Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 04:24 AM EDT

PDB ID	:	3ORZ
Title	:	PDK1 mutant bound to allosteric disulfide fragment activator 2A2
Authors	:	Sadowsky, J.D.; Wells, J.A.
Deposited on	:	2010-09-08
Resolution	:	2.00 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:

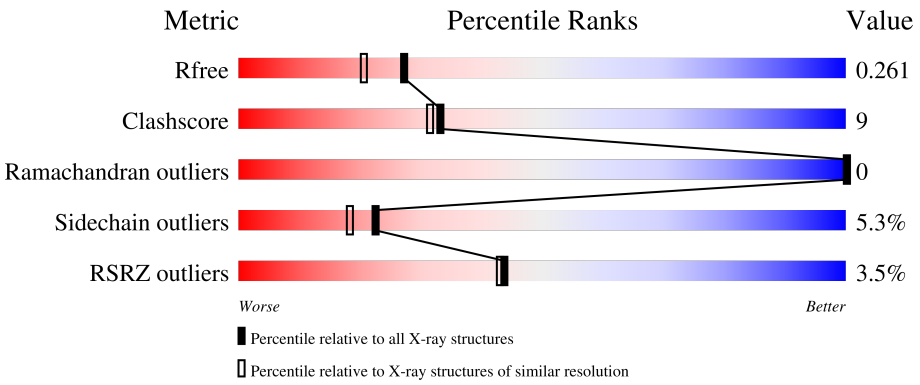
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	316	3% 75% 11% • 12%
1	B	316	2% 71% 14% • 12%
1	C	316	3% 74% 12% • 12%
1	D	316	4% 71% 16% • 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9976 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 3-phosphoinositide-dependent protein kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	277	2238	1456	362	411	1	8	0	1	0
1	B	279	2241	1457	365	410	1	8	0	0	0
1	C	277	2229	1451	362	407	1	8	0	0	0
1	D	279	2251	1461	367	414	1	8	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	GLY	-	expression tag	UNP O15530
A	45	ALA	-	expression tag	UNP O15530
A	46	MET	-	expression tag	UNP O15530
A	47	ASP	-	expression tag	UNP O15530
A	48	PRO	-	expression tag	UNP O15530
A	49	GLU	-	expression tag	UNP O15530
A	50	PHE	-	expression tag	UNP O15530
A	148	CYS	THR	engineered mutation	UNP O15530
B	44	GLY	-	expression tag	UNP O15530
B	45	ALA	-	expression tag	UNP O15530
B	46	MET	-	expression tag	UNP O15530
B	47	ASP	-	expression tag	UNP O15530
B	48	PRO	-	expression tag	UNP O15530
B	49	GLU	-	expression tag	UNP O15530
B	50	PHE	-	expression tag	UNP O15530
B	148	CYS	THR	engineered mutation	UNP O15530
C	44	GLY	-	expression tag	UNP O15530
C	45	ALA	-	expression tag	UNP O15530
C	46	MET	-	expression tag	UNP O15530
C	47	ASP	-	expression tag	UNP O15530
C	48	PRO	-	expression tag	UNP O15530

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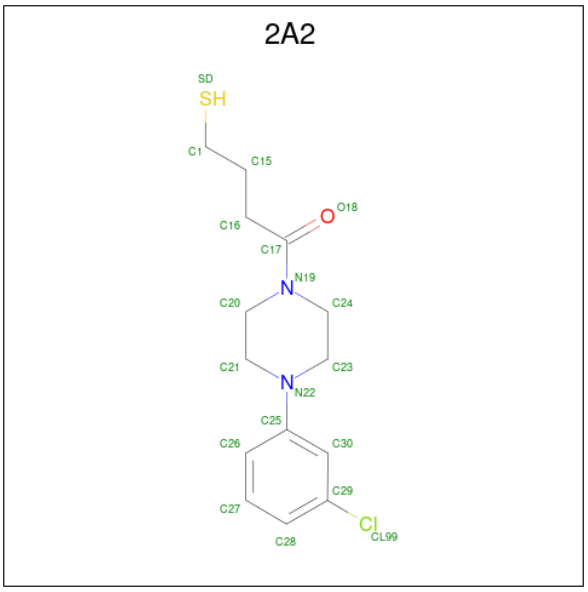
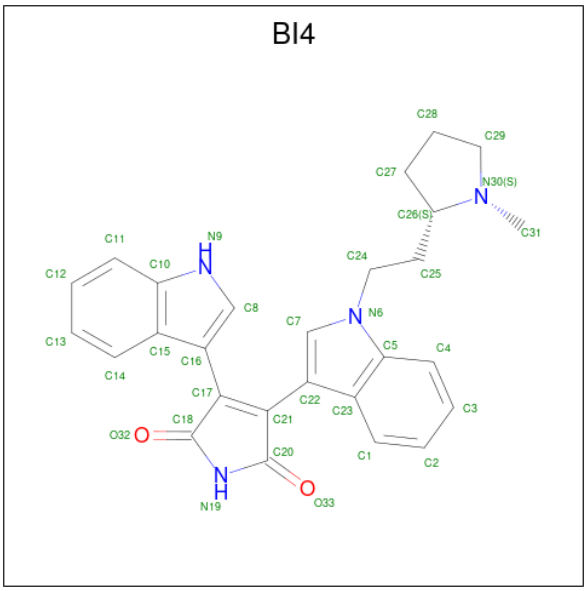
Chain	Residue	Modelled	Actual	Comment	Reference
C	49	GLU	-	expression tag	UNP O15530
C	50	PHE	-	expression tag	UNP O15530
C	148	CYS	THR	engineered mutation	UNP O15530
D	44	GLY	-	expression tag	UNP O15530
D	45	ALA	-	expression tag	UNP O15530
D	46	MET	-	expression tag	UNP O15530
D	47	ASP	-	expression tag	UNP O15530
D	48	PRO	-	expression tag	UNP O15530
D	49	GLU	-	expression tag	UNP O15530
D	50	PHE	-	expression tag	UNP O15530
D	148	CYS	THR	engineered mutation	UNP O15530

- Molecule 2 is 4-[4-(3-chlorophenyl)piperazin-1-yl]-4-oxobutane-1-thiol (three-letter code: 2A2) (formula: $C_{14}H_{19}ClN_2OS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
2	A	1	19	14	1	2	1	1	0	0
2	B	1	19	14	1	2	1	1	0	0
2	C	1	19	14	1	2	1	1	0	0
2	D	1	19	14	1	2	1	1	0	0

- Molecule 3 is 3-(1H-INDOL-3-YL)-4-{1-[2-(1-METHYLPYRROLIDIN-2-YL)ETHYL]-1H-INDOL-3-YL}-1H-PYRROLE-2,5-DIONE (three-letter code: BI4) (formula: $C_{27}H_{26}N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 33 27 4 2	0	0
3	B	1	Total C N O 33 27 4 2	0	0
3	C	1	Total C N O 33 27 4 2	0	0
3	D	1	Total C N O 33 27 4 2	0	0

- Molecule 4 is water.

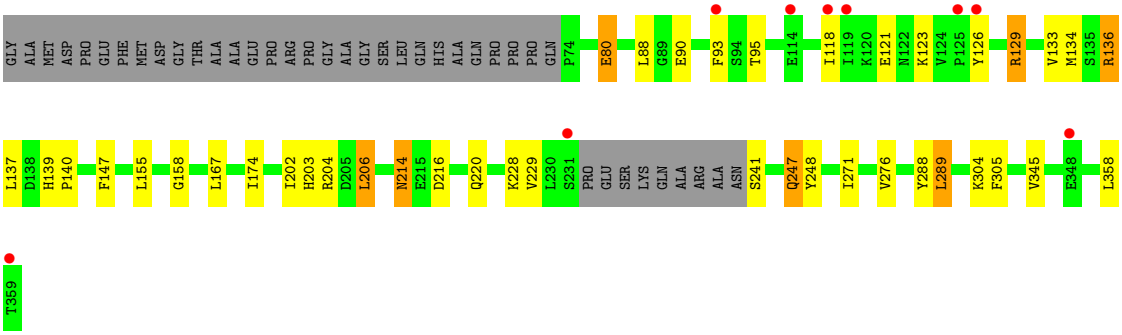
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	209	Total O 209 209	0	0
4	B	203	Total O 203 203	0	0
4	C	200	Total O 200 200	0	0
4	D	197	Total O 197 197	0	0

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.

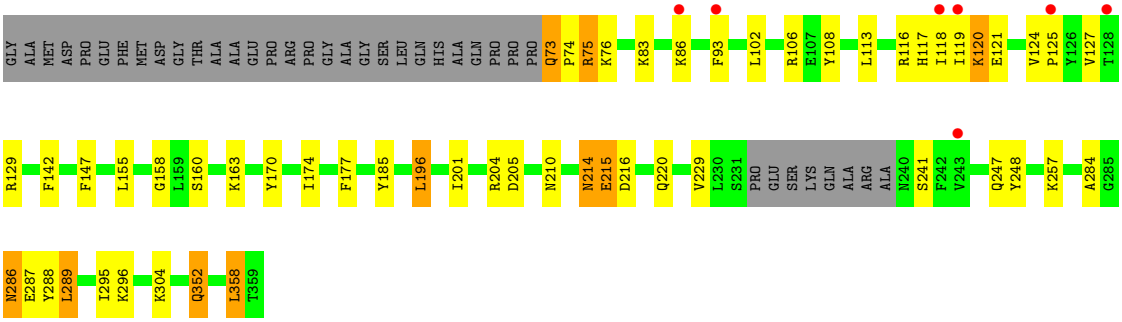
• Molecule 1: 3-phosphoinositide-dependent protein kinase 1

Chain A:



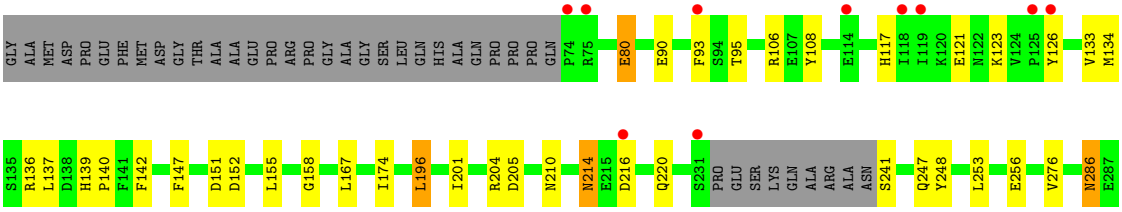
• Molecule 1: 3-phosphoinositide-dependent protein kinase 1

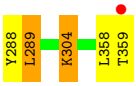
Chain B:



• Molecule 1: 3-phosphoinositide-dependent protein kinase 1

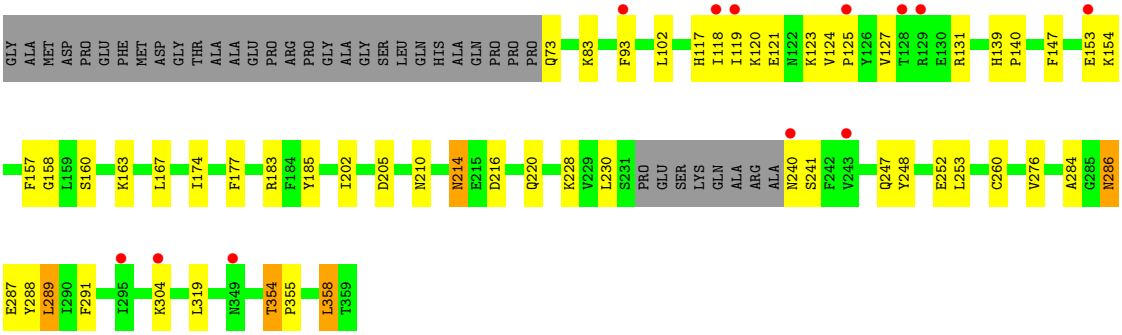
Chain C:





• Molecule 1: 3-phosphoinositide-dependent protein kinase 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	243.13Å 116.12Å 37.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.98 – 2.00 44.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (41.98-2.00) 98.8 (44.85-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.14 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 2010_01_09_2330)	Depositor
R, R_{free}	0.218 , 0.265 0.216 , 0.261	Depositor DCC
R_{free} test set	3525 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	19.5	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 36.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.458 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9976	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 99.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7895e-13. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: SEP, 2A2, BI4

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	0.48	0/2286	0.60	0/3087
1	B	0.49	0/2284	0.57	0/3082
1	C	0.46	0/2274	0.58	1/3071 (0.0%)
1	D	0.45	0/2294	0.57	0/3095
All	All	0.47	0/9138	0.58	1/12335 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	151	ASP	CB-CG-OD2	5.53	123.27	118.30

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	2238	0	2221	28	0
1	B	2241	0	2223	39	1
1	C	2229	0	2213	32	0
1	D	2251	0	2235	34	1
2	A	19	0	18	0	0
2	B	19	0	18	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	19	0	18	0	0
2	D	19	0	18	1	0
3	A	33	0	26	5	0
3	B	33	0	26	5	0
3	C	33	0	26	7	0
3	D	33	0	26	6	0
4	A	209	0	0	1	0
4	B	203	0	0	3	0
4	C	200	0	0	2	0
4	D	197	0	0	3	0
All	All	9976	0	9068	157	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (157) 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:73:GLN:HG2	1:B:74:PRO:HD2	1.50	0.91
1:A:202:ILE:HD12	1:A:228:LYS:HD2	1.67	0.76
1:C:214:ASN:ND2	1:C:216:ASP:OD2	2.21	0.72
1:C:276:VAL:O	1:C:304:LYS:HE2	1.91	0.71
1:B:129:ARG:HH11	1:B:229:VAL:H	1.39	0.70
1:B:116:ARG:O	1:B:120:LYS:HB2	1.93	0.69
1:B:214:ASN:ND2	1:B:216:ASP:OD1	2.26	0.69
3:B:360:BI4:H4	3:B:360:BI4:H251	1.75	0.69
3:D:360:BI4:H4	3:D:360:BI4:H251	1.75	0.68
3:A:360:BI4:H4	3:A:360:BI4:H251	1.77	0.66
1:C:359:THR:O	4:C:450:HOH:O	2.14	0.66
1:D:153:GLU:HG3	1:D:154:LYS:HG3	1.77	0.66
1:D:214:ASN:ND2	1:D:216:ASP:OD2	2.28	0.65
1:A:174:ILE:HD11	1:A:358:LEU:HB3	1.78	0.65
1:A:214:ASN:ND2	1:A:216[A]:ASP:OD1	2.29	0.64
3:C:360:BI4:H4	3:C:360:BI4:H251	1.79	0.64
1:B:163:LYS:HD2	1:B:215:GLU:HG3	1.78	0.64
1:D:93:PHE:HE1	1:D:121:GLU:HG3	1.64	0.63
1:C:174:ILE:CD1	1:C:358:LEU:HB3	2.29	0.62
1:C:214:ASN:HD22	1:C:214:ASN:C	2.02	0.62
1:C:214:ASN:HB3	1:C:220:GLN:NE2	2.15	0.62
1:A:247:GLN:HE21	1:A:247:GLN:HA	1.63	0.62
1:C:214:ASN:HB3	1:C:220:GLN:HE21	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:ASN:C	1:C:286:ASN:HD22	2.04	0.61
1:A:214:ASN:HB3	1:A:220:GLN:NE2	2.15	0.61
1:A:174:ILE:CD1	1:A:358:LEU:HB3	2.30	0.61
1:A:93:PHE:HE1	1:A:121:GLU:HG3	1.65	0.61
1:A:123:LYS:O	1:A:126:TYR:HB3	2.00	0.60
1:A:214:ASN:C	1:A:214:ASN:HD22	2.04	0.60
3:D:360:BI4:H252	4:D:378:HOH:O	2.00	0.60
1:C:139:HIS:CG	1:C:140:PRO:HD2	2.36	0.59
1:A:214:ASN:HB3	1:A:220:GLN:HE21	1.68	0.58
1:D:286:ASN:HD22	1:D:286:ASN:C	2.06	0.58
1:C:123:LYS:O	1:C:126:TYR:HB3	2.03	0.58
1:B:286:ASN:C	1:B:286:ASN:HD22	2.06	0.58
3:B:360:BI4:H252	4:B:375:HOH:O	2.02	0.58
1:C:93:PHE:CZ	1:C:121:GLU:HG2	2.39	0.58
1:C:174:ILE:HD11	1:C:358:LEU:HB3	1.84	0.57
1:B:118:ILE:HG21	2:B:1:2A2:CL99	2.42	0.57
1:D:286:ASN:ND2	1:D:289:LEU:H	2.02	0.57
3:D:360:BI4:H251	3:D:360:BI4:C4	2.35	0.56
3:B:360:BI4:H251	3:B:360:BI4:C4	2.35	0.56
1:C:286:ASN:ND2	1:C:289:LEU:H	2.04	0.55
1:B:286:ASN:ND2	1:B:289:LEU:H	2.03	0.55
1:C:93:PHE:HZ	1:C:121:GLU:HG2	1.70	0.55
1:C:106:ARG:HG3	1:C:108:TYR:CE2	2.40	0.55
4:A:748:HOH:O	1:B:352:GLN:HG3	2.06	0.55
1:B:118:ILE:CG2	2:B:1:2A2:CL99	2.92	0.54
1:C:196:LEU:HD22	1:C:201:ILE:HB	1.90	0.54
1:B:124:VAL:O	1:B:127:VAL:N	2.41	0.52
1:D:118:ILE:HB	2:D:1:2A2:CL99	2.46	0.52
3:A:360:BI4:H251	3:A:360:BI4:C4	2.40	0.51
1:A:93:PHE:CE1	1:A:121:GLU:HG3	2.45	0.51
1:A:276:VAL:O	1:A:304:LYS:HE2	2.10	0.51
1:B:214:ASN:HB3	1:B:220:GLN:HE21	1.75	0.51
1:D:288:TYR:HD2	1:D:289:LEU:HD13	1.75	0.51
1:C:142:PHE:CZ	1:C:196:LEU:HG	2.46	0.51
1:D:214:ASN:C	1:D:214:ASN:HD22	2.13	0.51
1:B:214:ASN:C	1:B:214:ASN:HD22	2.14	0.50
1:C:133:VAL:HA	1:C:136:ARG:HD3	1.93	0.50
1:B:196:LEU:HD22	1:B:201:ILE:HB	1.93	0.50
1:C:247:GLN:HB2	1:C:248:TYR:CE2	2.46	0.50
1:A:90:GLU:HG2	1:A:95:THR:HG23	1.93	0.50
3:C:360:BI4:H251	3:C:360:BI4:C4	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ARG:HD2	1:A:228:LYS:HB2	1.95	0.49
3:D:360:BI4:O33	3:D:360:BI4:H1	2.13	0.49
1:A:247:GLN:HB2	1:A:248:TYR:CE2	2.48	0.49
3:B:360:BI4:O33	3:B:360:BI4:H1	2.13	0.49
3:D:360:BI4:H13	3:D:360:BI4:H271	1.95	0.48
1:D:174:ILE:HD11	1:D:177:PHE:CE1	2.49	0.48
1:B:174:ILE:HD11	1:B:177:PHE:CE1	2.49	0.47
1:A:118:ILE:HG23	1:A:123:LYS:HB2	1.96	0.47
1:B:142:PHE:CZ	1:B:196:LEU:HG	2.50	0.47
1:B:124:VAL:N	1:B:125:PRO:CD	2.77	0.47
1:D:93:PHE:CE1	1:D:121:GLU:HG3	2.45	0.47
1:A:139:HIS:CG	1:A:140:PRO:HD2	2.49	0.47
1:D:214:ASN:HB3	1:D:220:GLN:HE21	1.79	0.47
1:B:304:LYS:CB	4:B:709:HOH:O	2.64	0.46
3:A:360:BI4:O33	3:A:360:BI4:H1	2.15	0.46
1:B:119:ILE:HG13	1:B:120:LYS:N	2.31	0.46
1:B:284:ALA:HB1	1:B:289:LEU:HB3	1.98	0.46
1:B:163:LYS:HE3	4:B:444:HOH:O	2.15	0.46
1:C:117:HIS:O	1:C:121:GLU:HB2	2.16	0.46
1:C:142:PHE:CE1	1:C:196:LEU:HG	2.51	0.46
1:A:129:ARG:HH21	1:A:229:VAL:H	1.63	0.45
1:B:288:TYR:HD2	1:B:289:LEU:HD13	1.80	0.45
1:A:206:LEU:HD13	1:A:271:ILE:CD1	2.47	0.45
1:B:83:LYS:HB2	1:B:102:LEU:HD21	1.99	0.45
1:C:205:ASP:O	1:C:210:ASN:ND2	2.49	0.45
1:B:75:ARG:HG2	1:B:76:LYS:O	2.17	0.45
1:B:286:ASN:HD22	1:B:289:LEU:H	1.64	0.45
1:D:93:PHE:CE1	1:D:117:HIS:CE1	3.04	0.45
1:B:247:GLN:HB2	1:B:248:TYR:CE2	2.52	0.45
3:B:360:BI4:H271	3:B:360:BI4:H13	1.98	0.45
1:A:134:MET:HA	1:A:137:LEU:HD12	1.97	0.45
1:A:203:HIS:O	1:A:204:ARG:HB2	2.16	0.45
1:D:247:GLN:HB2	1:D:248:TYR:CE2	2.52	0.45
3:C:360:BI4:H1	3:C:360:BI4:O33	2.17	0.44
1:D:83:LYS:HB2	1:D:102:LEU:HD21	1.99	0.44
1:B:93:PHE:CE1	1:B:117:HIS:CE1	3.05	0.44
1:C:90:GLU:HG2	1:C:95:THR:HG23	1.98	0.44
1:D:124:VAL:O	1:D:127:VAL:N	2.51	0.44
1:D:205:ASP:O	1:D:210:ASN:ND2	2.51	0.44
1:C:80:GLU:H	1:C:80:GLU:CD	2.20	0.44
1:B:170:TYR:O	1:B:174:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:ARG:HG3	1:D:157:PHE:CE1	2.53	0.44
1:D:276:VAL:O	1:D:304:LYS:HE2	2.17	0.44
1:D:284:ALA:HB1	1:D:289:LEU:HB3	2.00	0.44
1:A:133:VAL:O	1:A:136:ARG:HG2	2.17	0.44
1:B:113:LEU:HB3	1:B:118:ILE:HD11	2.00	0.43
1:A:147:PHE:CE1	1:A:158:GLY:HA3	2.53	0.43
1:A:288:TYR:CD2	1:A:289:LEU:HD13	2.53	0.43
1:C:134:MET:HA	1:C:137:LEU:HD12	1.99	0.43
1:D:121:GLU:O	1:D:123:LYS:HG2	2.18	0.43
1:D:287:GLU:HG2	1:D:291:PHE:CZ	2.54	0.43
1:D:354:THR:HA	1:D:355:PRO:HD3	1.88	0.43
1:B:295:ILE:HD12	1:B:296:LYS:HG3	1.99	0.43
1:A:288:TYR:HD2	1:A:289:LEU:HD13	1.83	0.43
1:B:205:ASP:O	1:B:210:ASN:ND2	2.52	0.43
1:C:147:PHE:CE1	1:C:158:GLY:HA3	2.54	0.43
1:C:288:TYR:HD2	1:C:289:LEU:HD13	1.83	0.43
1:D:183:ARG:NH1	4:D:777:HOH:O	2.41	0.43
1:A:80:GLU:H	1:A:80:GLU:CD	2.21	0.43
1:D:260:CYS:SG	4:D:457:HOH:O	2.55	0.43
1:B:86:LYS:O	1:B:86:LYS:HG3	2.18	0.42
1:D:163:LYS:HE2	1:D:163:LYS:HB2	1.89	0.42
1:D:124:VAL:O	1:D:125:PRO:C	2.56	0.42
1:D:139:HIS:CG	1:D:140:PRO:HD2	2.54	0.42
1:A:129:ARG:NH2	1:A:229:VAL:H	2.16	0.42
1:B:106:ARG:HG3	1:B:108:TYR:CE2	2.54	0.42
2:B:1:2A2:H20	2:B:1:2A2:H15A	2.01	0.42
1:C:288:TYR:CD2	1:C:289:LEU:HD13	2.55	0.42
3:C:360:BI4:H272	3:C:360:BI4:C5	2.49	0.42
1:D:202:ILE:HD12	1:D:228:LYS:HE3	2.02	0.42
1:B:295:ILE:HD12	1:B:296:LYS:N	2.34	0.42
1:C:147:PHE:CZ	1:C:158:GLY:HA3	2.54	0.42
1:D:124:VAL:N	1:D:125:PRO:CD	2.83	0.42
1:B:129:ARG:NH1	1:B:229:VAL:H	2.14	0.42
1:D:147:PHE:CZ	1:D:158:GLY:HA3	2.55	0.42
1:B:147:PHE:CZ	1:B:158:GLY:HA3	2.55	0.42
3:A:360:BI4:H271	3:A:360:BI4:H13	2.02	0.41
3:C:360:BI4:H252	4:C:823:HOH:O	2.19	0.41
1:D:185:TYR:CE2	1:D:358:LEU:HD11	2.55	0.41
3:C:360:BI4:C7	3:C:360:BI4:C14	2.98	0.41
1:D:286:ASN:HD22	1:D:289:LEU:H	1.66	0.41
1:C:139:HIS:CD2	1:C:140:PRO:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:PHE:CZ	1:A:158:GLY:HA3	2.55	0.41
1:B:257:LYS:HE3	1:B:257:LYS:HB2	1.86	0.41
1:C:93:PHE:CE1	1:C:117:HIS:CE1	3.09	0.41
1:D:119:ILE:HG22	1:D:120:LYS:N	2.33	0.41
1:D:174:ILE:HD11	1:D:177:PHE:CD1	2.56	0.40
3:D:360:BI4:H252	3:D:360:BI4:H312	1.85	0.40
3:A:360:BI4:H272	3:A:360:BI4:C5	2.51	0.40
1:B:352:GLN:HE21	1:B:352:GLN:HB3	1.65	0.40
3:C:360:BI4:H13	3:C:360:BI4:H271	2.03	0.40
1:C:174:ILE:HD13	1:C:358:LEU:HB3	2.03	0.40
1:B:185:TYR:CE2	1:B:358:LEU:HD11	2.56	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:GLU:OE1	1:D:287:GLU:OE1[4_554]	2.15	0.05

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	274/316 (87%)	262 (96%)	12 (4%)	0	100	100
1	B	274/316 (87%)	266 (97%)	8 (3%)	0	100	100
1	C	273/316 (86%)	266 (97%)	7 (3%)	0	100	100
1	D	274/316 (87%)	266 (97%)	8 (3%)	0	100	100
All	All	1095/1264 (87%)	1060 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	239/273 (88%)	227 (95%)	12 (5%)	24	20
1	B	238/273 (87%)	224 (94%)	14 (6%)	19	15
1	C	237/273 (87%)	225 (95%)	12 (5%)	24	19
1	D	241/273 (88%)	228 (95%)	13 (5%)	22	18
All	All	955/1092 (88%)	904 (95%)	51 (5%)	22	18

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	88	LEU
1	A	129	ARG
1	A	136	ARG
1	A	155	LEU
1	A	167	LEU
1	A	206	LEU
1	A	214	ASN
1	A	247	GLN
1	A	289	LEU
1	A	305	PHE
1	A	345	VAL
1	B	73	GLN
1	B	75	ARG
1	B	120	LYS
1	B	121	GLU
1	B	155	LEU
1	B	160	SER
1	B	196	LEU
1	B	204	ARG
1	B	214	ASN
1	B	215	GLU
1	B	286	ASN
1	B	289	LEU

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Mol	Chain	Res	Type
1	B	352	GLN
1	B	358	LEU
1	C	80	GLU
1	C	152	ASP
1	C	155	LEU
1	C	167	LEU
1	C	196	LEU
1	C	204	ARG
1	C	214	ASN
1	C	253	LEU
1	C	256	GLU
1	C	286	ASN
1	C	289	LEU
1	C	304	LYS
1	D	73	GLN
1	D	160	SER
1	D	167	LEU
1	D	214	ASN
1	D	230	LEU
1	D	240	ASN
1	D	252	GLU
1	D	253	LEU
1	D	286	ASN
1	D	289	LEU
1	D	319	LEU
1	D	354	THR
1	D	358	LEU

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

Mol	Chain	Res	Type
1	A	214	ASN
1	A	220	GLN
1	A	247	GLN
1	A	349	ASN
1	B	73	GLN
1	B	214	ASN
1	B	220	GLN
1	B	247	GLN
1	B	286	ASN
1	B	352	GLN
1	C	214	ASN

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Mol	Chain	Res	Type
1	C	220	GLN
1	C	286	ASN
1	D	214	ASN
1	D	220	GLN
1	D	240	ASN
1	D	247	GLN
1	D	286	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	SEP	D	241	1	8,9,10	1.58	1 (12%)	8,12,14	1.47	2 (25%)
1	SEP	A	241	1	8,9,10	1.62	1 (12%)	8,12,14	1.73	2 (25%)
1	SEP	C	241	1	8,9,10	1.62	1 (12%)	8,12,14	1.57	2 (25%)
1	SEP	B	241	1	8,9,10	1.61	1 (12%)	8,12,14	1.43	2 (25%)

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
1	SEP	D	241	1	-	0/5/8/10	-
1	SEP	A	241	1	-	1/5/8/10	-
1	SEP	C	241	1	-	3/5/8/10	-
1	SEP	B	241	1	-	3/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	241	SEP	P-O1P	3.50	1.61	1.50
1	C	241	SEP	P-O1P	3.48	1.61	1.50
1	A	241	SEP	P-O1P	3.46	1.61	1.50
1	D	241	SEP	P-O1P	3.46	1.61	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	241	SEP	OG-CB-CA	3.63	111.67	108.14
1	C	241	SEP	OG-CB-CA	3.24	111.30	108.14
1	D	241	SEP	P-OG-CB	-2.71	110.83	118.30
1	B	241	SEP	OG-CB-CA	2.64	110.71	108.14
1	A	241	SEP	P-OG-CB	-2.61	111.11	118.30
1	D	241	SEP	OG-CB-CA	2.55	110.63	108.14
1	B	241	SEP	P-OG-CB	-2.51	111.37	118.30
1	C	241	SEP	P-OG-CB	-2.31	111.93	118.30

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	241	SEP	N-CA-CB-OG
1	B	241	SEP	CB-OG-P-O2P
1	C	241	SEP	CB-OG-P-O1P
1	B	241	SEP	CB-OG-P-O1P
1	B	241	SEP	CB-OG-P-O3P
1	C	241	SEP	N-CA-CB-OG
1	C	241	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	2A2	D	1	1	20,20,20	0.83	1 (5%)	26,26,26	1.42	4 (15%)
3	BI4	A	360	-	35,38,38	1.85	7 (20%)	35,56,56	3.43	10 (28%)
2	2A2	C	1	1	20,20,20	0.86	1 (5%)	26,26,26	1.46	5 (19%)
2	2A2	A	1	1	20,20,20	0.85	1 (5%)	26,26,26	1.46	5 (19%)
3	BI4	C	360	-	35,38,38	1.87	7 (20%)	35,56,56	3.44	10 (28%)
3	BI4	D	360	-	35,38,38	1.85	7 (20%)	35,56,56	3.35	9 (25%)
2	2A2	B	1	1	20,20,20	0.83	1 (5%)	26,26,26	1.46	5 (19%)
3	BI4	B	360	-	35,38,38	1.85	7 (20%)	35,56,56	3.35	8 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2A2	D	1	1	-	0/12/22/22	0/2/2/2
3	BI4	A	360	-	-	2/5/39/39	0/6/6/6
2	2A2	C	1	1	-	0/12/22/22	0/2/2/2
2	2A2	A	1	1	-	0/12/22/22	0/2/2/2
3	BI4	C	360	-	-	2/5/39/39	0/6/6/6
3	BI4	D	360	-	-	2/5/39/39	0/6/6/6
2	2A2	B	1	1	-	1/12/22/22	0/2/2/2
3	BI4	B	360	-	-	2/5/39/39	0/6/6/6

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	360	BI4	C22-C23	-5.38	1.37	1.42
3	A	360	BI4	C22-C23	-5.36	1.37	1.42
3	D	360	BI4	C16-C15	-4.94	1.38	1.42
3	B	360	BI4	C22-C23	-4.88	1.38	1.42
3	C	360	BI4	C16-C15	-4.83	1.38	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	360	BI4	C16-C15	-4.80	1.38	1.42
3	A	360	BI4	C16-C15	-4.77	1.38	1.42
3	D	360	BI4	C22-C23	-4.72	1.38	1.42
3	C	360	BI4	C21-C17	4.66	1.48	1.37
3	A	360	BI4	C21-C17	4.65	1.48	1.37
3	D	360	BI4	C21-C17	4.57	1.48	1.37
3	B	360	BI4	C21-C17	4.51	1.47	1.37
3	B	360	BI4	C5-N6	-3.18	1.35	1.39
3	A	360	BI4	C5-N6	-3.07	1.35	1.39
3	D	360	BI4	C5-N6	-3.06	1.35	1.39
3	C	360	BI4	C5-N6	-3.04	1.35	1.39
3	B	360	BI4	C7-N6	-2.85	1.34	1.38
3	D	360	BI4	C7-N6	-2.83	1.34	1.38
2	C	1	2A2	C29-CL99	2.80	1.80	1.74
2	A	1	2A2	C29-CL99	2.79	1.80	1.74
3	C	360	BI4	C7-N6	-2.79	1.35	1.38
3	B	360	BI4	O32-C18	2.75	1.28	1.23
2	B	1	2A2	C29-CL99	2.71	1.80	1.74
3	D	360	BI4	O32-C18	2.71	1.28	1.23
2	D	1	2A2	C29-CL99	2.68	1.80	1.74
3	A	360	BI4	C7-N6	-2.62	1.35	1.38
3	A	360	BI4	O33-C20	2.58	1.28	1.23
3	C	360	BI4	O33-C20	2.51	1.28	1.23
3	D	360	BI4	O33-C20	2.43	1.28	1.23
3	B	360	BI4	O33-C20	2.43	1.28	1.23
3	C	360	BI4	O32-C18	2.36	1.28	1.23
3	A	360	BI4	O32-C18	2.33	1.28	1.23

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	360	BI4	C17-C18-N19	12.24	114.04	106.62
3	C	360	BI4	C17-C18-N19	12.15	113.98	106.62
3	C	360	BI4	C21-C20-N19	12.04	113.92	106.62
3	B	360	BI4	C17-C18-N19	11.89	113.82	106.62
3	A	360	BI4	C21-C20-N19	11.88	113.82	106.62
3	D	360	BI4	C21-C20-N19	11.82	113.78	106.62
3	D	360	BI4	C17-C18-N19	11.69	113.70	106.62
3	B	360	BI4	C21-C20-N19	11.63	113.67	106.62
3	C	360	BI4	C20-N19-C18	-5.77	105.19	111.29
3	A	360	BI4	C20-N19-C18	-5.77	105.19	111.29
3	B	360	BI4	C20-N19-C18	-5.64	105.33	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	360	BI4	C20-N19-C18	-5.63	105.34	111.29
2	D	1	2A2	C23-N22-C21	4.39	121.22	111.52
2	C	1	2A2	C23-N22-C21	4.36	121.14	111.52
2	A	1	2A2	C23-N22-C21	4.36	121.14	111.52
2	B	1	2A2	C23-N22-C21	4.35	121.11	111.52
3	D	360	BI4	O33-C20-C21	-3.99	122.75	128.17
3	A	360	BI4	O32-C18-C17	-3.98	122.76	128.17
3	B	360	BI4	O32-C18-C17	-3.86	122.92	128.17
3	D	360	BI4	O32-C18-C17	-3.85	122.94	128.17
3	C	360	BI4	O32-C18-C17	-3.81	122.99	128.17
3	B	360	BI4	O33-C20-C21	-3.77	123.05	128.17
3	A	360	BI4	C14-C15-C10	3.74	123.12	118.17
3	C	360	BI4	C14-C15-C10	3.70	123.08	118.17
3	D	360	BI4	C14-C15-C10	3.48	122.79	118.17
3	B	360	BI4	C14-C15-C10	3.47	122.77	118.17
3	C	360	BI4	O33-C20-C21	-3.33	123.64	128.17
3	D	360	BI4	C31-N30-C29	3.23	122.84	112.70
3	A	360	BI4	O33-C20-C21	-3.23	123.78	128.17
3	B	360	BI4	C31-N30-C29	3.23	122.82	112.70
3	A	360	BI4	C31-N30-C29	3.04	122.22	112.70
3	C	360	BI4	C31-N30-C29	3.01	122.14	112.70
2	D	1	2A2	C24-N19-C20	2.65	117.72	112.62
2	A	1	2A2	C30-C25-N22	-2.61	118.52	121.33
2	B	1	2A2	C24-N19-C20	2.60	117.63	112.62
2	B	1	2A2	C30-C25-N22	-2.59	118.55	121.33
2	C	1	2A2	C23-C24-N19	-2.54	104.99	110.44
2	A	1	2A2	C24-N19-C20	2.54	117.50	112.62
2	C	1	2A2	C30-C25-N22	-2.50	118.64	121.33
2	C	1	2A2	C24-N19-C20	2.50	117.43	112.62
2	D	1	2A2	C30-C25-N22	-2.48	118.66	121.33
2	A	1	2A2	C23-C24-N19	-2.44	105.20	110.44
3	A	360	BI4	C13-C14-C15	-2.39	117.58	120.89
3	C	360	BI4	C13-C14-C15	-2.32	117.68	120.89
3	C	360	BI4	C16-C8-N9	-2.26	104.54	108.91
2	C	1	2A2	C24-C23-N22	-2.26	106.30	110.70
2	B	1	2A2	C23-C24-N19	-2.26	105.60	110.44
2	A	1	2A2	C24-C23-N22	-2.24	106.34	110.70
3	A	360	BI4	C16-C8-N9	-2.24	104.58	108.91
3	D	360	BI4	C16-C8-N9	-2.21	104.64	108.91
2	B	1	2A2	C24-C23-N22	-2.18	106.46	110.70
3	B	360	BI4	C16-C8-N9	-2.18	104.70	108.91
3	A	360	BI4	C14-C15-C16	-2.09	132.65	135.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	360	BI4	C14-C15-C16	-2.09	132.65	135.63
2	D	1	2A2	C20-C21-N22	-2.05	106.73	110.70
3	D	360	BI4	C13-C14-C15	-2.01	118.11	120.89

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	360	BI4	C25-C24-N6-C7
3	A	360	BI4	C25-C24-N6-C5
3	B	360	BI4	C25-C24-N6-C7
3	B	360	BI4	C25-C24-N6-C5
3	C	360	BI4	C25-C24-N6-C7
3	C	360	BI4	C25-C24-N6-C5
3	D	360	BI4	C25-C24-N6-C7
3	D	360	BI4	C25-C24-N6-C5
2	B	1	2A2	C15-C16-C17-O18

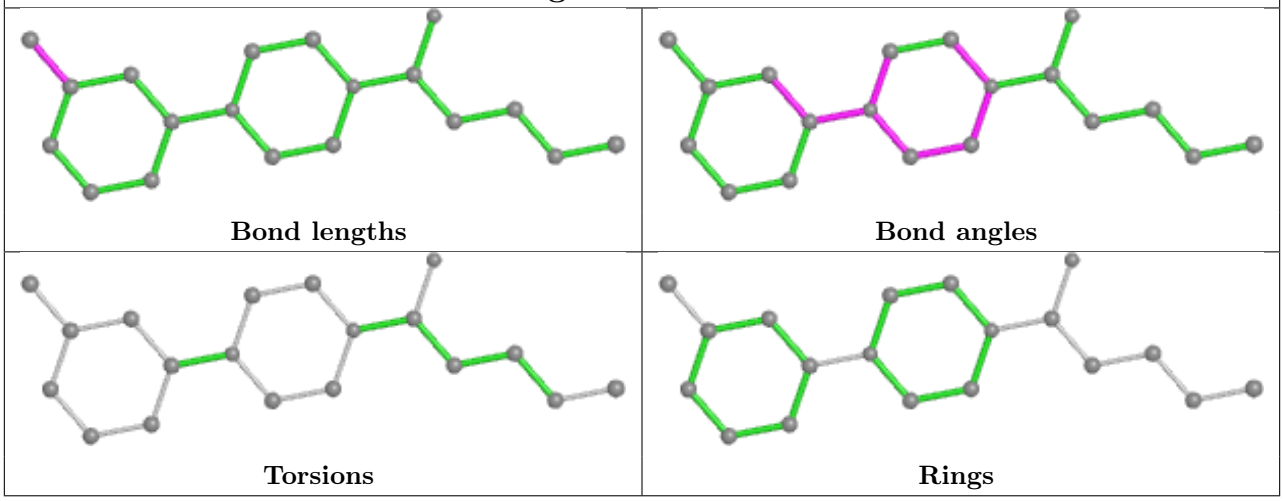
There are no ring outliers.

6 monomers are involved in 27 short contacts:

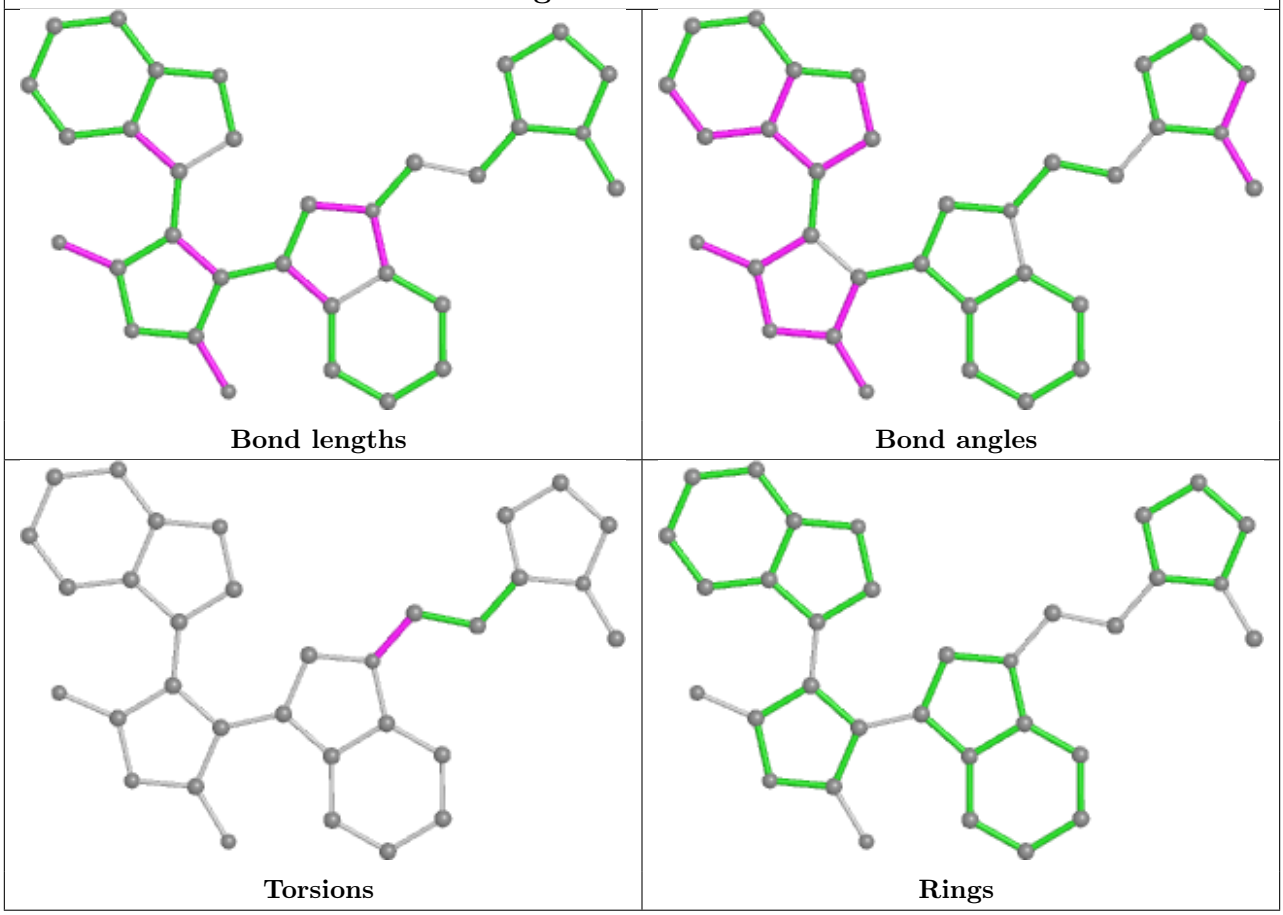
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	2A2	1	0
3	A	360	BI4	5	0
3	C	360	BI4	7	0
3	D	360	BI4	6	0
2	B	1	2A2	3	0
3	B	360	BI4	5	0

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.

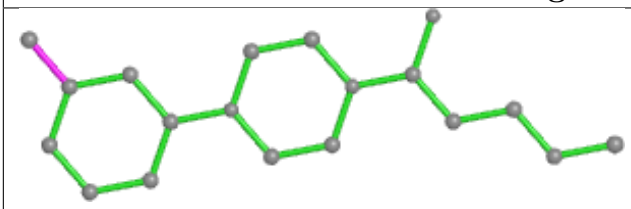
Ligand 2A2 D 1



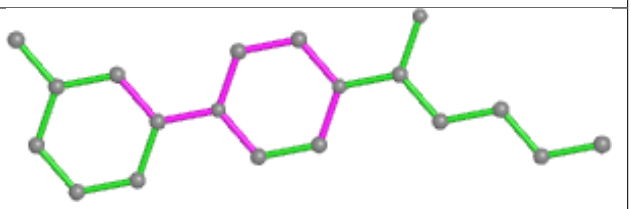
Ligand BI4 A 360



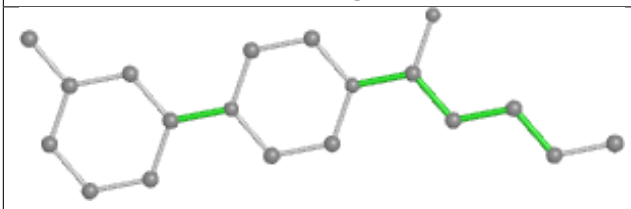
Ligand 2A2 C 1



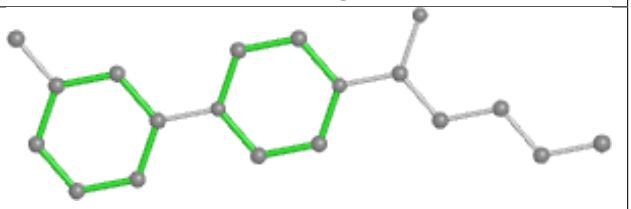
Bond lengths



Bond angles

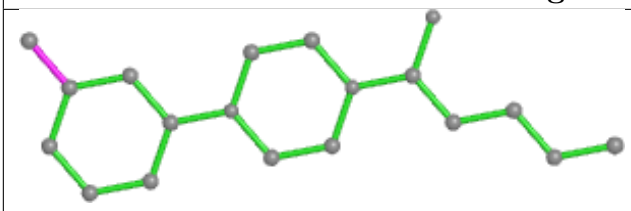


Torsions

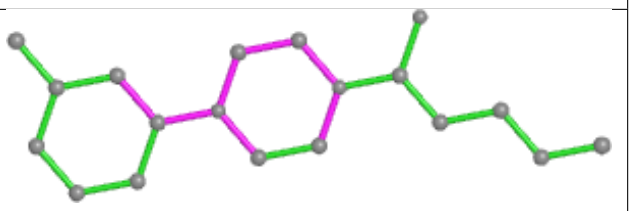


Rings

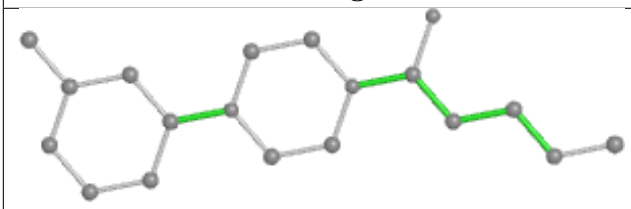
Ligand 2A2 A 1



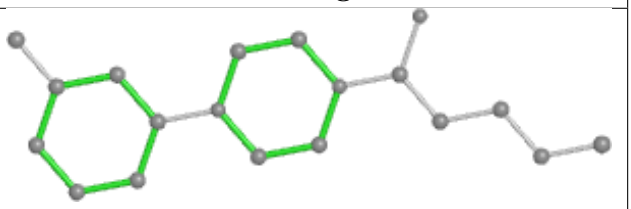
Bond lengths



Bond angles

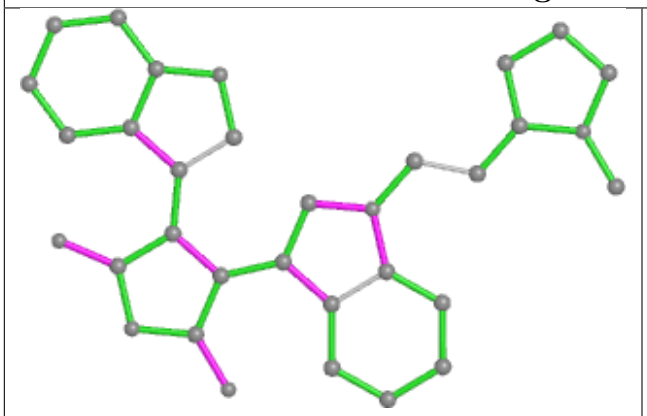


Torsions

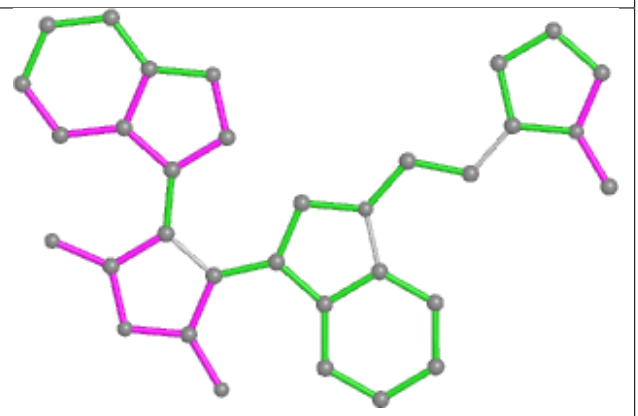


Rings

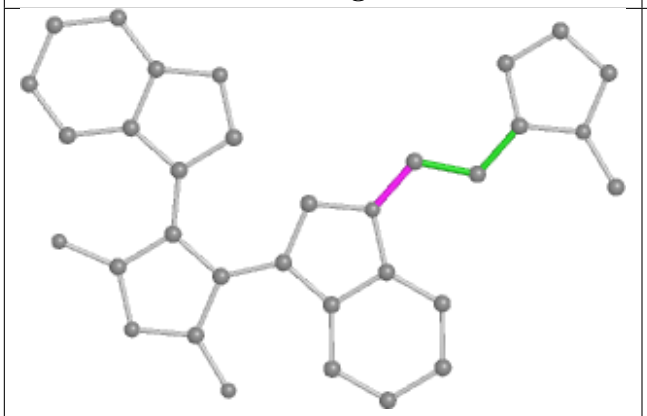
Ligand BI4 C 360



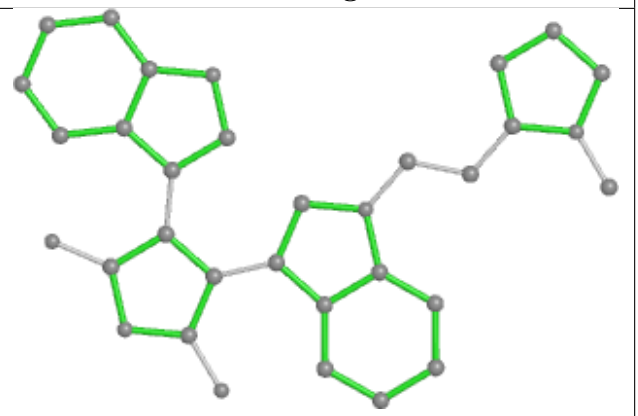
Bond lengths



Bond angles

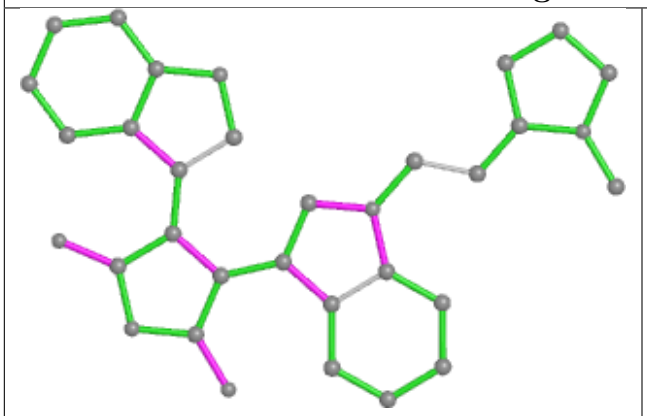


Torsions

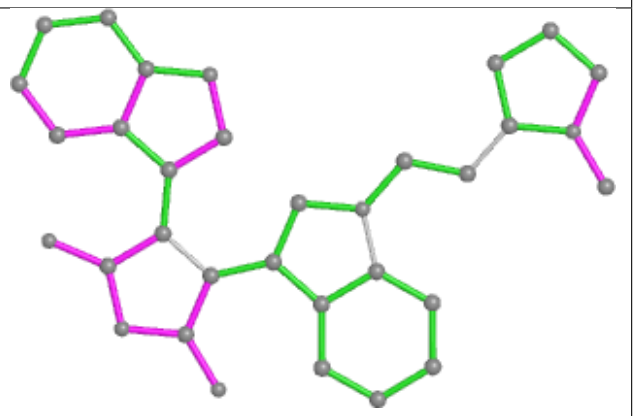


Rings

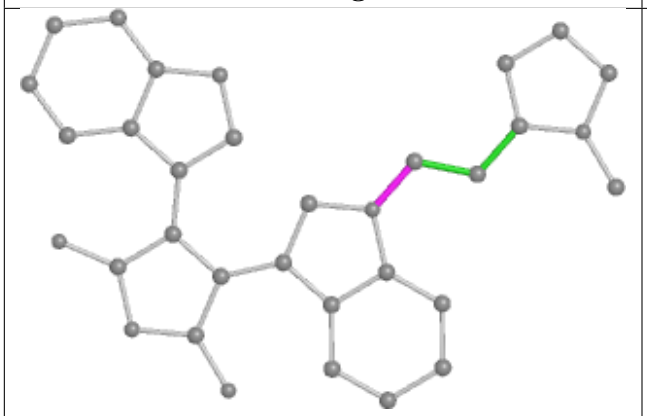
Ligand BI4 D 360



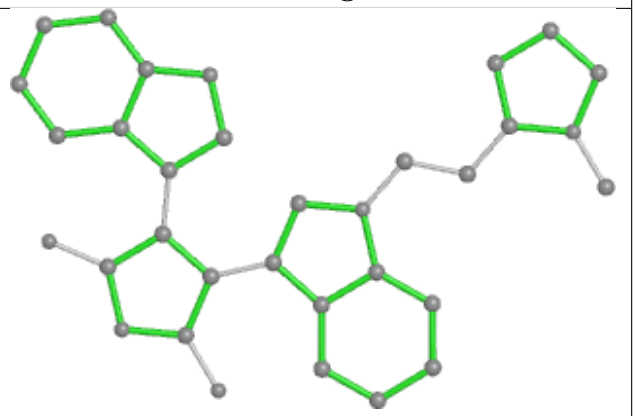
Bond lengths



Bond angles

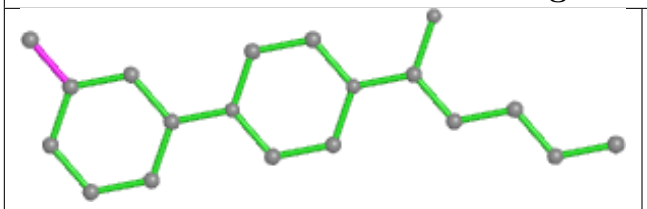


Torsions

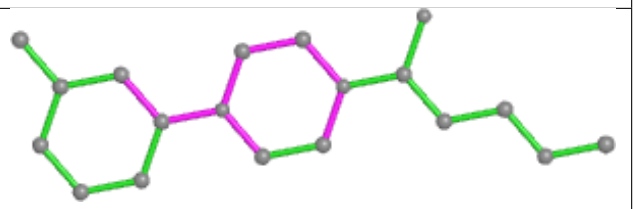


Rings

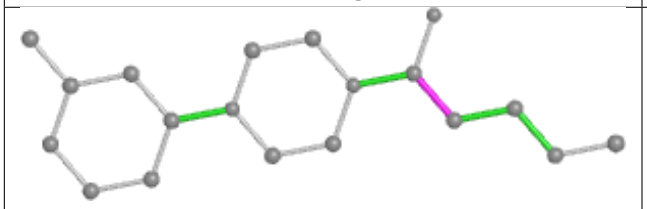
Ligand 2A2 B 1



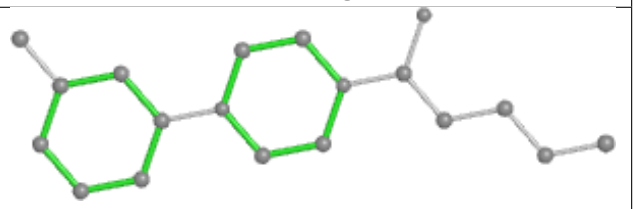
Bond lengths



Bond angles

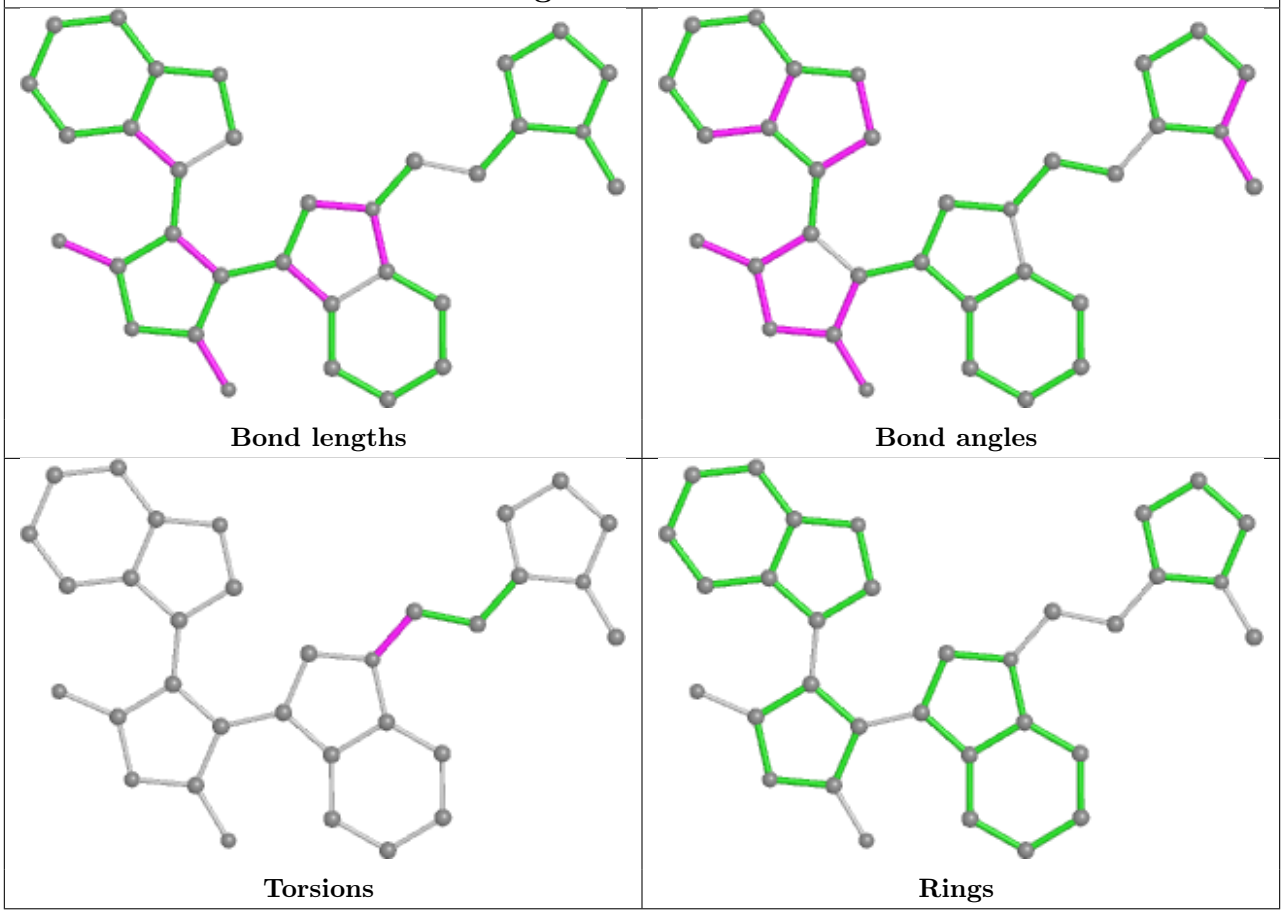


Torsions



Rings

Ligand BI4 B 360



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	276/316 (87%)	0.00	9 (3%)	46	45	10, 20, 40, 49	0
1	B	278/316 (87%)	0.06	7 (2%)	57	56	11, 21, 42, 52	0
1	C	276/316 (87%)	0.01	11 (3%)	38	37	10, 20, 40, 48	0
1	D	278/316 (87%)	0.10	12 (4%)	35	34	11, 21, 43, 52	0
All	All	1108/1264 (87%)	0.04	39 (3%)	44	43	10, 20, 42, 52	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	240	ASN	4.1
1	D	349	ASN	4.0
1	B	118	ILE	3.8
1	C	359	THR	3.5
1	A	119	ILE	3.4
1	C	125	PRO	3.3
1	A	348	GLU	3.3
1	B	243	VAL	3.2
1	D	118	ILE	3.2
1	C	119	ILE	3.0
1	A	125	PRO	3.0
1	C	114	GLU	2.9
1	A	126	TYR	2.9
1	A	359	THR	2.8
1	C	231	SER	2.8
1	D	129	ARG	2.7
1	A	114	GLU	2.7
1	C	216	ASP	2.6
1	C	93	PHE	2.6
1	C	126	TYR	2.6
1	C	118	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	153	GLU	2.6
1	A	93	PHE	2.5
1	D	93	PHE	2.5
1	B	93	PHE	2.5
1	D	119	ILE	2.5
1	B	128	THR	2.5
1	D	295	ILE	2.5
1	B	86	LYS	2.4
1	A	118	ILE	2.4
1	B	119	ILE	2.4
1	D	125	PRO	2.4
1	B	125	PRO	2.4
1	D	243	VAL	2.3
1	A	231	SER	2.2
1	D	304	LYS	2.2
1	C	74	PRO	2.1
1	C	75	ARG	2.1
1	D	128	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	SEP	C	241	10/11	0.66	0.24	33,49,69,78	0
1	SEP	A	241	10/11	0.75	0.19	32,49,66,75	0
1	SEP	D	241	10/11	0.91	0.14	33,43,66,67	0
1	SEP	B	241	10/11	0.93	0.16	31,42,64,65	0

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,

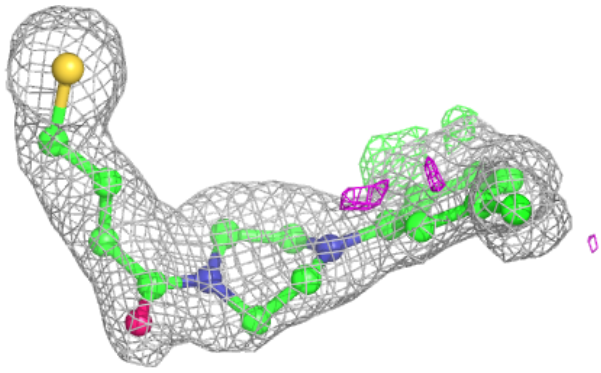
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

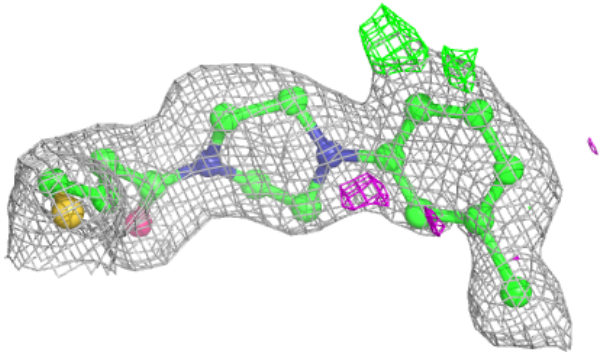
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	2A2	A	1	19/19	0.85	0.16	31,36,43,55	0
2	2A2	B	1	19/19	0.85	0.14	29,35,41,51	0
2	2A2	D	1	19/19	0.85	0.15	30,35,42,51	0
2	2A2	C	1	19/19	0.86	0.15	31,35,44,54	0
3	BI4	A	360	33/33	0.94	0.12	13,19,30,32	0
3	BI4	B	360	33/33	0.94	0.13	15,19,30,36	0
3	BI4	C	360	33/33	0.94	0.12	13,19,31,33	0
3	BI4	D	360	33/33	0.94	0.13	15,19,29,34	0

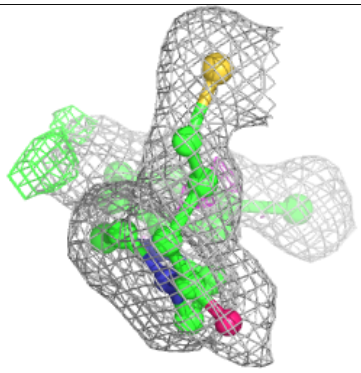
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 2A2 A 1:

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

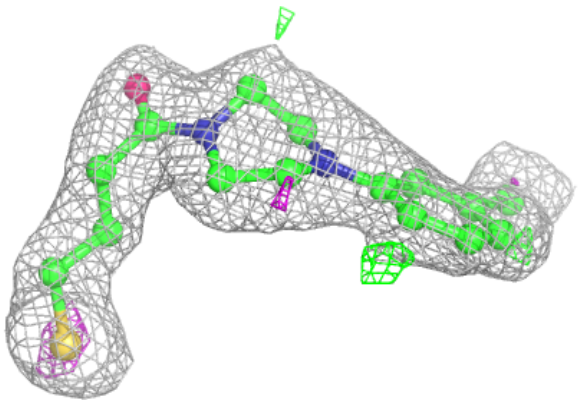


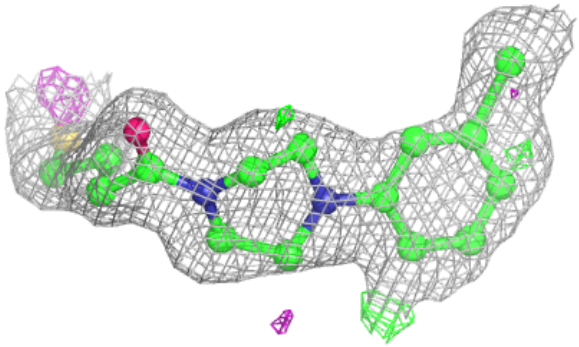


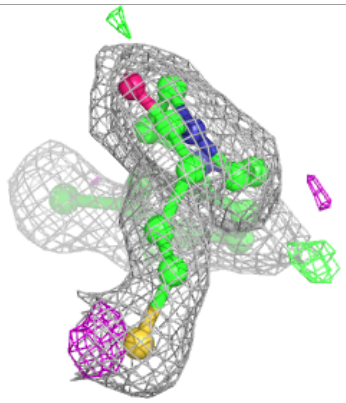


Electron density around 2A2 B 1:

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

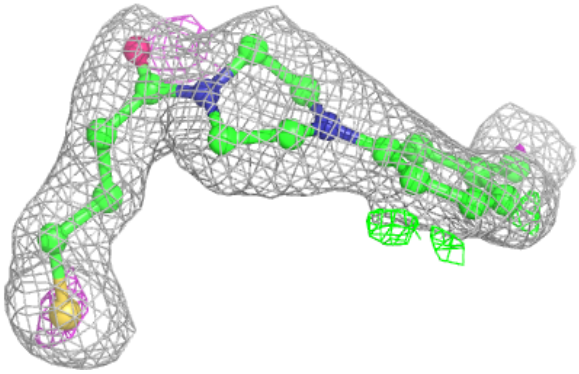


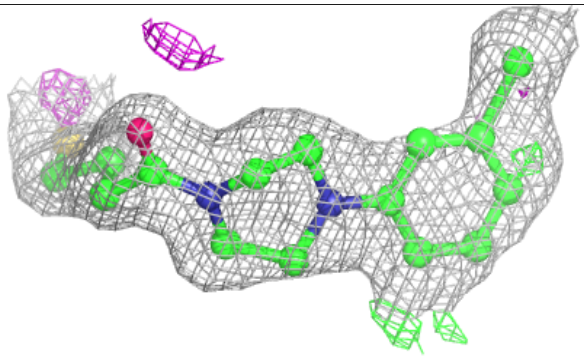


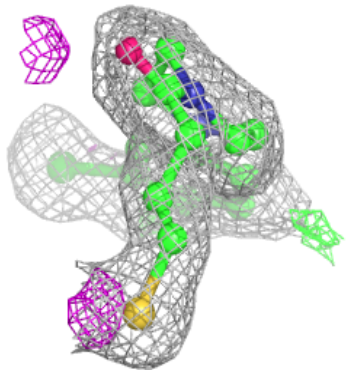


Electron density around 2A2 D 1:

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

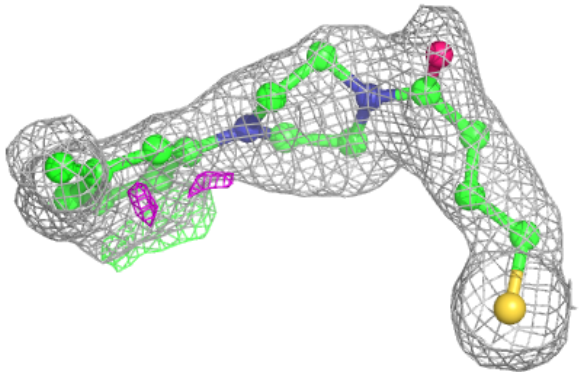


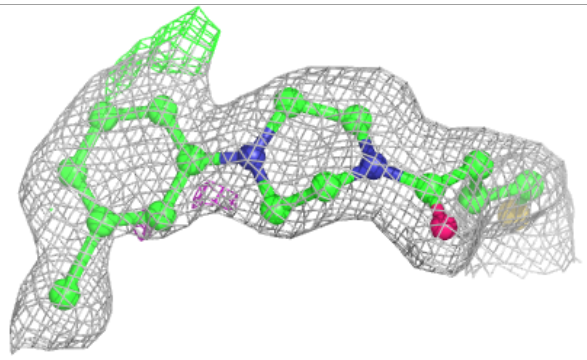




Electron density around 2A2 C 1:

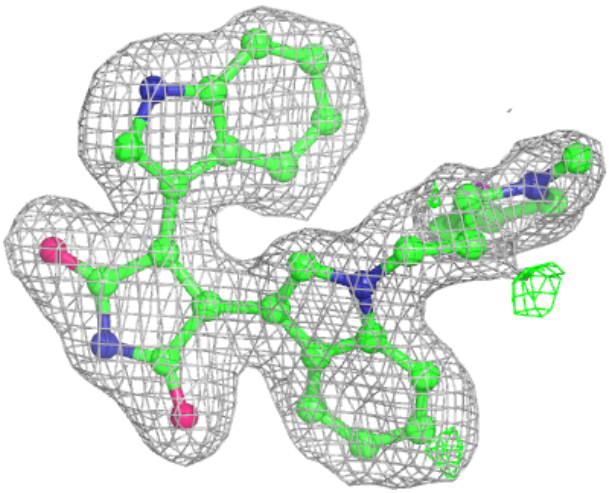
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

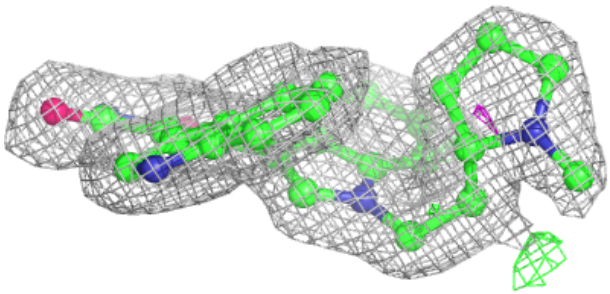


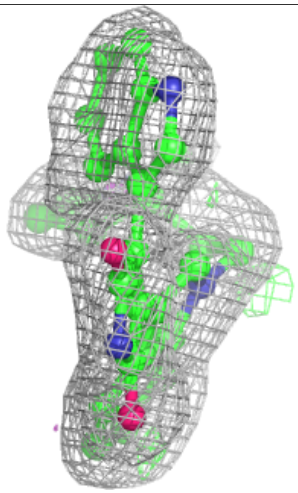


Electron density around BI4 A 360:

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

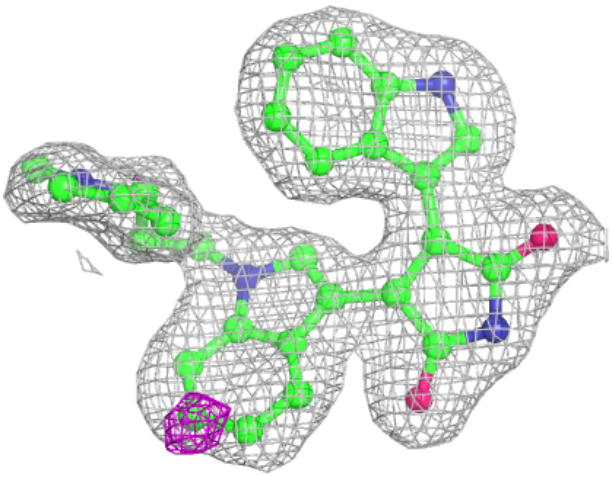


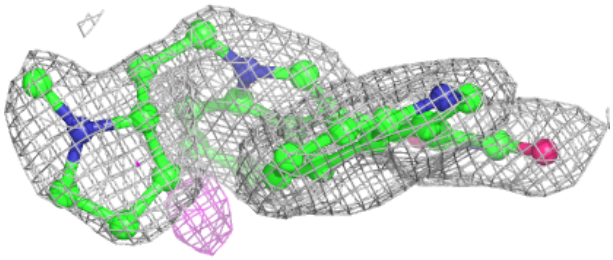


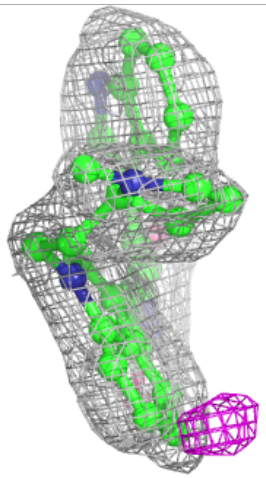


Electron density around BI4 B 360:

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

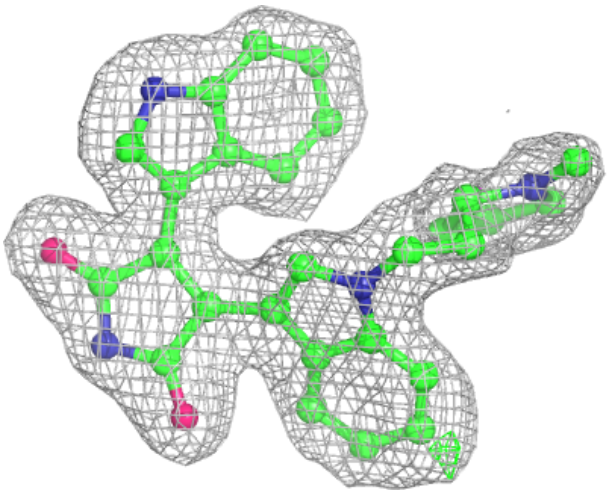


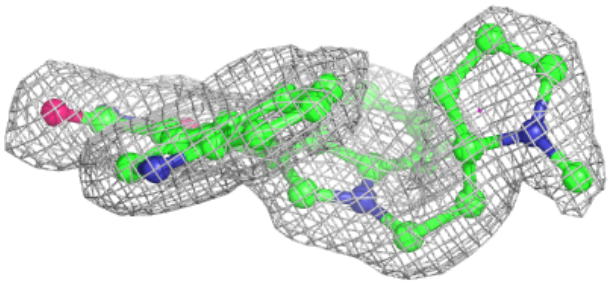


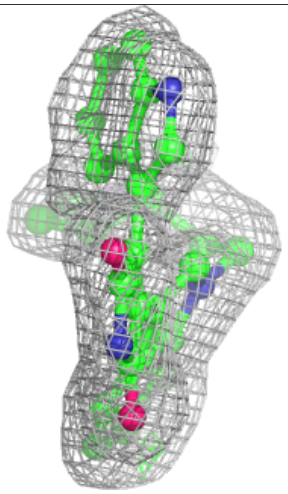


Electron density around BI4 C 360:

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

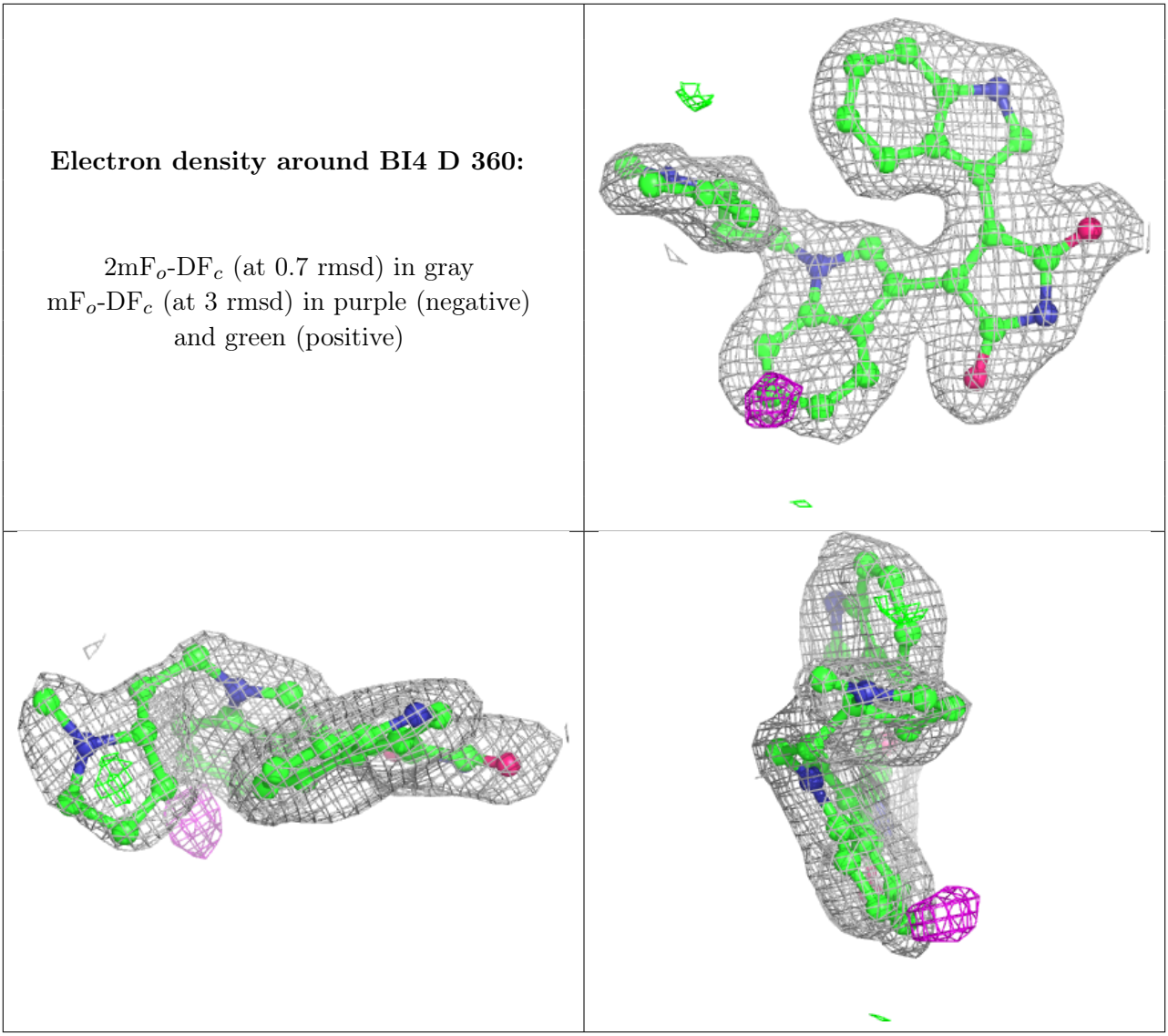






Electron density around BI4 D 360:

$2mF_o$-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.