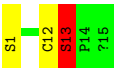
• Molecule 2: THIOCILLIN GE2270

Chain C:



• Molecule 2: THIOCILLIN GE2270

Chain D: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.47Å 45.17Å 144.00Å 90.00° 94.64° 90.00°	Depositor
Resolution (Å)	24.44 – 2.35	Depositor
% Data completeness (in resolution range)	86.3 (24.44-2.35)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6718	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, NH2, MEN, ACT, MH6, BB9, BB8, BB7, BB6

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	0.37	0/3084	0.68	0/4173
1	B	0.34	0/3018	0.65	0/4086
2	C	2.02	1/23 (4.3%)	2.05	1/26 (3.8%)
2	D	1.95	1/23 (4.3%)	2.10	0/26
All	All	0.39	2/6148 (0.0%)	0.68	1/8311 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	2	0
2	D	2	0
All	All	4	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	SER	CA-CB	-6.38	1.43	1.52
2	D	1	SER	CA-CB	-6.33	1.43	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	13	SER	CB-CA-C	5.10	119.79	110.10

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	SER	CA
2	C	8	BB8	CB
2	D	1	SER	CA
2	D	8	BB8	CB

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3024	0	3030	118	0
1	B	2963	0	2974	95	0
2	C	87	0	56	2	0
2	D	87	0	56	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	28	0	12	1	0
4	B	28	0	12	0	0
5	A	76	0	57	7	0
5	B	44	0	33	3	0
6	A	227	0	0	6	0
6	B	146	0	0	2	0
6	C	4	0	0	0	0
6	D	2	0	0	0	0
All	All	6718	0	6230	213	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (213) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:327:ARG:O	1:B:327:ARG:HD2	1.46	1.13
1:B:327:ARG:HD3	1:B:338:THR:HG23	1.28	1.11
1:B:348:GLU:CD	1:B:348:GLU:H	1.72	0.93
1:A:279:ARG:HE	1:A:280:GLY:H	1.20	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:11:HIS:HD2	1:A:75:HIS:HD2	1.18	0.86
1:A:11:HIS:CD2	1:A:75:HIS:HD2	1.99	0.81
1:B:327:ARG:C	1:B:327:ARG:HD2	2.06	0.76
1:B:327:ARG:CD	1:B:338:THR:HG23	2.12	0.75
1:A:4:LYS:HG3	1:A:8:THR:H	1.53	0.74
1:B:381:ARG:HD3	1:B:382:THR:N	2.03	0.73
1:B:288:ARG:HG2	1:B:335:THR:CG2	2.18	0.73
1:A:147:GLU:O	1:A:151:MET:HG3	1.89	0.72
1:A:281:ILE:HG21	1:A:286:ILE:HD11	1.72	0.71
1:B:218:PHE:HB2	1:B:226:VAL:HG13	1.72	0.71
1:B:282:LYS:HB2	1:B:285:GLU:OE2	1.90	0.71
1:A:279:ARG:NE	1:A:279:ARG:HA	2.05	0.70
1:B:282:LYS:HE3	1:B:283:ARG:H	1.57	0.70
1:B:327:ARG:HD3	1:B:338:THR:CG2	2.16	0.69
1:B:258:VAL:O	1:B:264:LEU:HD23	1.91	0.68
1:A:237:LYS:HG2	1:A:240:GLU:CD	2.14	0.68
1:A:3:GLU:OE1	1:A:4:LYS:HD3	1.94	0.67
1:B:381:ARG:HD3	1:B:382:THR:H	1.59	0.67
1:A:204:ARG:HB2	1:A:207:ASP:OD2	1.95	0.66
1:A:11:HIS:HD2	1:A:75:HIS:CD2	2.09	0.66
1:A:3:GLU:O	1:A:5:PHE:CD2	2.49	0.66
1:B:218:PHE:HB2	1:B:226:VAL:CG1	2.26	0.66
1:A:150:GLU:O	1:A:154:ARG:HG3	1.95	0.66
1:A:324:LYS:HE3	1:A:347:VAL:O	1.97	0.65
1:B:204:ARG:HB2	1:B:207:ASP:OD2	1.94	0.65
1:B:56:LYS:HD2	1:B:56:LYS:O	1.96	0.65
1:A:163:PRO:O	1:A:167:THR:HG22	1.96	0.65
1:A:148:LEU:HA	1:A:151:MET:HE2	1.79	0.64
1:B:235:ILE:CD1	1:B:269:ARG:HG2	2.27	0.64
1:A:4:LYS:CG	1:A:8:THR:H	2.10	0.64
1:B:205:ALA:HA	1:B:208:LYS:HD2	1.79	0.64
1:A:282:LYS:HE3	1:A:284:GLU:OE2	1.98	0.64
1:A:192:ALA:HB3	5:A:3030:ACT:H3	1.79	0.63
1:B:235:ILE:HD12	1:B:268:GLY:O	1.99	0.62
1:A:303:LYS:HB3	1:A:393:GLY:HA3	1.81	0.62
1:A:3:GLU:CD	1:A:3:GLU:C	2.58	0.62
1:A:331:TYR:HB2	1:A:377:ARG:HD2	1.82	0.62
1:A:19:HIS:ND1	1:A:114:GLN:HB2	2.14	0.62
1:A:155:GLU:O	1:A:159:GLN:HG3	2.00	0.61
1:B:230:ARG:HB2	1:B:273:ASN:ND2	2.16	0.61
1:B:99:ASP:OD1	1:B:202:PRO:HB3	2.01	0.60
1:A:284:GLU:H	1:A:284:GLU:CD	2.04	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:327:ARG:CG	1:A:340:THR:HG22	2.32	0.60
1:A:336:ASP:OD1	1:A:377:ARG:HD3	2.01	0.60
1:B:16:THR:HG23	1:B:78:HIS:CE1	2.36	0.59
1:A:4:LYS:HD2	1:A:8:THR:OG1	2.03	0.59
1:B:282:LYS:HE3	1:B:283:ARG:N	2.17	0.59
1:A:223:ARG:HH11	2:C:12:BB9:HN1	1.51	0.59
1:A:69:TYR:OH	1:A:78:HIS:HD2	1.85	0.59
1:A:154:ARG:NH2	1:A:167:THR:O	2.36	0.58
1:A:356:ILE:HG13	1:A:357:LYS:N	2.20	0.57
1:A:288:ARG:HG2	1:A:335:THR:CG2	2.35	0.56
1:A:237:LYS:HG2	1:A:240:GLU:HG3	1.87	0.56
1:B:56:LYS:C	1:B:56:LYS:HD2	2.25	0.56
1:B:107:ALA:HB2	1:B:134:LEU:HD22	1.87	0.56
1:A:257:GLY:HA3	2:C:13:SER:OG	2.05	0.56
1:B:140:VAL:HG13	5:B:3011:ACT:H3	1.87	0.56
1:B:331:TYR:HB2	1:B:377:ARG:HD2	1.87	0.56
1:B:338:THR:HB	1:B:363:ILE:HD13	1.88	0.56
1:A:4:LYS:CE	1:A:8:THR:OG1	2.54	0.55
1:A:313:LYS:HG3	1:A:319:HIS:CD2	2.40	0.55
1:A:4:LYS:HE2	1:A:8:THR:OG1	2.07	0.55
1:A:205:ALA:HA	1:A:208:LYS:HD2	1.88	0.55
1:B:348:GLU:N	1:B:348:GLU:CD	2.50	0.55
1:A:237:LYS:HG2	1:A:240:GLU:CG	2.36	0.55
1:A:279:ARG:HE	1:A:280:GLY:N	1.97	0.54
1:B:128:PRO:HB2	1:B:129:TYR:CD2	2.43	0.54
1:B:96:ALA:HB2	6:B:2029:HOH:O	2.07	0.54
1:B:241:GLU:OE1	1:B:252:LYS:HE2	2.07	0.54
1:B:312:SER:OG	1:B:315:GLU:HG3	2.07	0.54
1:B:260:MET:HE2	1:B:272:GLU:HB3	1.90	0.53
1:B:356:ILE:HG13	1:B:357:LYS:N	2.22	0.53
1:A:212:LEU:HD23	1:A:212:LEU:C	2.29	0.53
1:A:286:ILE:HG22	1:A:287:GLU:N	2.24	0.53
1:B:223:ARG:HH11	2:D:13:SER:H	1.57	0.53
1:A:88:VAL:O	1:A:92:ILE:HG12	2.09	0.52
1:B:301:HIS:CE1	1:B:391:VAL:HG11	2.45	0.52
1:A:296:GLY:HA2	6:A:2146:HOH:O	2.09	0.52
1:A:356:ILE:HG13	1:A:357:LYS:H	1.75	0.52
1:A:381:ARG:HD2	1:A:382:THR:H	1.73	0.52
1:A:4:LYS:CD	1:A:8:THR:OG1	2.58	0.51
1:B:341:ILE:O	1:B:341:ILE:HG13	2.10	0.51
1:A:10:PRO:HD2	1:A:73:THR:O	2.10	0.51
1:A:20:VAL:HG22	1:A:114:GLN:OE1	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:60:ILE:HG12	1:A:311:LEU:CD2	2.41	0.51
1:B:61:THR:HG23	6:B:2018:HOH:O	2.11	0.50
1:B:356:ILE:HG13	1:B:357:LYS:H	1.76	0.50
1:A:165:ASP:O	5:A:3004:ACT:H2	2.11	0.50
1:B:16:THR:HG23	1:B:78:HIS:NE2	2.27	0.50
1:A:312:SER:OG	1:A:315:GLU:HG3	2.11	0.50
1:A:282:LYS:NZ	6:A:2164:HOH:O	2.45	0.50
1:A:140:VAL:HG11	1:A:145:LEU:HD23	1.93	0.49
1:A:146:LEU:O	1:A:150:GLU:HG3	2.12	0.49
1:A:112:MET:HB3	1:A:113:PRO:HD2	1.94	0.49
1:B:237:LYS:HB2	1:B:240:GLU:OE2	2.12	0.49
1:B:256:THR:HG21	1:B:279:ARG:HB3	1.94	0.49
1:B:288:ARG:NH1	1:B:334:THR:HB	2.29	0.48
1:B:19:HIS:ND1	1:B:114:GLN:HB2	2.28	0.48
1:A:163:PRO:O	1:A:167:THR:CG2	2.62	0.48
1:A:288:ARG:NH1	1:A:334:THR:O	2.47	0.48
1:A:261:PHE:O	1:A:262:ARG:HB2	2.12	0.48
1:A:3:GLU:O	1:A:3:GLU:CG	2.61	0.48
1:A:279:ARG:NE	1:A:279:ARG:CA	2.74	0.48
1:B:209:PRO:HB3	1:B:297:THR:HG21	1.95	0.48
1:B:181:ASP:O	1:B:185:GLU:HG3	2.12	0.48
1:A:6:GLU:HB3	6:A:2005:HOH:O	2.13	0.48
1:A:140:VAL:CG1	1:A:145:LEU:HD23	2.44	0.48
1:A:206:ILE:CG1	1:A:235:ILE:HD11	2.44	0.47
1:B:319:HIS:H	5:B:3009:ACT:H2	1.79	0.47
1:A:209:PRO:HB3	1:A:297:THR:HG21	1.97	0.47
1:B:260:MET:CE	1:B:274:VAL:HG12	2.44	0.47
1:B:57:ALA:C	1:B:59:GLY:H	2.17	0.47
1:A:82:PRO:HB3	5:A:3021:ACT:H1	1.96	0.47
1:A:251:GLN:HE22	1:A:285:GLU:HB3	1.80	0.47
1:B:288:ARG:HG2	1:B:335:THR:HG22	1.96	0.47
1:B:305:GLU:CD	1:B:357:LYS:HE3	2.35	0.47
1:B:237:LYS:HD3	1:B:240:GLU:OE2	2.15	0.47
1:A:107:ALA:HB2	1:A:134:LEU:HD22	1.96	0.47
1:A:3:GLU:O	1:A:5:PHE:N	2.48	0.47
1:A:4:LYS:NZ	6:A:2001:HOH:O	2.48	0.47
1:A:148:LEU:HA	1:A:151:MET:CE	2.45	0.47
1:A:98:MET:HB2	5:A:3007:ACT:H2	1.97	0.47
1:A:236:ILE:O	1:A:267:GLU:HA	2.15	0.47
1:A:381:ARG:HD2	1:A:382:THR:N	2.30	0.46
1:B:60:ILE:HG22	1:B:61:THR:N	2.30	0.46
1:B:237:LYS:HG3	1:B:267:GLU:CB	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:10:PRO:HD2	1:B:73:THR:O	2.15	0.46
1:A:60:ILE:HG12	1:A:311:LEU:HD21	1.96	0.46
1:A:192:ALA:CB	5:A:3030:ACT:H3	2.45	0.46
1:B:13:ASN:OD1	1:B:77:ALA:HB3	2.16	0.46
1:A:4:LYS:HG2	1:A:9:LYS:HG3	1.98	0.46
1:B:112:MET:HB3	1:B:113:PRO:CD	2.46	0.46
1:B:245:VAL:HG13	1:B:300:PRO:HD3	1.97	0.46
1:A:55:GLU:OE2	1:A:66:HIS:NE2	2.39	0.46
1:A:303:LYS:HB3	1:A:393:GLY:CA	2.45	0.45
1:A:27:LEU:O	1:A:31:ILE:HG13	2.16	0.45
1:B:236:ILE:O	1:B:267:GLU:HA	2.16	0.45
1:A:120:LEU:HD23	1:A:120:LEU:C	2.37	0.45
1:A:301:HIS:CE1	1:A:391:VAL:HG11	2.51	0.45
1:A:336:ASP:OD2	1:A:377:ARG:NH1	2.50	0.45
1:A:221:SER:HA	5:A:3028:ACT:O	2.17	0.45
1:A:127:VAL:HG22	5:A:3007:ACT:H3	1.99	0.45
1:B:237:LYS:HG3	1:B:267:GLU:HB2	1.99	0.45
1:A:256:THR:CG2	1:A:279:ARG:HB2	2.47	0.45
1:B:349:MET:HE3	1:B:351:MET:SD	2.56	0.45
1:B:167:THR:HA	1:B:168:PRO:HD3	1.79	0.45
1:B:282:LYS:CE	1:B:283:ARG:H	2.29	0.45
1:B:354:ASP:OD1	1:B:355:ASN:N	2.46	0.44
1:A:112:MET:HB3	1:A:113:PRO:CD	2.47	0.44
1:B:257:GLY:HA3	2:D:13:SER:OG	2.18	0.44
1:B:52:ALA:HA	1:B:53:PRO:HD3	1.79	0.44
1:B:286:ILE:HG22	1:B:287:GLU:N	2.33	0.44
1:A:308:VAL:HG12	1:A:309:TYR:N	2.33	0.44
1:B:99:ASP:CG	1:B:202:PRO:HB3	2.38	0.44
1:A:253:SER:HB2	1:A:281:ILE:HD11	1.99	0.43
1:A:343:LEU:HD13	1:A:347:VAL:HG12	2.00	0.43
1:B:381:ARG:CD	1:B:382:THR:N	2.78	0.43
1:A:308:VAL:CG1	1:A:309:TYR:N	2.81	0.43
1:A:283:ARG:HB3	1:A:284:GLU:OE2	2.17	0.43
1:A:3:GLU:O	1:A:3:GLU:CD	2.57	0.43
1:A:4:LYS:HG2	1:A:9:LYS:H	1.82	0.43
1:A:327:ARG:HH11	1:A:340:THR:CG2	2.31	0.43
1:A:327:ARG:HD2	1:A:340:THR:HG22	1.98	0.43
1:A:37:LYS:HE3	1:A:185:GLU:OE2	2.17	0.43
1:B:288:ARG:HH12	5:B:3012:ACT:H3	1.84	0.43
1:B:264:LEU:HD11	2:D:13:SER:N	2.34	0.43
1:B:143:GLU:O	1:B:147:GLU:HG3	2.19	0.43
1:B:223:ARG:HH11	2:D:12:BB9:HN1	1.67	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:341:ILE:HG23	1:A:358:MET:HB2	2.00	0.43
1:B:212:LEU:HD23	1:B:212:LEU:C	2.40	0.42
1:B:58:ARG:HG3	1:B:58:ARG:O	2.19	0.42
1:B:261:PHE:O	1:B:261:PHE:CG	2.72	0.42
1:A:85:ALA:O	1:A:89:LYS:HG3	2.19	0.42
1:A:125:VAL:HB	1:A:373:ARG:NH2	2.34	0.42
1:A:167:THR:HA	1:A:168:PRO:HD3	1.91	0.42
1:A:37:LYS:HB3	1:A:37:LYS:NZ	2.34	0.42
1:A:260:MET:HG3	1:A:273:ASN:O	2.20	0.42
1:A:324:LYS:NZ	6:A:2188:HOH:O	2.52	0.42
1:A:324:LYS:HE2	1:A:343:LEU:HB2	2.01	0.42
1:A:351:MET:O	1:A:354:ASP:HB2	2.20	0.42
1:B:327:ARG:CD	1:B:338:THR:CG2	2.90	0.42
1:A:3:GLU:OE1	1:A:4:LYS:CD	2.67	0.42
1:A:136:LYS:HG2	4:A:999:GDP:C6	2.55	0.42
1:B:260:MET:HE3	1:B:274:VAL:HG12	2.01	0.41
1:B:112:MET:HB3	1:B:113:PRO:HD2	2.00	0.41
1:B:277:LEU:HB2	2:D:12:BB9:CB	2.50	0.41
1:A:58:ARG:HH11	1:A:58:ARG:HG2	1.84	0.41
1:B:303:LYS:HB3	1:B:393:GLY:H	1.85	0.41
1:B:81:CYS:HA	1:B:82:PRO:HD3	1.81	0.41
1:A:212:LEU:HD23	1:A:212:LEU:O	2.20	0.41
1:B:318:ARG:NH1	1:B:378:GLU:OE2	2.44	0.41
1:A:25:THR:HG23	1:A:49:ILE:HG22	2.02	0.41
1:B:327:ARG:C	1:B:327:ARG:CD	2.85	0.41
1:B:69:TYR:OH	1:B:78:HIS:HD2	2.04	0.41
1:B:303:LYS:HA	1:B:360:VAL:O	2.20	0.41
1:A:206:ILE:HG13	1:A:235:ILE:HG13	2.02	0.41
1:A:37:LYS:HE2	6:A:2024:HOH:O	2.20	0.41
1:B:303:LYS:HG2	1:B:392:LEU:HB2	2.02	0.41
1:A:213:PRO:HG3	1:A:333:ARG:HD3	2.03	0.41
1:B:67:VAL:CG2	1:B:78:HIS:HB3	2.51	0.41
1:B:92:ILE:O	1:B:373:ARG:NE	2.53	0.41
1:B:282:LYS:HA	1:B:282:LYS:HD2	1.82	0.40
1:B:9:LYS:HA	1:B:10:PRO:HD3	1.98	0.40
1:A:292:LEU:HD12	1:A:292:LEU:HA	1.91	0.40
1:B:214:ILE:HD11	1:B:292:LEU:HD13	2.02	0.40
1:B:336:ASP:OD1	1:B:377:ARG:HD3	2.21	0.40
1:A:230:ARG:HB2	1:A:273:ASN:ND2	2.36	0.40
1:A:225:THR:O	1:A:277:LEU:HD12	2.22	0.40
1:B:57:ALA:C	1:B:59:GLY:N	2.75	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	390/393 (99%)	378 (97%)	10 (3%)	2 (0%)	38	45
1	B	383/393 (98%)	371 (97%)	10 (3%)	2 (0%)	38	45
2	C	4/15 (27%)	2 (50%)	1 (25%)	1 (25%)	0	0
2	D	4/15 (27%)	2 (50%)	1 (25%)	1 (25%)	0	0
All	All	781/816 (96%)	753 (96%)	22 (3%)	6 (1%)	27	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
2	C	13	SER
2	D	13	SER
1	B	261	PHE
1	A	247	ILE
1	B	247	ILE

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	324/325 (100%)	304 (94%)	20 (6%)	26	29
1	B	317/325 (98%)	298 (94%)	19 (6%)	27	32
2	C	3/4 (75%)	1 (33%)	2 (67%)	0	0
2	D	3/4 (75%)	2 (67%)	1 (33%)	0	0
All	All	647/658 (98%)	605 (94%)	42 (6%)	25	27

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	4	LYS
1	A	16	THR
1	A	20	VAL
1	A	37	LYS
1	A	70	ASP
1	A	117	GLU
1	A	134	LEU
1	A	144	GLU
1	A	167	THR
1	A	206	ILE
1	A	262	ARG
1	A	282	LYS
1	A	288	ARG
1	A	292	LEU
1	A	303	LYS
1	A	345[A]	GLU
1	A	345[B]	GLU
1	A	354	ASP
1	A	357	LYS
1	B	20	VAL
1	B	48	GLN
1	B	56	LYS
1	B	65	SER
1	B	134	LEU
1	B	144	GLU
1	B	155	GLU
1	B	204	ARG
1	B	221	SER
1	B	237	LYS
1	B	261	PHE
1	B	263	LYS
1	B	264	LEU
1	B	284	GLU
1	B	292	LEU
1	B	303	LYS
1	B	327	ARG
1	B	348	GLU
1	B	381	ARG
2	C	5	VAL
2	C	13	SER
2	D	13	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	75	HIS
1	A	78	HIS
1	A	251	GLN
1	A	273	ASN
1	A	329	GLN
1	B	11	HIS
1	B	75	HIS
1	B	78	HIS
1	B	273	ASN
1	B	329	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

18 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
2	BB9	C	10	2	2,4,6	4.90	2 (100%)	1,4,7	4.15	1 (100%)
2	MH6	C	11	2	2,3,6	1.04	0	0,3,7	0.00	-
2	BB9	C	12	2	2,4,6	3.62	1 (50%)	1,4,7	3.11	1 (100%)
2	BB9	C	2	2	3,5,6	1.77	1 (33%)	1,5,7	4.38	1 (100%)
2	MEN	C	3	2	7,7,9	2.33	2 (28%)	6,8,11	2.33	1 (16%)
2	BB6	C	4	2	5,6,7	2.43	3 (60%)	2,7,9	2.07	1 (50%)
2	BB7	C	6	2	7,8,9	2.20	3 (42%)	3,9,11	1.71	1 (33%)
2	BB8	C	8	2	11,11,13	2.08	4 (36%)	12,14,17	0.88	1 (8%)
2	BB9	C	9	2	2,4,6	3.93	1 (50%)	1,4,7	3.46	1 (100%)
2	BB9	D	10	2	2,4,6	5.25	2 (100%)	1,4,7	3.94	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MH6	D	11	2	2,3,6	1.01	0	0,3,7	0.00	-
2	BB9	D	12	2	2,4,6	3.50	1 (50%)	1,4,7	3.15	1 (100%)
2	BB9	D	2	2	3,5,6	1.92	2 (66%)	1,5,7	4.44	1 (100%)
2	MEN	D	3	2	7,7,9	1.99	3 (42%)	6,8,11	2.03	1 (16%)
2	BB6	D	4	2	5,6,7	2.19	3 (60%)	2,7,9	2.10	1 (50%)
2	BB7	D	6	2	7,8,9	2.51	3 (42%)	3,9,11	1.45	1 (33%)
2	BB8	D	8	2	11,11,13	2.99	6 (54%)	12,14,17	1.87	4 (33%)
2	BB9	D	9	2	2,4,6	3.23	1 (50%)	1,4,7	3.45	1 (100%)

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
2	BB9	C	10	2	-	0/0/2/6	0/0/0/0
2	MH6	C	11	2	-	0/0/0/6	0/0/0/0
2	BB9	C	12	2	-	0/0/2/6	0/0/0/0
2	BB9	C	2	2	-	0/0/4/6	0/0/0/0
2	MEN	C	3	2	-	0/6/6/10	0/0/0/0
2	BB6	C	4	2	-	0/0/6/8	0/0/0/0
2	BB7	C	6	2	-	0/1/9/11	0/0/0/0
2	BB8	C	8	2	1/1/2/3	0/8/8/12	0/1/1/1
2	BB9	C	9	2	-	0/0/2/6	0/0/0/0
2	BB9	D	10	2	-	0/0/2/6	0/0/0/0
2	MH6	D	11	2	-	0/0/0/6	0/0/0/0
2	BB9	D	12	2	-	0/0/2/6	0/0/0/0
2	BB9	D	2	2	-	0/0/4/6	0/0/0/0
2	MEN	D	3	2	-	0/6/6/10	0/0/0/0
2	BB6	D	4	2	-	0/0/6/8	0/0/0/0
2	BB7	D	6	2	-	0/1/9/11	0/0/0/0
2	BB8	D	8	2	1/1/2/3	0/8/8/12	0/1/1/1
2	BB9	D	9	2	-	0/0/2/6	0/0/0/0

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	10	BB9	CB-CA	7.14	1.40	1.33
2	D	8	BB8	CD1-CG	6.68	1.50	1.39
2	C	10	BB9	CB-CA	6.60	1.39	1.33
2	C	9	BB9	CB-CA	5.32	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	6	BB7	CA-CB	5.16	1.41	1.33
2	C	12	BB9	CB-CA	4.82	1.38	1.33
2	D	12	BB9	CB-CA	4.64	1.37	1.33
2	D	8	BB8	CG-CB	4.51	1.58	1.51
2	D	9	BB9	CB-CA	4.41	1.37	1.33
2	C	4	BB6	CA-CB	4.31	1.40	1.33
2	C	3	MEN	CB-CA	4.28	1.57	1.52
2	C	6	BB7	CA-CB	4.07	1.40	1.33
2	D	4	BB6	CA-CB	3.69	1.39	1.33
2	C	8	BB8	CG-CB	3.68	1.57	1.51
2	C	3	MEN	CB-CG	3.55	1.57	1.51
2	D	3	MEN	CB-CA	3.43	1.56	1.52
2	D	8	BB8	CA-N	3.28	1.53	1.47
2	C	8	BB8	CD1-CG	3.06	1.44	1.39
2	D	3	MEN	CB-CG	2.80	1.56	1.51
2	C	8	BB8	CD2-CG	2.60	1.43	1.39
2	C	6	BB7	CB1-CB	2.54	1.55	1.50
2	D	6	BB7	CB1-CB	2.50	1.55	1.50
2	D	8	BB8	CA-CB	2.38	1.57	1.53
2	D	8	BB8	C-CA	2.36	1.56	1.51
2	D	2	BB9	O-C	2.31	1.24	1.17
2	D	2	BB9	CB-CA	2.29	1.38	1.34
2	C	2	BB9	O-C	2.28	1.24	1.17
2	C	6	BB7	O-C	2.26	1.24	1.17
2	D	4	BB6	O-C	2.22	1.24	1.17
2	D	6	BB7	O-C	2.22	1.24	1.17
2	C	4	BB6	O-C	2.16	1.24	1.17
2	D	8	BB8	CE1-CD1	2.16	1.44	1.39
2	C	10	BB9	CA-N	2.13	1.38	1.34
2	C	8	BB8	CA-CB	2.10	1.57	1.53
2	D	3	MEN	C-CA	2.10	1.55	1.51
2	C	4	BB6	CD-CB	2.09	1.55	1.50
2	D	10	BB9	CA-N	2.07	1.38	1.34
2	D	4	BB6	CD-CB	2.01	1.55	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	MEN	CA-CB-CG	5.55	121.59	112.04
2	D	3	MEN	CA-CB-CG	4.75	120.20	112.04
2	D	2	BB9	CB-CA-N	-4.44	113.58	123.34
2	C	2	BB9	CB-CA-N	-4.38	113.71	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	10	BB9	CB-CA-N	-4.15	112.56	122.77
2	D	10	BB9	CB-CA-N	-3.94	113.09	122.77
2	C	9	BB9	CB-CA-N	-3.46	114.25	122.77
2	D	9	BB9	CB-CA-N	-3.45	114.29	122.77
2	D	12	BB9	CB-CA-N	-3.15	115.03	122.77
2	C	12	BB9	CB-CA-N	-3.11	115.11	122.77
2	D	8	BB8	CD2-CG-CB	-3.03	116.43	120.75
2	D	8	BB8	CD1-CG-CB	3.02	125.06	120.75
2	D	8	BB8	CG-CB-CA	2.91	115.26	111.49
2	D	8	BB8	CB-CA-N	2.76	114.71	109.41
2	C	6	BB7	CB1-CB-SG	2.65	121.97	115.41
2	D	4	BB6	CD-CB-SG	2.52	122.63	116.57
2	C	4	BB6	CD-CB-SG	2.48	122.53	116.57
2	D	6	BB7	CB1-CB-SG	2.23	120.93	115.41
2	C	8	BB8	OB-CB-CA	2.02	110.88	108.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	8	BB8	CB
2	C	8	BB8	CB

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 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
5	ACT	A	3002	-	1,3,3	2.27	1 (100%)	0,3,3	0.00	-
5	ACT	A	3003	-	1,3,3	2.52	1 (100%)	0,3,3	0.00	-
5	ACT	A	3004	-	1,3,3	1.71	0	0,3,3	0.00	-
5	ACT	A	3005	-	1,3,3	2.46	1 (100%)	0,3,3	0.00	-
5	ACT	A	3006	-	1,3,3	2.68	1 (100%)	0,3,3	0.00	-
5	ACT	A	3007	-	1,3,3	2.38	1 (100%)	0,3,3	0.00	-
5	ACT	A	3010	-	1,3,3	2.62	1 (100%)	0,3,3	0.00	-
5	ACT	A	3013	-	1,3,3	2.69	1 (100%)	0,3,3	0.00	-
5	ACT	A	3016	-	1,3,3	2.65	1 (100%)	0,3,3	0.00	-
5	ACT	A	3017	-	1,3,3	2.60	1 (100%)	0,3,3	0.00	-
5	ACT	A	3019	-	1,3,3	2.67	1 (100%)	0,3,3	0.00	-
5	ACT	A	3020	-	1,3,3	2.86	1 (100%)	0,3,3	0.00	-
5	ACT	A	3021	-	1,3,3	2.52	1 (100%)	0,3,3	0.00	-
5	ACT	A	3022	-	1,3,3	2.37	1 (100%)	0,3,3	0.00	-
5	ACT	A	3023	-	1,3,3	2.45	1 (100%)	0,3,3	0.00	-
5	ACT	A	3025	-	1,3,3	1.94	0	0,3,3	0.00	-
5	ACT	A	3026	-	1,3,3	2.40	1 (100%)	0,3,3	0.00	-
5	ACT	A	3028	-	1,3,3	2.57	1 (100%)	0,3,3	0.00	-
5	ACT	A	3030	-	1,3,3	2.84	1 (100%)	0,3,3	0.00	-
4	GDP	A	999	3	30,30,30	0.87	0	44,47,47	4.23	7 (15%)
5	ACT	B	3001	-	1,3,3	2.56	1 (100%)	0,3,3	0.00	-
5	ACT	B	3008	-	1,3,3	2.31	1 (100%)	0,3,3	0.00	-
5	ACT	B	3009	-	1,3,3	2.65	1 (100%)	0,3,3	0.00	-
5	ACT	B	3011	-	1,3,3	2.42	1 (100%)	0,3,3	0.00	-
5	ACT	B	3012	-	1,3,3	2.76	1 (100%)	0,3,3	0.00	-
5	ACT	B	3014	-	1,3,3	2.19	1 (100%)	0,3,3	0.00	-
5	ACT	B	3015	-	1,3,3	2.66	1 (100%)	0,3,3	0.00	-
5	ACT	B	3018	-	1,3,3	2.57	1 (100%)	0,3,3	0.00	-
5	ACT	B	3024	-	1,3,3	2.44	1 (100%)	0,3,3	0.00	-
5	ACT	B	3027	-	1,3,3	3.15	1 (100%)	0,3,3	0.00	-
5	ACT	B	3029	-	1,3,3	2.85	1 (100%)	0,3,3	0.00	-
4	GDP	B	999	3	30,30,30	0.93	0	44,47,47	3.68	9 (20%)

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. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ACT	A	3002	-	-	0/0/0/0	0/0/0/0
5	ACT	A	3003	-	-	0/0/0/0	0/0/0/0
5	ACT	A	3004	-	-	0/0/0/0	0/0/0/0
5	ACT	A	3005	-	-	0/0/0/0	0/0/0/0
5	ACT	A	3006	-	-	0/0/0/0	0/0/0/0
5	ACT	A	3007	-	-	0/0/0/0	0/0/0/0
5	ACT	A	3010	-	-	0/0/0/0	0/0/0/0
5	ACT	A	3013	-	-	0/0/0/0	0/0/0/0
5	ACT	A	3016	-	-	0/0/0/0	0/0/0/0
5	ACT	A	3017	-	-	0/0/0/0	0/0/0/0
5	ACT	A	3019	-	-	0/0/0/0	0/0/0/0
5	ACT	A	3020	-	-	0/0/0/0	0/0/0/0
5	ACT	A	3021	-	-	0/0/0/0	0/0/0/0
5	ACT	A	3022	-	-	0/0/0/0	0/0/0/0
5	ACT	A	3023	-	-	0/0/0/0	0/0/0/0
5	ACT	A	3025	-	-	0/0/0/0	0/0/0/0
5	ACT	A	3026	-	-	0/0/0/0	0/0/0/0
5	ACT	A	3028	-	-	0/0/0/0	0/0/0/0
5	ACT	A	3030	-	-	0/0/0/0	0/0/0/0
4	GDP	A	999	3	-	0/16/32/32	0/1/3/3
5	ACT	B	3001	-	-	0/0/0/0	0/0/0/0
5	ACT	B	3008	-	-	0/0/0/0	0/0/0/0
5	ACT	B	3009	-	-	0/0/0/0	0/0/0/0
5	ACT	B	3011	-	-	0/0/0/0	0/0/0/0
5	ACT	B	3012	-	-	0/0/0/0	0/0/0/0
5	ACT	B	3014	-	-	0/0/0/0	0/0/0/0
5	ACT	B	3015	-	-	0/0/0/0	0/0/0/0
5	ACT	B	3018	-	-	0/0/0/0	0/0/0/0
5	ACT	B	3024	-	-	0/0/0/0	0/0/0/0
5	ACT	B	3027	-	-	0/0/0/0	0/0/0/0
5	ACT	B	3029	-	-	0/0/0/0	0/0/0/0
4	GDP	B	999	3	-	0/16/32/32	0/1/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	3027	ACT	CH3-C	3.15	1.53	1.48
5	A	3020	ACT	CH3-C	2.86	1.52	1.48
5	B	3029	ACT	CH3-C	2.85	1.52	1.48
5	A	3030	ACT	CH3-C	2.84	1.52	1.48
5	B	3012	ACT	CH3-C	2.76	1.52	1.48
5	A	3013	ACT	CH3-C	2.69	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3006	ACT	CH3-C	2.68	1.52	1.48
5	A	3019	ACT	CH3-C	2.67	1.52	1.48
5	B	3015	ACT	CH3-C	2.66	1.52	1.48
5	B	3009	ACT	CH3-C	2.65	1.52	1.48
5	A	3016	ACT	CH3-C	2.65	1.52	1.48
5	A	3010	ACT	CH3-C	2.62	1.52	1.48
5	A	3017	ACT	CH3-C	2.60	1.52	1.48
5	A	3028	ACT	CH3-C	2.57	1.52	1.48
5	B	3018	ACT	CH3-C	2.57	1.52	1.48
5	B	3001	ACT	CH3-C	2.56	1.52	1.48
5	A	3003	ACT	CH3-C	2.52	1.52	1.48
5	A	3021	ACT	CH3-C	2.52	1.52	1.48
5	A	3005	ACT	CH3-C	2.46	1.52	1.48
5	A	3023	ACT	CH3-C	2.45	1.52	1.48
5	B	3024	ACT	CH3-C	2.44	1.52	1.48
5	B	3011	ACT	CH3-C	2.42	1.52	1.48
5	A	3026	ACT	CH3-C	2.40	1.52	1.48
5	A	3007	ACT	CH3-C	2.38	1.52	1.48
5	A	3022	ACT	CH3-C	2.37	1.52	1.48
5	B	3008	ACT	CH3-C	2.31	1.52	1.48
5	A	3002	ACT	CH3-C	2.27	1.52	1.48
5	B	3014	ACT	CH3-C	2.19	1.51	1.48

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	GDP	C6-C5-N7	-26.53	130.57	134.14
4	B	999	GDP	C6-C5-N7	-22.62	131.09	134.14
4	B	999	GDP	PA-O3A-PB	-3.31	121.99	131.68
4	A	999	GDP	C6-N1-C2	3.27	125.22	119.51
4	B	999	GDP	O3'-C3'-C4'	-3.19	101.68	111.08
4	A	999	GDP	O3'-C3'-C2'	-3.14	101.62	111.83
4	B	999	GDP	C6-N1-C2	3.11	124.94	119.51
4	A	999	GDP	PA-O3A-PB	-3.02	122.81	131.68
4	A	999	GDP	O3'-C3'-C4'	-2.97	102.33	111.08
4	B	999	GDP	O3'-C3'-C2'	-2.55	103.55	111.83
4	A	999	GDP	O4'-C1'-C2'	2.44	110.51	106.77
4	B	999	GDP	O4'-C1'-C2'	2.35	110.37	106.77
4	B	999	GDP	C5-C4-N3	2.24	129.20	125.94
4	A	999	GDP	C2-N3-C4	-2.08	112.17	115.09
4	B	999	GDP	C3'-C2'-C1'	2.06	104.14	100.91
4	B	999	GDP	C2-N3-C4	-2.04	112.22	115.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.