Full wwPDB X-ray Structure Validation Report (i)

Feb 11, 2024 – 04:14 PM EST

PDB ID	:	3DM5
Title	:	Structures of SRP54 and SRP19, the two proteins assembling the ribonucleic core of the Signal Recognition Particle from the archaeon Pyrococcus furiosus.
Authors	:	Egea, P.F.; Napetschnig, J.; Walter, P.; Stroud, R.M.
Deposited on	:	2008-06-30
Resolution	:	2.51 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:

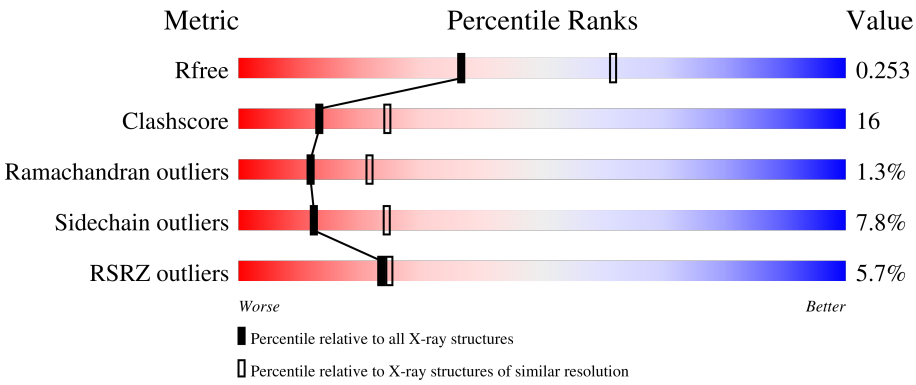
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.51 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	443	4% 65% 24% • 6%
1	B	443	7% 63% 26% • 7%

2 Entry composition (i)

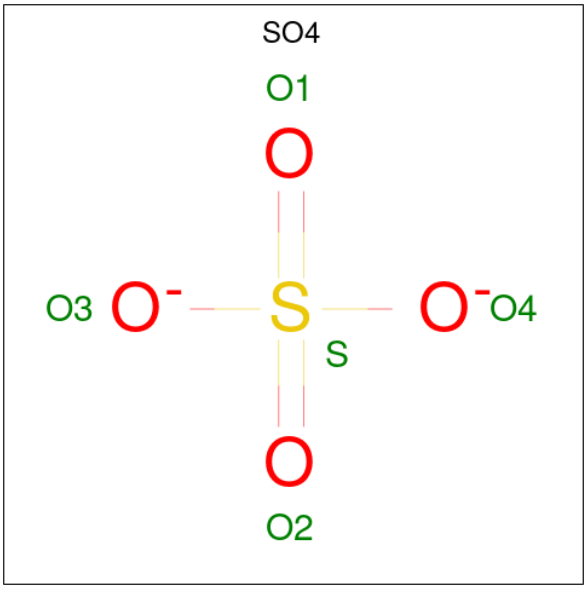
There are 5 unique types of molecules in this entry. The entry contains 6649 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Signal recognition 54 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	416	3192	2028	552	601	11	0	0	0
1	B	413	3196	2034	556	595	11	11	1	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



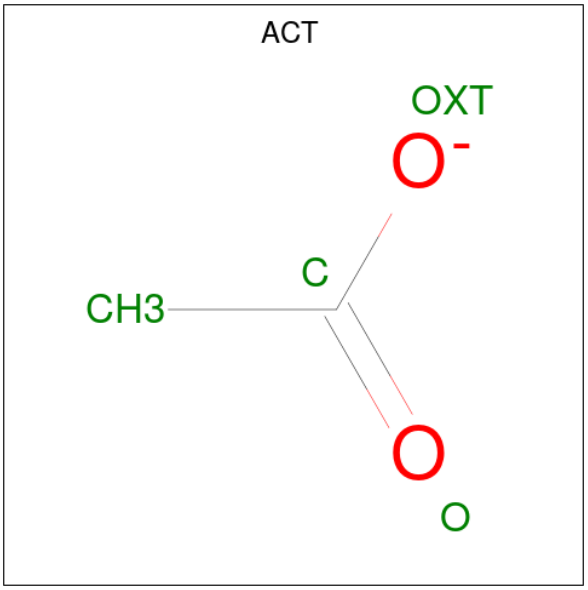
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

Continued on next page...

Continued from previous page...

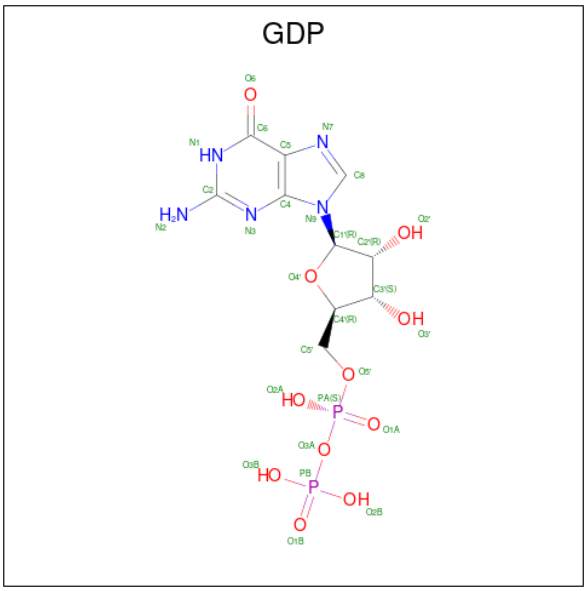
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 5 is water.

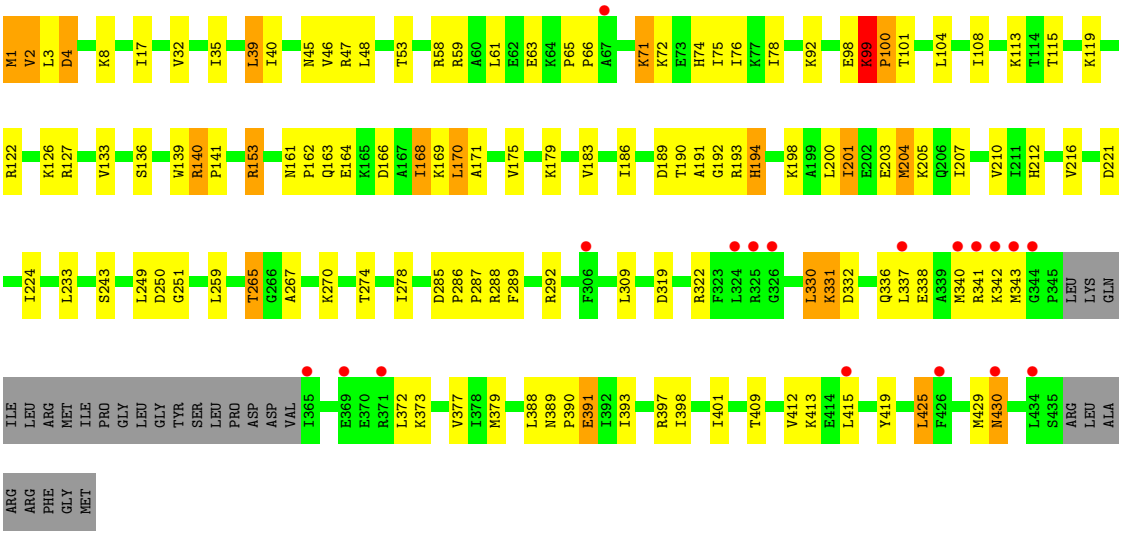
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	72	72	72	0	0
			Total	O		
5	B	70	70	70	0	0

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.

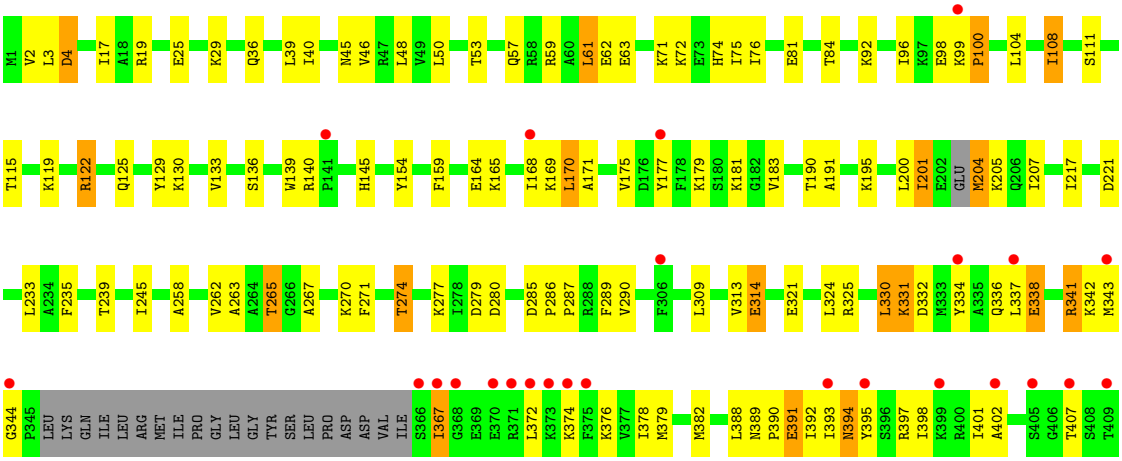
• Molecule 1: Signal recognition 54 kDa protein

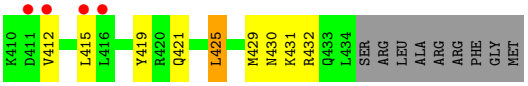
Chain A:



• Molecule 1: Signal recognition 54 kDa protein

Chain B:




K410
D411
V412
L415
L416
Y419
R420
Q421
L425
M429
N430
K431
R432
Q433
L434
SER
ARG
LEU
ALA
ARG
ARG
PHE
GLY
MET

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	127.01Å 127.01Å 186.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.74 – 2.51 64.74 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.5 (64.74-2.51) 99.5 (64.74-2.51)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine), ELVES	Depositor
R, R_{free}	0.222 , 0.259 0.214 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (3.80%)	wwPDB-VP
Wilson B-factor (Å^2)	55.2	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6649	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, GDP, SO4

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	0.40	0/3234	0.57	0/4357
1	B	0.40	0/3235	0.57	0/4348
All	All	0.40	0/6469	0.57	0/8705

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3192	0	3248	111	0
1	B	3196	0	3289	100	0
2	A	30	0	0	1	0
2	B	25	0	0	2	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	28	0	12	0	0
4	B	28	0	12	0	0
5	A	72	0	0	1	0
5	B	70	0	0	2	0
All	All	6649	0	6567	211	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 16.

All (211) 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:341:ARG:HG3	1:A:341:ARG:HH11	1.27	0.99
1:B:341:ARG:HG3	1:B:341:ARG:HH11	1.36	0.91
1:A:99:LYS:O	1:A:100:PRO:C	2.09	0.90
1:B:330:LEU:HD12	1:B:390:PRO:HG3	1.54	0.86
1:A:265:THR:HG22	1:A:267:ALA:H	1.40	0.85
1:B:324:LEU:HD22	1:B:429:MET:HB2	1.60	0.83
1:A:127:ARG:HG3	1:A:127:ARG:HH11	1.43	0.82
1:A:99:LYS:HG3	1:A:100:PRO:HD3	1.62	0.81
1:B:99:LYS:HG3	1:B:100:PRO:HD3	1.61	0.81
1:B:168:ILE:HD13	1:B:207:ILE:HG12	1.63	0.80
1:A:168:ILE:HD13	1:A:207:ILE:HG12	1.66	0.77
1:B:341:ARG:HG3	1:B:341:ARG:NH1	1.97	0.77
1:A:113:LYS:HE2	1:A:189:ASP:OD1	1.85	0.76
1:A:341:ARG:HG3	1:A:341:ARG:NH1	1.97	0.74
1:A:330:LEU:HD12	1:A:390:PRO:HG3	1.70	0.72
1:A:45:ASN:HD22	1:A:48:LEU:H	1.38	0.72
1:A:193:ARG:HG3	1:A:200:LEU:HD12	1.71	0.71
1:B:398:ILE:HG23	1:B:412:VAL:HG11	1.74	0.70
1:A:92:LYS:O	1:A:270:LYS:HD3	1.93	0.68
1:B:99:LYS:O	1:B:100:PRO:C	2.33	0.67
1:A:265:THR:CG2	1:A:267:ALA:H	2.07	0.67
1:A:153:ARG:HG2	5:A:505:HOH:O	1.95	0.66
1:A:2:VAL:H	1:A:250:ASP:HA	1.61	0.66
1:A:390:PRO:HG2	1:A:419:TYR:CZ	2.29	0.66
1:B:71:LYS:O	1:B:75:ILE:HG12	1.96	0.66
1:B:104:LEU:HD11	1:B:190:THR:CG2	2.26	0.66
1:B:111:SER:HA	1:B:221:ASP:HB2	1.77	0.66
1:B:334:TYR:OH	1:B:376:LYS:HE2	1.96	0.65
1:B:382:MET:HG2	1:B:401:ILE:HD13	1.79	0.65
1:A:136:SER:HA	1:A:170:LEU:HD13	1.79	0.65
1:B:330:LEU:HD21	1:B:415:LEU:HD21	1.80	0.64
1:A:164:GLU:OE1	1:A:164:GLU:HA	1.97	0.63
1:A:341:ARG:HD3	1:A:372:LEU:HD22	1.80	0.63
1:A:1:MET:O	1:A:2:VAL:HG12	1.99	0.62
1:B:136:SER:HA	1:B:170:LEU:HD13	1.81	0.62
1:A:59:ARG:O	1:A:63:GLU:HB2	1.98	0.62
1:A:32:VAL:HG13	1:A:53:THR:HB	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LYS:O	1:A:101:THR:N	2.32	0.62
1:B:245:ILE:HG12	1:B:271:PHE:HB2	1.81	0.62
1:A:203:GLU:O	1:A:207:ILE:HG13	1.99	0.62
1:B:100:PRO:HG2	1:B:179:LYS:HG3	1.81	0.61
1:B:324:LEU:CD2	1:B:429:MET:HB2	2.30	0.61
1:A:40:ILE:HD12	1:A:46:VAL:HG22	1.83	0.60
1:A:166:ASP:HB3	1:A:169:LYS:HB2	1.83	0.60
1:B:277:LYS:HE2	5:B:535:HOH:O	2.01	0.60
1:B:341:ARG:HH11	1:B:341:ARG:CG	2.14	0.60
1:B:398:ILE:HG23	1:B:412:VAL:CG1	2.32	0.60
1:A:127:ARG:HH11	1:A:127:ARG:CG	2.15	0.60
1:B:63:GLU:OE1	1:B:74:HIS:HE1	1.85	0.60
1:B:45:ASN:HD22	1:B:48:LEU:H	1.51	0.59
1:B:330:LEU:HD12	1:B:390:PRO:CG	2.31	0.59
1:A:285:ASP:OD1	1:A:287:PRO:HD2	2.03	0.59
1:B:337:LEU:HB3	1:B:372:LEU:HD12	1.85	0.58
1:A:71:LYS:HD2	1:A:71:LYS:H	1.68	0.58
1:A:286:PRO:HB2	1:A:287:PRO:HD3	1.85	0.58
1:A:139:TRP:HB2	1:A:191:ALA:HB1	1.85	0.57
1:A:58:ARG:HH12	1:A:59:ARG:HG2	1.69	0.57
1:A:99:LYS:CG	1:A:100:PRO:HD3	2.35	0.56
1:B:25:GLU:O	1:B:29:LYS:HG2	2.04	0.56
1:B:274:THR:HG22	1:B:280:ASP:HB3	1.87	0.56
1:A:127:ARG:HG3	1:A:127:ARG:NH1	2.19	0.56
1:B:29:LYS:HD2	1:B:57:GLN:HE21	1.71	0.55
1:B:59:ARG:O	1:B:63:GLU:HB2	2.05	0.55
1:A:340:MET:HA	1:A:343:MET:HE3	1.90	0.54
1:A:98:GLU:C	1:A:99:LYS:O	2.43	0.54
1:A:3:LEU:HD22	1:A:289:PHE:HZ	1.72	0.54
1:B:139:TRP:HB2	1:B:191:ALA:HB1	1.89	0.53
1:A:2:VAL:H	1:A:251:GLY:H	1.57	0.53
1:A:249:LEU:HD11	1:A:259:LEU:HD21	1.91	0.53
1:B:100:PRO:CG	1:B:179:LYS:HG3	2.38	0.53
1:A:100:PRO:HG2	1:A:179:LYS:HG3	1.90	0.52
1:B:96:ILE:HG21	1:B:129:TYR:CE1	2.45	0.52
1:A:99:LYS:HB3	1:A:100:PRO:CD	2.39	0.52
1:A:265:THR:HG22	1:A:267:ALA:N	2.18	0.52
1:B:334:TYR:HD1	1:B:379:MET:CE	2.23	0.52
1:B:130:LYS:HG2	1:B:183:VAL:HG12	1.90	0.52
1:A:104:LEU:HD11	1:A:190:THR:HG21	1.91	0.52
1:A:35:ILE:HG22	1:A:39:LEU:HD22	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ILE:CD1	1:A:46:VAL:HG22	2.40	0.51
1:A:192:GLY:O	1:A:193:ARG:HG2	2.10	0.51
1:B:394:ASN:O	1:B:398:ILE:HG13	2.10	0.51
1:B:262:VAL:O	1:B:265:THR:HG22	2.11	0.51
1:B:92:LYS:O	1:B:270:LYS:HD3	2.10	0.51
1:A:341:ARG:NH1	1:A:341:ARG:CG	2.72	0.51
1:A:288:ARG:O	1:A:292:ARG:HG2	2.10	0.51
1:B:164:GLU:HG2	1:B:170:LEU:HG	1.93	0.51
1:A:2:VAL:O	1:A:4:ASP:N	2.42	0.50
1:B:334:TYR:HE1	1:B:376:LYS:HG3	1.77	0.50
1:B:338:GLU:O	1:B:341:ARG:HG2	2.11	0.50
1:B:84:THR:HA	1:B:290:VAL:HG21	1.94	0.50
1:A:198:LYS:HE2	2:A:448:SO4:O4	2.11	0.50
1:B:36:GLN:OE1	1:B:53:THR:HG21	2.11	0.49
1:A:74:HIS:O	1:A:78:ILE:HG13	2.12	0.49
1:B:99:LYS:HG3	1:B:100:PRO:CD	2.37	0.49
1:B:235:PHE:O	1:B:239:THR:HG22	2.11	0.49
1:B:397:ARG:O	1:B:401:ILE:HG13	2.12	0.49
1:A:122:ARG:CZ	1:A:126:LYS:HG3	2.41	0.49
1:B:285:ASP:OD1	1:B:287:PRO:HD2	2.13	0.49
1:A:17:ILE:CD1	1:A:75:ILE:HG21	2.43	0.48
1:B:258:ALA:O	1:B:262:VAL:HG23	2.13	0.48
1:A:104:LEU:HD23	1:A:216:VAL:HG22	1.95	0.48
1:A:115:THR:HG22	1:A:119:LYS:HE3	1.95	0.48
1:B:36:GLN:CG	1:B:53:THR:HG21	2.44	0.48
1:B:342:LYS:C	1:B:344:GLY:H	2.16	0.48
1:A:164:GLU:CG	1:A:170:LEU:HG	2.43	0.48
1:A:127:ARG:CG	1:A:127:ARG:NH1	2.73	0.48
1:B:263:ALA:C	1:B:265:THR:H	2.17	0.48
1:B:430:ASN:C	1:B:432:ARG:H	2.16	0.48
1:B:331:LYS:HE3	1:B:388:LEU:HD21	1.96	0.47
1:B:390:PRO:HG2	1:B:419:TYR:CZ	2.50	0.47
1:A:99:LYS:HD2	1:A:99:LYS:HA	1.49	0.47
1:B:332:ASP:O	1:B:336:GLN:HG2	2.15	0.47
1:A:104:LEU:HD11	1:A:190:THR:CG2	2.44	0.47
1:A:397:ARG:O	1:A:401:ILE:HG13	2.15	0.47
1:A:71:LYS:H	1:A:71:LYS:CD	2.23	0.47
1:A:331:LYS:HE3	1:A:388:LEU:HD21	1.96	0.47
1:B:334:TYR:HD1	1:B:379:MET:HE3	1.80	0.47
1:B:390:PRO:O	1:B:393:ILE:HG13	2.15	0.47
1:A:161:ASN:O	1:A:163:GLN:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:MET:HG3	1:A:205:LYS:N	2.30	0.47
1:A:243:SER:HB3	1:A:270:LYS:HE3	1.97	0.47
1:B:99:LYS:HD2	1:B:99:LYS:HA	1.59	0.47
1:B:25:GLU:HG3	1:B:61:LEU:HD11	1.97	0.46
1:B:29:LYS:HD2	1:B:57:GLN:NE2	2.30	0.46
1:B:104:LEU:HD11	1:B:190:THR:HG21	1.97	0.46
1:A:1:MET:HG3	1:A:250:ASP:HB2	1.97	0.46
1:A:390:PRO:O	1:A:393:ILE:HG13	2.15	0.46
1:B:108:ILE:HG22	1:B:200:LEU:CD1	2.45	0.46
1:A:175:VAL:O	1:A:179:LYS:HB2	2.14	0.46
1:B:201:ILE:HA	1:B:204:MET:HG2	1.98	0.46
1:A:161:ASN:C	1:A:163:GLN:H	2.19	0.46
1:B:367:ILE:HD11	1:B:372:LEU:HB2	1.97	0.46
1:B:122:ARG:HD2	1:B:122:ARG:O	2.15	0.46
1:A:319:ASP:O	1:A:322:ARG:HB2	2.15	0.45
1:B:430:ASN:O	1:B:432:ARG:N	2.48	0.45
1:A:373:LYS:O	1:A:377:VAL:HG23	2.17	0.45
1:B:3:LEU:HD22	1:B:289:PHE:HZ	1.81	0.45
1:B:425:LEU:O	1:B:429:MET:HG2	2.16	0.45
1:A:3:LEU:HD22	1:A:289:PHE:CZ	2.52	0.45
1:A:99:LYS:CB	1:A:100:PRO:CD	2.94	0.45
1:A:164:GLU:OE2	1:A:169:LYS:HE2	2.16	0.45
1:B:59:ARG:HH12	1:B:81:GLU:CD	2.20	0.45
1:B:115:THR:HG22	1:B:119:LYS:HE3	1.99	0.45
1:B:374:LYS:O	1:B:378:ILE:HG13	2.17	0.45
1:B:145:HIS:HE1	2:B:445:SO4:O4	1.99	0.44
1:B:389:ASN:HB3	1:B:391:GLU:OE2	2.17	0.44
1:A:425:LEU:HD22	1:A:429:MET:CE	2.48	0.44
1:B:171:ALA:O	1:B:175:VAL:HG23	2.18	0.44
1:A:65:PRO:HG3	1:A:71:LYS:HA	1.99	0.44
1:A:99:LYS:HG3	1:A:100:PRO:CD	2.42	0.44
1:A:1:MET:HA	1:A:251:GLY:H	1.83	0.44
1:B:62:GLU:O	1:B:62:GLU:HG3	2.19	0.43
1:B:72:LYS:O	1:B:76:ILE:HG12	2.19	0.43
1:A:1:MET:HA	1:A:251:GLY:N	2.33	0.43
1:A:161:ASN:C	1:A:163:GLN:N	2.72	0.43
1:A:65:PRO:HA	1:A:66:PRO:HD2	1.86	0.43
1:A:72:LYS:O	1:A:76:ILE:HG12	2.18	0.43
1:B:313:VAL:HG13	1:B:314:GLU:H	1.82	0.43
1:B:342:LYS:C	1:B:344:GLY:N	2.72	0.43
1:A:2:VAL:N	1:A:250:ASP:HA	2.29	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ILE:HD13	1:B:75:ILE:HG21	2.00	0.43
1:A:243:SER:CB	1:A:270:LYS:HE3	2.49	0.43
1:B:279:ASP:HB2	5:B:545:HOH:O	2.18	0.43
1:A:164:GLU:HG3	1:A:170:LEU:HG	2.00	0.43
1:B:125:GLN:NE2	1:B:154:TYR:O	2.51	0.43
1:B:367:ILE:HD11	1:B:372:LEU:CA	2.49	0.43
1:A:274:THR:O	1:A:274:THR:CG2	2.67	0.43
1:A:343:MET:HG2	1:A:343:MET:O	2.19	0.42
1:A:221:ASP:O	1:A:224:ILE:HG12	2.18	0.42
1:A:415:LEU:HD23	1:A:415:LEU:O	2.19	0.42
1:A:164:GLU:OE1	1:A:164:GLU:CA	2.64	0.42
1:B:177:TYR:OH	1:B:181:LYS:HE2	2.19	0.42
1:B:195:LYS:HB3	1:B:195:LYS:HE2	1.76	0.42
1:B:389:ASN:O	1:B:392:ILE:HG12	2.20	0.42
1:A:183:VAL:HG21	1:A:186:ILE:HG12	2.02	0.42
1:A:278:ILE:O	1:A:278:ILE:HG13	2.19	0.42
1:B:337:LEU:HB3	1:B:372:LEU:CD1	2.49	0.42
1:A:389:ASN:HB3	1:A:391:GLU:OE2	2.20	0.42
1:B:50:LEU:HD23	1:B:50:LEU:HA	1.84	0.42
1:B:265:THR:CG2	1:B:267:ALA:H	2.33	0.42
1:B:313:VAL:HG13	1:B:314:GLU:N	2.35	0.42
1:B:177:TYR:C	1:B:177:TYR:CD2	2.92	0.42
1:A:168:ILE:HG21	1:A:210:VAL:HG21	2.02	0.41
1:A:171:ALA:O	1:A:175:VAL:HG23	2.20	0.41
1:A:337:LEU:HB3	1:A:372:LEU:HD11	2.02	0.41
1:A:198:LYS:HA	1:A:201:ILE:HD11	2.01	0.41
1:A:338:GLU:O	1:A:342:LYS:HD3	2.20	0.41
1:B:159:PHE:CD2	1:B:159:PHE:C	2.93	0.41
1:B:36:GLN:O	1:B:40:ILE:HG12	2.20	0.41
1:B:402:ALA:HB1	1:B:407:THR:O	2.20	0.41
1:B:71:LYS:HG3	2:B:448:SO4:O1	2.20	0.41
1:A:398:ILE:HG23	1:A:412:VAL:HG11	2.02	0.41
1:A:139:TRP:HH2	1:A:194:HIS:ND1	2.18	0.41
1:A:409:THR:O	1:A:413:LYS:HG3	2.20	0.41
1:A:99:LYS:HB3	1:A:100:PRO:HD3	2.02	0.41
1:B:98:GLU:C	1:B:99:LYS:O	2.58	0.41
1:B:204:MET:HG3	1:B:205:LYS:N	2.35	0.41
1:A:332:ASP:O	1:A:336:GLN:HG2	2.21	0.41
1:A:337:LEU:HB3	1:A:372:LEU:CD1	2.50	0.41
1:B:63:GLU:OE1	1:B:74:HIS:CE1	2.69	0.41
1:B:286:PRO:HB2	1:B:287:PRO:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:THR:HG22	1:B:280:ASP:CB	2.51	0.41
1:A:8:LYS:HE3	1:A:8:LYS:HB3	1.85	0.40
1:A:99:LYS:CB	1:A:100:PRO:HD3	2.51	0.40
1:A:2:VAL:O	1:A:2:VAL:HG13	2.20	0.40
1:A:98:GLU:O	1:A:99:LYS:O	2.39	0.40
1:A:140:ARG:HA	1:A:141:PRO:HD2	1.87	0.40
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.85	0.40
1:B:40:ILE:HD11	1:B:46:VAL:HG23	2.02	0.40
1:A:379:MET:HG3	1:A:415:LEU:HD11	2.03	0.40
1:B:321:GLU:O	1:B:325:ARG:HG3	2.22	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	412/443 (93%)	383 (93%)	23 (6%)	6 (2%)	10	18
1	B	408/443 (92%)	380 (93%)	23 (6%)	5 (1%)	13	24
All	All	820/886 (93%)	763 (93%)	46 (6%)	11 (1%)	12	21

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	LYS
1	B	4	ASP
1	B	100	PRO
1	B	394	ASN
1	A	430	ASN
1	B	431	LYS
1	A	4	ASP
1	B	421	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	100	PRO
1	A	2	VAL
1	A	162	PRO

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	332/378 (88%)	309 (93%)	23 (7%)	15	30
1	B	333/378 (88%)	304 (91%)	29 (9%)	10	20
All	All	665/756 (88%)	613 (92%)	52 (8%)	12	24

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	39	LEU
1	A	47	ARG
1	A	61	LEU
1	A	71	LYS
1	A	99	LYS
1	A	108	ILE
1	A	133	VAL
1	A	140	ARG
1	A	153	ARG
1	A	168	ILE
1	A	170	LEU
1	A	194	HIS
1	A	201	ILE
1	A	204	MET
1	A	212	HIS
1	A	233	LEU
1	A	265	THR
1	A	330	LEU
1	A	331	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	391	GLU
1	A	425	LEU
1	A	430	ASN
1	B	2	VAL
1	B	4	ASP
1	B	19	ARG
1	B	39	LEU
1	B	61	LEU
1	B	108	ILE
1	B	122	ARG
1	B	133	VAL
1	B	140	ARG
1	B	165	LYS
1	B	169	LYS
1	B	170	LEU
1	B	201	ILE
1	B	204	MET
1	B	217	ILE
1	B	233	LEU
1	B	265	THR
1	B	274	THR
1	B	309	LEU
1	B	314	GLU
1	B	330	LEU
1	B	331	LYS
1	B	338	GLU
1	B	341	ARG
1	B	343	MET
1	B	367	ILE
1	B	391	GLU
1	B	395	TYR
1	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	45	ASN
1	A	74	HIS
1	A	209	ASN
1	A	226	GLN
1	A	418	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	45	ASN
1	B	57	GLN
1	B	74	HIS
1	B	145	HIS
1	B	163	GLN
1	B	226	GLN
1	B	336	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)

15 ligands 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	SO4	B	448	-	4,4,4	0.12	0	6,6,6	0.23	0
2	SO4	A	445	-	4,4,4	0.14	0	6,6,6	0.12	0
3	ACT	B	449	-	3,3,3	0.73	0	3,3,3	1.39	0
2	SO4	A	444	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	A	447	-	4,4,4	0.17	0	6,6,6	0.39	0
2	SO4	A	449	-	4,4,4	0.12	0	6,6,6	0.14	0
4	GDP	B	501	-	24,30,30	0.87	1 (4%)	30,47,47	1.27	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	444	-	4,4,4	0.18	0	6,6,6	0.14	0
2	SO4	B	446	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	A	446	-	4,4,4	0.15	0	6,6,6	0.23	0
2	SO4	B	447	-	4,4,4	0.17	0	6,6,6	0.32	0
3	ACT	A	450	-	3,3,3	0.70	0	3,3,3	1.59	1 (33%)
2	SO4	B	445	-	4,4,4	0.19	0	6,6,6	0.38	0
2	SO4	A	448	-	4,4,4	0.19	0	6,6,6	0.11	0
4	GDP	A	501	-	24,30,30	1.06	2 (8%)	30,47,47	1.11	3 (10%)

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
4	GDP	B	501	-	-	0/12/32/32	0/3/3/3
4	GDP	A	501	-	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	GDP	C6-N1	-2.39	1.34	1.37
4	A	501	GDP	O4'-C1'	2.32	1.44	1.41
4	B	501	GDP	C6-N1	-2.05	1.34	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	501	GDP	O6-C6-C5	-2.72	119.05	124.37
4	B	501	GDP	C5-C6-N1	2.54	118.43	113.95
4	A	501	GDP	O3B-PB-O3A	2.39	112.65	104.64
4	A	501	GDP	C8-N7-C5	2.32	107.41	102.99
4	B	501	GDP	O4'-C1'-C2'	-2.22	103.69	106.93
4	B	501	GDP	C8-N7-C5	2.22	107.21	102.99
3	A	450	ACT	OXT-C-CH3	2.10	123.88	115.18
4	A	501	GDP	C5-C6-N1	2.03	117.55	113.95

There are no chirality outliers.

There are no torsion outliers.

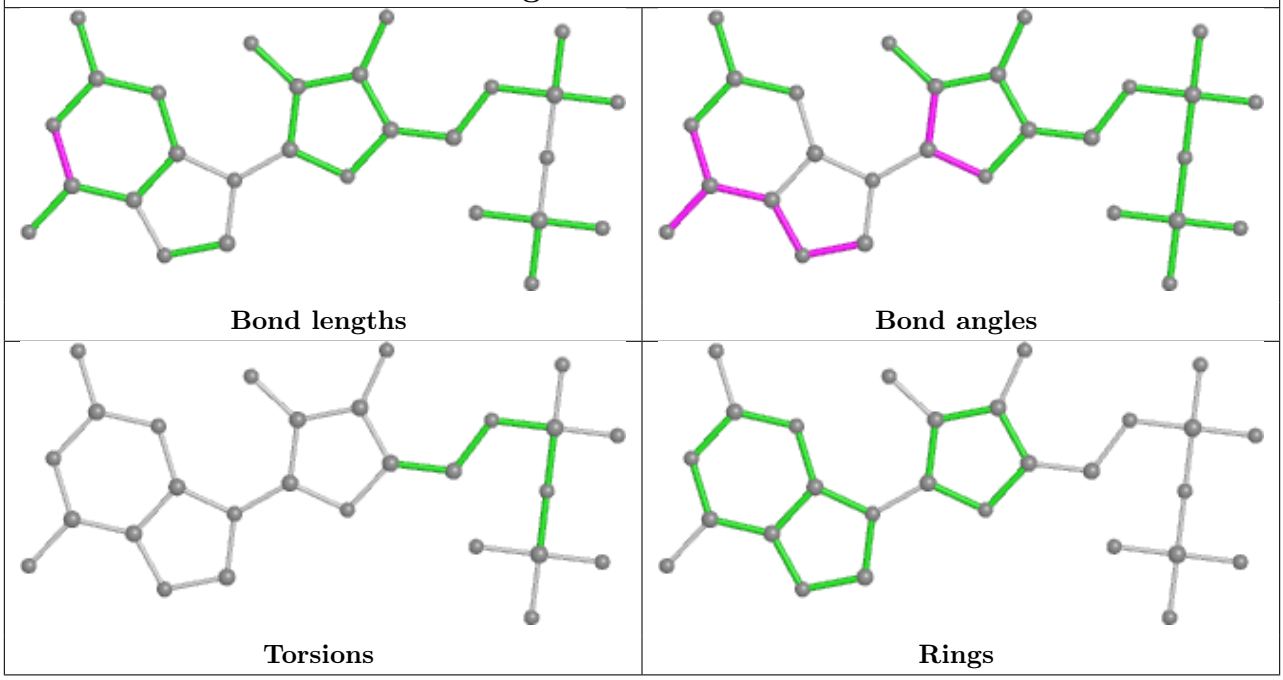
There are no ring outliers.

3 monomers are involved in 3 short contacts:

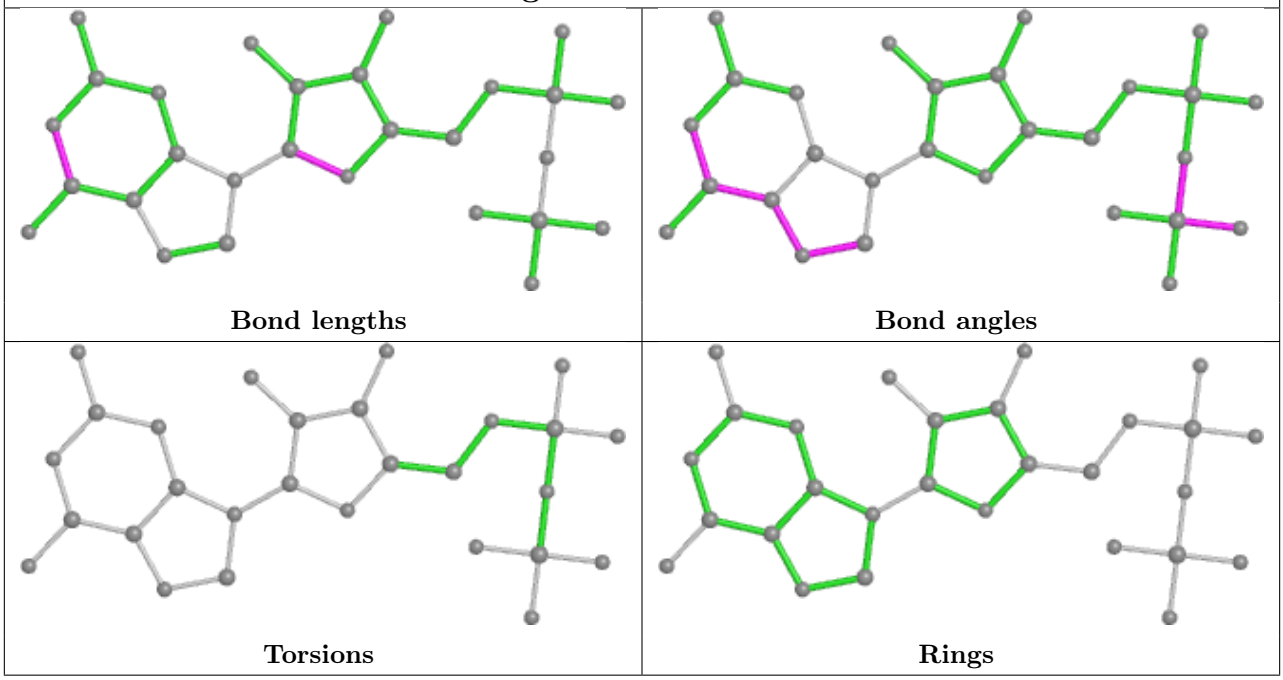
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	448	SO4	1	0
2	B	445	SO4	1	0
2	A	448	SO4	1	0

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 GDP B 501



Ligand GDP A 501



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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	416/443 (93%)	0.49	18 (4%)	35	38	35, 59, 112, 141	0
1	B	413/443 (93%)	0.52	29 (7%)	16	16	33, 64, 111, 132	0
All	All	829/886 (93%)	0.50	47 (5%)	23	25	33, 61, 112, 141	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	367	ILE	7.4
1	A	341	ARG	6.3
1	A	365	ILE	6.0
1	A	426	PHE	4.4
1	B	371	ARG	4.2
1	B	372	LEU	4.2
1	A	434	LEU	4.1
1	A	343	MET	4.0
1	B	415	LEU	4.0
1	B	373	LYS	3.9
1	B	334	TYR	3.8
1	B	407	THR	3.8
1	A	342	LYS	3.6
1	A	324	LEU	3.3
1	B	368	GLY	3.3
1	A	326	GLY	3.2
1	B	412	VAL	3.2
1	B	337	LEU	3.2
1	A	67	ALA	3.1
1	B	366	SER	3.1
1	A	430	ASN	3.1
1	A	340	MET	3.0
1	A	325	ARG	3.0
1	A	371	ARG	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	415	LEU	2.9
1	B	402	ALA	2.8
1	B	306	PHE	2.7
1	B	405	SER	2.5
1	B	141	PRO	2.5
1	A	344	GLY	2.5
1	A	369	GLU	2.5
1	B	411	ASP	2.4
1	B	344	GLY	2.4
1	B	393	ILE	2.4
1	B	409	THR	2.4
1	A	306	PHE	2.4
1	B	343	MET	2.3
1	B	374	LYS	2.3
1	A	337	LEU	2.3
1	B	416	LEU	2.3
1	B	375	PHE	2.2
1	B	370	GLU	2.2
1	B	177	TYR	2.2
1	B	168	ILE	2.1
1	B	99	LYS	2.1
1	B	395	TYR	2.1
1	B	399	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Continued on next page...

Continued from previous page...

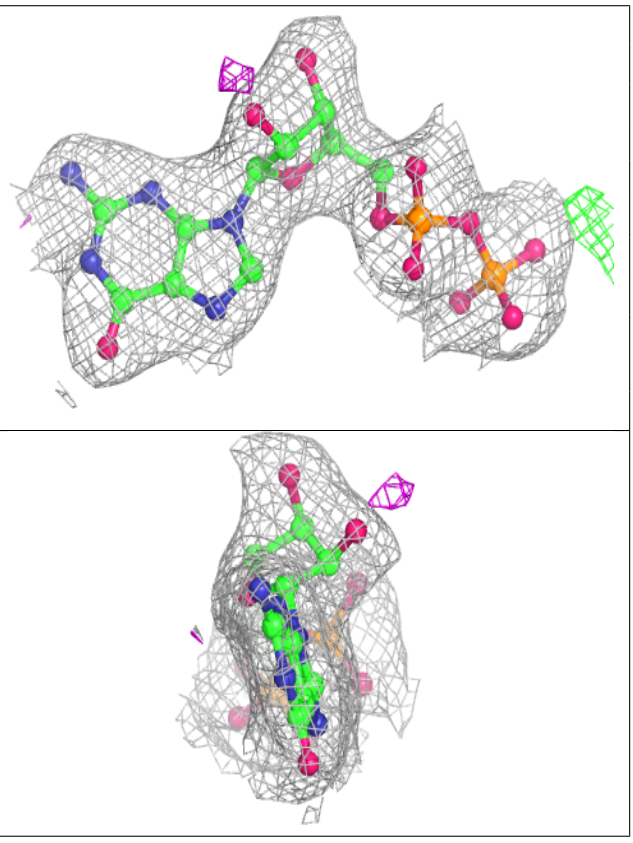
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACT	A	450	4/4	0.76	0.19	59,78,84,87	0
2	SO4	B	446	5/5	0.82	0.17	107,109,125,135	0
2	SO4	A	449	5/5	0.82	0.14	88,99,117,124	0
2	SO4	B	445	5/5	0.83	0.14	73,73,103,111	0
2	SO4	B	448	5/5	0.85	0.16	105,106,116,132	0
3	ACT	B	449	4/4	0.87	0.15	58,78,79,80	0
2	SO4	A	444	5/5	0.88	0.15	97,101,106,122	0
2	SO4	B	444	5/5	0.90	0.20	87,89,112,122	0
2	SO4	A	446	5/5	0.90	0.11	90,92,109,123	0
2	SO4	B	447	5/5	0.91	0.14	79,85,89,101	0
2	SO4	A	445	5/5	0.94	0.11	89,91,110,118	0
2	SO4	A	448	5/5	0.94	0.14	87,89,105,112	0
2	SO4	A	447	5/5	0.96	0.15	65,76,87,90	0
4	GDP	A	501	28/28	0.98	0.18	37,45,49,51	0
4	GDP	B	501	28/28	0.98	0.17	35,41,51,64	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.

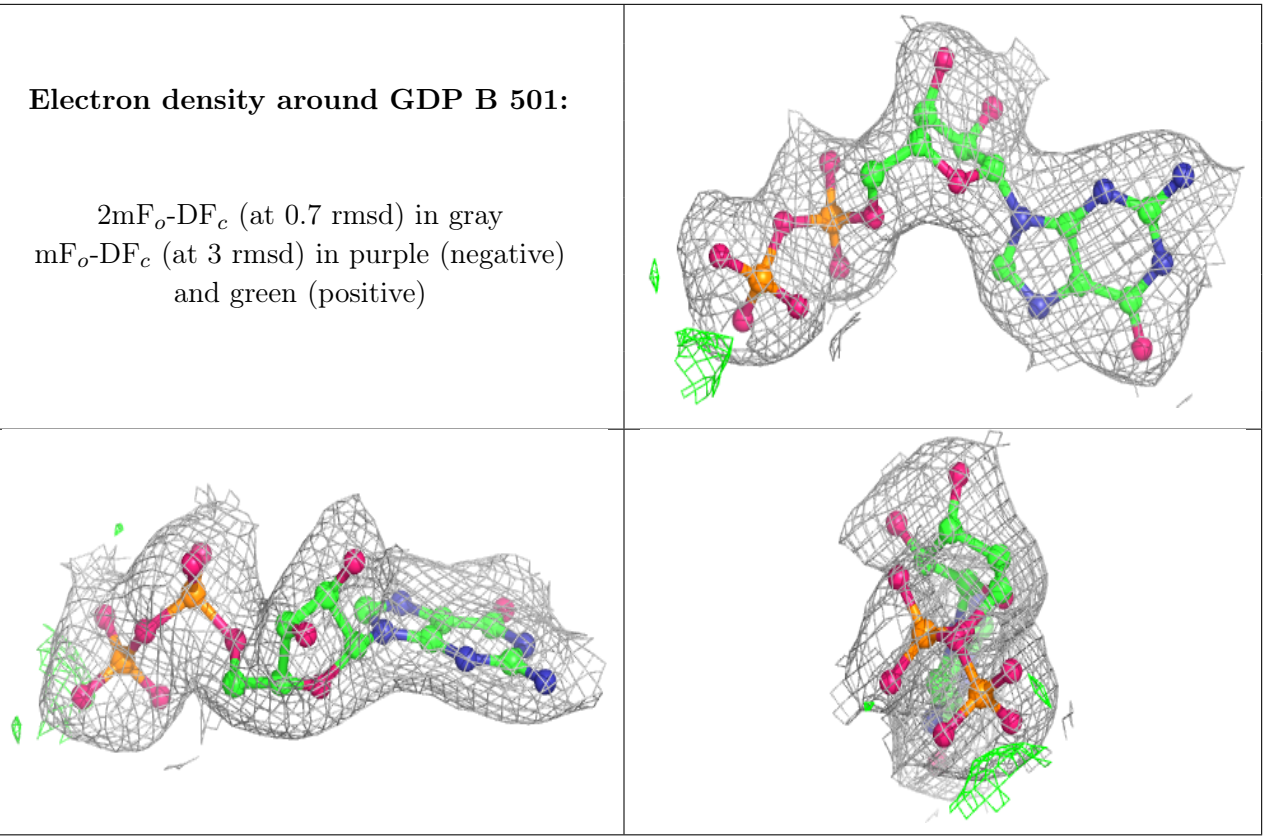
Electron density around GDP A 501:

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 GDP B 501:

$2mF_o$-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.