Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 02:15 PM EST

PDB ID	:	1EFC
Title	:	INTACT ELONGATION FACTOR FROM E.COLI
Authors	:	Song, H.; Parsons, M.R.; Rowsell, S.; Leonard, G.; Phillips, S.E.V.
Deposited on	:	1998-11-24
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 (i) 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 (i)) were used in the production of this report:

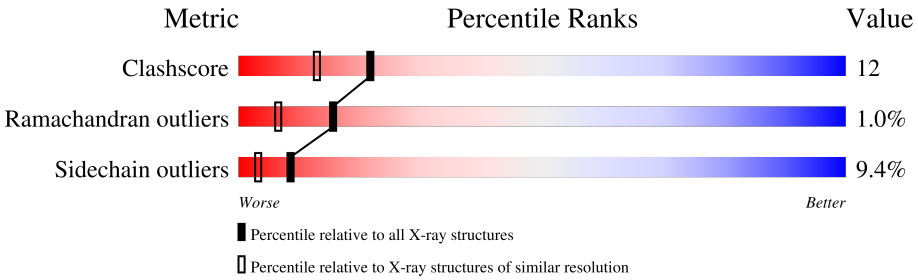
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.05 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))
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	393	71% 21% 5% • •
1	B	393	73% 19% 6% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6444 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.

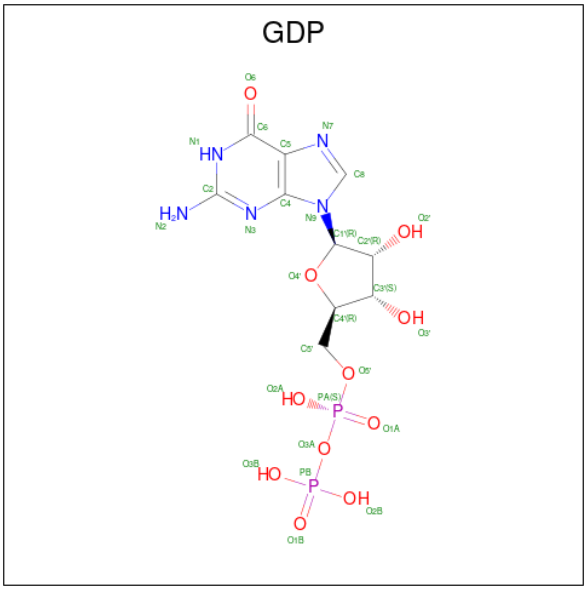
- Molecule 1 is a protein called PROTEIN (ELONGATION FACTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			2970	1877	511	569	13			
1	B	386	Total	C	N	O	S	0	0	0
			2970	1877	511	569	13			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	232	Total	O	0	0
			232	232		
4	B	214	Total	O	0	0
			214	214		

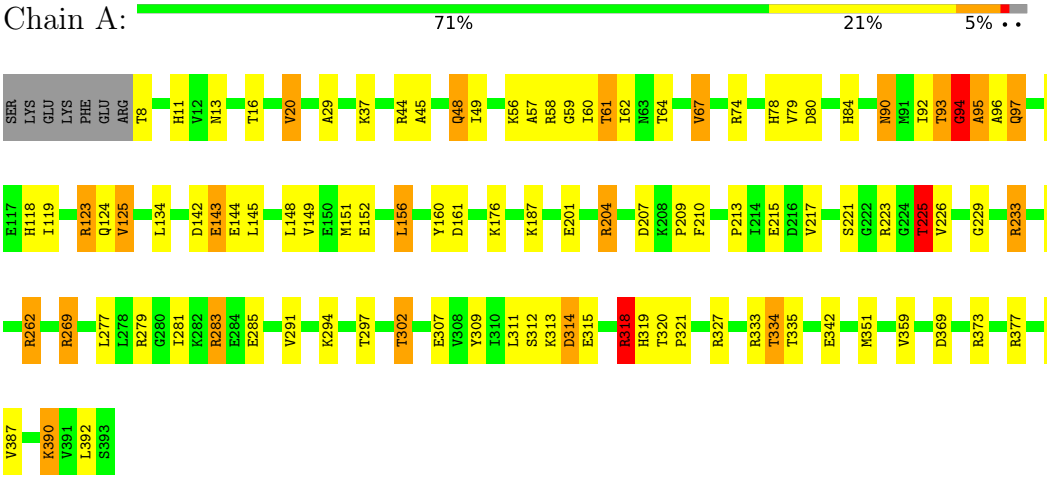
3 Residue-property plots (i)

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. 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. 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.

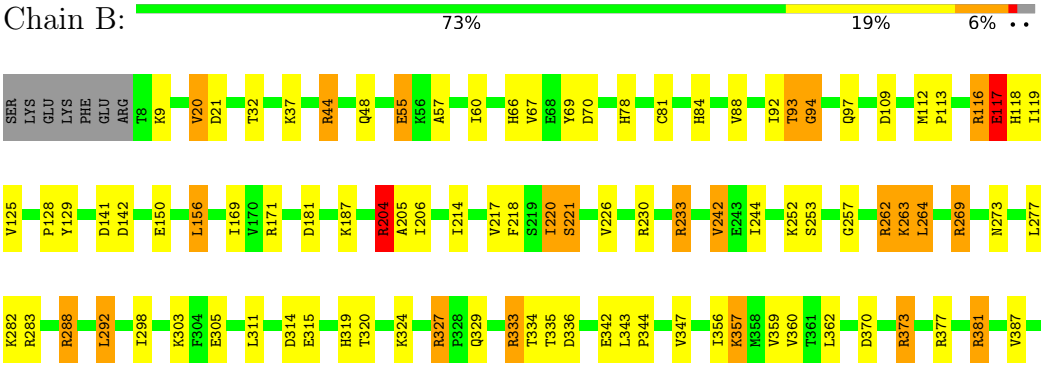
• Molecule 1: PROTEIN (ELONGATION FACTOR)

Chain A:



• Molecule 1: PROTEIN (ELONGATION FACTOR)

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	243.12Å 61.08Å 66.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.05	Depositor
% Data completeness (in resolution range)	90.5 (10.00-2.05)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6444	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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: MG, GDP

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	0.57	0/3025	1.38	26/4096 (0.6%)
1	B	0.53	0/3025	1.35	28/4096 (0.7%)
All	All	0.55	0/6050	1.37	54/8192 (0.7%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	116	ARG	NE-CZ-NH1	-20.99	109.80	120.30
1	A	327	ARG	CD-NE-CZ	19.72	151.20	123.60
1	A	327	ARG	NE-CZ-NH1	12.81	126.70	120.30
1	A	327	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	A	74	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	B	377	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	B	262	ARG	NE-CZ-NH1	-8.67	115.96	120.30
1	B	333	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	B	20	VAL	CB-CA-C	-8.33	95.57	111.40
1	B	269	ARG	CD-NE-CZ	8.22	135.11	123.60
1	A	334	THR	N-CA-CB	-8.12	94.88	110.30
1	A	20	VAL	CB-CA-C	-7.64	96.89	111.40
1	B	171	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	B	269	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	314	ASP	CB-CG-OD1	7.46	125.02	118.30
1	B	21	ASP	CB-CG-OD2	7.46	125.01	118.30
1	B	109	ASP	CB-CG-OD2	7.39	124.95	118.30
1	A	318	ARG	CD-NE-CZ	7.34	133.88	123.60
1	B	381	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	B	269	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	80	ASP	CB-CG-OD1	7.01	124.61	118.30
1	A	262	ARG	NE-CZ-NH1	6.87	123.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	327	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	B	116	ARG	NH1-CZ-NH2	6.59	126.66	119.40
1	B	116	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	B	288	ARG	CD-NE-CZ	6.43	132.60	123.60
1	A	369	ASP	CB-CG-OD1	6.35	124.02	118.30
1	B	117	GLU	OE1-CD-OE2	6.33	130.89	123.30
1	A	116	ARG	NE-CZ-NH2	6.31	123.46	120.30
1	B	181	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	302	THR	N-CA-CB	-6.21	98.50	110.30
1	A	318	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	204	ARG	CD-NE-CZ	6.17	132.24	123.60
1	B	69	TYR	CB-CG-CD1	6.15	124.69	121.00
1	A	204	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	207	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	B	171	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	369	ASP	N-CA-CB	5.85	121.14	110.60
1	B	373	ARG	CD-NE-CZ	5.84	131.78	123.60
1	A	225	THR	N-CA-CB	5.69	121.10	110.30
1	A	143	GLU	OE1-CD-OE2	-5.51	116.68	123.30
1	B	370	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	333	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	B	116	ARG	CD-NE-CZ	-5.30	116.19	123.60
1	A	94	GLY	N-CA-C	-5.29	99.89	113.10
1	B	288	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	A	279	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	A	377	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	B	204	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	95	ALA	CB-CA-C	5.23	117.94	110.10
1	A	381	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	264	LEU	CA-CB-CG	5.14	127.12	115.30
1	B	81	CYS	CA-CB-SG	5.12	123.21	114.00
1	B	55	GLU	N-CA-CB	5.05	119.69	110.60

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	2970	0	2979	75	0
1	B	2970	0	2979	68	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	0	12	0	0
3	B	28	0	12	0	0
4	A	232	0	0	11	0
4	B	214	0	0	7	1
All	All	6444	0	5982	143	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (143) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:VAL:HG23	1:A:387:VAL:HG11	1.37	1.07
1:B:288:ARG:HB3	1:B:335:THR:HG21	1.49	0.95
1:B:244:ILE:HD11	1:B:281:ILE:HD13	1.58	0.86
1:B:84:HIS:HD2	1:B:118:HIS:HE2	1.26	0.81
1:A:307:GLU:HG2	4:A:625:HOH:O	1.79	0.80
1:B:230:ARG:HE	1:B:273:ASN:ND2	1.79	0.80
1:A:151:MET:HG2	4:A:692:HOH:O	1.80	0.79
1:A:62:ILE:HG21	1:A:90:ASN:HD22	1.46	0.79
1:B:305:GLU:HG3	1:B:357:LYS:HD3	1.63	0.79
1:A:45:ALA:H	1:A:48:GLN:HE21	1.35	0.74
1:A:204:ARG:NH1	4:A:731:HOH:O	2.21	0.74
1:B:329:GLN:HE21	1:B:336:ASP:HB3	1.54	0.73
1:B:220:ILE:HG22	1:B:221:SER:H	1.53	0.73
1:B:257:GLY:HA3	1:B:277:LEU:HD12	1.71	0.71
1:B:125:VAL:HG23	1:B:387:VAL:HG11	1.73	0.71
1:A:123:ARG:NH1	1:A:124:GLN:HE21	1.88	0.70
1:A:294:LYS:NZ	1:A:297:THR:HG21	2.08	0.69
1:A:56:LYS:HD3	1:A:61:THR:HG22	1.73	0.68
1:A:84:HIS:HD2	1:A:118:HIS:HE2	1.43	0.67
1:A:64:THR:HG23	1:A:79:VAL:HG23	1.77	0.67
1:A:45:ALA:H	1:A:48:GLN:NE2	1.93	0.66
1:B:263:LYS:HG2	4:B:569:HOH:O	1.94	0.66
1:B:253:SER:HB2	1:B:281:ILE:HD11	1.77	0.66
1:B:214:ILE:HD11	1:B:292:LEU:HD13	1.79	0.65
1:A:123:ARG:HH11	1:A:124:GLN:HE21	1.45	0.65
1:B:253:SER:CB	1:B:281:ILE:HD11	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ALA:O	1:A:97:GLN:HB2	1.96	0.64
1:A:248:LYS:HE2	1:A:285:GLU:O	1.98	0.64
1:A:294:LYS:HZ3	1:A:297:THR:HG21	1.62	0.64
1:B:204:ARG:HE	1:B:205:ALA:H	1.44	0.64
1:B:230:ARG:HE	1:B:273:ASN:HD21	1.46	0.63
1:A:60:ILE:HD11	1:A:385:ALA:HB2	1.81	0.63
1:A:123:ARG:NH1	1:A:124:GLN:NE2	2.47	0.62
1:A:390:LYS:HE2	1:A:392:LEU:HD21	1.82	0.61
1:B:32:THR:HG21	1:B:67:VAL:HG21	1.82	0.61
1:A:313:LYS:HG3	1:A:319:HIS:CD2	2.35	0.61
1:A:313:LYS:HG3	1:A:319:HIS:HD2	1.66	0.61
1:A:152:GLU:OE1	4:A:632:HOH:O	2.16	0.61
1:A:92:ILE:HD12	1:A:309:TYR:HB2	1.84	0.60
1:A:125:VAL:CG2	1:A:387:VAL:HG11	2.24	0.60
1:B:214:ILE:HD11	1:B:292:LEU:CD1	2.32	0.60
1:B:305:GLU:CG	1:B:357:LYS:HD3	2.31	0.57
1:A:262:ARG:HD3	4:A:567:HOH:O	2.05	0.56
1:B:84:HIS:NE2	1:B:117:GLU:HG2	2.20	0.56
1:B:226:VAL:HB	1:B:277:LEU:HD23	1.87	0.56
1:A:209:PRO:HB3	1:A:294:LYS:NZ	2.21	0.55
1:B:84:HIS:HD2	1:B:118:HIS:NE2	2.02	0.55
1:B:278:LEU:HB3	1:B:281:ILE:HD12	1.87	0.55
1:B:119:ILE:HD12	1:B:156:LEU:HD13	1.89	0.55
1:A:312:SER:OG	1:A:315:GLU:HG3	2.06	0.55
1:A:84:HIS:CD2	1:A:118:HIS:HE2	2.24	0.55
1:B:97:GLN:HE21	1:B:373:ARG:NH1	2.05	0.54
1:B:57:ALA:HB3	4:B:653:HOH:O	2.09	0.54
1:A:64:THR:CG2	1:A:79:VAL:HG23	2.38	0.53
1:B:263:LYS:N	1:B:263:LYS:HE3	2.23	0.53
1:A:225:THR:HG23	1:A:281:ILE:O	2.09	0.53
1:A:269:ARG:NH1	4:A:714:HOH:O	2.35	0.52
1:A:64:THR:HG23	1:A:79:VAL:CG2	2.40	0.52
1:B:123:ARG:NH1	1:B:124:GLN:NE2	2.57	0.52
1:B:97:GLN:NE2	1:B:373:ARG:NH1	2.58	0.52
1:A:215:GLU:HG3	1:A:229:GLY:HA2	1.92	0.52
1:B:123:ARG:NH1	1:B:124:GLN:HE21	2.07	0.52
1:A:262:ARG:NE	4:A:623:HOH:O	2.36	0.51
1:B:120:LEU:C	1:B:120:LEU:HD23	2.30	0.51
1:B:278:LEU:CB	1:B:281:ILE:HD12	2.41	0.51
1:B:125:VAL:HG22	1:B:125:VAL:O	2.11	0.51
1:B:84:HIS:CD2	1:B:118:HIS:HE2	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ARG:HH11	1:B:279:ARG:HG3	1.76	0.51
1:A:29:ALA:HB2	1:A:49:ILE:HD12	1.93	0.50
1:A:134:LEU:HD11	1:A:149:VAL:HG11	1.93	0.50
1:B:88:VAL:O	1:B:92:ILE:HD13	2.11	0.50
1:B:67:VAL:HG12	1:B:78:HIS:HB3	1.93	0.50
1:B:204:ARG:NE	1:B:205:ALA:H	2.10	0.50
1:A:44:ARG:NH1	4:A:666:HOH:O	2.44	0.50
1:A:321:PRO:HG3	1:A:351:MET:CE	2.42	0.50
1:B:334:THR:C	1:B:335:THR:CG2	2.80	0.49
1:A:342:GLU:HB2	1:A:359:VAL:HB	1.93	0.49
1:B:342:GLU:HB2	1:B:359:VAL:HB	1.93	0.49
1:A:94:GLY:HA3	1:A:373:ARG:HH11	1.77	0.48
1:B:262:ARG:HG2	1:B:262:ARG:HH11	1.78	0.48
1:B:283:ARG:HD2	4:B:669:HOH:O	2.13	0.48
1:B:93:THR:HG23	1:B:94:GLY:H	1.77	0.48
1:B:44:ARG:NH1	4:B:699:HOH:O	2.45	0.48
1:B:262:ARG:C	1:B:263:LYS:HE3	2.34	0.48
1:A:311:LEU:HD22	1:A:315:GLU:CB	2.44	0.48
1:B:218:PHE:HA	1:B:283:ARG:NH2	2.30	0.47
1:A:45:ALA:N	1:A:48:GLN:HE21	2.09	0.47
1:B:343:LEU:HB3	1:B:344:PRO:HD2	1.95	0.47
1:A:112:MET:HB3	1:A:113:PRO:HD2	1.96	0.47
1:B:244:ILE:HD11	1:B:281:ILE:CD1	2.39	0.46
1:A:57:ALA:C	1:A:59:GLY:N	2.69	0.46
1:B:324:LYS:HB3	4:B:693:HOH:O	2.16	0.46
1:B:344:PRO:HG2	1:B:347:VAL:HG21	1.98	0.46
1:A:123:ARG:HH12	1:A:124:GLN:NE2	2.14	0.45
1:A:318:ARG:NH1	1:A:320:THR:O	2.46	0.45
1:A:318:ARG:HG2	4:A:585:HOH:O	2.16	0.45
1:A:187:LYS:HA	1:A:187:LYS:HD2	1.87	0.45
1:B:60:ILE:HG12	1:B:311:LEU:HD22	1.99	0.45
1:A:112:MET:HB3	1:A:113:PRO:CD	2.47	0.45
1:B:204:ARG:HA	1:B:204:ARG:HD2	1.70	0.45
1:A:67:VAL:HG12	1:A:78:HIS:HB3	1.98	0.45
1:B:262:ARG:NH1	4:B:545:HOH:O	2.49	0.44
1:A:90:ASN:CG	1:A:95:ALA:HB3	2.38	0.44
1:A:144:GLU:O	1:A:148:LEU:HG	2.17	0.44
1:A:209:PRO:HB3	1:A:294:LYS:HZ2	1.83	0.44
1:A:226:VAL:HB	1:A:277:LEU:HD23	2.00	0.43
1:A:84:HIS:HD2	1:A:118:HIS:NE2	2.11	0.43
1:B:187:LYS:HA	1:B:187:LYS:HD2	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:THR:OG1	1:A:94:GLY:N	2.48	0.43
1:A:294:LYS:HZ3	1:A:297:THR:CG2	2.31	0.43
1:B:356:ILE:HD12	1:B:357:LYS:O	2.18	0.43
1:A:57:ALA:C	1:A:59:GLY:H	2.21	0.43
1:A:119:ILE:HD12	1:A:156:LEU:HD13	2.01	0.42
1:A:97:GLN:HA	1:A:97:GLN:OE1	2.19	0.42
1:B:116:ARG:HH11	1:B:116:ARG:HD2	1.34	0.42
1:B:150:GLU:HG2	1:B:169:ILE:HG21	2.02	0.42
1:A:311:LEU:HD22	1:A:315:GLU:HB2	2.02	0.42
1:B:44:ARG:HA	1:B:44:ARG:HD3	1.85	0.42
1:A:251:GLN:HE22	1:A:285:GLU:HB3	1.83	0.42
1:B:303:LYS:HA	1:B:360:VAL:O	2.19	0.42
1:A:11:HIS:HE1	1:A:13:ASN:OD1	2.03	0.42
1:B:244:ILE:CD1	1:B:281:ILE:HD13	2.40	0.42
1:A:294:LYS:HD3	4:A:682:HOH:O	2.18	0.42
1:A:262:ARG:NH2	4:A:623:HOH:O	2.53	0.42
1:A:90:ASN:OD1	1:A:96:ALA:N	2.54	0.41
1:A:44:ARG:HG3	1:A:67:VAL:CG2	2.51	0.41
1:B:66:HIS:HD2	4:B:647:HOH:O	2.02	0.41
1:A:309:TYR:HE2	1:A:311:LEU:HD23	1.86	0.41
1:B:112:MET:HB3	1:B:113:PRO:CD	2.51	0.41
1:B:278:LEU:HD13	1:B:281:ILE:CD1	2.51	0.41
1:B:205:ALA:O	1:B:233:ARG:HB2	2.20	0.41
1:B:242:VAL:N	1:B:253:SER:O	2.53	0.41
1:A:90:ASN:ND2	1:A:95:ALA:HB3	2.36	0.41
1:A:160:TYR:O	1:A:161:ASP:HB2	2.20	0.41
1:A:269:ARG:HH11	1:A:269:ARG:HD3	1.63	0.41
1:B:311:LEU:HB3	1:B:315:GLU:HB2	2.03	0.41
1:B:334:THR:OG1	1:B:335:THR:HG23	2.20	0.41
1:A:97:GLN:NE2	1:A:373:ARG:NH1	2.68	0.40
1:A:217:VAL:HG22	1:A:283:ARG:HG2	2.02	0.40
1:A:210:PHE:HA	1:A:233:ARG:O	2.20	0.40
1:B:217:VAL:HG22	1:B:283:ARG:HG3	2.04	0.40
1:A:213:PRO:HA	1:A:291:VAL:HG12	2.03	0.40
1:B:128:PRO:HB2	1:B:129:TYR:CD1	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:702:HOH:O	4:B:702:HOH:O[2_585]	1.44	0.76

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	384/393 (98%)	364 (95%)	14 (4%)	6 (2%)	9 2
1	B	384/393 (98%)	367 (96%)	15 (4%)	2 (0%)	29 18
All	All	768/786 (98%)	731 (95%)	29 (4%)	8 (1%)	15 6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	THR
1	A	97	GLN
1	A	221	SER
1	A	223	ARG
1	B	94	GLY
1	A	94	GLY
1	A	142	ASP
1	B	333	ARG

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	318/326 (98%)	291 (92%)	27 (8%)	10 4
1	B	318/326 (98%)	285 (90%)	33 (10%)	7 2
All	All	636/652 (98%)	576 (91%)	60 (9%)	8 3

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	16	THR
1	A	20	VAL
1	A	37	LYS
1	A	48	GLN
1	A	58	ARG
1	A	61	THR
1	A	67	VAL
1	A	90	ASN
1	A	123	ARG
1	A	125	VAL
1	A	143	GLU
1	A	145	LEU
1	A	156	LEU
1	A	176	LYS
1	A	201	GLU
1	A	225	THR
1	A	233	ARG
1	A	249	GLU
1	A	269	ARG
1	A	283	ARG
1	A	302	THR
1	A	314	ASP
1	A	318	ARG
1	A	334	THR
1	A	335	THR
1	A	390	LYS
1	B	9	LYS
1	B	20	VAL
1	B	37	LYS
1	B	44	ARG
1	B	48	GLN
1	B	55	GLU
1	B	70	ASP
1	B	93	THR
1	B	117	GLU
1	B	123	ARG
1	B	141	ASP
1	B	142	ASP
1	B	156	LEU
1	B	204	ARG
1	B	206	ILE
1	B	220	ILE

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Mol	Chain	Res	Type
1	B	221	SER
1	B	233	ARG
1	B	242	VAL
1	B	252	LYS
1	B	263	LYS
1	B	264	LEU
1	B	269	ARG
1	B	282	LYS
1	B	292	LEU
1	B	298	ILE
1	B	314	ASP
1	B	319	HIS
1	B	320	THR
1	B	327	ARG
1	B	357	LYS
1	B	362	LEU
1	B	381	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	48	GLN
1	A	66	HIS
1	A	84	HIS
1	A	124	GLN
1	A	251	GLN
1	A	319	HIS
1	A	364	HIS
1	B	63	ASN
1	B	66	HIS
1	B	84	HIS
1	B	90	ASN
1	B	97	GLN
1	B	124	GLN
1	B	251	GLN
1	B	273	ASN
1	B	319	HIS
1	B	329	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GDP	B	514	2	24,30,30	1.18	3 (12%)	30,47,47	1.24	1 (3%)
3	GDP	A	513	2	24,30,30	1.23	2 (8%)	30,47,47	1.19	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GDP	B	514	2	-	2/12/32/32	0/3/3/3
3	GDP	A	513	2	-	2/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	513	GDP	PB-O2B	-3.06	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	514	GDP	C8-N7	-2.98	1.29	1.35
3	A	513	GDP	C8-N7	-2.82	1.30	1.35
3	B	514	GDP	C5-C4	-2.46	1.36	1.43
3	B	514	GDP	C5-C6	-2.05	1.43	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	514	GDP	O6-C6-N1	4.40	125.84	120.65
3	A	513	GDP	PA-O3A-PB	-2.61	123.86	132.83
3	A	513	GDP	O3B-PB-O2B	2.48	117.10	107.64
3	A	513	GDP	O3'-C3'-C2'	-2.18	104.78	111.82
3	A	513	GDP	O6-C6-N1	-2.11	118.16	120.65

There are no chirality outliers.

All (4) torsion outliers are listed below:

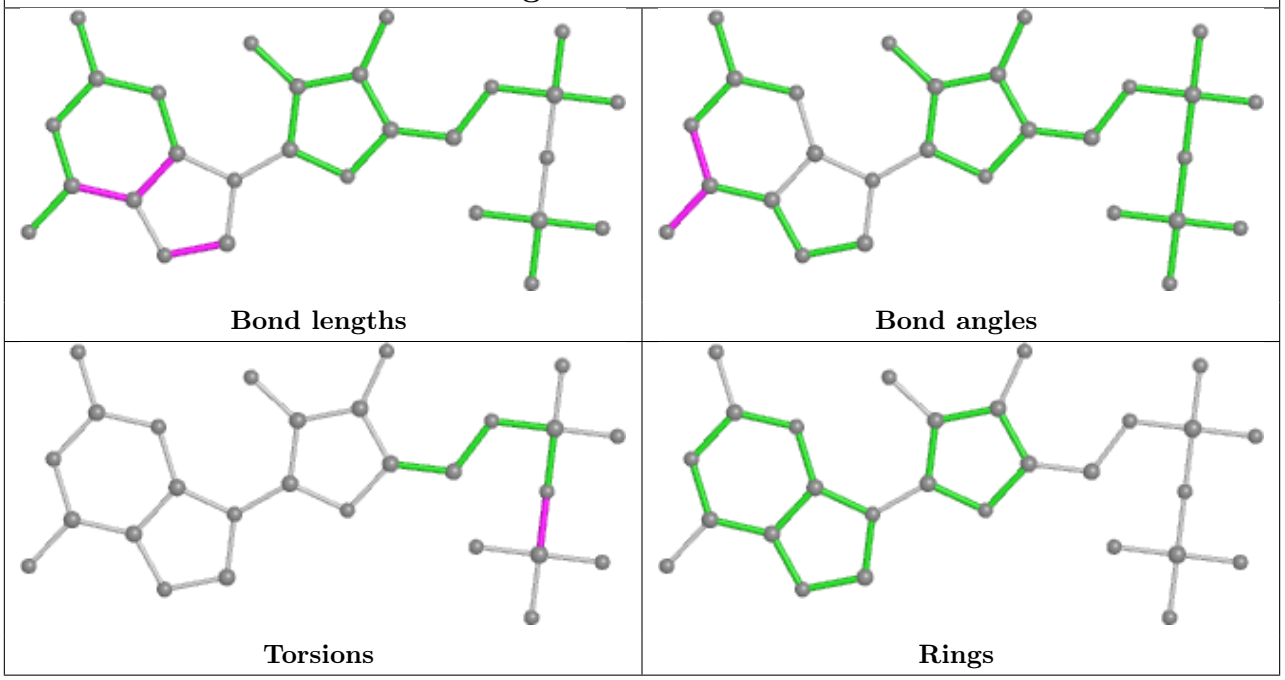
Mol	Chain	Res	Type	Atoms
3	A	513	GDP	PA-O3A-PB-O2B
3	B	514	GDP	PA-O3A-PB-O2B
3	B	514	GDP	PA-O3A-PB-O1B
3	A	513	GDP	PA-O3A-PB-O1B

There are no ring outliers.

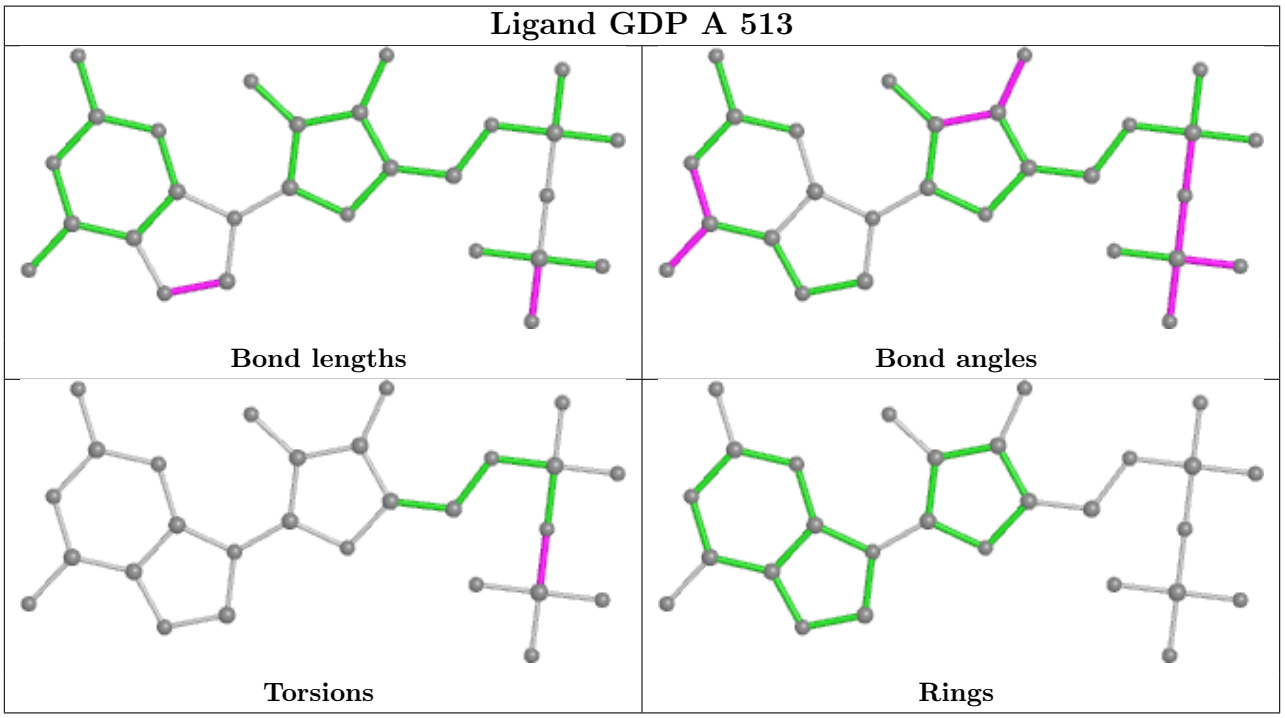
No monomer is involved in short contacts.

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 GDP B 514



Ligand GDP A 513



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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.