Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2024 – 04:03 PM EST

PDB ID	:	1M52
Title	:	Crystal Structure of the c-Abl Kinase domain in complex with PD173955
Authors	:	Nagar, B.; Bornmann, W.; Pellicena, P.; Schindler, T.; Veach, D.; Miller, W.T.; Clarkson, B.; Kuriyan, J.
Deposited on	:	2002-07-08
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

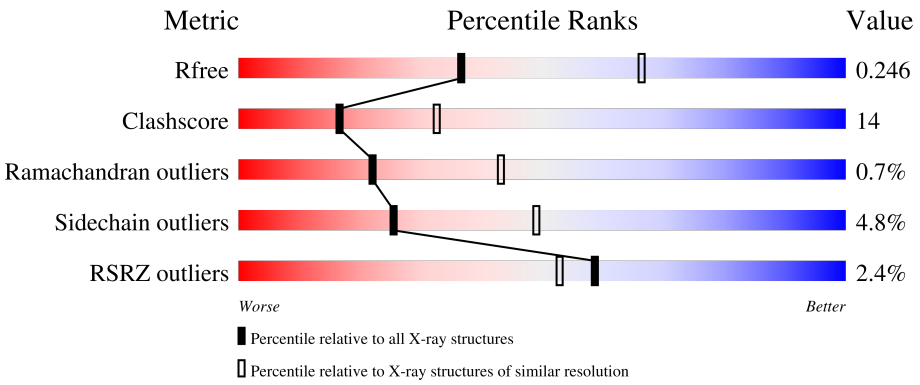
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	293	4% 65% 26% • 8%
1	B	293	% 66% 24% • 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4620 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.

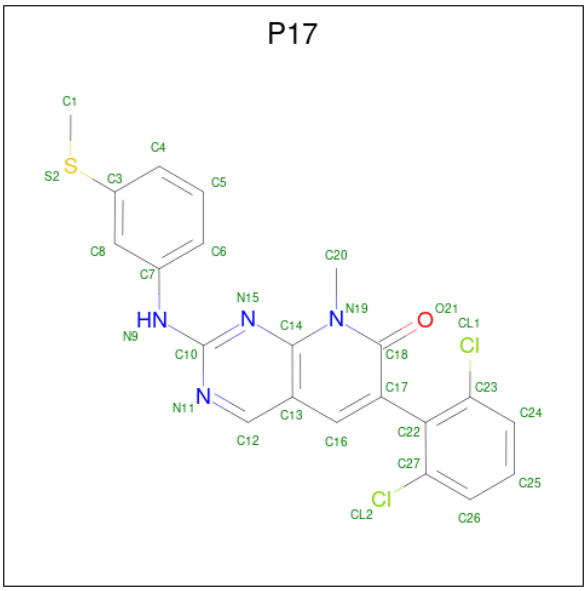
- Molecule 1 is a protein called PROTO-ONCOGENE TYROSINE-PROTEIN KINASE ABL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	271	2208	1423	358	410	17	0	0	0
1	B	272	2214	1426	359	412	17	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

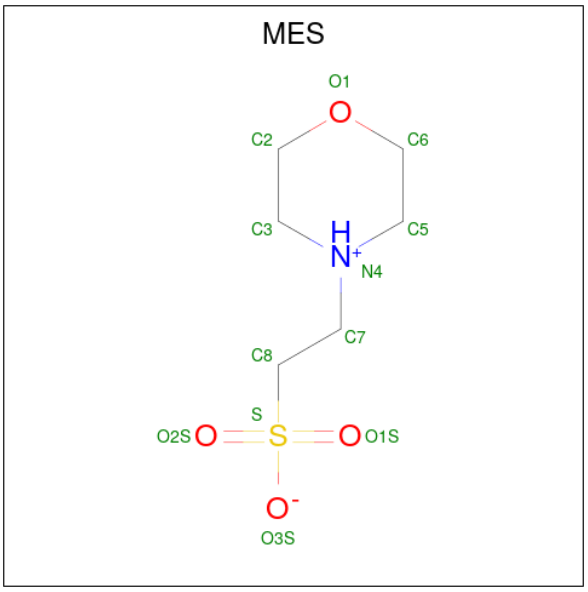
Chain	Residue	Modelled	Actual	Comment	Reference
A	223	GLY	-	cloning artifact	UNP P00520
A	224	ALA	-	cloning artifact	UNP P00520
A	225	MET	-	cloning artifact	UNP P00520
A	226	ASP	-	cloning artifact	UNP P00520
A	227	PRO	-	cloning artifact	UNP P00520
A	228	SER	-	cloning artifact	UNP P00520
B	223	GLY	-	cloning artifact	UNP P00520
B	224	ALA	-	cloning artifact	UNP P00520
B	225	MET	-	cloning artifact	UNP P00520
B	226	ASP	-	cloning artifact	UNP P00520
B	227	PRO	-	cloning artifact	UNP P00520
B	228	SER	-	cloning artifact	UNP P00520

- Molecule 2 is 6-(2,6-DICHLORO-PHENYL)-8-METHYL-2-(3-METHYLSULFANYL-PHENYLAMINO)-8H-PYRIDO[2,3-D]PYRIMIDIN-7-ONE (three-letter code: P17) (formula: $C_{21}H_{16}Cl_2N_4OS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
2	A	1	29	21	2	4	1	1	0	0
			Total	C	Cl	N	O	S		
2	B	1	29	21	2	4	1	1	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	B	1	12	6	1	4	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	B	1	12	6	1	4	1	0	0

- Molecule 4 is water.

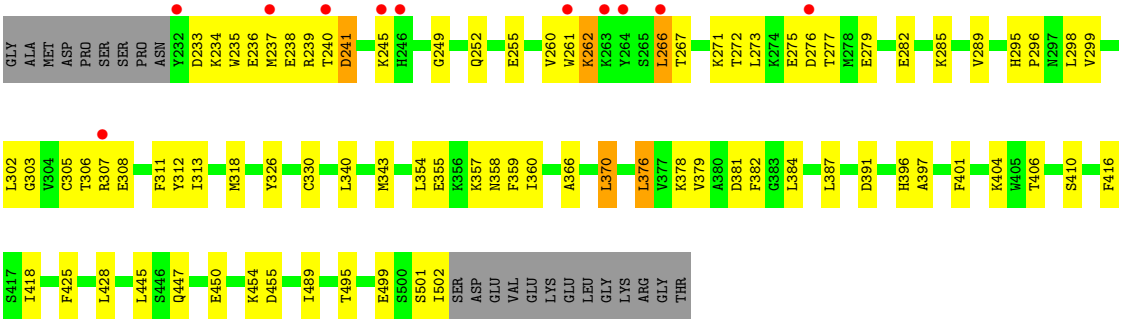
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	47	47	47	0	0
			Total	O		
4	B	69	69	69	0	0

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.

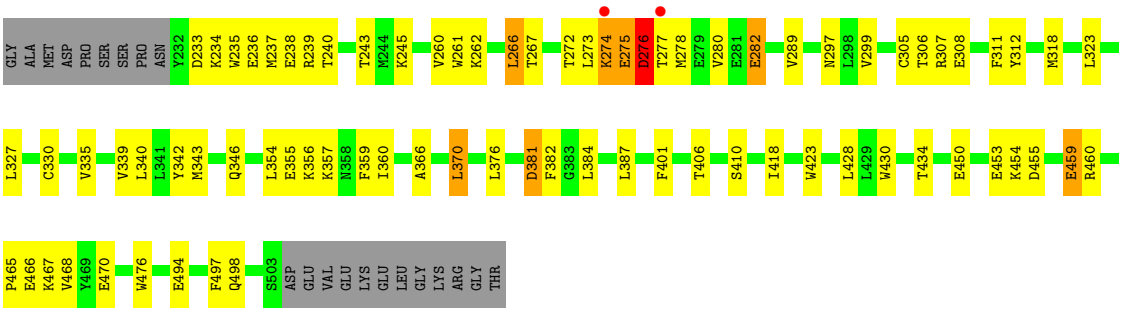
• Molecule 1: PROTO-ONCOGENE TYROSINE-PROTEIN KINASE ABL1

Chain A:



• Molecule 1: PROTO-ONCOGENE TYROSINE-PROTEIN KINASE ABL1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	115.85Å 125.71Å 56.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.25 – 2.60 55.25 – 2.49	Depositor EDS
% Data completeness (in resolution range)	94.7 (55.25-2.60) 93.4 (55.25-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.254 0.202 , 0.246	Depositor DCC
R_{free} test set	2743 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4620	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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: P17, MES

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	0.37	0/2265	0.62	0/3065
1	B	0.41	0/2271	0.65	0/3073
All	All	0.39	0/4536	0.63	0/6138

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2208	0	2162	63	0
1	B	2214	0	2167	59	0
2	A	29	0	16	2	0
2	B	29	0	16	2	0
3	B	24	0	26	0	0
4	A	47	0	0	0	0
4	B	69	0	0	1	0
All	All	4620	0	4387	126	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 14.

All (126) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:CYS:HB2	1:A:312:TYR:HB2	1.58	0.84
1:B:299:VAL:HB	1:B:381:ASP:OD1	1.80	0.81
1:B:305:CYS:HB2	1:B:312:TYR:HB2	1.64	0.79
1:A:340:LEU:HA	1:A:343:MET:HE2	1.67	0.75
1:B:276:ASP:CG	1:B:276:ASP:O	2.25	0.74
1:B:340:LEU:HA	1:B:343:MET:HE2	1.71	0.73
1:B:357:LYS:HB3	1:B:359:PHE:HD1	1.54	0.72
1:A:495:THR:O	1:A:499:GLU:HG2	1.93	0.69
2:A:119:P17:N15	2:A:119:P17:H16	2.08	0.68
1:A:360:ILE:HG23	1:A:387:LEU:HD21	1.74	0.66
1:A:235:TRP:O	1:A:237:MET:HG3	1.96	0.66
1:A:318:MET:HG3	1:A:370:LEU:HB3	1.78	0.66
1:B:459:GLU:CD	1:B:459:GLU:H	2.00	0.65
1:B:239:ARG:HG3	1:B:312:TYR:CE1	2.32	0.64
1:B:355:GLU:HG3	1:B:418:ILE:HG12	1.80	0.64
1:B:360:ILE:HG23	1:B:387:LEU:HD21	1.81	0.63
1:B:357:LYS:HB3	1:B:359:PHE:CD1	2.33	0.63
1:A:238:GLU:HB3	1:A:241:ASP:OD1	1.99	0.63
1:A:239:ARG:HG3	1:A:312:TYR:CE1	2.34	0.62
1:B:306:THR:HA	1:B:311:PHE:HD2	1.65	0.62
1:A:276:ASP:O	1:A:277:THR:HG23	2.00	0.61
1:A:238:GLU:HG3	1:A:240:THR:H	1.65	0.61
2:B:120:P17:H16	2:B:120:P17:N15	2.17	0.60
1:B:318:MET:HG3	1:B:370:LEU:HB3	1.84	0.60
1:B:381:ASP:O	1:B:384:LEU:HG	2.01	0.60
1:A:273:LEU:HD11	1:A:279:GLU:HB2	1.83	0.60
1:B:282:GLU:HA	1:B:282:GLU:OE1	2.03	0.58
1:A:306:THR:HA	1:A:311:PHE:HD2	1.68	0.58
1:A:275:GLU:HG3	1:A:276:ASP:N	2.19	0.58
1:A:406:THR:CG2	1:A:410:SER:HB2	2.34	0.57
1:A:357:LYS:HB3	1:A:359:PHE:HD1	1.69	0.57
1:A:299:VAL:HB	1:A:381:ASP:OD1	2.05	0.56
1:B:245:LYS:HD2	1:B:260:VAL:CG2	2.36	0.56
1:B:245:LYS:HD2	1:B:260:VAL:HG23	1.88	0.55
1:B:498:GLN:NE2	1:B:498:GLN:HA	2.22	0.54
1:A:255:GLU:HB2	1:A:272:THR:O	2.09	0.53
1:A:454:LYS:O	1:A:455:ASP:HB2	2.09	0.53
1:B:498:GLN:HA	1:B:498:GLN:HE21	1.73	0.53
1:B:307:ARG:HH11	1:B:307:ARG:HG2	1.73	0.53
1:A:296:PRO:O	1:A:378:LYS:HE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:HD23	1:A:343:MET:HE1	1.91	0.53
2:A:119:P17:N15	2:A:119:P17:C6	2.72	0.53
1:B:467:LYS:HB2	4:B:34:HOH:O	2.07	0.53
1:B:465:PRO:HG2	1:B:468:VAL:CG2	2.40	0.52
1:B:238:GLU:HG3	1:B:240:THR:H	1.74	0.52
1:A:376:LEU:HD11	1:A:378:LYS:HE3	1.91	0.52
1:A:318:MET:HG3	1:A:370:LEU:CB	2.39	0.51
1:B:237:MET:SD	1:B:261:TRP:CH2	3.04	0.51
1:B:238:GLU:HG3	1:B:240:THR:HB	1.92	0.51
1:B:274:LYS:HG3	1:B:275:GLU:HG2	1.91	0.51
1:A:237:MET:CE	1:A:303:GLY:HA3	2.40	0.51
1:B:342:TYR:HB2	1:B:497:PHE:CE1	2.46	0.50
1:A:366:ALA:N	1:A:428:LEU:HD13	2.27	0.50
1:B:274:LYS:CG	1:B:275:GLU:H	2.24	0.50
1:A:298:LEU:HD23	1:A:379:VAL:HB	1.92	0.50
1:B:340:LEU:HD23	1:B:343:MET:HE1	1.92	0.50
1:A:245:LYS:HE3	1:A:260:VAL:CG2	2.43	0.49
2:B:120:P17:N15	2:B:120:P17:C6	2.75	0.49
1:B:450:GLU:O	1:B:454:LYS:HG2	2.12	0.49
1:A:340:LEU:HD23	1:A:343:MET:CE	2.43	0.49
1:A:305:CYS:CB	1:A:312:TYR:HB2	2.36	0.49
1:A:233:ASP:HB3	1:A:236:GLU:HG2	1.95	0.48
1:B:318:MET:HG3	1:B:370:LEU:CB	2.43	0.48
1:B:406:THR:CG2	1:B:410:SER:HB2	2.43	0.48
1:B:233:ASP:OD1	1:B:235:TRP:HB2	2.14	0.48
1:A:295:HIS:CG	1:A:296:PRO:HD2	2.49	0.47
1:B:274:LYS:HG3	1:B:275:GLU:H	1.79	0.47
1:B:494:GLU:O	1:B:498:GLN:HG2	2.13	0.47
1:B:243:THR:OG1	1:B:262:LYS:HE2	2.14	0.47
1:B:453:GLU:C	1:B:455:ASP:H	2.17	0.47
1:A:326:TYR:O	1:A:330:CYS:HB3	2.14	0.47
1:A:355:GLU:HG3	1:A:418:ILE:HG12	1.96	0.47
1:B:274:LYS:CG	1:B:275:GLU:N	2.78	0.47
1:B:274:LYS:HG3	1:B:275:GLU:N	2.30	0.47
1:B:307:ARG:HG2	1:B:307:ARG:NH1	2.30	0.46
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.79	0.46
1:A:357:LYS:HB3	1:A:359:PHE:CD1	2.48	0.46
1:A:307:ARG:HG2	1:A:307:ARG:NH1	2.31	0.46
1:A:266:LEU:HD23	1:A:267:THR:N	2.30	0.46
1:A:501:SER:O	1:A:502:ILE:HG13	2.16	0.46
1:A:404:LYS:HE2	1:A:445:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ASP:HB3	1:B:236:GLU:HG2	1.98	0.45
1:A:236:GLU:OE2	1:A:306:THR:OG1	2.34	0.45
1:B:273:LEU:HD23	1:B:280:VAL:HG22	1.98	0.45
1:B:339:VAL:O	1:B:343:MET:HG3	2.15	0.45
1:A:382:PHE:C	1:A:382:PHE:CD1	2.90	0.45
1:A:396:HIS:O	1:A:397:ALA:C	2.55	0.45
1:A:450:GLU:O	1:A:454:LYS:HG2	2.16	0.45
1:A:245:LYS:HE3	1:A:260:VAL:HG23	1.99	0.44
1:B:340:LEU:HD23	1:B:343:MET:CE	2.47	0.44
1:A:425:PHE:CE2	1:A:489:ILE:HG21	2.52	0.44
1:A:416:PHE:CD1	1:A:416:PHE:N	2.85	0.44
1:A:237:MET:SD	1:A:261:TRP:CH2	3.11	0.44
1:B:266:LEU:HD23	1:B:267:THR:N	2.32	0.44
1:B:455:ASP:O	1:B:455:ASP:CG	2.56	0.44
1:B:330:CYS:HB2	1:B:335:VAL:HG21	1.99	0.44
1:A:273:LEU:HD11	1:A:279:GLU:CB	2.46	0.43
1:A:381:ASP:O	1:A:384:LEU:HG	2.17	0.43
1:B:366:ALA:N	1:B:428:LEU:HD13	2.34	0.43
1:A:357:LYS:O	1:A:358:ASN:HB2	2.18	0.43
1:B:278:MET:O	1:B:278:MET:HG3	2.19	0.43
1:A:285:LYS:O	1:A:289:VAL:HG23	2.19	0.42
1:A:406:THR:HG22	1:A:410:SER:HB2	2.01	0.42
1:A:275:GLU:HG3	1:A:276:ASP:H	1.82	0.42
1:B:423:TRP:CE3	1:B:476:TRP:HA	2.55	0.42
1:A:391:ASP:OD2	1:A:391:ASP:N	2.51	0.42
1:B:382:PHE:C	1:B:382:PHE:CD1	2.93	0.42
1:B:237:MET:SD	1:B:261:TRP:CZ2	3.12	0.42
1:B:289:VAL:HG13	1:B:359:PHE:CE2	2.54	0.42
1:A:450:GLU:OE2	1:A:454:LYS:HE3	2.19	0.42
1:A:360:ILE:HG23	1:A:387:LEU:CD2	2.47	0.42
1:A:249:GLY:O	1:A:252:GLN:HG2	2.20	0.41
1:A:273:LEU:HD12	1:A:273:LEU:HA	1.87	0.41
1:A:261:TRP:O	1:A:262:LYS:C	2.58	0.41
1:A:261:TRP:HZ3	1:A:302:LEU:HB3	1.86	0.41
1:A:233:ASP:OD1	1:A:235:TRP:HB2	2.21	0.41
1:B:466:GLU:O	1:B:470:GLU:HG3	2.21	0.41
1:A:271:LYS:HB3	1:A:313:ILE:HB	2.03	0.40
1:B:272:THR:HG22	1:B:273:LEU:N	2.37	0.40
1:A:239:ARG:NH1	1:A:239:ARG:CB	2.84	0.40
1:A:360:ILE:O	1:A:360:ILE:HG13	2.19	0.40
1:B:238:GLU:HG3	1:B:240:THR:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ASN:ND2	1:B:346:GLN:HB3	2.36	0.40
1:B:323:LEU:O	1:B:327:LEU:HG	2.22	0.40
1:B:356:LYS:HB2	1:B:356:LYS:HE3	1.85	0.40
1:B:430:TRP:O	1:B:434:THR:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	269/293 (92%)	253 (94%)	15 (6%)	1 (0%)	34	57
1	B	270/293 (92%)	255 (94%)	12 (4%)	3 (1%)	14	30
All	All	539/586 (92%)	508 (94%)	27 (5%)	4 (1%)	22	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	276	ASP
1	B	277	THR
1	A	262	LYS
1	B	274	LYS

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	237/255 (93%)	227 (96%)	10 (4%)	30	55
1	B	238/255 (93%)	225 (94%)	13 (6%)	21	43
All	All	475/510 (93%)	452 (95%)	23 (5%)	25	49

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	LYS
1	A	241	ASP
1	A	266	LEU
1	A	282	GLU
1	A	308	GLU
1	A	354	LEU
1	A	370	LEU
1	A	376	LEU
1	A	401	PHE
1	A	447	GLN
1	B	234	LYS
1	B	266	LEU
1	B	275	GLU
1	B	276	ASP
1	B	282	GLU
1	B	308	GLU
1	B	354	LEU
1	B	370	LEU
1	B	376	LEU
1	B	381	ASP
1	B	401	PHE
1	B	459	GLU
1	B	460	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	GLN
1	B	498	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)

4 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	$\#\|Z\| > 2$
3	MES	B	117	-	12,12,12	3.24	6 (50%)	14,16,16	1.86	3 (21%)
2	P17	B	120	-	30,32,32	2.12	8 (26%)	36,46,46	2.13	10 (27%)
3	MES	B	118	-	12,12,12	3.28	6 (50%)	14,16,16	1.90	6 (42%)
2	P17	A	119	-	30,32,32	2.21	8 (26%)	36,46,46	2.21	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
3	MES	B	117	-	-	4/6/14/14	0/1/1/1
2	P17	B	120	-	-	0/6/10/10	0/4/4/4
3	MES	B	118	-	-	0/6/14/14	0/1/1/1
2	P17	A	119	-	-	2/6/10/10	0/4/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	118	MES	O2S-S	7.39	1.66	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	117	MES	O2S-S	7.12	1.66	1.45
2	A	119	P17	C16-C13	6.79	1.52	1.39
2	B	120	P17	C16-C13	6.33	1.51	1.39
2	A	119	P17	C17-C18	4.96	1.50	1.41
2	B	120	P17	C17-C18	4.90	1.50	1.41
3	B	118	MES	O1S-S	4.13	1.57	1.45
3	B	117	MES	O1S-S	4.01	1.56	1.45
3	B	117	MES	C3-N4	3.80	1.57	1.46
2	B	120	P17	C6-C7	3.73	1.45	1.39
3	B	118	MES	C5-N4	3.63	1.56	1.46
3	B	118	MES	C3-N4	3.53	1.56	1.46
3	B	117	MES	O3S-S	3.49	1.60	1.47
3	B	117	MES	C7-N4	3.44	1.55	1.47
3	B	117	MES	C5-N4	3.33	1.56	1.46
2	A	119	P17	C6-C7	3.30	1.44	1.39
3	B	118	MES	O3S-S	3.21	1.59	1.47
3	B	118	MES	C7-N4	3.07	1.54	1.47
2	B	120	P17	C18-N19	-2.99	1.34	1.38
2	A	119	P17	C18-N19	-2.83	1.34	1.38
2	A	119	P17	C24-C23	2.80	1.42	1.36
2	A	119	P17	C26-C27	2.56	1.42	1.36
2	A	119	P17	C12-N11	2.48	1.37	1.32
2	B	120	P17	C24-C23	2.44	1.41	1.36
2	B	120	P17	C26-C27	2.42	1.41	1.36
2	B	120	P17	C5-C6	2.30	1.43	1.38
2	A	119	P17	C4-C3	2.25	1.43	1.39
2	B	120	P17	C4-C3	2.08	1.43	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	119	P17	N11-C10-N15	-7.11	119.65	126.52
2	A	119	P17	C10-N15-C14	6.66	122.84	115.28
2	B	120	P17	C10-N15-C14	6.44	122.59	115.28
2	B	120	P17	N11-C10-N15	-6.30	120.43	126.52
2	B	120	P17	C13-C14-N15	-4.26	117.83	123.37
2	A	119	P17	C13-C14-N15	-4.17	117.96	123.37
3	B	117	MES	O2S-S-C8	4.15	111.91	106.92
3	B	118	MES	O2S-S-C8	4.15	111.91	106.92
2	A	119	P17	C17-C18-N19	3.45	120.64	116.33
3	B	117	MES	O3S-S-C8	3.26	111.04	105.77
2	B	120	P17	C17-C18-N19	3.17	120.29	116.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	119	P17	C12-N11-C10	3.16	120.57	115.88
3	B	118	MES	O3S-S-C8	3.05	110.70	105.77
2	B	120	P17	C12-N11-C10	3.01	120.34	115.88
2	B	120	P17	C17-C16-C13	-2.72	118.23	122.27
2	A	119	P17	C17-C16-C13	-2.69	118.28	122.27
2	A	119	P17	C27-C22-C23	-2.64	119.38	125.49
2	B	120	P17	C27-C22-C23	-2.49	119.73	125.49
3	B	118	MES	O1S-S-C8	2.48	109.91	106.92
3	B	118	MES	C5-N4-C3	2.38	114.20	108.83
2	B	120	P17	C13-C12-N11	-2.37	119.63	124.08
3	B	118	MES	C6-O1-C2	2.28	117.51	109.89
2	A	119	P17	C13-C12-N11	-2.24	119.87	124.08
3	B	117	MES	C6-O1-C2	2.20	117.23	109.89
2	B	120	P17	C26-C27-C22	-2.08	119.33	122.58
3	B	118	MES	O2S-S-O1S	-2.04	106.90	113.95
2	B	120	P17	C7-C8-C3	2.01	121.25	119.57

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	117	MES	C8-C7-N4-C3
3	B	117	MES	C7-C8-S-O1S
3	B	117	MES	C7-C8-S-O3S
2	A	119	P17	C8-C3-S2-C1
2	A	119	P17	C4-C3-S2-C1
3	B	117	MES	C7-C8-S-O2S

There are no ring outliers.

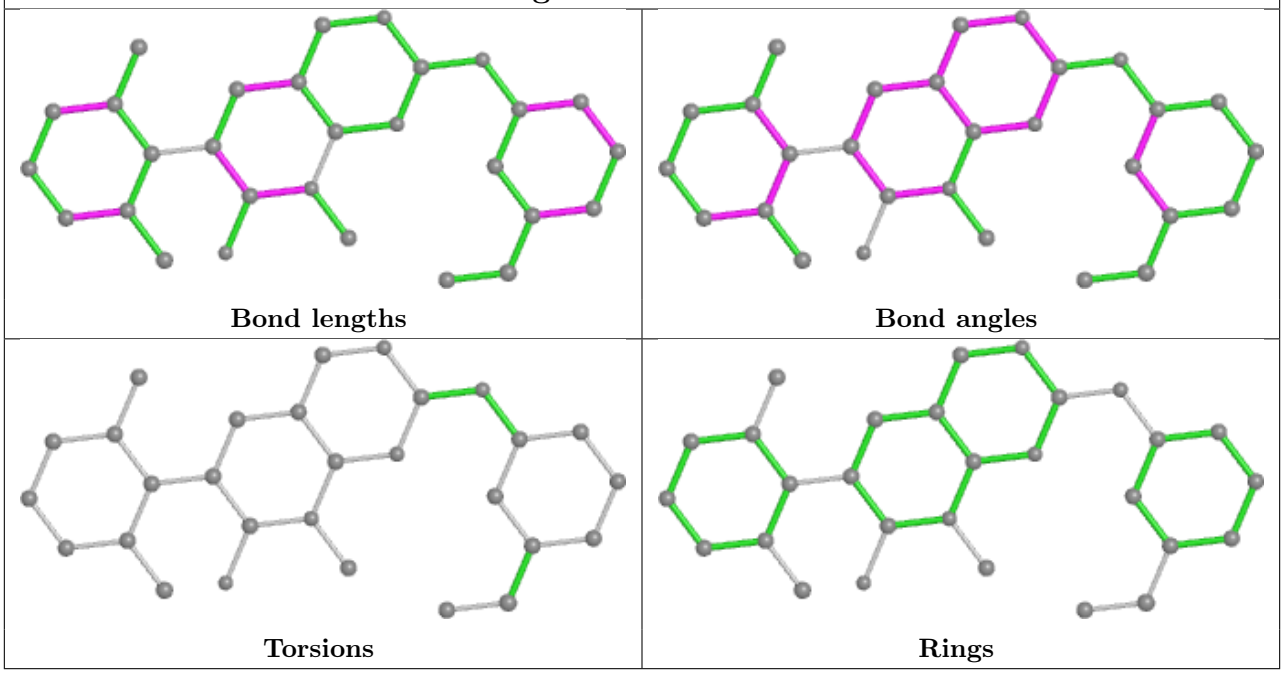
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	120	P17	2	0
2	A	119	P17	2	0

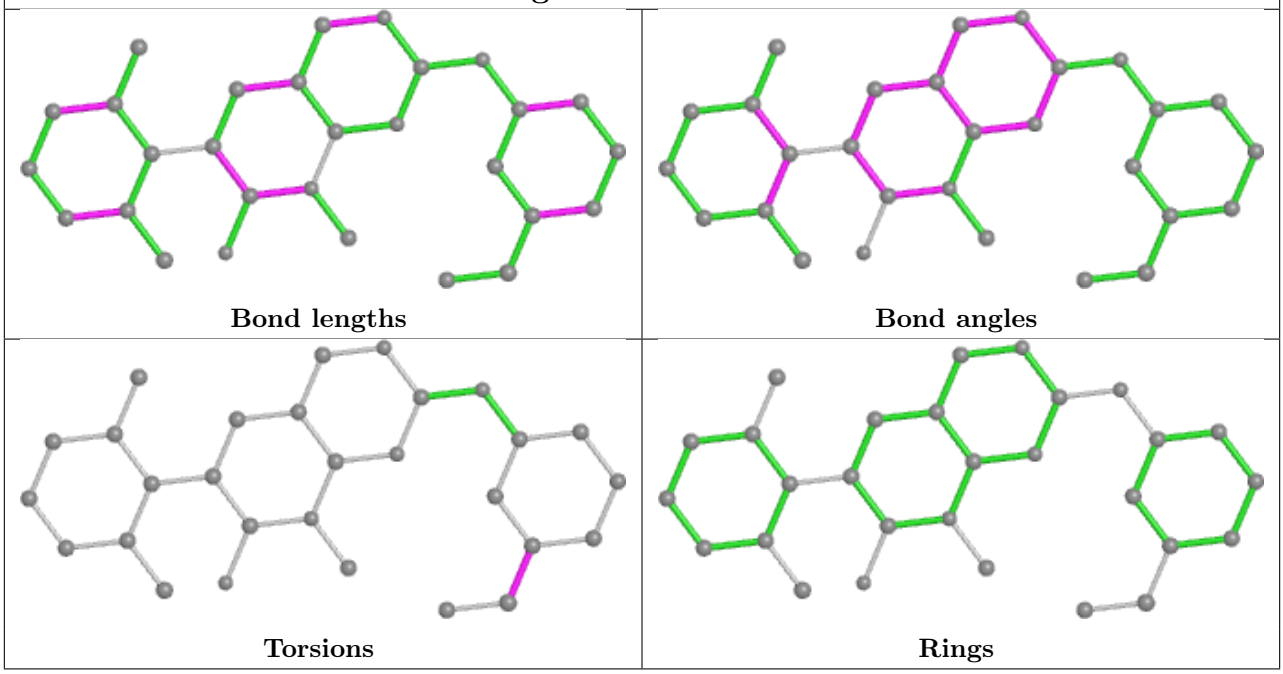
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 P17 B 120



Ligand P17 A 119



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	271/293 (92%)	-0.03	11 (4%)	37	30	15, 39, 84, 115	0
1	B	272/293 (92%)	-0.36	2 (0%)	87	86	14, 29, 69, 100	0
All	All	543/586 (92%)	-0.20	13 (2%)	59	53	14, 34, 76, 115	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	MET	4.7
1	B	274	LYS	3.4
1	A	261	TRP	3.3
1	B	277	THR	3.3
1	A	264	TYR	3.2
1	A	263	LYS	3.1
1	A	232	TYR	2.8
1	A	245	LYS	2.5
1	A	246	HIS	2.5
1	A	240	THR	2.4
1	A	266	LEU	2.4
1	A	276	ASP	2.1
1	A	307	ARG	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)

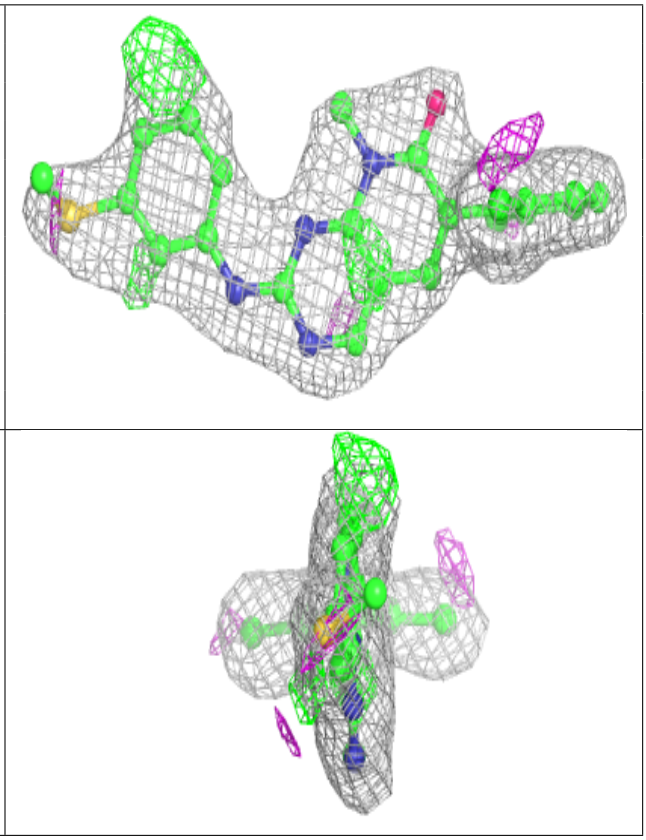
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	P17	A	119	29/29	0.91	0.18	38,41,46,50	0
3	MES	B	118	12/12	0.92	0.20	50,52,52,53	0
2	P17	B	120	29/29	0.94	0.14	25,28,32,37	0
3	MES	B	117	12/12	0.95	0.27	52,53,55,56	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.

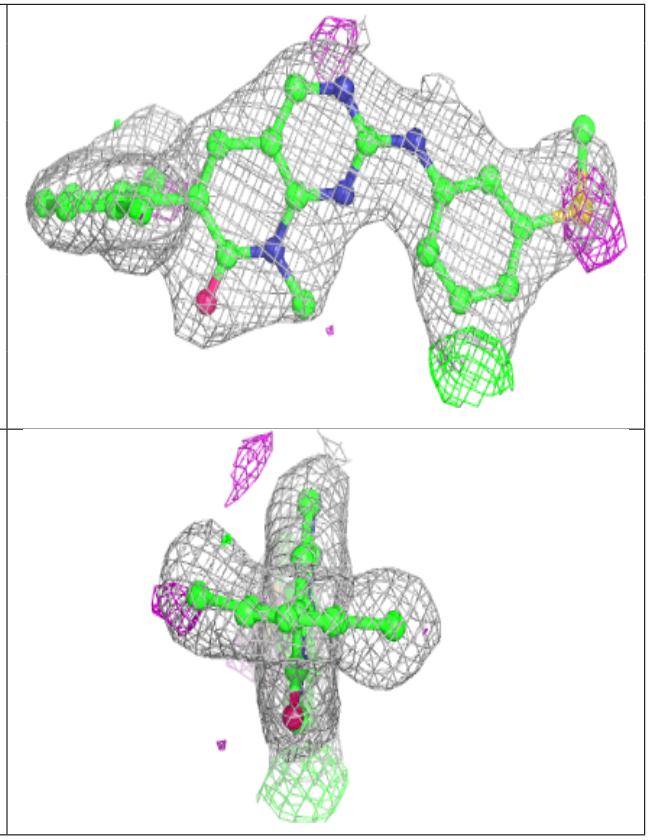
Electron density around P17 A 119:

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 P17 B 120:

$2mF_o$-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.