Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 11:21 pm GMT

PDB ID	:	2WTK
Title	:	Structure of the heterotrimeric LKB1-STRADalpha-MO25alpha complex
Authors	:	Zeqiraj, E.; van Aalten, D.M.F.
Deposited on	:	2009-09-16
Resolution	:	2.65 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:

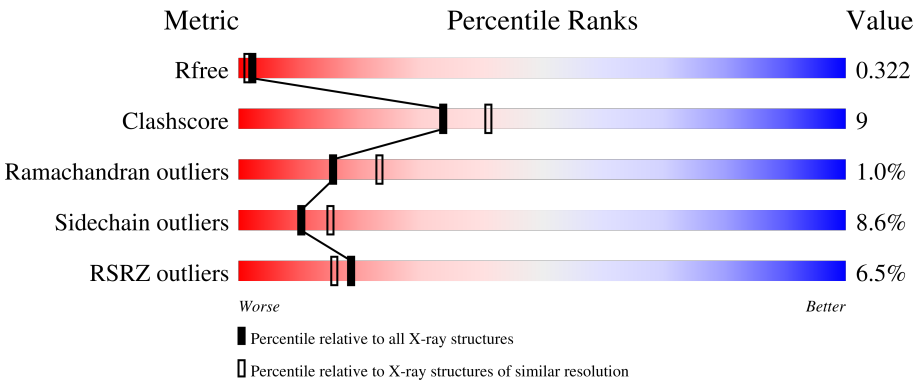
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	341	2%, 80%, 13%, • 6%
1	D	341	3%, 77%, 16%, • 5%
2	B	373	5%, 59%, 22%, • 17%
2	E	373	6%, 58%, 22%, • 17%
3	C	305	6%, 68%, 21%, • 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	305	13% 68% 17% • 12%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14850 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 CALCIUM-BINDING PROTEIN 39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	2655	1708	448	488	11	0	0	0
1	D	325	2681	1721	450	499	11	0	0	0

- Molecule 2 is a protein called STE20-RELATED KINASE ADAPTER PROTEIN ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	311	2473	1588	422	448	15	0	0	0
2	E	308	2454	1576	419	444	15	0	0	0

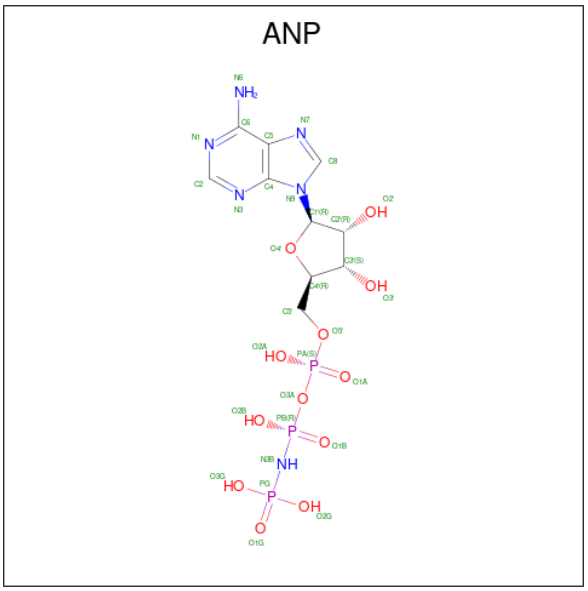
- Molecule 3 is a protein called SERINE/THREONINE-PROTEIN KINASE 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	285	2254	1448	386	406	14	0	0	0
3	F	268	2110	1360	363	374	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

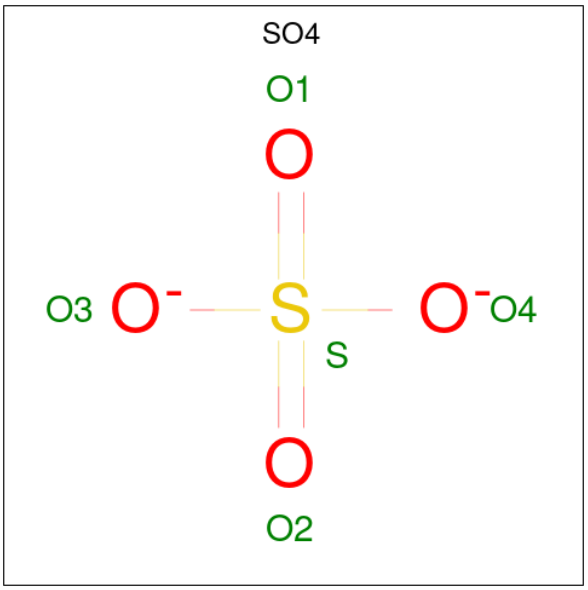
Chain	Residue	Modelled	Actual	Comment	Reference
C	194	ALA	ASP	engineered mutation	UNP Q15831
F	194	ALA	ASP	engineered mutation	UNP Q15831

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	B	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
4	C	1	27	10	6	9	2	0	0
			Total	C	N	O	P		
4	E	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
4	F	1	27	10	6	9	2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is water.

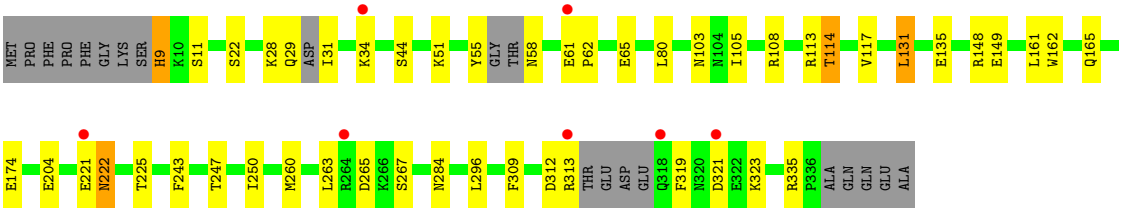
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	24	24	24	0	0
6	B	8	8	8	0	0
6	C	18	18	18	0	0
6	D	26	26	26	0	0
6	E	18	18	18	0	0
6	F	8	8	8	0	0

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.

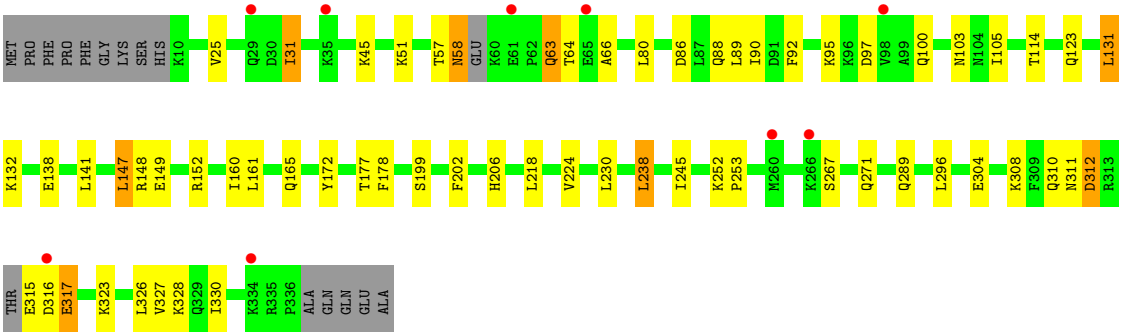
• Molecule 1: CALCIUM-BINDING PROTEIN 39

Chain A:



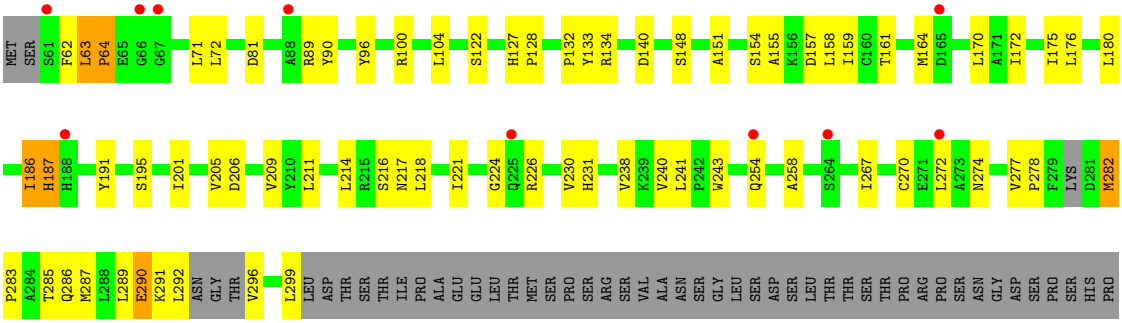
• Molecule 1: CALCIUM-BINDING PROTEIN 39

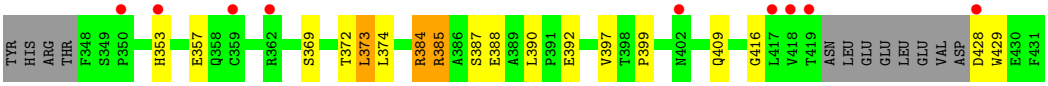
Chain D:



• Molecule 2: STE20-RELATED KINASE ADAPTER PROTEIN ALPHA

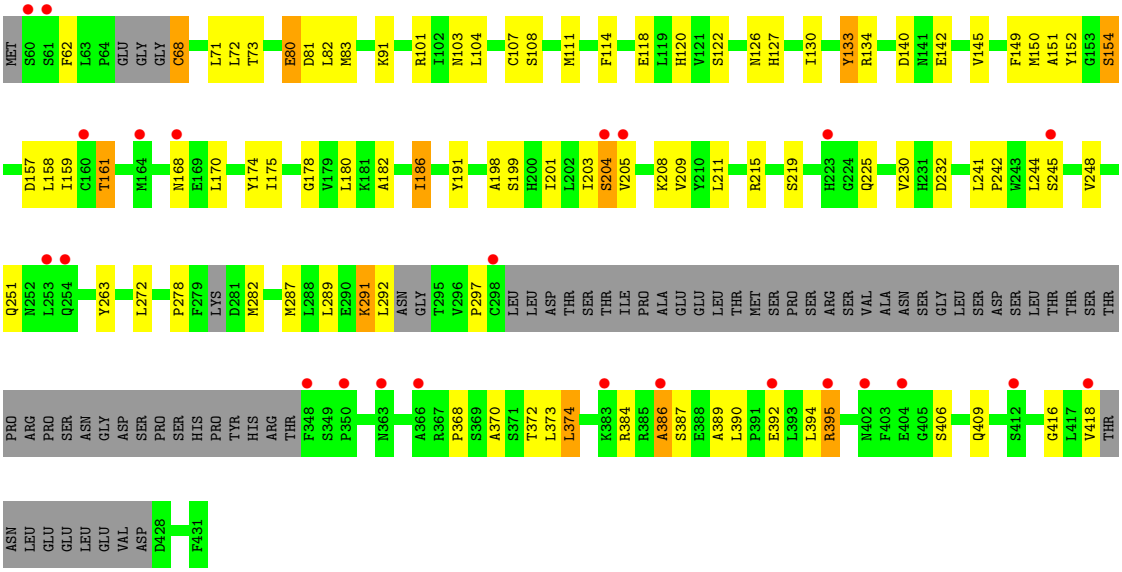
Chain B:





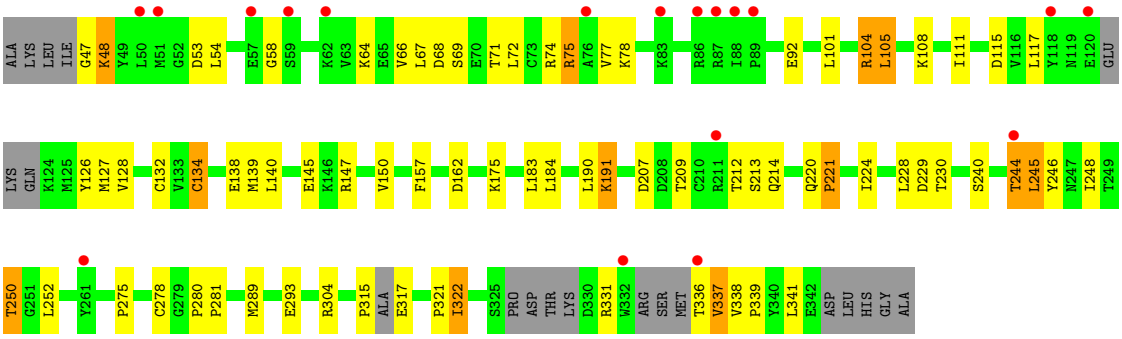
• Molecule 2: STE20-RELATED KINASE ADAPTER PROTEIN ALPHA

Chain E:



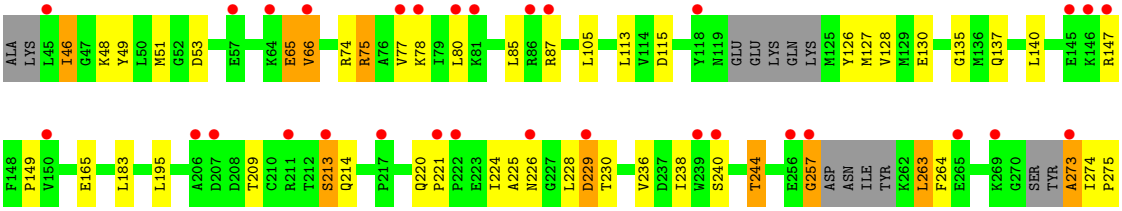
• Molecule 3: SERINE/THREONINE-PROTEIN KINASE 11

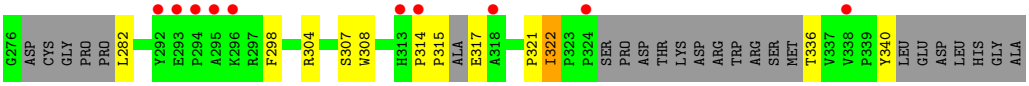
Chain C:



• Molecule 3: SERINE/THREONINE-PROTEIN KINASE 11

Chain F:




G276
ASP
CYS
GLY
PRO
PRO
L282
Y292
E293
P294
A295
K296
R297
F298
R304
S307
W308
H313
P314
P315
ALA
E317
A318
P321
I322
P323
P324
SER
PRO
ASP
THR
LYS
ASP
ARG
TRP
ARG
SER
MET
T336
V337
V338
P339
Y340
LEU
GLU
ASP
LEU
HIS
GLY
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	118.36Å 118.36Å 390.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.90 – 2.65 19.96 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.90-2.65) 99.2 (19.96-2.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.67Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.240 , 0.291 0.287 , 0.322	Depositor DCC
R_{free} test set	919 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	60.4	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 60.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14850	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: SO4, ANP

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	0.54	0/2700	0.62	0/3627
1	D	0.56	0/2726	0.62	0/3664
2	B	0.55	0/2534	0.69	0/3432
2	E	0.57	0/2514	0.67	0/3404
3	C	0.48	0/2305	0.62	1/3110 (0.0%)
3	F	0.68	5/2153 (0.2%)	0.62	0/2899
All	All	0.56	5/14932 (0.0%)	0.64	1/20136 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	273	ALA	CA-CB	15.55	1.85	1.52
3	F	273	ALA	N-CA	8.80	1.64	1.46
3	F	273	ALA	C-N	8.24	1.52	1.34
3	F	273	ALA	C-O	7.15	1.36	1.23
3	F	257	GLY	CA-C	6.12	1.61	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	105	LEU	CA-CB-CG	5.13	127.10	115.30

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	2655	0	2710	30	0
1	D	2681	0	2728	31	0
2	B	2473	0	2439	52	0
2	E	2454	0	2420	53	0
3	C	2254	0	2280	54	0
3	F	2110	0	2162	37	0
4	B	31	0	13	2	0
4	C	27	0	12	3	0
4	E	31	0	13	1	0
4	F	27	0	12	0	0
5	D	5	0	0	1	0
6	A	24	0	0	0	0
6	B	8	0	0	1	0
6	C	18	0	0	1	0
6	D	26	0	0	0	0
6	E	18	0	0	0	0
6	F	8	0	0	1	0
All	All	14850	0	14789	252	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 9.

All (252) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:273:ALA:CB	3:F:273:ALA:CA	1.85	1.50
3:C:104:ARG:HG3	3:C:104:ARG:HH11	1.11	1.10
2:B:161:THR:HG21	2:B:416:GLY:HA3	1.07	1.05
2:B:384:ARG:HG2	2:B:384:ARG:HH11	1.26	1.01
2:B:161:THR:CG2	2:B:416:GLY:HA3	1.95	0.97
3:F:75:ARG:HG3	3:F:75:ARG:HH11	1.35	0.89
1:D:63:GLN:HG3	1:D:66:ALA:HB3	1.55	0.87
3:C:104:ARG:HG3	3:C:104:ARG:NH1	1.87	0.82
3:C:331:ARG:HG2	3:C:331:ARG:HH11	1.46	0.81
3:F:75:ARG:HH11	3:F:75:ARG:CG	1.93	0.80
3:F:240:SER:O	3:F:244:THR:HG23	1.83	0.79
1:A:114:THR:CG2	1:A:117:VAL:HB	2.14	0.77
3:C:240:SER:O	3:C:244:THR:HG23	1.86	0.75
1:A:80:LEU:HD11	1:A:105:ILE:HD11	1.69	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:321:PRO:O	3:F:322:ILE:HB	1.86	0.74
1:D:90:ILE:O	1:D:95:LYS:HE3	1.88	0.74
2:B:254:GLN:HB2	3:C:331:ARG:HD3	1.71	0.73
1:D:63:GLN:CG	1:D:66:ALA:HB3	2.19	0.71
3:C:175:LYS:NZ	3:C:212:THR:OG1	2.22	0.71
2:E:127:HIS:HB3	2:E:130:ILE:HD12	1.73	0.71
3:C:250:THR:HG22	3:C:252:LEU:H	1.55	0.71
1:A:221:GLU:O	1:A:222:ASN:HB2	1.89	0.70
1:D:63:GLN:HG3	1:D:66:ALA:CB	2.19	0.70
3:F:228:LEU:O	3:F:229:ASP:HB2	1.90	0.70
1:A:108:ARG:HG3	1:A:108:ARG:HH11	1.57	0.69
2:B:384:ARG:HH11	2:B:384:ARG:CG	2.04	0.69
2:B:299:LEU:HD13	2:B:353:HIS:ND1	2.08	0.69
3:F:75:ARG:HD3	6:F:2001:HOH:O	1.95	0.67
2:B:195:SER:HB3	2:B:216:SER:OG	1.95	0.66
3:C:315:PRO:O	3:C:317:GLU:N	2.28	0.66
1:D:88:GLN:HE22	1:D:138:GLU:HG3	1.60	0.66
3:F:282:LEU:HB2	3:F:308:TRP:CD1	2.32	0.64
1:A:114:THR:HG23	1:A:117:VAL:HB	1.78	0.64
2:E:242:PRO:O	2:E:291:LYS:NZ	2.31	0.64
2:B:282:MET:HB2	2:B:283:PRO:HD2	1.81	0.63
3:C:250:THR:CG2	3:C:252:LEU:H	2.12	0.63
1:D:80:LEU:HD11	1:D:105:ILE:HD11	1.81	0.63
2:B:290:GLU:O	2:B:292:LEU:N	2.32	0.62
3:C:134:CYS:SG	3:C:138:GLU:HG3	2.38	0.62
1:A:309:PHE:O	1:A:323:LYS:NZ	2.26	0.62
1:A:55:TYR:HE1	2:B:224:GLY:O	1.83	0.62
2:B:133:TYR:N	2:B:133:TYR:HD1	1.97	0.62
2:B:385:ARG:NH2	6:B:2008:HOH:O	2.33	0.62
3:C:246:TYR:O	3:C:250:THR:HB	1.99	0.61
3:C:78:LYS:HB3	3:C:127:MET:HB2	1.83	0.61
4:C:2:ANP:O5'	4:C:2:ANP:H8	2.01	0.61
3:C:66:VAL:HG13	3:C:67:LEU:N	2.16	0.60
3:C:75:ARG:NH2	6:C:2001:HOH:O	2.34	0.60
2:B:187:HIS:CD2	2:B:258:ALA:HB1	2.37	0.60
2:B:369:SER:O	2:B:373:LEU:HB2	2.01	0.60
2:B:133:TYR:N	2:B:133:TYR:CD1	2.68	0.59
3:C:111:ILE:HD13	3:C:183:LEU:HD12	1.84	0.59
3:C:338:VAL:HB	3:C:339:PRO:HD3	1.84	0.59
2:E:174:TYR:CD1	2:E:386:ALA:HB2	2.37	0.58
3:F:137:GLN:HA	3:F:140:LEU:HD12	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:209:THR:HG23	3:F:230:THR:HB	1.86	0.58
2:E:161:THR:CG2	2:E:416:GLY:HA3	2.34	0.58
2:E:159:ILE:HD11	2:E:272:LEU:HA	1.85	0.57
2:B:384:ARG:HG2	2:B:384:ARG:NH1	2.06	0.57
3:C:104:ARG:HH11	3:C:104:ARG:CG	2.00	0.57
3:C:321:PRO:O	3:C:322:ILE:HB	2.05	0.57
1:A:319:PHE:CE2	1:A:323:LYS:HD2	2.40	0.57
2:B:186:ILE:HD12	2:B:191:TYR:CB	2.35	0.57
3:C:207:ASP:OD2	3:C:209:THR:OG1	2.18	0.57
2:B:122:SER:HB2	2:B:214:LEU:HD12	1.87	0.57
3:C:221:PRO:HD2	3:C:224:ILE:HD12	1.86	0.56
3:F:213:SER:HB3	3:F:224:ILE:HG21	1.88	0.56
1:A:114:THR:CG2	1:A:114:THR:O	2.53	0.56
2:B:238:VAL:HG22	3:C:71:THR:HB	1.86	0.56
1:D:63:GLN:H	1:D:63:GLN:HE21	1.52	0.56
2:B:186:ILE:HD12	2:B:191:TYR:HB2	1.87	0.56
3:F:228:LEU:O	3:F:229:ASP:CB	2.52	0.56
2:B:158:LEU:HD21	2:B:397:VAL:HG11	1.86	0.56
1:D:92:PHE:CE2	2:E:126:ASN:HB2	2.40	0.56
3:C:245:LEU:HD12	3:C:289:MET:CE	2.35	0.55
2:B:151:ALA:HB2	2:B:205:VAL:HG22	1.87	0.55
2:B:157:ASP:OD2	4:B:432:ANP:O2'	2.25	0.55
3:C:77:VAL:HG22	3:C:128:VAL:HG22	1.89	0.55
1:D:152:ARG:NH2	5:D:342:SO4:O1	2.35	0.55
2:E:182:ALA:O	2:E:186:ILE:HG23	2.06	0.55
2:B:221:ILE:HG12	2:B:226:ARG:HG3	1.89	0.55
2:B:172:ILE:HG22	2:B:176:LEU:HD12	1.89	0.54
3:C:213:SER:OG	3:C:214:GLN:N	2.40	0.54
3:C:331:ARG:HG2	3:C:331:ARG:NH1	2.18	0.54
3:C:250:THR:OG1	3:C:275:PRO:HG2	2.08	0.54
1:A:103:ASN:CG	1:A:149:GLU:HG3	2.28	0.54
3:F:336:THR:HG22	3:F:336:THR:O	2.08	0.54
1:D:267:SER:O	1:D:271:GLN:HG2	2.07	0.54
2:E:244:LEU:O	2:E:291:LYS:HE3	2.06	0.54
3:F:66:VAL:HB	3:F:77:VAL:HG23	1.90	0.54
2:B:158:LEU:CD2	2:B:397:VAL:HG11	2.38	0.53
1:D:316:ASP:O	1:D:317:GLU:HB2	2.08	0.53
3:C:229:ASP:O	3:C:230:THR:HG23	2.08	0.53
2:E:158:LEU:HD13	2:E:394:LEU:HD22	1.90	0.53
2:E:186:ILE:HD12	2:E:191:TYR:HB2	1.90	0.53
2:E:186:ILE:HD12	2:E:191:TYR:CB	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:GLY:HA3	4:C:2:ANP:O2B	2.08	0.53
1:A:221:GLU:O	1:A:222:ASN:CB	2.55	0.52
3:C:47:GLY:O	3:C:48:LYS:HB3	2.09	0.52
3:C:157:PHE:CD2	3:C:245:LEU:HG	2.44	0.52
3:F:80:LEU:HD22	3:F:85:LEU:HD21	1.92	0.52
3:C:250:THR:HG23	3:C:252:LEU:HB2	1.92	0.52
1:D:86:ASP:HB3	1:D:89:LEU:HD12	1.92	0.52
1:A:131:LEU:HB3	1:A:165:GLN:OE1	2.09	0.51
2:B:132:PRO:C	2:B:133:TYR:HD1	2.13	0.51
3:C:117:LEU:HB2	3:C:126:TYR:HB2	1.92	0.51
3:C:280:PRO:HB2	3:C:281:PRO:HD3	1.91	0.51
3:F:53:ASP:H	3:F:336:THR:CG2	2.24	0.51
1:A:108:ARG:HG3	1:A:108:ARG:NH1	2.23	0.51
2:E:107:CYS:HB3	2:E:111:MET:HB2	1.93	0.51
3:F:165:GLU:CD	3:F:304:ARG:HH12	2.14	0.51
1:A:312:ASP:O	1:A:313:ARG:HG2	2.11	0.51
1:A:319:PHE:CZ	1:A:323:LYS:HD2	2.46	0.51
2:E:149:PHE:CE2	2:E:151:ALA:HA	2.46	0.51
3:F:336:THR:O	3:F:336:THR:CG2	2.59	0.51
3:C:66:VAL:CG1	3:C:67:LEU:N	2.74	0.50
3:C:108:LYS:O	3:C:191:LYS:HE3	2.11	0.50
2:B:428:ASP:CG	2:B:429:TRP:H	2.14	0.50
2:E:191:TYR:CE1	2:E:219:SER:HB2	2.46	0.50
2:E:178:GLY:HA3	2:E:209:VAL:CG2	2.42	0.50
2:B:89:ARG:HB2	2:B:96:TYR:CE2	2.47	0.50
3:C:66:VAL:HG13	3:C:67:LEU:H	1.77	0.50
1:D:218:LEU:HD22	1:D:230:LEU:HD13	1.94	0.50
1:D:103:ASN:CG	1:D:149:GLU:HG3	2.32	0.49
3:F:257:GLY:HA3	3:F:263:LEU:HD22	1.94	0.49
3:C:68:ASP:O	3:C:72:LEU:HA	2.12	0.49
2:E:175:ILE:HG23	2:E:201:ILE:HG21	1.95	0.49
2:E:108:SER:OG	2:E:111:MET:HG3	2.13	0.49
1:D:202:PHE:CD1	1:D:206:HIS:ND1	2.80	0.49
2:B:240:VAL:O	2:B:243:TRP:HE3	1.96	0.49
2:E:161:THR:HG23	2:E:416:GLY:HA3	1.95	0.49
1:A:260:MET:HA	1:A:263:LEU:HD12	1.94	0.49
2:B:206:ASP:O	2:B:387:SER:HA	2.13	0.49
3:C:140:LEU:HD11	3:C:248:ILE:HG22	1.94	0.49
1:D:141:LEU:HD11	2:E:120:HIS:ND1	2.26	0.48
3:F:78:LYS:HE2	3:F:80:LEU:HD21	1.93	0.48
3:C:132:CYS:O	4:C:2:ANP:H2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:224:ILE:C	3:F:226:ASN:H	2.16	0.48
2:E:133:TYR:CD2	2:E:145:VAL:HG11	2.48	0.48
3:C:48:LYS:O	3:C:69:SER:HB3	2.14	0.48
2:B:122:SER:O	2:B:122:SER:OG	2.25	0.48
2:E:384:ARG:HD2	2:E:389:ALA:HB2	1.96	0.48
1:A:80:LEU:HD11	1:A:105:ILE:CD1	2.43	0.47
2:E:154:SER:HA	2:E:201:ILE:O	2.14	0.47
3:F:113:LEU:HD13	3:F:127:MET:HE3	1.96	0.47
3:F:221:PRO:HG3	3:F:236:VAL:HG22	1.95	0.47
1:D:147:LEU:HD21	1:D:160:ILE:HD11	1.96	0.47
3:C:53:ASP:HB2	3:C:336:THR:HG21	1.96	0.47
1:D:25:VAL:O	1:D:31:ILE:HD11	2.14	0.47
2:E:83:MET:HA	2:E:101:ARG:O	2.14	0.47
2:E:133:TYR:HD2	2:E:145:VAL:HG11	1.80	0.47
1:A:51:LYS:HG2	1:A:55:TYR:CD2	2.49	0.47
3:F:213:SER:HB3	3:F:224:ILE:CG2	2.44	0.47
1:D:51:LYS:HE3	1:D:97:ASP:OD1	2.15	0.47
3:C:67:LEU:HG	3:C:337:VAL:HG11	1.96	0.47
2:E:157:ASP:O	2:E:161:THR:HB	2.14	0.47
2:B:134:ARG:NH1	2:B:148:SER:OG	2.46	0.46
1:A:114:THR:HG23	1:A:114:THR:O	2.16	0.46
1:D:310:GLN:C	1:D:312:ASP:H	2.19	0.46
1:A:243:PHE:O	1:A:247:THR:HG23	2.16	0.46
2:E:204:SER:HB2	2:E:208:LYS:HB2	1.96	0.46
2:B:151:ALA:HB1	2:B:399:PRO:HB2	1.98	0.46
1:D:316:ASP:O	1:D:317:GLU:CB	2.64	0.46
2:E:370:ALA:O	2:E:374:LEU:HD22	2.15	0.46
1:D:131:LEU:HD22	1:D:172:TYR:HE2	1.81	0.46
2:E:114:PHE:CE2	2:E:215:ARG:HG2	2.51	0.45
2:E:122:SER:OG	2:E:133:TYR:CD1	2.58	0.45
2:E:133:TYR:CD1	2:E:133:TYR:N	2.83	0.45
1:A:131:LEU:HD13	1:A:165:GLN:HB3	1.97	0.45
3:C:321:PRO:O	3:C:322:ILE:CB	2.64	0.45
3:F:135:GLY:HA2	3:F:183:LEU:HA	1.97	0.45
2:B:296:VAL:O	2:B:296:VAL:HG12	2.15	0.45
3:F:75:ARG:HG3	3:F:75:ARG:NH1	2.13	0.45
2:B:63:LEU:HA	2:B:64:PRO:HD3	1.84	0.45
2:E:62:PHE:HZ	2:E:134:ARG:HH11	1.65	0.45
3:F:149:PRO:HB3	3:F:317:GLU:OE1	2.17	0.45
2:B:299:LEU:HD12	2:B:299:LEU:H	1.80	0.45
2:E:118:GLU:HG3	2:E:215:ARG:HA	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:150:MET:O	4:E:432:ANP:H2	2.17	0.44
3:F:65:GLU:OE1	3:F:74:ARG:NH1	2.50	0.44
2:B:155:ALA:O	2:B:159:ILE:HG12	2.17	0.44
2:B:175:ILE:HG23	2:B:201:ILE:HG21	1.99	0.44
3:C:245:LEU:HD12	3:C:289:MET:HE1	1.99	0.44
2:E:133:TYR:HD2	2:E:145:VAL:CG1	2.29	0.44
3:F:314:PRO:HA	3:F:315:PRO:HD3	1.83	0.44
1:D:252:LYS:HA	1:D:253:PRO:HD2	1.67	0.44
2:E:244:LEU:HD22	2:E:248:VAL:HG11	1.99	0.44
3:F:225:ALA:HB1	3:F:264:PHE:O	2.17	0.44
3:C:250:THR:CG2	3:C:252:LEU:HB2	2.48	0.44
3:C:47:GLY:O	3:C:48:LYS:CB	2.66	0.44
2:E:161:THR:HG21	2:E:416:GLY:CA	2.48	0.44
2:E:198:ALA:HA	2:E:201:ILE:HD12	2.00	0.44
3:F:77:VAL:HG11	3:F:126:TYR:HB3	2.00	0.44
3:C:162:ASP:OD1	3:C:304:ARG:NH2	2.51	0.43
2:B:154:SER:HA	2:B:201:ILE:O	2.18	0.43
3:C:190:LEU:C	3:C:190:LEU:HD23	2.39	0.43
1:A:174:GLU:HG3	1:A:225:THR:HG21	2.00	0.43
3:C:245:LEU:HD12	3:C:289:MET:HE3	1.99	0.43
1:D:88:GLN:NE2	1:D:138:GLU:HG3	2.28	0.43
3:C:48:LYS:O	3:C:69:SER:CB	2.66	0.43
3:F:49:TYR:HB3	3:F:66:VAL:CG2	2.49	0.43
1:A:61:GLU:HA	1:A:62:PRO:HD2	1.73	0.43
3:F:46:ILE:N	3:F:49:TYR:O	2.49	0.43
2:B:230:VAL:HG22	2:B:231:HIS:N	2.34	0.43
2:E:161:THR:CG2	2:E:416:GLY:CA	2.97	0.43
1:A:114:THR:HG22	1:A:117:VAL:HB	1.99	0.43
1:D:57:THR:OG1	1:D:58:ASN:N	2.52	0.43
2:E:82:LEU:CD1	2:E:111:MET:CE	2.97	0.43
2:E:82:LEU:HD13	2:E:111:MET:HE1	1.99	0.43
2:E:230:VAL:HG22	2:E:232:ASP:H	1.83	0.43
2:E:392:GLU:O	2:E:395:ARG:HB2	2.18	0.43
1:A:265:ASP:OD2	1:A:267:SER:HB3	2.19	0.42
2:B:159:ILE:O	2:B:164:MET:HA	2.18	0.42
1:A:51:LYS:HG2	1:A:55:TYR:HD2	1.83	0.42
1:A:114:THR:HG23	1:A:117:VAL:CB	2.47	0.42
2:B:214:LEU:O	2:B:217:ASN:HB2	2.19	0.42
1:D:326:LEU:O	1:D:330:ILE:HG12	2.19	0.42
1:A:9:HIS:HD1	1:A:9:HIS:N	2.17	0.42
2:E:62:PHE:HZ	2:E:134:ARG:NH1	2.16	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:245:SER:HA	2:E:263:TYR:CD2	2.55	0.42
2:E:373:LEU:HD23	2:E:373:LEU:HA	1.90	0.42
1:D:245:ILE:HD12	1:D:245:ILE:H	1.85	0.42
2:B:63:LEU:HB2	2:B:90:TYR:OH	2.19	0.42
1:D:238:LEU:HD12	1:D:238:LEU:HA	1.81	0.42
2:E:80:GLU:O	2:E:81:ASP:HB2	2.19	0.42
1:A:28:LYS:HG2	1:A:29:GLN:OE1	2.19	0.42
2:B:155:ALA:HB1	2:B:272:LEU:HD21	2.01	0.42
2:B:267:ILE:HG23	2:B:278:PRO:HG2	2.02	0.42
2:E:251:GLN:HB2	3:F:74:ARG:HG3	2.00	0.41
2:B:282:MET:CB	2:B:283:PRO:HD2	2.50	0.41
2:B:230:VAL:HG22	2:B:231:HIS:H	1.85	0.41
2:B:270:CYS:O	2:B:274:ASN:HB2	2.20	0.41
1:A:250:ILE:HD12	1:A:284:ASN:HB2	2.03	0.41
3:C:67:LEU:HG	3:C:337:VAL:CG1	2.50	0.41
2:E:161:THR:HG21	2:E:416:GLY:HA3	2.02	0.41
2:B:100:ARG:NH1	4:B:432:ANP:O1A	2.37	0.41
1:D:178:PHE:CE1	1:D:224:VAL:HG11	2.56	0.41
2:E:103:ASN:HA	2:E:142:GLU:HG2	2.02	0.41
3:F:77:VAL:HG22	3:F:128:VAL:HG22	2.03	0.41
3:C:139:MET:SD	3:C:184:LEU:HD12	2.60	0.41
1:D:304:GLU:O	1:D:308:LYS:HG2	2.21	0.41
2:E:368:PRO:HG2	2:E:373:LEU:HG	2.03	0.41
3:C:54:LEU:HA	3:C:64:LYS:HG2	2.03	0.40
2:E:152:TYR:HB2	2:E:203:ILE:O	2.21	0.40
2:E:278:PRO:HB3	2:E:297:PRO:HG3	2.03	0.40
3:F:238:ILE:HD13	3:F:298:PHE:O	2.21	0.40
2:B:127:HIS:CG	2:B:128:PRO:HD2	2.56	0.40
1:D:323:LYS:O	1:D:327:VAL:HG23	2.21	0.40
2:E:68:CYS:N	2:E:91:LYS:HZ2	2.18	0.40
2:B:277:VAL:HG22	2:B:278:PRO:O	2.22	0.40
3:C:101:LEU:O	3:C:104:ARG:HG2	2.20	0.40
3:F:65:GLU:HG3	3:F:66:VAL:N	2.34	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	313/341 (92%)	300 (96%)	11 (4%)	2 (1%)	25	37
1	D	319/341 (94%)	301 (94%)	16 (5%)	2 (1%)	25	37
2	B	301/373 (81%)	277 (92%)	20 (7%)	4 (1%)	12	18
2	E	296/373 (79%)	270 (91%)	22 (7%)	4 (1%)	11	16
3	C	275/305 (90%)	258 (94%)	15 (6%)	2 (1%)	22	33
3	F	254/305 (83%)	235 (92%)	15 (6%)	4 (2%)	9	14
All	All	1758/2038 (86%)	1641 (93%)	99 (6%)	18 (1%)	15	23

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
2	B	62	PHE
1	D	317	GLU
2	E	387	SER
3	F	214	GLN
3	F	229	ASP
2	B	64	PRO
3	C	48	LYS
2	E	73	THR
3	F	275	PRO
2	B	290	GLU
3	C	322	ILE
2	E	205	VAL
3	F	322	ILE
2	B	291	LYS
2	E	386	ALA
1	D	311	ASN
1	A	11	SER

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	296/312 (95%)	278 (94%)	18 (6%)	18	29
1	D	299/312 (96%)	277 (93%)	22 (7%)	13	21
2	B	274/331 (83%)	245 (89%)	29 (11%)	6	10
2	E	273/331 (82%)	243 (89%)	30 (11%)	6	9
3	C	246/262 (94%)	225 (92%)	21 (8%)	10	15
3	F	230/262 (88%)	211 (92%)	19 (8%)	11	16
All	All	1618/1810 (89%)	1479 (91%)	139 (9%)	10	15

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	22	SER
1	A	31	ILE
1	A	34	LYS
1	A	44	SER
1	A	58	ASN
1	A	65	GLU
1	A	113	ARG
1	A	114	THR
1	A	131	LEU
1	A	135	GLU
1	A	148	ARG
1	A	161	LEU
1	A	162	TRP
1	A	204	GLU
1	A	296	LEU
1	A	321	ASP
1	A	335	ARG
2	B	63	LEU
2	B	71	LEU
2	B	72	LEU
2	B	81	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	104	LEU
2	B	140	ASP
2	B	170	LEU
2	B	180	LEU
2	B	186	ILE
2	B	187	HIS
2	B	209	VAL
2	B	211	LEU
2	B	218	LEU
2	B	241	LEU
2	B	282	MET
2	B	285	THR
2	B	286	GLN
2	B	287	MET
2	B	289	LEU
2	B	357	GLU
2	B	372	THR
2	B	373	LEU
2	B	374	LEU
2	B	384	ARG
2	B	385	ARG
2	B	388	GLU
2	B	390	LEU
2	B	392	GLU
2	B	409	GLN
3	C	74	ARG
3	C	75	ARG
3	C	92	GLU
3	C	104	ARG
3	C	105	LEU
3	C	115	ASP
3	C	134	CYS
3	C	145	GLU
3	C	147	ARG
3	C	150	VAL
3	C	191	LYS
3	C	220	GLN
3	C	221	PRO
3	C	228	LEU
3	C	244	THR
3	C	245	LEU
3	C	250	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	278	CYS
3	C	293	GLU
3	C	337	VAL
3	C	341	LEU
1	D	31	ILE
1	D	45	LYS
1	D	58	ASN
1	D	63	GLN
1	D	64	THR
1	D	100	GLN
1	D	114	THR
1	D	123	GLN
1	D	131	LEU
1	D	132	LYS
1	D	147	LEU
1	D	148	ARG
1	D	161	LEU
1	D	165	GLN
1	D	177	THR
1	D	199	SER
1	D	238	LEU
1	D	289	GLN
1	D	296	LEU
1	D	312	ASP
1	D	315	GLU
1	D	328	LYS
2	E	68	CYS
2	E	71	LEU
2	E	72	LEU
2	E	80	GLU
2	E	104	LEU
2	E	133	TYR
2	E	140	ASP
2	E	154	SER
2	E	161	THR
2	E	168	ASN
2	E	170	LEU
2	E	180	LEU
2	E	186	ILE
2	E	199	SER
2	E	204	SER
2	E	211	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	225	GLN
2	E	241	LEU
2	E	282	MET
2	E	287	MET
2	E	289	LEU
2	E	291	LYS
2	E	292	LEU
2	E	372	THR
2	E	374	LEU
2	E	390	LEU
2	E	395	ARG
2	E	406	SER
2	E	409	GLN
2	E	418	VAL
3	F	46	ILE
3	F	48	LYS
3	F	51	MET
3	F	65	GLU
3	F	66	VAL
3	F	75	ARG
3	F	87	ARG
3	F	105	LEU
3	F	115	ASP
3	F	130	GLU
3	F	147	ARG
3	F	195	LEU
3	F	213	SER
3	F	220	GLN
3	F	244	THR
3	F	263	LEU
3	F	274	ILE
3	F	307	SER
3	F	340	TYR

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

Mol	Chain	Res	Type
2	B	168	ASN
2	B	254	GLN
3	C	226	ASN
1	D	63	GLN
1	D	100	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	205	GLN
1	D	228	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)

5 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	$\#\|Z\| > 2$
4	ANP	B	432	-	29,33,33	1.77	6 (20%)	31,52,52	1.69	8 (25%)
4	ANP	E	432	-	29,33,33	1.85	7 (24%)	31,52,52	1.73	8 (25%)
5	SO4	D	342	-	4,4,4	0.13	0	6,6,6	0.13	0
4	ANP	C	2	-	24,29,33	1.36	4 (16%)	25,45,52	1.44	5 (20%)
4	ANP	F	4	-	24,29,33	1.42	4 (16%)	25,45,52	1.36	4 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	B	432	-	-	7/14/38/38	0/3/3/3
4	ANP	E	432	-	-	3/14/38/38	0/3/3/3
4	ANP	C	2	-	-	2/9/32/38	0/3/3/3
4	ANP	F	4	-	-	4/9/32/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	432	ANP	PG-N3B	4.40	1.74	1.63
4	E	432	ANP	PG-N3B	4.34	1.74	1.63
4	E	432	ANP	PB-N3B	4.03	1.73	1.63
4	E	432	ANP	PG-O1G	3.83	1.52	1.46
4	B	432	ANP	PG-O1G	3.81	1.52	1.46
4	C	2	ANP	PB-O1B	3.63	1.51	1.46
4	B	432	ANP	PB-N3B	3.59	1.72	1.63
4	F	4	ANP	PB-O1B	3.46	1.51	1.46
4	B	432	ANP	PB-O1B	3.21	1.51	1.46
4	E	432	ANP	PB-O1B	3.11	1.51	1.46
4	E	432	ANP	C5-C4	3.05	1.49	1.40
4	F	4	ANP	PB-O3A	3.03	1.62	1.59
4	F	4	ANP	C5-C4	2.78	1.48	1.40
4	B	432	ANP	C5-C4	2.69	1.48	1.40
4	C	2	ANP	C5-C4	2.57	1.47	1.40
4	C	2	ANP	PB-O3A	2.33	1.62	1.59
4	E	432	ANP	PB-O3A	2.30	1.62	1.59
4	B	432	ANP	PB-O2B	-2.26	1.50	1.56
4	F	4	ANP	C2-N3	2.23	1.35	1.32
4	E	432	ANP	PB-O2B	-2.19	1.50	1.56
4	C	2	ANP	C2-N3	2.01	1.35	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	432	ANP	O1G-PG-N3B	-4.40	105.29	111.77
4	E	432	ANP	N3-C2-N1	-3.81	122.73	128.68
4	B	432	ANP	N3-C2-N1	-3.54	123.14	128.68
4	B	432	ANP	O1B-PB-N3B	-3.46	106.68	111.77
4	F	4	ANP	C4-C5-N7	-3.18	106.08	109.40
4	C	2	ANP	N3-C2-N1	-3.18	123.71	128.68
4	F	4	ANP	N3-C2-N1	-3.05	123.91	128.68
4	B	432	ANP	PB-O3A-PA	-3.03	121.94	132.62
4	C	2	ANP	O2B-PB-O1B	3.02	118.08	110.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	2	ANP	PB-O3A-PA	-2.97	123.14	132.56
4	E	432	ANP	O2G-PG-O3G	2.96	115.51	107.64
4	E	432	ANP	O2B-PB-O1B	2.94	116.08	109.92
4	F	4	ANP	O2B-PB-O1B	2.91	117.80	110.25
4	B	432	ANP	O1G-PG-N3B	-2.76	107.70	111.77
4	B	432	ANP	O2B-PB-O1B	2.73	115.65	109.92
4	C	2	ANP	C4-C5-N7	-2.68	106.61	109.40
4	B	432	ANP	O2A-PA-O1A	2.52	124.72	112.24
4	C	2	ANP	C3'-C2'-C1'	2.42	104.63	100.98
4	F	4	ANP	C3'-C2'-C1'	2.32	104.47	100.98
4	B	432	ANP	O3A-PB-N3B	2.23	112.77	106.59
4	E	432	ANP	PB-O3A-PA	-2.21	124.83	132.62
4	E	432	ANP	C4-C5-N7	-2.20	107.10	109.40
4	E	432	ANP	O2B-PB-O3A	2.17	111.88	104.64
4	E	432	ANP	C2-N1-C6	2.11	122.37	118.75
4	B	432	ANP	O2G-PG-O3G	2.06	113.12	107.64

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	432	ANP	PB-N3B-PG-O1G
4	B	432	ANP	PG-N3B-PB-O1B
4	B	432	ANP	PG-N3B-PB-O3A
4	E	432	ANP	PB-N3B-PG-O1G
4	E	432	ANP	PG-N3B-PB-O1B
4	F	4	ANP	C5'-O5'-PA-O2A
4	B	432	ANP	O4'-C4'-C5'-O5'
4	B	432	ANP	PB-O3A-PA-O1A
4	F	4	ANP	C5'-O5'-PA-O3A
4	F	4	ANP	C5'-O5'-PA-O1A
4	B	432	ANP	PB-O3A-PA-O2A
4	B	432	ANP	C3'-C4'-C5'-O5'
4	C	2	ANP	PB-O3A-PA-O2A
4	F	4	ANP	PB-O3A-PA-O2A
4	E	432	ANP	PB-O3A-PA-O1A
4	C	2	ANP	O4'-C4'-C5'-O5'

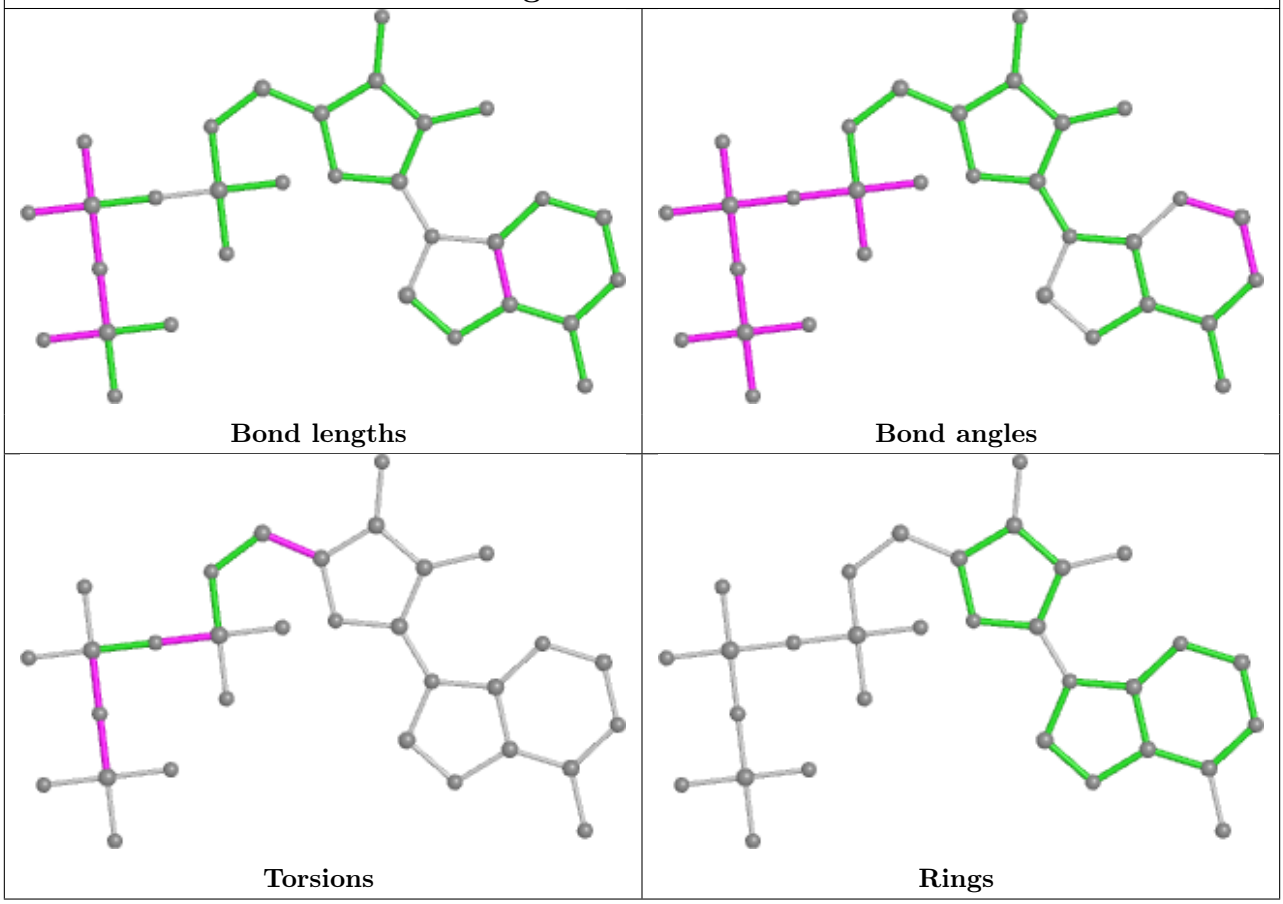
There are no ring outliers.

4 monomers are involved in 7 short contacts:

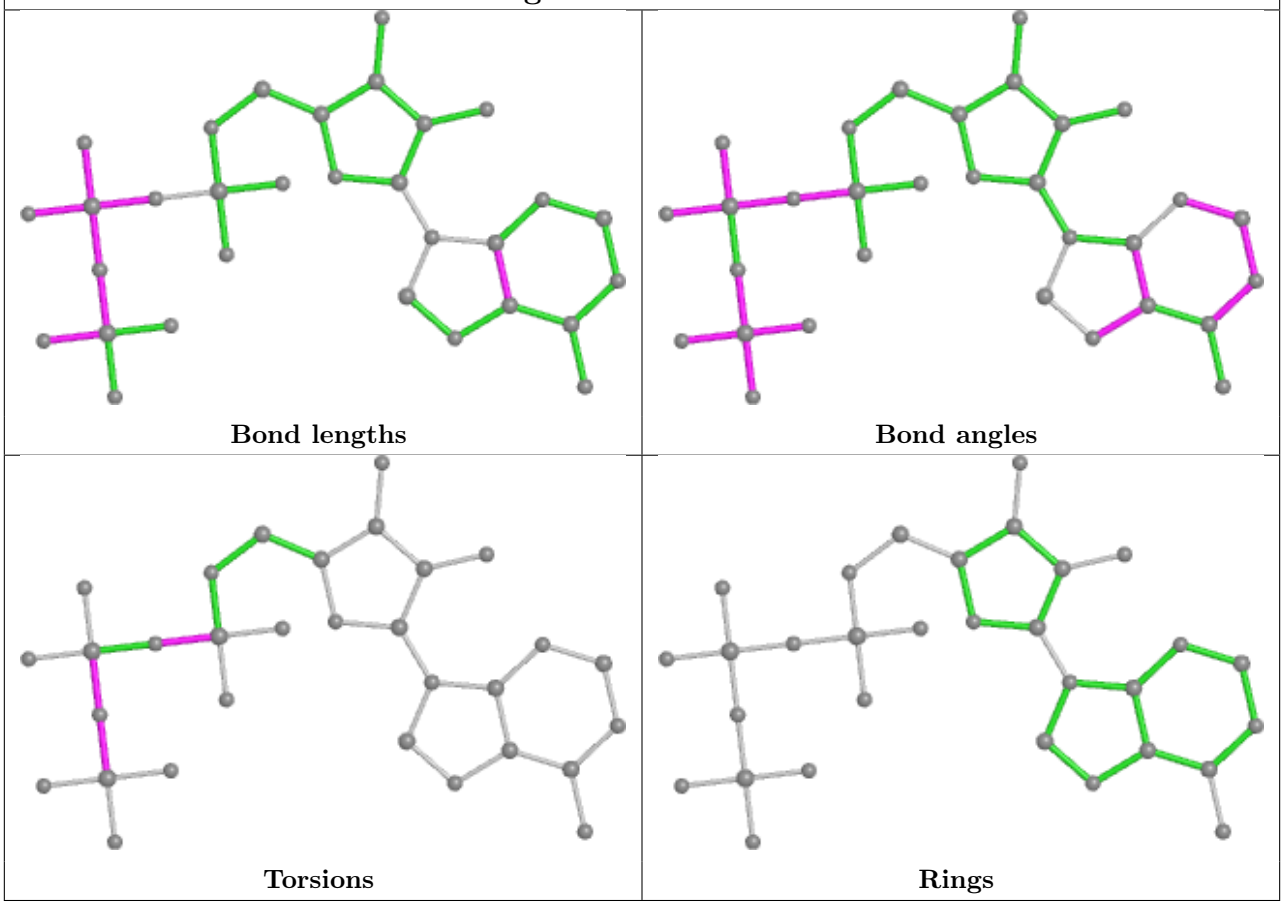
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	432	ANP	2	0
4	E	432	ANP	1	0
5	D	342	SO4	1	0
4	C	2	ANP	3	0

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.

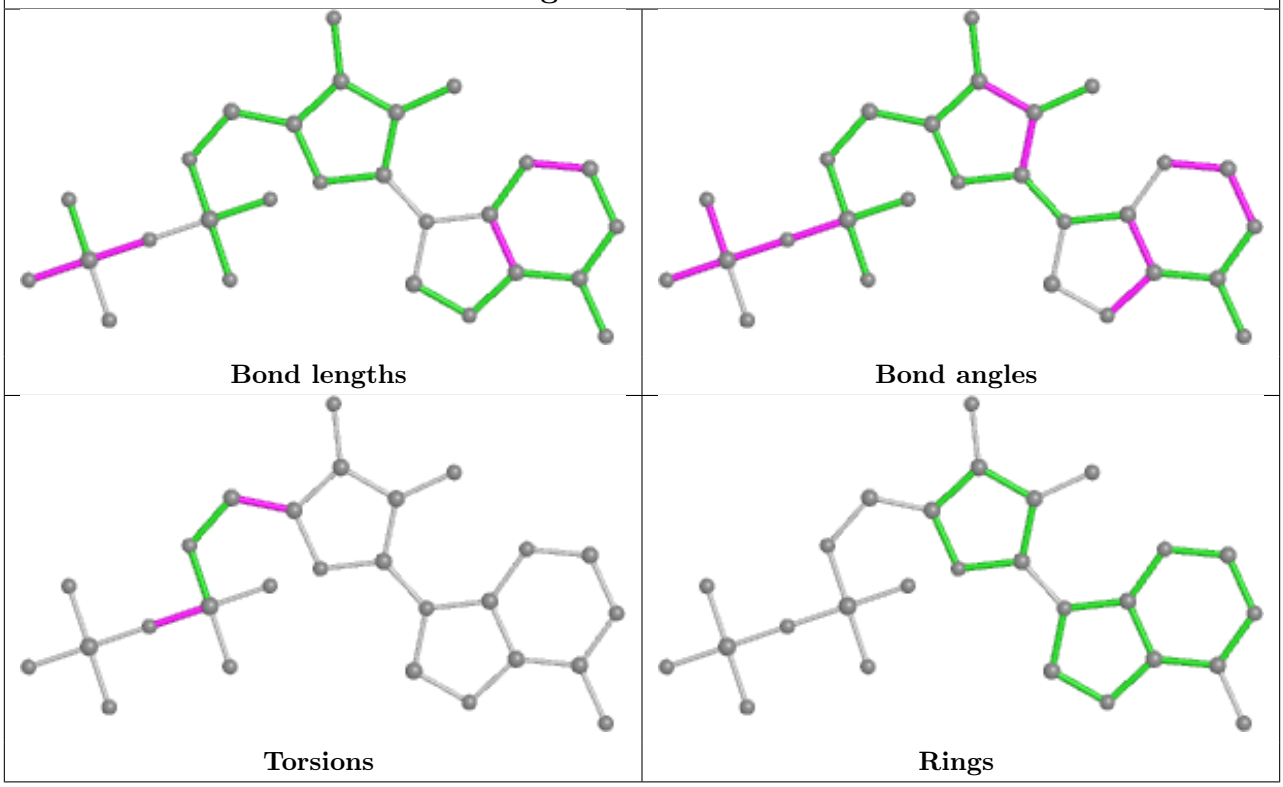
Ligand ANP B 432



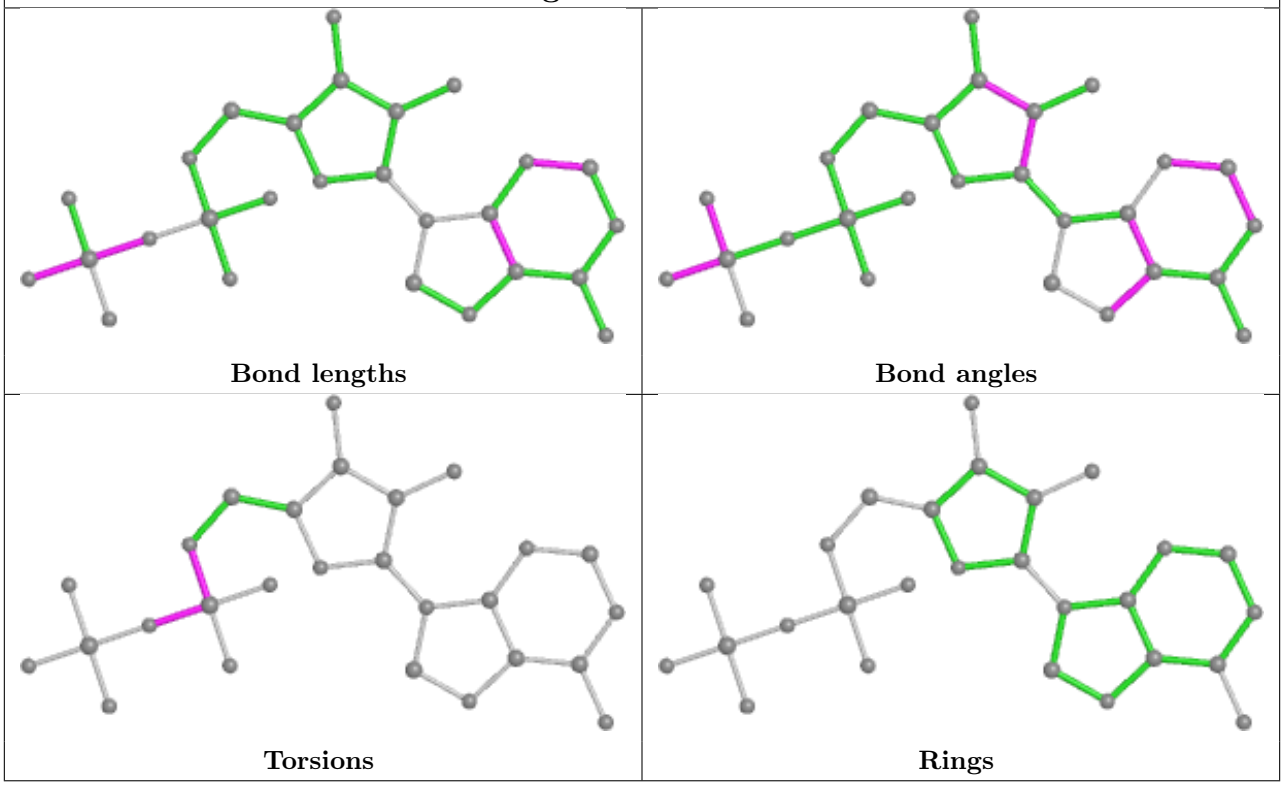
Ligand ANP E 432



Ligand ANP C 2



Ligand ANP F 4



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	321/341 (94%)	0.09	7 (2%)	62	57	28, 57, 107, 145	0
1	D	325/341 (95%)	0.10	9 (2%)	53	49	30, 61, 105, 155	0
2	B	311/373 (83%)	0.66	19 (6%)	21	18	51, 72, 106, 139	0
2	E	308/373 (82%)	0.56	24 (7%)	13	10	51, 74, 114, 146	0
3	C	285/305 (93%)	0.41	18 (6%)	20	17	39, 75, 128, 194	0
3	F	268/305 (87%)	0.87	41 (15%)	2	1	47, 95, 137, 171	0
All	All	1818/2038 (89%)	0.43	118 (6%)	18	16	28, 71, 121, 194	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	206	ALA	5.4
2	E	348	PHE	5.4
3	C	332	TRP	4.8
2	E	253	LEU	4.8
2	E	350	PRO	4.6
2	B	428	ASP	4.5
3	F	86	ARG	4.4
2	E	223	HIS	4.4
1	D	29	GLN	4.2
3	F	256	GLU	4.2
2	B	165	ASP	4.0
2	E	386	ALA	4.0
3	F	294	PRO	3.9
3	F	150	VAL	3.8
3	F	78	LYS	3.8
2	E	60	SER	3.8
3	C	89	PRO	3.7
1	A	61	GLU	3.7
3	F	269	LYS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	87	ARG	3.7
2	E	205	VAL	3.7
3	F	324	PRO	3.6
3	F	217	PRO	3.6
3	F	77	VAL	3.6
2	B	350	PRO	3.5
3	F	295	ALA	3.5
3	C	59	SER	3.5
2	B	359	CYS	3.5
3	F	292	TYR	3.5
2	B	67	GLY	3.3
2	E	254	GLN	3.2
3	F	265	GLU	3.2
2	E	383	LYS	3.2
2	B	66	GLY	3.2
1	D	316	ASP	3.1
2	E	404	GLU	3.1
3	F	221	PRO	3.1
3	C	261	TYR	3.0
2	E	61	SER	3.0
2	E	418	VAL	3.0
2	E	160	CYS	3.0
1	A	318	GLN	2.9
3	F	293	GLU	2.9
3	C	83	LYS	2.9
3	F	207	ASP	2.9
2	B	254	GLN	2.9
3	C	88	ILE	2.9
3	F	314	PRO	2.8
1	A	264	ARG	2.8
3	F	145	GLU	2.7
3	C	51	MET	2.7
3	C	118	TYR	2.7
2	E	298	CYS	2.7
3	F	318	ALA	2.7
2	B	353	HIS	2.6
3	F	338	VAL	2.6
2	E	363	ASN	2.6
1	D	35	LYS	2.6
3	C	57	GLU	2.6
2	E	366	ALA	2.6
3	F	147	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	334	LYS	2.6
2	B	362	ARG	2.6
3	F	80	LEU	2.5
2	E	402	ASN	2.5
3	F	57	GLU	2.5
1	A	221	GLU	2.5
1	D	260	MET	2.5
3	F	87	ARG	2.5
3	F	229	ASP	2.5
1	D	98	VAL	2.4
2	B	402	ASN	2.4
2	B	61	SER	2.4
2	E	392	GLU	2.4
2	B	418	VAL	2.4
3	F	273	ALA	2.4
3	F	222	PRO	2.4
2	B	225	GLN	2.4
2	E	168	ASN	2.4
1	D	65	GLU	2.4
3	F	45	LEU	2.3
3	C	244	THR	2.3
1	A	321	ASP	2.3
1	A	313	ARG	2.3
2	E	395	ARG	2.3
3	F	211	ARG	2.3
1	D	61	GLU	2.3
3	F	240	SER	2.3
3	F	257	GLY	2.3
3	C	76	ALA	2.3
3	F	118	TYR	2.3
3	C	62	LYS	2.3
2	E	204	SER	2.3
1	D	266	LYS	2.2
3	C	211	ARG	2.2
1	A	34	LYS	2.2
3	F	296	LYS	2.2
3	F	81	LYS	2.2
3	F	146	LYS	2.2
2	B	264	SER	2.1
3	F	226	ASN	2.1
2	B	272	LEU	2.1
3	C	120	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	419	THR	2.1
3	C	50	LEU	2.1
3	F	64	LYS	2.1
2	B	188	HIS	2.1
2	B	88	ALA	2.1
3	C	86	ARG	2.1
3	F	213	SER	2.1
2	E	245	SER	2.1
2	E	412	SER	2.1
2	B	417	LEU	2.0
3	F	66	VAL	2.0
3	F	239	TRP	2.0
2	E	164	MET	2.0
3	F	313	HIS	2.0
3	C	336	THR	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.

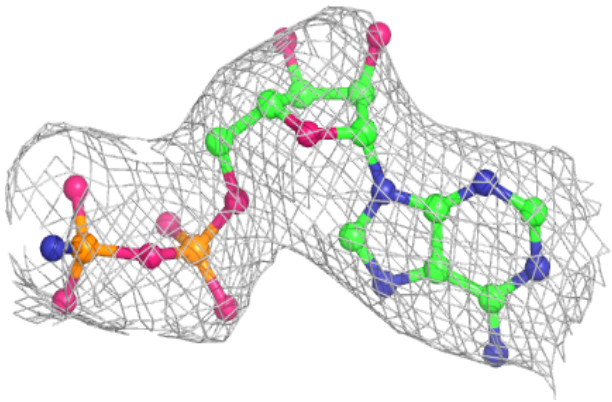
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ANP	C	2	27/31	0.85	0.17	82,102,121,123	0
4	ANP	F	4	27/31	0.85	0.24	89,98,102,103	0
4	ANP	B	432	31/31	0.90	0.20	44,56,69,73	0
4	ANP	E	432	31/31	0.93	0.17	48,59,81,83	0
5	SO4	D	342	5/5	0.95	0.29	69,75,78,79	0

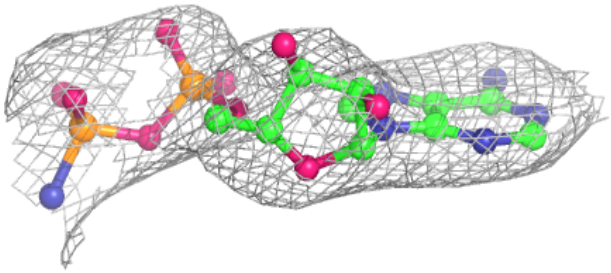
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

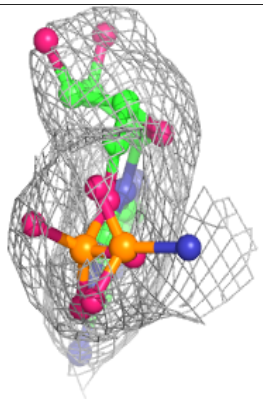
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ANP C 2:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

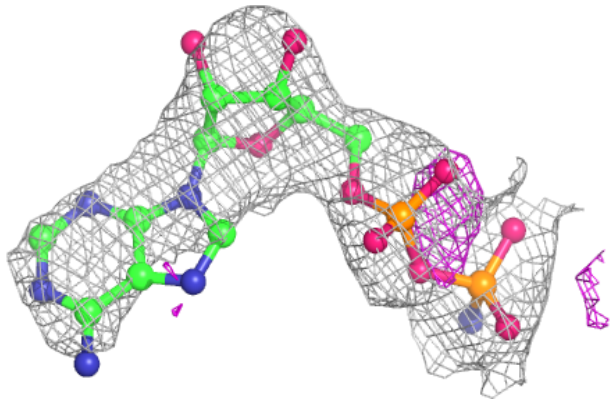


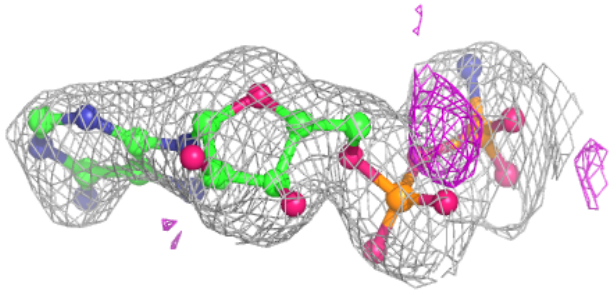


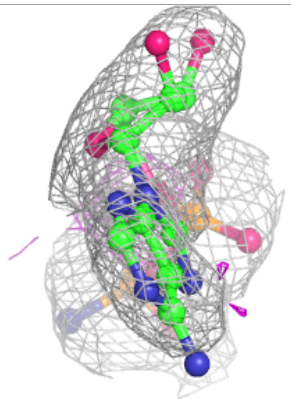


Electron density around ANP F 4:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

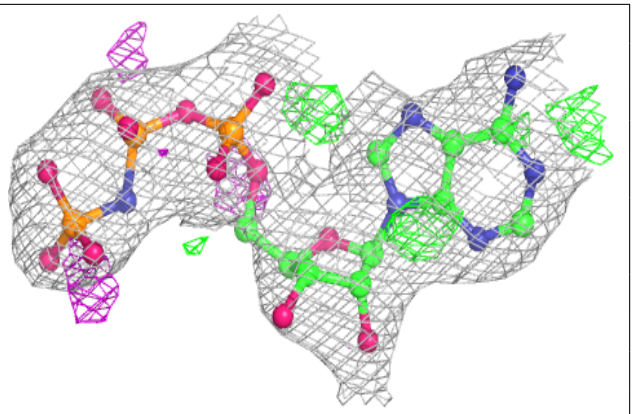


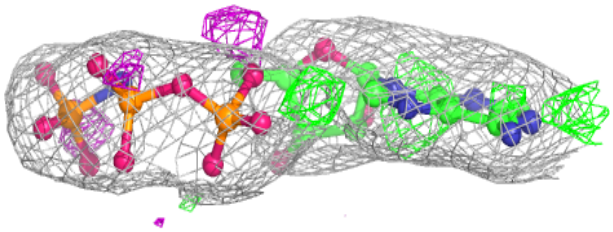


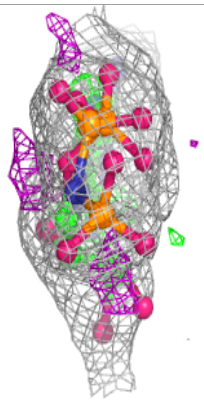


Electron density around ANP B 432:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

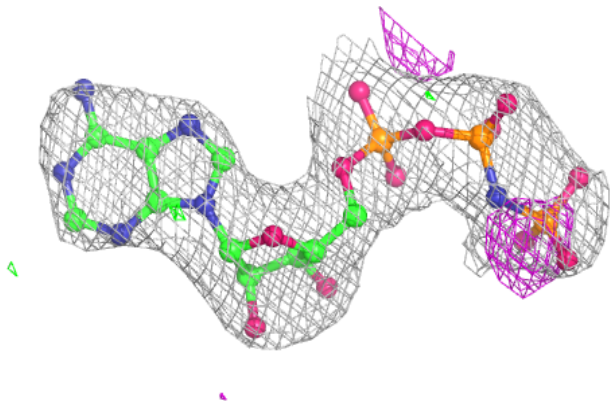


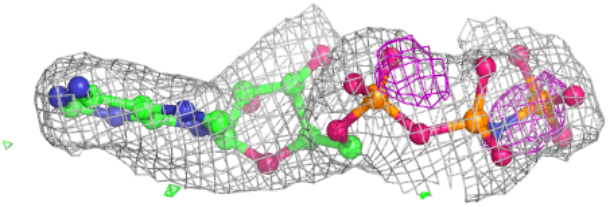


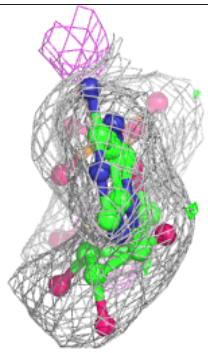


Electron density around ANP E 432:

$2mF_o$-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.