Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 09:43 PM EDT

PDB ID	:	1SKQ
Title	:	The crystal structure of Sulfolobus solfataricus elongation factor 1-alpha in complex with magnesium and GDP
Authors	:	Vitagliano, L.; Ruggiero, A.; Masullo, M.; Cantiello, P.; Arcari, P.; Zagari, A.
Deposited on	:	2004-03-05
Resolution	:	1.80 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:

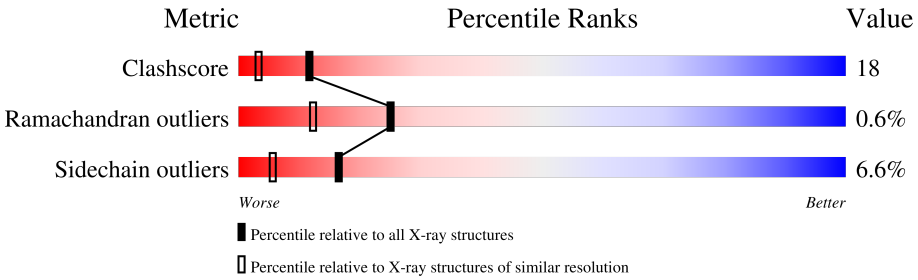
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.80 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	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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	435	73% 18%
1	B	435	67% 24%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6916 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 Elongation factor 1-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3253	2076	564	599	14			
1	B	416	Total	C	N	O	S	0	0	0
			3253	2076	564	599	14			

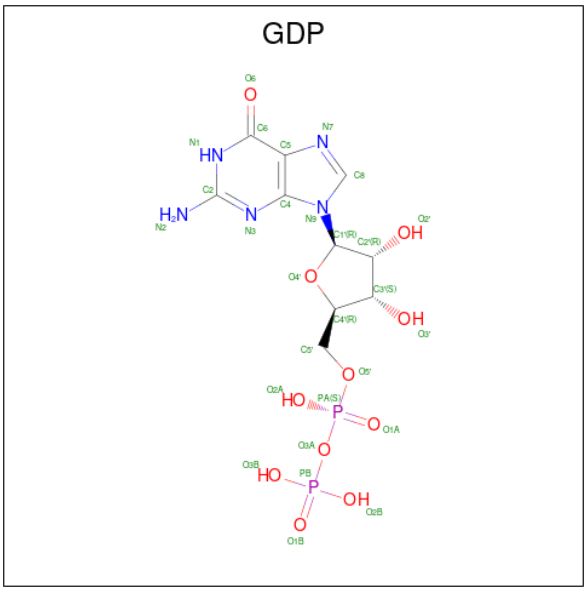
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	VAL	ILE	SEE REMARK 999	UNP P35021
A	196	SER	ALA	SEE REMARK 999	UNP P35021
A	203	LYS	ARG	SEE REMARK 999	UNP P35021
A	347	LEU	ILE	SEE REMARK 999	UNP P35021
B	15	VAL	ILE	SEE REMARK 999	UNP P35021
B	196	SER	ALA	SEE REMARK 999	UNP P35021
B	203	LYS	ARG	SEE REMARK 999	UNP P35021
B	347	LEU	ILE	SEE REMARK 999	UNP P35021

- 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		

- 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	241	Total	O	0	0
			241	241		
4	B	112	Total	O	0	0
			112	112		

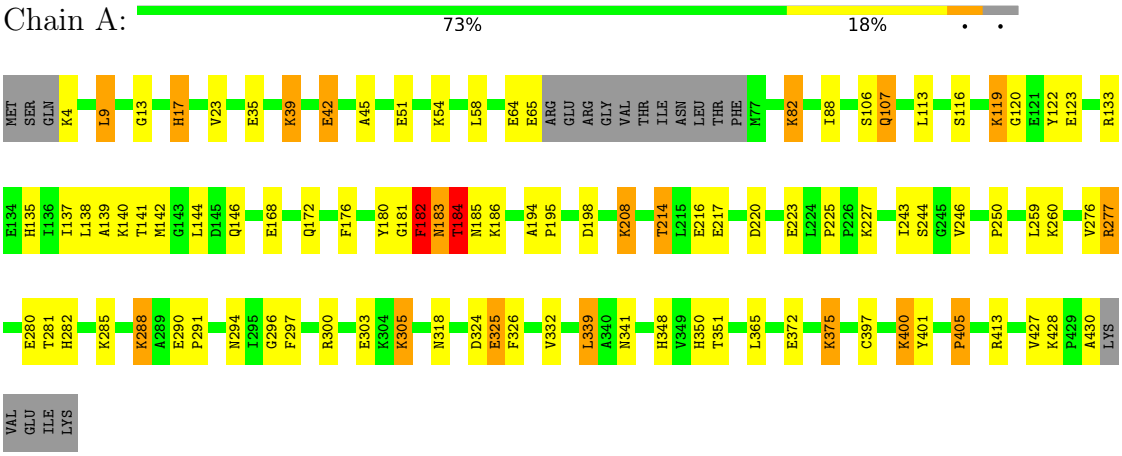
3 Residue-property plots (i)

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.

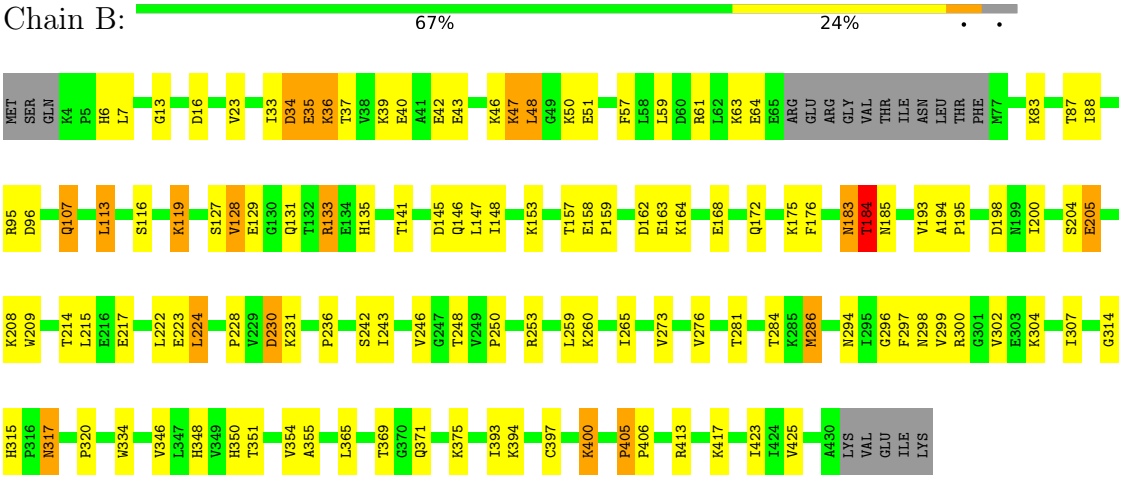
• Molecule 1: Elongation factor 1-alpha

Chain A:



• Molecule 1: Elongation factor 1-alpha

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 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.95Å 113.83Å 81.08Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-1.80)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6916	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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

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	0.91	3/3321 (0.1%)	0.94	4/4486 (0.1%)
1	B	0.78	0/3321	0.91	2/4486 (0.0%)
All	All	0.85	3/6642 (0.0%)	0.92	6/8972 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	PHE	CB-CG	-5.67	1.41	1.51
1	A	325	GLU	CG-CD	5.23	1.59	1.51
1	A	332	VAL	CB-CG1	5.14	1.63	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	339	LEU	CA-CB-CG	9.47	137.07	115.30
1	A	400	LYS	CD-CE-NZ	8.30	130.79	111.70
1	A	9	LEU	CA-CB-CG	7.03	131.46	115.30
1	B	296	GLY	N-CA-C	-6.82	96.06	113.10
1	A	296	GLY	N-CA-C	-5.88	98.41	113.10
1	B	145	ASP	N-CA-CB	-5.04	101.53	110.60

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	3253	0	3321	101	0
1	B	3253	0	3322	131	0
2	A	1	0	0	0	0
3	A	28	0	12	0	0
3	B	28	0	12	0	0
4	A	241	0	0	9	0
4	B	112	0	0	8	0
All	All	6916	0	6667	232	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 18.

All (232) 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:B:224:LEU:HD22	1:B:224:LEU:H	1.07	1.09
1:B:164:LYS:NZ	1:B:168:GLU:HB2	1.70	1.07
1:A:208:LYS:H	1:A:208:LYS:CE	1.68	1.06
1:B:131:GLN:HG3	4:B:541:HOH:O	1.56	1.03
1:A:42:GLU:HG3	1:A:54:LYS:HE2	1.42	1.01
1:A:146:GLN:HE22	1:A:223:GLU:H	1.04	1.00
1:A:119:LYS:HE2	1:A:119:LYS:HA	1.44	1.00
1:A:39:LYS:HE3	1:A:39:LYS:HA	1.43	0.99
1:A:183:ASN:HD21	1:A:185:ASN:ND2	1.63	0.96
1:A:208:LYS:H	1:A:208:LYS:CD	1.81	0.94
1:A:214:THR:HG21	4:A:666:HOH:O	1.69	0.93
1:B:393:ILE:HG13	1:B:394:LYS:HD3	1.51	0.92
1:B:23:VAL:HG13	1:B:88:ILE:HD13	1.51	0.92
1:B:224:LEU:H	1:B:224:LEU:CD2	1.83	0.91
1:B:405:PRO:HG2	1:B:406:PRO:HD3	1.54	0.89
1:B:224:LEU:HD22	1:B:224:LEU:N	1.87	0.88
1:A:214:THR:HG22	1:A:217:GLU:H	1.38	0.88
1:B:164:LYS:HZ1	1:B:168:GLU:HB2	1.29	0.87
1:B:183:ASN:C	1:B:183:ASN:HD22	1.77	0.87
1:A:183:ASN:HB3	4:A:601:HOH:O	1.75	0.85
1:A:281:THR:HG23	1:A:294:ASN:O	1.77	0.85
1:B:146:GLN:HE22	1:B:223:GLU:H	1.20	0.85
1:A:13:GLY:H	1:A:135:HIS:HD2	1.20	0.84
1:B:148:ILE:HG21	1:B:215:LEU:CD2	2.08	0.83
1:B:183:ASN:ND2	1:B:185:ASN:H	1.78	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LYS:HD3	1:A:120:GLY:N	1.98	0.78
1:A:208:LYS:CD	1:A:208:LYS:N	2.46	0.78
1:B:243:ILE:HB	1:B:246:VAL:HB	1.66	0.78
1:B:405:PRO:CG	1:B:406:PRO:HD3	2.14	0.77
1:A:303:GLU:HB3	1:A:305:LYS:HE3	1.66	0.77
1:B:164:LYS:HZ3	1:B:168:GLU:HB2	1.49	0.77
1:B:13:GLY:H	1:B:135:HIS:HD2	1.34	0.76
1:B:35:GLU:C	1:B:37:THR:H	1.89	0.75
1:B:183:ASN:O	1:B:184:THR:HB	1.86	0.74
1:B:400:LYS:HE2	4:B:558:HOH:O	1.88	0.73
1:B:348:HIS:CD2	1:B:413:ARG:HG3	2.24	0.72
1:B:242:SER:C	1:B:243:ILE:HD13	2.10	0.72
1:A:119:LYS:NZ	1:A:123:GLU:OE2	2.22	0.71
1:A:42:GLU:HG3	1:A:54:LYS:CE	2.19	0.71
1:A:350:HIS:CD2	1:A:351:THR:H	2.10	0.70
1:B:6:HIS:HE1	1:B:87:THR:OG1	1.75	0.70
1:A:119:LYS:HA	1:A:119:LYS:CE	2.22	0.70
1:A:208:LYS:N	1:A:208:LYS:HD3	2.07	0.69
1:B:183:ASN:C	1:B:183:ASN:ND2	2.46	0.69
1:B:39:LYS:N	1:B:39:LYS:HD2	2.07	0.69
1:A:430:ALA:C	4:A:567:HOH:O	2.30	0.69
1:B:350:HIS:CD2	1:B:351:THR:H	2.10	0.69
1:B:141:THR:HG23	1:B:425:VAL:HG12	1.76	0.68
1:A:17:HIS:CD2	1:A:116:SER:H	2.11	0.68
1:B:35:GLU:O	1:B:37:THR:N	2.25	0.68
1:A:208:LYS:H	1:A:208:LYS:HE2	1.57	0.68
1:B:107:GLN:HB3	4:B:565:HOH:O	1.94	0.68
1:B:405:PRO:CD	1:B:406:PRO:HD3	2.24	0.68
1:A:45:ALA:HB2	1:A:54:LYS:HG3	1.76	0.67
1:B:127:SER:O	1:B:133:ARG:HD2	1.95	0.67
1:B:35:GLU:O	1:B:36:LYS:HG3	1.95	0.66
1:B:116:SER:OG	1:B:153:LYS:HD2	1.95	0.66
1:B:13:GLY:H	1:B:135:HIS:CD2	2.14	0.66
1:B:228:PRO:CB	1:B:231:LYS:HD3	2.26	0.66
1:A:135:HIS:HE1	4:A:639:HOH:O	1.78	0.65
1:A:288:LYS:NZ	1:A:288:LYS:HB3	2.11	0.65
1:A:183:ASN:C	1:A:183:ASN:HD22	2.01	0.64
1:B:36:LYS:HA	1:B:39:LYS:HD3	1.78	0.64
1:B:355:ALA:HB3	1:B:393:ILE:CD1	2.28	0.64
1:A:324:ASP:OD2	1:A:428:LYS:HE3	1.97	0.64
1:A:82:LYS:HB2	1:A:220:ASP:OD1	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ASP:O	1:B:35:GLU:HB3	1.98	0.63
1:A:350:HIS:HD2	1:A:351:THR:H	1.44	0.63
1:B:405:PRO:HG2	1:B:406:PRO:CD	2.27	0.63
1:B:159:PRO:O	1:B:162:ASP:HB2	1.99	0.63
1:A:183:ASN:ND2	1:A:185:ASN:ND2	2.43	0.62
1:B:128:VAL:HG12	1:B:129:GLU:OE2	1.98	0.62
1:B:163:GLU:HB2	1:B:209:TRP:CE2	2.34	0.62
1:B:400:LYS:CE	4:B:558:HOH:O	2.46	0.62
1:B:43:GLU:HG2	1:B:46:LYS:NZ	2.14	0.62
1:B:42:GLU:O	1:B:46:LYS:HG3	2.00	0.62
1:A:139:ALA:HA	1:A:142:MET:HE2	1.82	0.62
1:A:277:ARG:HA	1:A:277:ARG:NH1	2.15	0.62
1:A:400:LYS:HE2	4:A:584:HOH:O	2.00	0.61
1:A:142:MET:HE3	1:A:144:LEU:HD12	1.82	0.61
1:A:208:LYS:CE	1:A:208:LYS:N	2.53	0.60
1:B:253:ARG:NH1	1:B:294:ASN:HB2	2.17	0.60
1:A:277:ARG:HG3	1:A:300:ARG:CG	2.32	0.60
1:A:350:HIS:HE1	1:A:397:CYS:O	1.84	0.60
1:A:305:LYS:HD3	1:A:305:LYS:N	2.16	0.60
1:B:393:ILE:CG1	1:B:394:LYS:HD3	2.29	0.59
1:B:133:ARG:HB2	1:B:176:PHE:CZ	2.38	0.59
1:B:259:LEU:HD11	1:B:276:VAL:HG21	1.83	0.59
1:B:131:GLN:HE22	1:B:371:GLN:HB3	1.67	0.58
1:A:288:LYS:NZ	1:A:288:LYS:CB	2.66	0.58
1:A:142:MET:HE3	1:A:144:LEU:CD1	2.34	0.58
1:B:39:LYS:O	1:B:43:GLU:HG3	2.04	0.58
1:B:131:GLN:HE22	1:B:371:GLN:CB	2.17	0.57
1:B:164:LYS:HD3	1:B:164:LYS:C	2.24	0.57
1:B:183:ASN:HD22	1:B:185:ASN:H	1.50	0.57
1:A:288:LYS:HB3	1:A:288:LYS:HZ3	1.69	0.57
1:A:39:LYS:HE3	1:A:39:LYS:CA	2.26	0.57
1:A:280:GLU:OE1	1:A:285:LYS:HE3	2.04	0.57
1:B:39:LYS:HD2	1:B:39:LYS:H	1.69	0.57
1:B:119:LYS:HZ1	1:B:158:GLU:H	1.53	0.57
1:B:148:ILE:HG21	1:B:215:LEU:HD22	1.86	0.57
1:B:33:ILE:O	1:B:35:GLU:N	2.37	0.56
1:A:140:LYS:HD3	1:A:182:PHE:HA	1.87	0.56
1:B:204:SER:O	1:B:205:GLU:HB2	2.04	0.56
1:B:43:GLU:O	1:B:47:LYS:HD3	2.06	0.56
1:A:45:ALA:CB	1:A:54:LYS:HG3	2.35	0.55
1:A:400:LYS:NZ	1:A:427:VAL:H	2.03	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ASN:O	1:A:184:THR:HB	2.05	0.55
1:A:186:LYS:NZ	1:A:223:GLU:OE2	2.39	0.55
1:B:405:PRO:HD2	1:B:406:PRO:HD3	1.88	0.55
1:A:133:ARG:HG3	1:A:176:PHE:CZ	2.42	0.55
1:B:214:THR:OG1	1:B:217:GLU:HG3	2.07	0.55
1:A:277:ARG:HA	1:A:277:ARG:CZ	2.36	0.55
1:A:372:GLU:OE1	1:A:375:LYS:HG2	2.06	0.55
1:A:303:GLU:HB3	1:A:305:LYS:CE	2.34	0.55
1:B:43:GLU:HA	1:B:46:LYS:HD2	1.87	0.55
1:B:369:THR:OG1	1:B:371:GLN:HG2	2.07	0.54
1:B:298:ASN:HD21	1:B:300:ARG:HE	1.56	0.54
1:B:141:THR:CG2	1:B:425:VAL:HG12	2.38	0.54
1:B:260:LYS:HG3	4:B:593:HOH:O	2.07	0.54
1:A:51:GLU:OE2	1:A:54:LYS:HD2	2.08	0.54
1:B:193:VAL:HB	1:B:198:ASP:HB2	1.89	0.54
1:B:35:GLU:C	1:B:37:THR:N	2.56	0.54
1:B:57:PHE:CE1	1:B:61:ARG:HG3	2.43	0.53
1:A:277:ARG:HG3	1:A:300:ARG:HG2	1.89	0.53
1:B:43:GLU:HG2	1:B:46:LYS:HZ2	1.74	0.53
1:A:168:GLU:HG3	4:A:739:HOH:O	2.08	0.53
1:B:350:HIS:HD2	1:B:351:THR:H	1.55	0.53
1:A:4:LYS:HE2	1:A:82:LYS:O	2.08	0.53
1:A:208:LYS:H	1:A:208:LYS:HD3	1.62	0.53
1:A:82:LYS:HB2	1:A:82:LYS:HZ3	1.74	0.53
1:B:243:ILE:HD13	1:B:243:ILE:N	2.24	0.53
1:B:236:PRO:HB3	1:B:350:HIS:CD2	2.44	0.53
1:B:13:GLY:N	1:B:135:HIS:HD2	2.03	0.52
1:B:281:THR:HB	1:B:286:MET:HE3	1.89	0.52
1:B:284:THR:O	1:B:286:MET:HE2	2.09	0.52
1:B:119:LYS:NZ	1:B:158:GLU:H	2.06	0.52
1:B:304:LYS:O	1:B:304:LYS:HG2	2.08	0.52
1:A:281:THR:O	1:A:282:HIS:HB2	2.10	0.52
1:B:228:PRO:HB2	1:B:231:LYS:HD3	1.90	0.52
1:A:138:LEU:HG	1:A:142:MET:HE1	1.92	0.51
1:B:350:HIS:HE1	1:B:397:CYS:O	1.93	0.51
1:A:277:ARG:HG3	1:A:300:ARG:HG3	1.93	0.51
1:B:242:SER:O	1:B:243:ILE:HD13	2.11	0.50
1:B:228:PRO:HB3	1:B:231:LYS:HD3	1.94	0.50
1:A:119:LYS:HE2	1:A:119:LYS:CA	2.30	0.50
1:A:183:ASN:C	1:A:183:ASN:ND2	2.64	0.50
1:B:265:ILE:O	1:B:273:VAL:HA	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:GLU:HA	1:B:46:LYS:CD	2.42	0.50
1:B:355:ALA:HB3	1:B:393:ILE:HD11	1.94	0.50
1:B:250:PRO:HD2	1:B:297:PHE:O	2.12	0.49
1:B:135:HIS:HE1	1:B:369:THR:O	1.95	0.49
1:B:317:ASN:OD1	1:B:317:ASN:N	2.42	0.49
1:A:350:HIS:CD2	1:A:351:THR:N	2.78	0.49
1:B:131:GLN:NE2	1:B:371:GLN:CD	2.66	0.49
1:A:214:THR:CG2	1:A:217:GLU:H	2.20	0.49
1:A:137:ILE:O	1:A:141:THR:HG23	2.13	0.48
1:A:277:ARG:CD	1:A:300:ARG:HG3	2.43	0.48
1:A:401:TYR:O	1:A:405:PRO:HG3	2.13	0.48
1:B:119:LYS:HZ3	1:B:157:THR:HA	1.78	0.48
1:B:48:LEU:HB3	1:B:50:LYS:HG2	1.95	0.48
1:A:277:ARG:CG	1:A:300:ARG:HG3	2.44	0.48
1:B:131:GLN:NE2	1:B:371:GLN:HB3	2.29	0.48
1:B:350:HIS:CD2	1:B:351:THR:N	2.81	0.48
1:B:36:LYS:CA	1:B:39:LYS:HD3	2.41	0.48
1:A:243:ILE:HB	1:A:246:VAL:HB	1.96	0.47
1:A:23:VAL:HG13	1:A:88:ILE:HD13	1.97	0.47
1:B:7:LEU:HD21	1:B:224:LEU:CD1	2.44	0.47
1:B:230:ASP:OD1	1:B:230:ASP:N	2.42	0.47
1:B:354:VAL:HG13	1:B:394:LYS:HE2	1.96	0.47
1:A:277:ARG:HD3	1:A:300:ARG:HG3	1.97	0.47
1:B:164:LYS:HD3	1:B:164:LYS:O	2.13	0.47
1:B:253:ARG:HH12	1:B:294:ASN:HB2	1.80	0.47
1:A:194:ALA:HB3	1:A:195:PRO:HD3	1.97	0.47
1:B:183:ASN:HD22	1:B:184:THR:N	2.11	0.46
1:B:194:ALA:HA	1:B:200:ILE:CD1	2.45	0.46
1:B:34:ASP:HB3	1:B:37:THR:OG1	2.16	0.46
1:A:119:LYS:CE	1:A:119:LYS:CA	2.91	0.46
1:A:138:LEU:HG	1:A:142:MET:CE	2.46	0.46
1:A:181:GLY:O	1:A:183:ASN:N	2.48	0.46
1:B:59:LEU:HG	1:B:63:LYS:HE3	1.96	0.46
1:B:248:THR:HG21	1:B:307:ILE:HD12	1.97	0.46
1:B:37:THR:HA	1:B:40:GLU:OE1	2.16	0.46
1:B:95:ARG:NH1	1:B:96:ASP:OD2	2.48	0.46
1:A:318:ASN:HB3	4:A:547:HOH:O	2.15	0.45
1:A:259:LEU:HD11	1:A:276:VAL:HG21	1.97	0.45
1:A:140:LYS:HE2	1:A:181:GLY:C	2.36	0.45
1:A:208:LYS:H	1:A:208:LYS:HE3	1.72	0.45
1:B:34:ASP:C	1:B:35:GLU:O	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:GLU:O	1:B:64:GLU:HG2	2.16	0.45
1:A:227:LYS:HE3	1:A:227:LYS:HB3	1.76	0.45
1:A:17:HIS:HE1	4:A:635:HOH:O	2.00	0.45
1:B:7:LEU:HD21	1:B:224:LEU:HD12	1.99	0.45
1:A:119:LYS:HD3	1:A:119:LYS:C	2.38	0.45
1:A:180:TYR:C	1:A:182:PHE:H	2.20	0.45
1:B:334:TRP:CD2	1:B:417:LYS:HE2	2.52	0.44
1:A:58:LEU:HA	1:A:58:LEU:HD23	1.63	0.44
1:A:168:GLU:O	1:A:172:GLN:HG3	2.17	0.44
1:B:172:GLN:HA	1:B:175:LYS:HB2	2.00	0.44
1:B:59:LEU:O	1:B:63:LYS:HG3	2.18	0.44
1:B:113:LEU:HB2	1:B:147:LEU:HD11	2.00	0.44
1:B:334:TRP:CE2	1:B:417:LYS:HE2	2.53	0.43
1:B:183:ASN:O	1:B:184:THR:CB	2.64	0.43
1:A:400:LYS:HZ3	1:A:427:VAL:H	1.65	0.43
1:B:194:ALA:HB3	1:B:195:PRO:HD3	2.00	0.43
1:A:305:LYS:N	1:A:305:LYS:CD	2.82	0.43
1:A:348:HIS:CD2	1:A:413:ARG:HG3	2.54	0.43
1:A:225:PRO:HD3	4:A:730:HOH:O	2.19	0.43
1:A:42:GLU:HA	1:A:54:LYS:HE2	2.01	0.42
1:A:82:LYS:NZ	1:A:216:GLU:OE1	2.49	0.42
1:A:325:GLU:HG2	1:A:326:PHE:N	2.34	0.42
1:B:286:MET:HG2	4:B:519:HOH:O	2.18	0.42
1:A:116:SER:O	1:A:122:TYR:HB2	2.20	0.42
1:B:299:VAL:HG13	1:B:302:VAL:HG12	2.01	0.42
1:B:375:LYS:HE3	1:B:375:LYS:HB2	1.84	0.42
1:B:163:GLU:HB2	1:B:209:TRP:CD2	2.55	0.42
1:B:83:LYS:HB3	1:B:83:LYS:HE2	1.85	0.41
1:B:205:GLU:HA	1:B:208:LYS:HE3	2.02	0.41
1:A:186:LYS:NZ	1:A:223:GLU:CD	2.73	0.41
1:A:250:PRO:HD2	1:A:297:PHE:O	2.19	0.41
1:A:260:LYS:HG3	1:A:288:LYS:HG3	2.02	0.41
1:B:131:GLN:HE22	1:B:371:GLN:CD	2.24	0.41
1:B:315:HIS:HD2	4:B:535:HOH:O	2.03	0.41
1:B:346:VAL:HA	1:B:355:ALA:HA	2.02	0.41
1:A:39:LYS:HA	1:A:39:LYS:CE	2.29	0.41
1:B:6:HIS:CE1	1:B:87:THR:OG1	2.65	0.41
1:B:314:GLY:HA3	1:B:320:PRO:HD3	2.03	0.41
1:B:405:PRO:CD	1:B:406:PRO:CD	2.98	0.41
1:A:106:SER:O	1:A:107:GLN:HB2	2.21	0.40
1:B:405:PRO:HB2	4:B:574:HOH:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLU:HB3	1:A:291:PRO:CD	2.51	0.40
1:B:47:LYS:HD3	1:B:47:LYS:H	1.86	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	412/435 (95%)	401 (97%)	9 (2%)	2 (0%)	29	15
1	B	412/435 (95%)	394 (96%)	15 (4%)	3 (1%)	22	10
All	All	824/870 (95%)	795 (96%)	24 (3%)	5 (1%)	25	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	34	ASP
1	A	184	THR
1	B	205	GLU
1	B	184	THR
1	A	182	PHE

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	357/375 (95%)	332 (93%)	25 (7%)	15 5
1	B	357/375 (95%)	335 (94%)	22 (6%)	18 6
All	All	714/750 (95%)	667 (93%)	47 (7%)	16 5

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	17	HIS
1	A	35	GLU
1	A	39	LYS
1	A	42	GLU
1	A	64	GLU
1	A	65	GLU
1	A	82	LYS
1	A	107	GLN
1	A	113	LEU
1	A	119	LYS
1	A	183	ASN
1	A	184	THR
1	A	198	ASP
1	A	208	LYS
1	A	214	THR
1	A	244	SER
1	A	277	ARG
1	A	288	LYS
1	A	305	LYS
1	A	339	LEU
1	A	341	ASN
1	A	365	LEU
1	A	375	LYS
1	A	405	PRO
1	B	16	ASP
1	B	35	GLU
1	B	36	LYS
1	B	47	LYS
1	B	48	LEU
1	B	51	GLU
1	B	107	GLN
1	B	113	LEU
1	B	119	LYS
1	B	128	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	133	ARG
1	B	183	ASN
1	B	184	THR
1	B	222	LEU
1	B	224	LEU
1	B	230	ASP
1	B	286	MET
1	B	317	ASN
1	B	365	LEU
1	B	400	LYS
1	B	405	PRO
1	B	423	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	100	ASN
1	A	135	HIS
1	A	146	GLN
1	A	183	ASN
1	A	202	HIS
1	A	294	ASN
1	A	317	ASN
1	A	341	ASN
1	A	350	HIS
1	B	6	HIS
1	B	14	HIS
1	B	131	GLN
1	B	135	HIS
1	B	146	GLN
1	B	172	GLN
1	B	183	ASN
1	B	202	HIS
1	B	221	GLN
1	B	298	ASN
1	B	315	HIS
1	B	348	HIS
1	B	350	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is 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	501	-	24,30,30	2.60	12 (50%)	30,47,47	3.92	18 (60%)
3	GDP	A	500	2	24,30,30	1.84	7 (29%)	30,47,47	1.67	7 (23%)

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	501	-	-	0/12/32/32	0/3/3/3
3	GDP	A	500	2	-	1/12/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	GDP	O4'-C1'	5.77	1.49	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	GDP	O6-C6	5.67	1.34	1.23
3	B	501	GDP	C2-N1	4.09	1.47	1.37
3	A	500	GDP	C8-N7	-4.01	1.28	1.35
3	A	500	GDP	C6-N1	4.00	1.43	1.37
3	B	501	GDP	O3'-C3'	3.68	1.51	1.43
3	B	501	GDP	C8-N7	3.30	1.40	1.35
3	B	501	GDP	C2-N3	-3.16	1.25	1.33
3	B	501	GDP	PB-O2B	-3.15	1.42	1.54
3	B	501	GDP	O4'-C4'	2.76	1.51	1.45
3	A	500	GDP	C2-N3	2.73	1.39	1.33
3	B	501	GDP	C5-C6	-2.63	1.42	1.47
3	A	500	GDP	O6-C6	-2.59	1.18	1.23
3	A	500	GDP	C2'-C1'	-2.55	1.49	1.53
3	B	501	GDP	C3'-C4'	2.36	1.59	1.53
3	A	500	GDP	O4'-C1'	-2.27	1.37	1.41
3	B	501	GDP	PB-O3B	2.22	1.63	1.54
3	B	501	GDP	C2'-C3'	2.09	1.59	1.53
3	A	500	GDP	C5-C4	-2.04	1.37	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	GDP	C8-N7-C5	11.51	124.91	102.99
3	B	501	GDP	O4'-C1'-C2'	-8.90	93.92	106.93
3	B	501	GDP	O6-C6-N1	-5.53	114.12	120.65
3	B	501	GDP	C5-C6-N1	5.35	123.40	113.95
3	B	501	GDP	N2-C2-N3	5.11	129.69	119.74
3	B	501	GDP	C2-N1-C6	-4.80	116.26	125.10
3	A	500	GDP	O3'-C3'-C4'	-4.56	97.87	111.05
3	B	501	GDP	O3'-C3'-C2'	4.50	126.38	111.82
3	B	501	GDP	O2'-C2'-C3'	4.14	125.23	111.82
3	B	501	GDP	C3'-C2'-C1'	3.91	106.86	100.98
3	B	501	GDP	N2-C2-N1	-3.90	108.41	116.71
3	B	501	GDP	O4'-C4'-C3'	-3.82	97.55	105.11
3	B	501	GDP	O3'-C3'-C4'	3.50	121.17	111.05
3	A	500	GDP	O2A-PA-O5'	2.85	120.99	107.75
3	A	500	GDP	C2'-C3'-C4'	2.82	108.12	102.64
3	B	501	GDP	O3B-PB-O2B	2.77	118.21	107.64
3	A	500	GDP	O6-C6-N1	-2.35	117.88	120.65
3	B	501	GDP	O5'-C5'-C4'	2.29	116.88	108.99
3	B	501	GDP	O2B-PB-O1B	-2.23	101.94	110.68
3	B	501	GDP	O3B-PB-O1B	2.20	119.30	110.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	GDP	PA-O3A-PB	-2.19	125.32	132.83
3	B	501	GDP	C5'-C4'-C3'	2.09	123.02	115.18
3	A	500	GDP	O4'-C1'-C2'	2.09	109.97	106.93
3	A	500	GDP	C3'-C2'-C1'	2.08	104.11	100.98
3	A	500	GDP	O2B-PB-O3A	-2.02	97.87	104.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

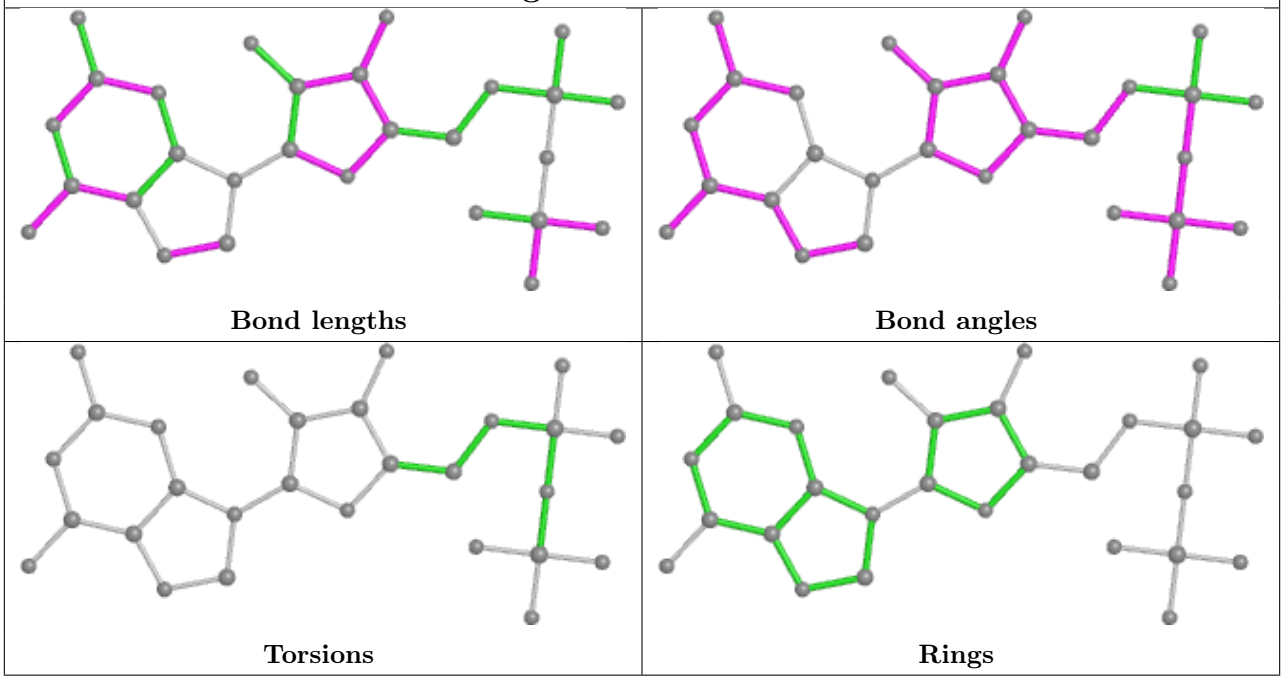
Mol	Chain	Res	Type	Atoms
3	A	500	GDP	PB-O3A-PA-O2A

There are no ring outliers.

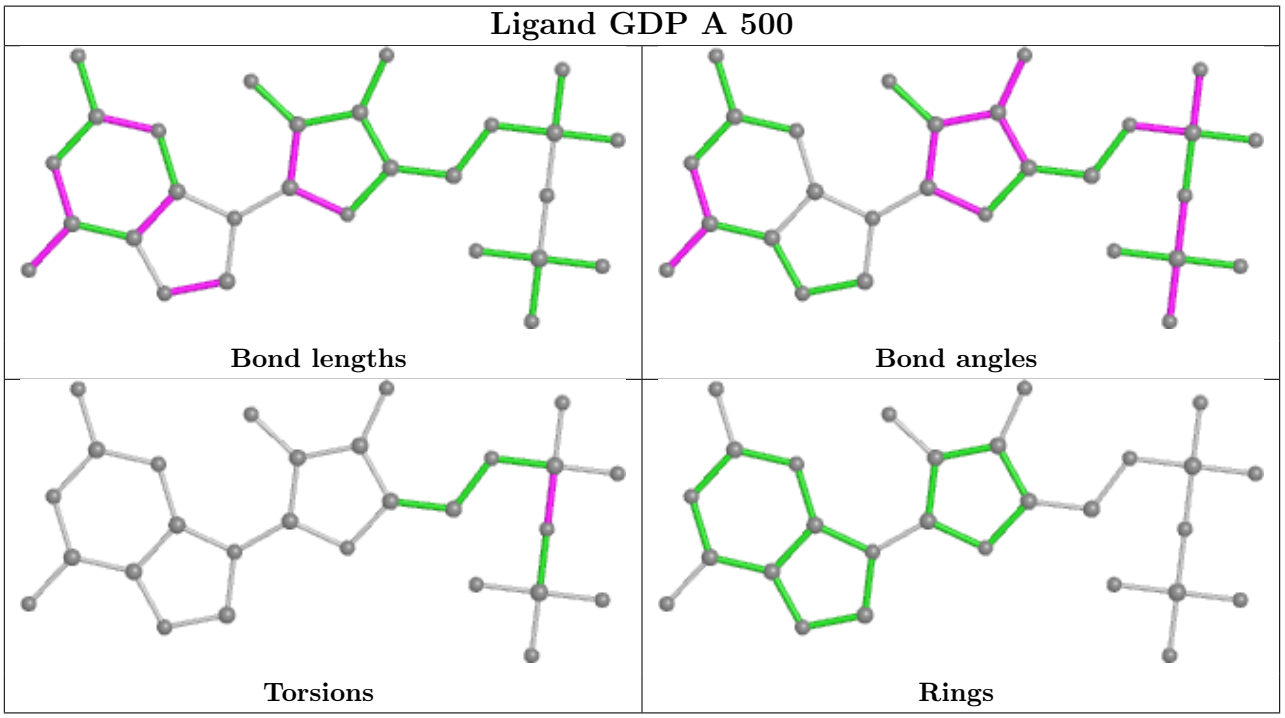
No monomer is involved in short contacts.

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 501



Ligand GDP A 500



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.