



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 09:27 PM JST

PDB ID : 6JWY
Title : Crystal structure of Plasmodium falciparum HPPK-DHPS A437G with SDX-DHP
Authors : Chitnumsub, P.; Jaruwat, A.; Yuthavong, Y.
Deposited on : 2019-04-21
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 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

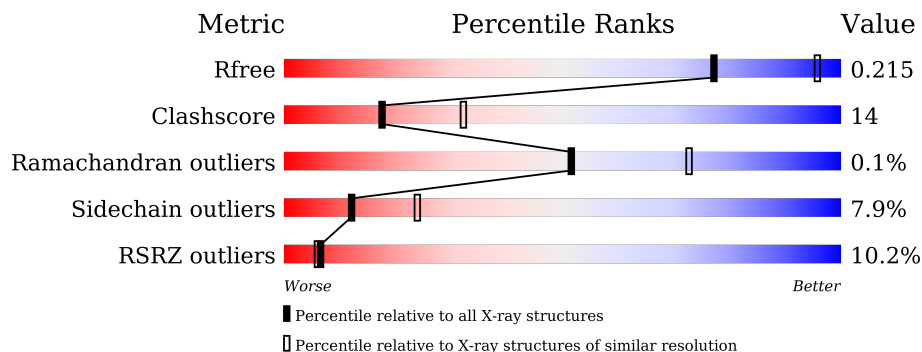
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	728	 4% 56% 16% 26%
1	B	728	 11% 46% 23% 27%

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 9241 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 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihydropteroate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	538	Total	C	N	O	S	0	0	0
			4459	2873	737	826	23			
1	B	529	Total	C	N	O	S	0	0	0
			4364	2812	720	811	21			

There are 46 discrepancies between the modelled and reference sequences:

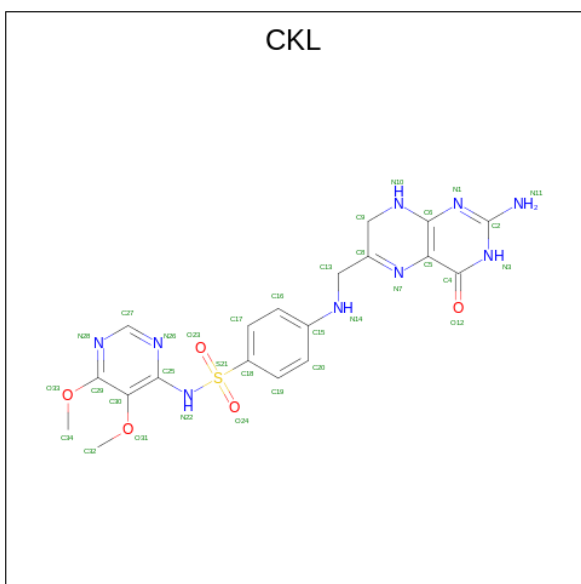
Chain	Residue	Modelled	Actual	Comment	Reference
A	437	GLY	ALA	engineered mutation	UNP Q25704
A	707	LYS	-	expression tag	UNP Q25704
A	708	ASP	-	expression tag	UNP Q25704
A	709	PRO	-	expression tag	UNP Q25704
A	710	ASN	-	expression tag	UNP Q25704
A	711	SER	-	expression tag	UNP Q25704
A	712	SER	-	expression tag	UNP Q25704
A	713	SER	-	expression tag	UNP Q25704
A	714	VAL	-	expression tag	UNP Q25704
A	715	ASP	-	expression tag	UNP Q25704
A	716	LYS	-	expression tag	UNP Q25704
A	717	LEU	-	expression tag	UNP Q25704
A	718	ALA	-	expression tag	UNP Q25704
A	719	ALA	-	expression tag	UNP Q25704
A	720	ALA	-	expression tag	UNP Q25704
A	721	LEU	-	expression tag	UNP Q25704
A	722	GLU	-	expression tag	UNP Q25704
A	723	HIS	-	expression tag	UNP Q25704
A	724	HIS	-	expression tag	UNP Q25704
A	725	HIS	-	expression tag	UNP Q25704
A	726	HIS	-	expression tag	UNP Q25704
A	727	HIS	-	expression tag	UNP Q25704
A	728	HIS	-	expression tag	UNP Q25704
B	437	GLY	ALA	engineered mutation	UNP Q25704

Continued on next page...

Continued from previous page...

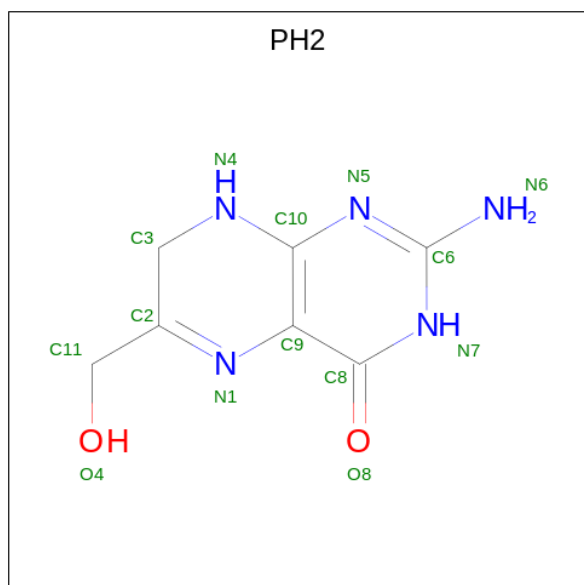
Chain	Residue	Modelled	Actual	Comment	Reference
B	707	LYS	-	expression tag	UNP Q25704
B	708	ASP	-	expression tag	UNP Q25704
B	709	PRO	-	expression tag	UNP Q25704
B	710	ASN	-	expression tag	UNP Q25704
B	711	SER	-	expression tag	UNP Q25704
B	712	SER	-	expression tag	UNP Q25704
B	713	SER	-	expression tag	UNP Q25704
B	714	VAL	-	expression tag	UNP Q25704
B	715	ASP	-	expression tag	UNP Q25704
B	716	LYS	-	expression tag	UNP Q25704
B	717	LEU	-	expression tag	UNP Q25704
B	718	ALA	-	expression tag	UNP Q25704
B	719	ALA	-	expression tag	UNP Q25704
B	720	ALA	-	expression tag	UNP Q25704
B	721	LEU	-	expression tag	UNP Q25704
B	722	GLU	-	expression tag	UNP Q25704
B	723	HIS	-	expression tag	UNP Q25704
B	724	HIS	-	expression tag	UNP Q25704
B	725	HIS	-	expression tag	UNP Q25704
B	726	HIS	-	expression tag	UNP Q25704
B	727	HIS	-	expression tag	UNP Q25704
B	728	HIS	-	expression tag	UNP Q25704

- Molecule 2 is 4-[(2-azanyl-4-oxidanylidene-7,8-dihydro-3 {H}-pteridin-6-yl)methylamino]-{N}-(5,6-dimethoxypyrimidin-4-yl)benzenesulfonamide (three-letter code: CKL) (formula: C₁₉H₂₁N₉O₅S) (labeled as "Ligand of Interest" by depositor).



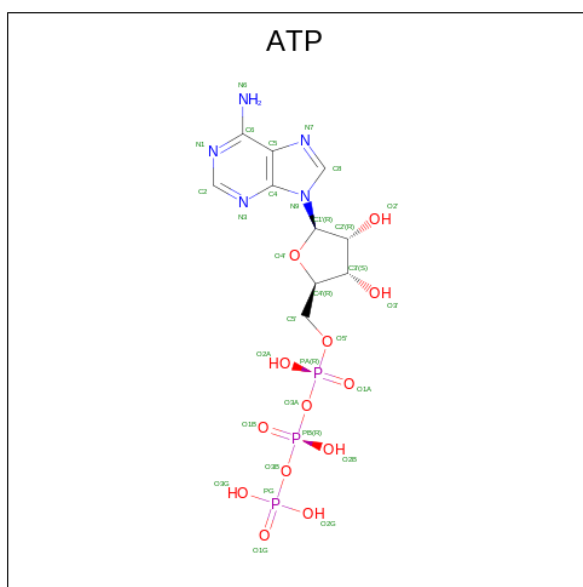
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	34	19	9	5	1	0	0
2	B	1	34	19	9	5	1	0	0

- Molecule 3 is 2-AMINO-6-HYDROXYMETHYL-7,8-DIHYDRO-3H-PTERIDIN-4-ONE (three-letter code: PH2) (formula: C₇H₉N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	7	5	2	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

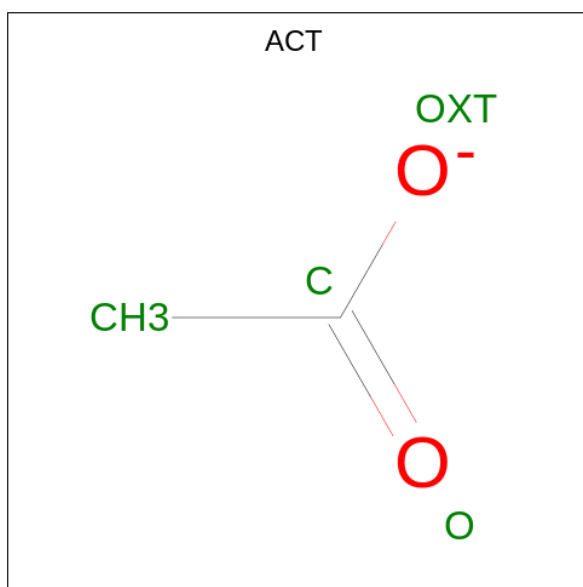
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

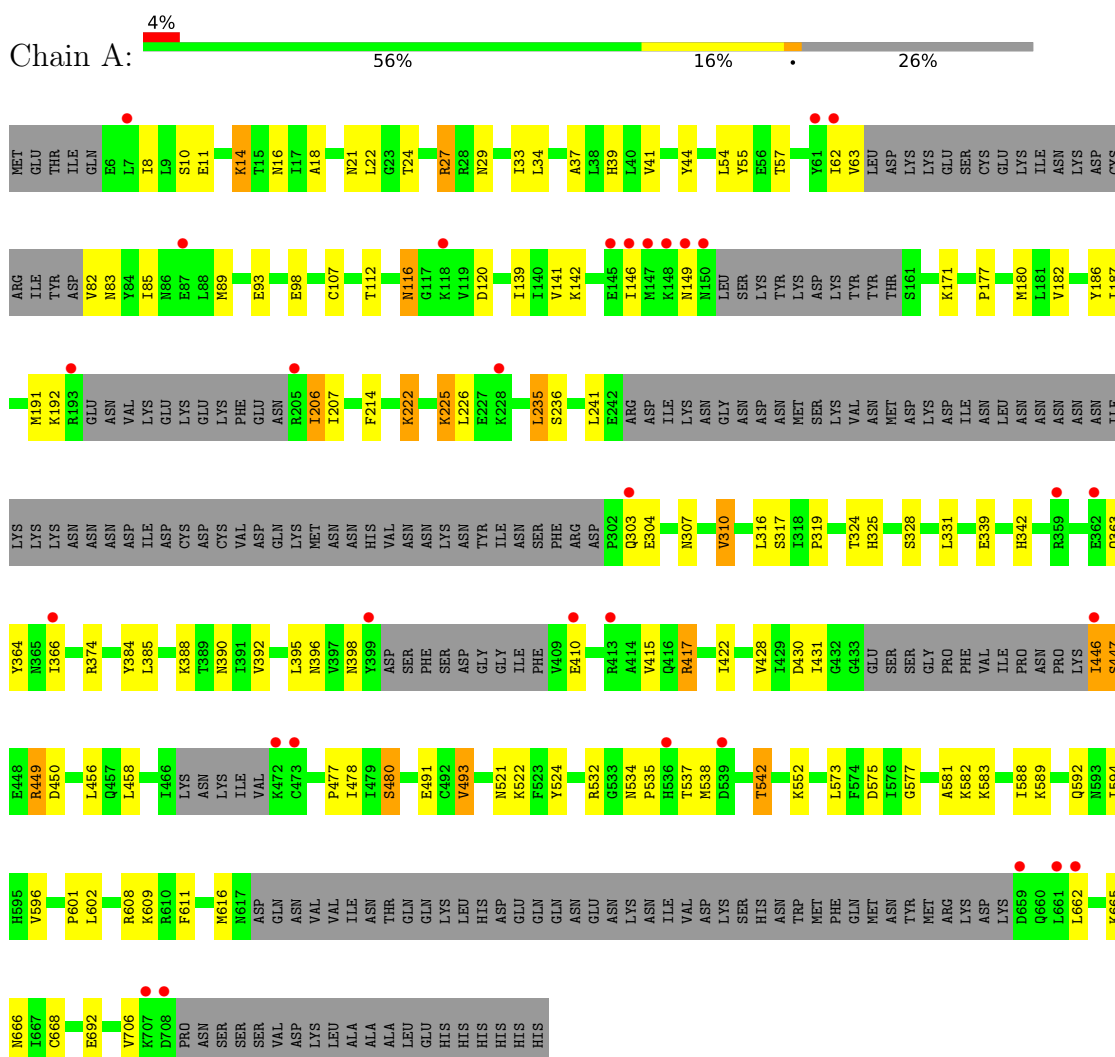
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	166	Total O 166 166	0	0
8	B	84	Total O 84 84	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: 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihydropteroate synthase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.43Å 137.15Å 137.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.95 – 2.50 28.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	82.8 (28.95-2.50) 82.9 (28.94-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.92 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.209 , 0.221 0.200 , 0.215	Depositor DCC
R_{free} test set	2680 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtrriage
Anisotropy	0.417	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.008 for -h,l,k	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9241	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: PH2, CA, ATP, CKL, MG, ACT

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	0.36	0/4527	0.76	1/6103 (0.0%)
1	B	0.32	0/4432	0.72	0/5977
All	All	0.34	0/8959	0.74	1/12080 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	THR	CA-CB-OG1	-5.02	98.46	109.00

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	4459	0	4558	97	0
1	B	4364	0	4451	152	0
2	A	34	0	0	2	0
2	B	34	0	0	0	0
3	A	14	0	9	0	0
4	A	31	0	12	2	0
4	B	31	0	12	3	0
5	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	A	1	0	0	0	0
7	A	8	0	6	1	0
7	B	12	0	9	0	0
8	A	166	0	0	4	0
8	B	84	0	0	3	0
All	All	9241	0	9057	248	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 (248) 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:107:CYS:SG	1:A:171:LYS:HE3	1.78	1.22
1:B:337:ILE:HG23	1:B:340:TYR:HB2	1.38	1.04
1:A:107:CYS:SG	1:A:171:LYS:CE	2.48	1.00
1:B:527:VAL:HG22	1:B:573:LEU:HD12	1.40	0.99
1:B:337:ILE:CG2	1:B:340:TYR:HB2	1.99	0.93
1:A:552:LYS:HD2	1:A:596:VAL:HG13	1.53	0.91
1:A:27:ARG:HG3	1:A:27:ARG:HH11	1.37	0.89
1:A:225:LYS:HE3	1:A:225:LYS:HA	1.54	0.89
1:A:665:LYS:HE3	8:B:928:HOH:O	1.74	0.88
1:B:534:ASN:HB2	1:B:535:PRO:HD2	1.57	0.86
1:B:96:LYS:HG3	1:B:240:HIS:CD2	2.11	0.86
1:B:422:ILE:HG12	1:B:477:PRO:HG3	1.58	0.84
1:A:107:CYS:HG	1:A:171:LYS:HE3	1.39	0.84
1:B:449:ARG:HG3	1:B:449:ARG:HH11	1.46	0.80
1:B:315:PHE:HB3	4:B:802:ATP:H1'	1.62	0.80
1:B:179:SER:O	1:B:183:VAL:HG23	1.83	0.79
1:B:608:ARG:HA	1:B:666:ASN:ND2	1.98	0.79
1:B:392:VAL:HG22	1:B:428:VAL:HB	1.65	0.77
1:B:127:VAL:HG13	1:B:131:ASN:HB3	1.66	0.77
1:B:113:PHE:O	1:B:116:ASN:HB3	1.84	0.77
1:B:419:PHE:HA	1:B:422:ILE:HD12	1.66	0.76
1:B:337:ILE:CG2	1:B:340:TYR:CB	2.63	0.75
1:A:39:HIS:CE1	1:A:521:ASN:HA	2.21	0.75
1:B:42:GLU:OE2	1:B:47:LYS:HA	1.86	0.74
1:B:178:LEU:O	1:B:182:VAL:HG23	1.89	0.72
1:B:534:ASN:HB2	1:B:535:PRO:CD	2.19	0.71
1:B:333:LEU:HD13	1:B:349:ILE:CD1	2.20	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:ARG:HA	1:B:666:ASN:HD21	1.55	0.71
1:B:180:MET:HG3	1:B:214:PHE:HE2	1.55	0.70
1:B:186:TYR:CE2	1:B:190:LEU:HD11	2.27	0.70
1:B:337:ILE:HG22	1:B:337:ILE:O	1.92	0.69
1:A:431:ILE:HG21	1:A:456:LEU:HD21	1.73	0.69
1:B:208:ASP:OD2	4:B:802:ATP:O1B	2.10	0.69
1:B:333:LEU:HD13	1:B:349:ILE:HD13	1.75	0.69
1:B:187:ILE:HA	1:B:190:LEU:HD12	1.75	0.68
1:B:184:ILE:O	1:B:187:ILE:HB	1.94	0.68
1:B:668:CYS:SG	8:B:984:HOH:O	1.94	0.67
1:B:373:LYS:O	1:B:375:ILE:HD12	1.95	0.66
1:B:14:LYS:NZ	1:B:120:ASP:HB2	2.10	0.66
1:B:177:PRO:HB3	1:B:318:ILE:CD1	2.26	0.66
1:B:108:GLU:CD	1:B:108:GLU:H	1.98	0.65
1:B:127:VAL:CG1	1:B:131:ASN:HB3	2.26	0.65
1:A:668:CYS:SG	8:A:1059:HOH:O	1.98	0.64
1:B:96:LYS:NZ	1:B:236:SER:O	2.28	0.64
1:B:167:THR:HG21	1:B:333:LEU:HD23	1.81	0.62
1:B:395:LEU:HD22	1:B:418:MET:HG3	1.81	0.62
1:A:27:ARG:HH11	1:A:27:ARG:CG	2.10	0.62
1:B:46:GLY:HA3	1:B:171:LYS:O	1.99	0.62
1:B:449:ARG:HH11	1:B:449:ARG:CG	2.11	0.61
1:B:45:LEU:HD22	1:B:180:MET:SD	2.40	0.61
1:A:18:ALA:HB1	1:A:180:MET:HE1	1.82	0.61
1:B:167:THR:OG1	1:B:332:CYS:HB3	2.00	0.60
1:B:534:ASN:CB	1:B:535:PRO:HD2	2.31	0.60
1:B:123:ILE:O	1:B:123:ILE:HG13	2.01	0.60
1:B:113:PHE:O	1:B:116:ASN:CB	2.50	0.59
1:B:388:LYS:HE3	1:B:390:ASN:OD1	2.02	0.59
1:B:227:GLU:HB2	1:B:230:MET:HB2	1.85	0.59
1:A:177:PRO:HD3	1:A:214:PHE:CD1	2.38	0.59
1:B:361:LYS:O	1:B:365:ASN:HA	2.03	0.59
1:B:132:TYR:OH	1:B:319:PRO:O	2.19	0.58
1:B:493:VAL:HG22	1:B:524:TYR:CZ	2.38	0.58
1:B:577:GLY:O	1:B:582:LYS:HE2	2.03	0.58
1:B:17:ILE:HG21	1:B:113:PHE:CD2	2.39	0.58
1:A:18:ALA:CB	1:A:180:MET:HE1	2.34	0.57
1:A:37:ALA:O	1:A:41:VAL:HG23	2.04	0.57
1:B:318:ILE:HA	1:B:319:PRO:C	2.25	0.56
1:B:527:VAL:CG2	1:B:573:LEU:HD12	2.26	0.56
1:A:396:ASN:OD1	7:A:808:ACT:H3	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:PRO:HD3	1:A:214:PHE:CE1	2.41	0.56
1:A:142:LYS:O	1:A:146:ILE:HD12	2.05	0.56
1:B:506:ALA:HB1	1:B:558:ARG:HG2	1.88	0.56
1:A:319:PRO:HD3	1:A:342:HIS:CE1	2.41	0.55
1:B:20:LEU:HD21	1:B:180:MET:HE1	1.88	0.55
1:A:89:MET:HE2	1:A:521:ASN:HB2	1.88	0.55
1:B:454:PRO:O	1:B:457:GLN:HB2	2.07	0.55
1:B:14:LYS:HZ3	1:B:120:ASP:HB2	1.72	0.55
1:A:89:MET:HG3	1:A:521:ASN:ND2	2.22	0.55
1:A:493:VAL:HG22	1:A:524:TYR:CZ	2.42	0.54
1:A:316:LEU:HA	4:A:803:ATP:C8	2.42	0.54
1:A:317:SER:N	4:A:803:ATP:N7	2.49	0.54
1:B:166:LEU:HG	1:B:166:LEU:O	2.06	0.54
1:B:425:GLY:HA3	1:B:694:LYS:HD3	1.89	0.54
1:A:182:VAL:HG12	1:A:235:LEU:HD13	1.89	0.54
1:B:433:GLY:O	1:B:434:GLU:HB2	2.07	0.54
1:B:227:GLU:HB2	1:B:230:MET:CB	2.38	0.54
1:A:39:HIS:CE1	1:A:521:ASN:CA	2.90	0.53
1:A:616:MET:CE	1:A:665:LYS:O	2.57	0.53
1:B:449:ARG:HE	1:B:491:GLU:CD	2.12	0.53
1:B:241:LEU:HD12	1:B:241:LEU:H	1.73	0.53
1:B:521:ASN:N	1:B:521:ASN:HD22	2.07	0.53
1:A:534:ASN:HB2	1:A:535:PRO:HD3	1.91	0.52
1:B:446:ILE:HG13	1:B:447:SER:H	1.74	0.52
1:B:337:ILE:CG2	1:B:337:ILE:O	2.56	0.52
1:B:21:ASN:C	1:B:21:ASN:HD22	2.13	0.52
1:B:31:VAL:HG12	1:B:32:LEU:N	2.24	0.52
1:B:410:GLU:HG3	1:B:410:GLU:O	2.10	0.52
1:A:449:ARG:HH11	1:A:449:ARG:CG	2.23	0.52
1:A:534:ASN:HB2	1:A:535:PRO:CD	2.39	0.52
1:B:333:LEU:HD13	1:B:349:ILE:HD11	1.91	0.52
1:A:177:PRO:HB2	1:A:316:LEU:HD21	1.91	0.52
1:B:395:LEU:HD23	1:B:431:ILE:HD12	1.92	0.51
1:B:231:ILE:O	1:B:235:LEU:HB2	2.09	0.51
1:A:27:ARG:HG3	1:A:27:ARG:NH1	2.17	0.51
1:B:449:ARG:HG3	1:B:449:ARG:NH1	2.17	0.51
1:B:167:THR:O	1:B:168:VAL:HG23	2.10	0.51
1:B:327:TYR:HB2	1:B:356:TYR:CZ	2.45	0.51
1:A:392:VAL:HG22	1:A:428:VAL:HB	1.93	0.51
1:B:55:TYR:CD1	1:B:331:LEU:HD21	2.46	0.51
1:A:225:LYS:HA	1:A:225:LYS:CE	2.33	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ILE:HG13	1:B:85:ILE:O	2.11	0.50
1:B:112:THR:O	1:B:116:ASN:HA	2.11	0.50
1:A:63:VAL:HG11	1:A:325:HIS:HB3	1.92	0.50
1:B:40:LEU:HD12	1:B:187:ILE:HG23	1.92	0.50
1:B:431:ILE:HG21	1:B:456:LEU:HD21	1.92	0.50
1:A:542:THR:HG21	1:A:583:LYS:HE2	1.91	0.50
1:A:395:LEU:HD23	1:A:431:ILE:HD12	1.92	0.50
1:A:449:ARG:NE	1:A:491:GLU:OE1	2.42	0.50
1:A:616:MET:HE1	1:A:665:LYS:O	2.12	0.50
1:B:552:LYS:HD2	1:B:596:VAL:HG13	1.94	0.50
1:A:57:THR:HG21	1:A:328:SER:HB2	1.93	0.49
1:A:141:VAL:CG2	1:A:142:LYS:N	2.75	0.49
1:A:93:GLU:OE2	1:A:186:TYR:OH	2.25	0.49
1:A:107:CYS:SG	1:A:171:LYS:HE2	2.48	0.49
1:A:206:ILE:HG23	1:A:207:ILE:HG22	1.94	0.49
1:A:449:ARG:HH11	1:A:449:ARG:HG3	1.77	0.49
1:B:395:LEU:HD22	1:B:418:MET:CG	2.43	0.49
1:A:446:ILE:HD13	1:A:450:ASP:HB2	1.95	0.49
1:B:175:ASN:N	1:B:175:ASN:HD22	2.10	0.49
1:B:337:ILE:HG22	1:B:340:TYR:HB3	1.95	0.48
1:B:96:LYS:HG3	1:B:240:HIS:HD2	1.68	0.48
1:A:374:ARG:HD2	1:A:385:LEU:HD22	1.95	0.48
1:A:222:LYS:HE3	1:A:222:LYS:HB2	1.61	0.48
1:B:17:ILE:HG21	1:B:113:PHE:CG	2.48	0.48
1:B:337:ILE:HG22	1:B:340:TYR:CB	2.41	0.48
1:A:21:ASN:C	1:A:22:LEU:HD12	2.33	0.48
1:B:111:GLU:O	1:B:115:LYS:HG2	2.14	0.48
1:A:609:LYS:NZ	2:A:801:CKL:O12	2.46	0.48
1:A:304:GLU:H	1:A:304:GLU:CD	2.16	0.48
1:B:96:LYS:HB2	1:B:238:TYR:O	2.14	0.48
1:A:27:ARG:CG	1:A:27:ARG:NH1	2.73	0.48
1:B:189:GLU:HG2	1:B:305:ILE:HB	1.96	0.48
1:B:336:MET:HE3	1:B:337:ILE:HD12	1.96	0.47
1:B:21:ASN:OD1	1:B:329:ILE:HG12	2.14	0.47
1:A:55:TYR:CD2	1:A:331:LEU:HD21	2.49	0.47
1:B:37:ALA:HB2	1:B:207:ILE:HD11	1.97	0.47
1:B:177:PRO:HB2	1:B:316:LEU:HD11	1.95	0.47
1:A:29:ASN:O	1:A:33:ILE:HG12	2.15	0.47
1:B:27:ARG:HG2	1:B:164:TYR:OH	2.15	0.46
1:B:307:ASN:C	1:B:309:MET:H	2.19	0.46
1:B:417:ARG:HH11	1:B:421:MET:HG3	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:PHE:C	1:B:116:ASN:HB3	2.35	0.46
1:B:21:ASN:HD22	1:B:22:LEU:N	2.13	0.46
1:B:27:ARG:CG	1:B:164:TYR:OH	2.63	0.46
1:A:363:GLN:O	1:A:363:GLN:HG2	2.16	0.46
1:A:588:ILE:CD1	1:A:611:PHE:HD1	2.29	0.46
1:B:96:LYS:HG3	1:B:240:HIS:NE2	2.28	0.46
1:A:112:THR:O	1:A:116:ASN:HA	2.16	0.46
1:A:398:ASN:HD22	1:A:398:ASN:HA	1.63	0.46
1:A:573:LEU:HD23	1:A:601:PRO:HB2	1.96	0.46
1:A:34:LEU:CD1	1:A:54:LEU:HD11	2.45	0.46
1:B:608:ARG:HH21	1:B:667:ILE:HD11	1.81	0.46
1:A:447:SER:HB2	1:A:450:ASP:OD2	2.15	0.46
1:B:56:GLU:O	1:B:372:ASN:HA	2.16	0.46
1:B:608:ARG:HH21	1:B:667:ILE:CD1	2.29	0.45
1:A:187:ILE:HG22	1:A:191:MET:HE3	1.97	0.45
1:B:542:THR:HG21	1:B:583:LYS:HE2	1.98	0.45
1:B:186:TYR:HB2	1:B:235:LEU:HD21	1.98	0.45
1:B:54:LEU:HB3	1:B:375:ILE:HB	1.99	0.45
1:B:45:LEU:O	1:B:172:THR:HA	2.16	0.45
1:A:573:LEU:HD23	1:A:601:PRO:CB	2.46	0.45
1:B:241:LEU:H	1:B:241:LEU:CD1	2.29	0.45
1:B:30:ALA:O	1:B:34:LEU:HB2	2.17	0.45
1:A:236:SER:OG	1:A:241:LEU:HD12	2.17	0.45
1:B:135:GLU:OE2	1:B:222:LYS:HD2	2.18	0.44
1:B:139:ILE:HG21	1:B:315:PHE:HE2	1.82	0.44
1:A:542:THR:HG23	1:A:542:THR:O	2.17	0.44
1:B:394:ILE:O	1:B:421:MET:HE1	2.17	0.44
1:A:388:LYS:HD2	1:A:390:ASN:OD1	2.18	0.44
1:B:123:ILE:HG12	1:B:176:ASP:HB3	1.99	0.44
1:A:27:ARG:CZ	1:A:384:TYR:OH	2.66	0.44
1:B:182:VAL:HG12	1:B:235:LEU:HD11	2.00	0.44
1:B:307:ASN:O	1:B:309:MET:N	2.51	0.44
1:A:588:ILE:CD1	1:A:611:PHE:CD1	3.01	0.44
1:B:18:ALA:HB3	1:B:170:VAL:HB	1.98	0.44
1:B:449:ARG:CD	1:B:491:GLU:OE1	2.65	0.44
1:A:417:ARG:HD2	1:A:417:ARG:O	2.17	0.44
1:A:662:LEU:O	1:A:666:ASN:HB2	2.18	0.44
1:B:317:SER:O	4:B:802:ATP:N6	2.43	0.44
1:B:422:ILE:HG12	1:B:477:PRO:CG	2.39	0.44
1:A:430:ASP:OD1	1:A:480:SER:OG	2.36	0.43
1:A:446:ILE:CG2	1:A:446:ILE:O	2.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:ARG:HE	1:A:491:GLU:CD	2.21	0.43
1:B:118:LYS:HA	1:B:118:LYS:HD2	1.70	0.43
1:A:422:ILE:HD11	1:A:477:PRO:HG3	2.00	0.43
1:A:522:LYS:HE2	8:A:974:HOH:O	2.18	0.43
1:A:575:ASP:OD2	2:A:801:CKL:N3	2.52	0.43
1:A:592:GLN:HG2	1:B:703:ILE:O	2.17	0.43
1:B:182:VAL:HG12	1:B:235:LEU:CD1	2.49	0.43
1:A:449:ARG:HD2	1:A:491:GLU:OE1	2.18	0.43
1:B:538:MET:O	1:B:581:ALA:HA	2.18	0.43
1:B:333:LEU:CD1	1:B:349:ILE:HD13	2.46	0.43
1:B:337:ILE:N	1:B:338:PRO:CD	2.81	0.43
1:B:364:TYR:HB3	1:B:366:ILE:HG13	2.01	0.43
1:B:181:LEU:HD12	1:B:181:LEU:O	2.18	0.43
1:B:309:MET:O	1:B:313:ILE:HG13	2.18	0.43
1:B:54:LEU:HD12	1:B:54:LEU:HA	1.87	0.42
1:B:413:ARG:O	1:B:416:GLN:N	2.52	0.42
1:B:309:MET:HB3	1:B:313:ILE:HD11	2.01	0.42
1:A:14:LYS:HD3	1:A:16:ASN:HD21	1.83	0.42
1:A:415:VAL:HG21	1:A:458:LEU:HG	2.01	0.42
1:B:333:LEU:CD1	1:B:349:ILE:CD1	2.96	0.42
1:B:504:ILE:HA	1:B:529:MET:HB3	2.01	0.42
1:A:594:ILE:CG1	1:A:602:LEU:HD21	2.50	0.42
1:B:305:ILE:HA	1:B:308:ASN:CG	2.39	0.42
1:B:320:HIS:ND1	1:B:321:VAL:N	2.68	0.42
1:A:39:HIS:ND1	1:A:521:ASN:HA	2.32	0.42
1:A:449:ARG:CD	1:A:491:GLU:OE1	2.68	0.42
1:B:534:ASN:CB	1:B:535:PRO:CD	2.86	0.41
1:A:304:GLU:O	1:A:307:ASN:HB2	2.20	0.41
1:A:235:LEU:HB3	1:A:241:LEU:HD11	2.02	0.41
1:A:44:TYR:HA	8:A:961:HOH:O	2.18	0.41
1:B:385:LEU:HG	1:B:386:LYS:HG2	2.02	0.41
1:A:226:LEU:O	1:A:310:VAL:HG13	2.20	0.41
1:A:692:GLU:OE1	1:A:692:GLU:N	2.43	0.41
1:B:594:ILE:HD11	1:B:602:LEU:HD21	2.02	0.41
1:A:577:GLY:O	1:A:582:LYS:HE2	2.20	0.41
1:B:35:GLU:O	1:B:38:LEU:HB2	2.20	0.41
1:B:57:THR:HG21	1:B:328:SER:CB	2.51	0.41
1:A:82:VAL:HG23	1:A:83:ASN:ND2	2.35	0.41
1:A:374:ARG:CD	1:A:385:LEU:HD22	2.51	0.41
1:A:428:VAL:HG22	1:A:478:ILE:HB	2.03	0.41
1:A:538:MET:O	1:A:581:ALA:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:SER:C	1:B:97:TYR:H	2.24	0.41
1:B:241:LEU:HD12	1:B:241:LEU:N	2.35	0.41
1:A:364:TYR:HB3	1:A:366:ILE:HG13	2.03	0.41
1:B:446:ILE:HD12	1:B:446:ILE:HA	1.95	0.40
1:B:342:HIS:ND1	1:B:344:VAL:HG12	2.36	0.40
1:B:394:ILE:O	1:B:421:MET:CE	2.69	0.40
1:A:532:ARG:HB2	1:A:581:ALA:CB	2.51	0.40
1:A:581:ALA:N	8:A:905:HOH:O	2.40	0.40
1:B:55:TYR:O	1:B:164:TYR:HA	2.21	0.40
1:B:110:TYR:CE1	1:B:169:VAL:HG11	2.56	0.40
1:B:353:TYR:OH	1:B:369:LYS:NZ	2.54	0.40
1:B:670:GLY:HA3	8:B:910:HOH:O	2.21	0.40
1:A:608:ARG:HA	1:A:666:ASN:OD1	2.22	0.40
1:B:37:ALA:O	1:B:41:VAL:HG23	2.21	0.40
1:B:45:LEU:CD2	1:B:180:MET:SD	3.08	0.40
1:B:542:THR:HG21	1:B:583:LYS:CE	2.52	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	520/728 (71%)	488 (94%)	31 (6%)	1 (0%)	47	68
1	B	511/728 (70%)	460 (90%)	51 (10%)	0	100	100
All	All	1031/1456 (71%)	948 (92%)	82 (8%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	ASP

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	513/696 (74%)	482 (94%)	31 (6%)	19	37
1	B	501/696 (72%)	452 (90%)	49 (10%)	8	15
All	All	1014/1392 (73%)	934 (92%)	80 (8%)	12	24

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	10	SER
1	A	11	GLU
1	A	14	LYS
1	A	27	ARG
1	A	62	ILE
1	A	85	ILE
1	A	98	GLU
1	A	116	ASN
1	A	139	ILE
1	A	149	ASN
1	A	192	LYS
1	A	206	ILE
1	A	222	LYS
1	A	225	LYS
1	A	235	LEU
1	A	303	GLN
1	A	310	VAL
1	A	324	THR
1	A	339	GLU
1	A	410	GLU
1	A	417	ARG
1	A	446	ILE
1	A	447	SER
1	A	449	ARG
1	A	480	SER
1	A	493	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	537	THR
1	A	542	THR
1	A	589	LYS
1	A	706	VAL
1	B	21	ASN
1	B	32	LEU
1	B	43	LYS
1	B	84	TYR
1	B	85	ILE
1	B	91	ASN
1	B	93	GLU
1	B	101	LYS
1	B	102	GLU
1	B	105	ASP
1	B	123	ILE
1	B	142	LYS
1	B	144	ASP
1	B	171	LYS
1	B	175	ASN
1	B	178	LEU
1	B	180	MET
1	B	207	ILE
1	B	220	PHE
1	B	222	LYS
1	B	224	ILE
1	B	241	LEU
1	B	308	ASN
1	B	316	LEU
1	B	321	VAL
1	B	323	THR
1	B	341	LYS
1	B	345	LEU
1	B	360	MET
1	B	361	LYS
1	B	363	GLN
1	B	381	ARG
1	B	410	GLU
1	B	416	GLN
1	B	417	ARG
1	B	449	ARG
1	B	462	GLU
1	B	518	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	521	ASN
1	B	542	THR
1	B	562	LEU
1	B	573	LEU
1	B	582	LYS
1	B	596	VAL
1	B	617	ASN
1	B	660	GLN
1	B	667	ILE
1	B	694	LYS
1	B	723	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	83	ASN
1	A	308	ASN
1	A	343	ASN
1	A	398	ASN
1	A	521	ASN
1	A	664	GLN
1	B	21	ASN
1	B	90	GLN
1	B	91	ASN
1	B	165	ASN
1	B	175	ASN
1	B	240	HIS
1	B	308	ASN
1	B	363	GLN
1	B	521	ASN
1	B	660	GLN
1	B	664	GLN
1	B	666	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](#)

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](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ACT	B	805	-	3,3,3	0.92	0	3,3,3	0.76	0
3	PH2	A	802	-	10,15,15	1.21	1 (10%)	10,21,21	3.05	6 (60%)
2	CKL	B	801	-	32,37,37	2.01	3 (9%)	37,53,53	2.98	17 (45%)
4	ATP	B	802	5	26,33,33	0.65	0	31,52,52	0.91	2 (6%)
7	ACT	B	806	-	3,3,3	1.17	0	3,3,3	0.62	0
2	CKL	A	801	-	32,37,37	2.10	4 (12%)	37,53,53	2.91	12 (32%)
7	ACT	A	807	-	3,3,3	0.83	0	3,3,3	0.84	0
4	ATP	A	803	5	26,33,33	0.64	0	31,52,52	0.84	1 (3%)
7	ACT	A	808	-	3,3,3	1.15	0	3,3,3	0.69	0
7	ACT	B	804	-	3,3,3	1.01	0	3,3,3	0.90	0

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PH2	A	802	-	-	0/0/11/11	0/2/2/2
2	CKL	B	801	-	-	3/18/29/29	0/4/4/4
4	ATP	B	802	5	-	2/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CKL	A	801	-	-	6/18/29/29	0/4/4/4
4	ATP	A	803	5	-	4/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	CKL	C18-S21	-9.79	1.61	1.76
2	B	801	CKL	C18-S21	-9.50	1.61	1.76
2	A	801	CKL	C5-C6	3.11	1.47	1.40
3	A	802	PH2	C8-N7	2.79	1.37	1.33
2	B	801	CKL	C25-N22	-2.22	1.36	1.40
2	A	801	CKL	C25-N22	-2.21	1.36	1.40
2	B	801	CKL	C5-C6	2.12	1.45	1.40
2	A	801	CKL	O33-C29	2.01	1.38	1.35

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	CKL	O23-S21-O24	-11.45	105.47	119.55
2	A	801	CKL	O23-S21-O24	-11.03	105.99	119.55
3	A	802	PH2	C10-C9-C8	6.55	118.81	114.53
2	A	801	CKL	O23-S21-C18	6.12	115.51	107.97
2	A	801	CKL	N26-C27-N28	-5.17	120.51	128.60
2	B	801	CKL	O24-S21-C18	5.12	114.28	107.97
2	B	801	CKL	N26-C27-N28	-4.98	120.81	128.60
2	B	801	CKL	C2-N1-C6	4.78	122.07	113.43
2	A	801	CKL	C34-O33-C29	4.76	121.93	117.21
3	A	802	PH2	C9-C8-N7	-4.43	117.38	123.43
2	A	801	CKL	O24-S21-N22	4.35	117.61	106.73
2	B	801	CKL	C18-S21-N22	4.24	112.16	106.83
2	B	801	CKL	O12-C4-C5	-3.76	116.62	126.60
2	A	801	CKL	C2-N1-C6	3.65	120.02	113.43
3	A	802	PH2	C6-N7-C8	3.63	121.70	115.93
2	A	801	CKL	C27-N28-C29	3.32	121.44	115.88
2	A	801	CKL	C18-S21-N22	-3.27	102.72	106.83
2	B	801	CKL	C5-C4-N3	2.96	120.71	113.19
2	B	801	CKL	C27-N28-C29	2.96	120.84	115.88
2	B	801	CKL	C34-O33-C29	2.93	120.12	117.21
4	B	802	ATP	PA-O3A-PB	2.84	142.59	132.83
2	A	801	CKL	C5-C4-N3	2.79	120.27	113.19
2	A	801	CKL	C13-N14-C15	2.72	127.85	122.49
2	B	801	CKL	C2-N3-C4	-2.69	120.20	125.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	CKL	C20-C19-C18	2.69	122.23	119.45
2	A	801	CKL	O12-C4-C5	-2.64	119.59	126.60
2	B	801	CKL	C17-C18-S21	2.55	122.54	119.77
3	A	802	PH2	N5-C6-N7	-2.38	121.68	125.42
2	B	801	CKL	C25-N22-S21	2.30	128.35	124.16
2	B	801	CKL	C5-N7-C8	2.30	120.81	116.24
3	A	802	PH2	C6-N5-C10	2.30	119.68	114.54
4	A	803	ATP	C5-C6-N6	2.27	123.80	120.35
2	B	801	CKL	O24-S21-N22	2.21	112.27	106.73
3	A	802	PH2	N6-C6-N5	2.21	120.68	117.25
2	A	801	CKL	C32-O31-C30	2.15	120.67	114.78
4	B	802	ATP	C5-C6-N6	2.11	123.56	120.35
2	B	801	CKL	O33-C29-C30	2.11	121.04	116.95
2	B	801	CKL	N22-C25-N26	2.06	122.64	118.66

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	CKL	C25-N22-S21-O23
2	B	801	CKL	C30-C29-O33-C34
2	B	801	CKL	N28-C29-O33-C34
4	B	802	ATP	PB-O3A-PA-O5'
2	A	801	CKL	N28-C29-O33-C34
2	A	801	CKL	C30-C29-O33-C34
2	A	801	CKL	C25-N22-S21-O24
2	A	801	CKL	C25-N22-S21-C18
4	A	803	ATP	O4'-C4'-C5'-O5'
2	B	801	CKL	C8-C13-N14-C15
4	A	803	ATP	PB-O3A-PA-O1A
4	A	803	ATP	PA-O3A-PB-O1B
2	A	801	CKL	C8-C13-N14-C15
4	B	802	ATP	O4'-C4'-C5'-O5'
4	A	803	ATP	PA-O3A-PB-O2B

There are no ring outliers.

4 monomers are involved in 8 short contacts:

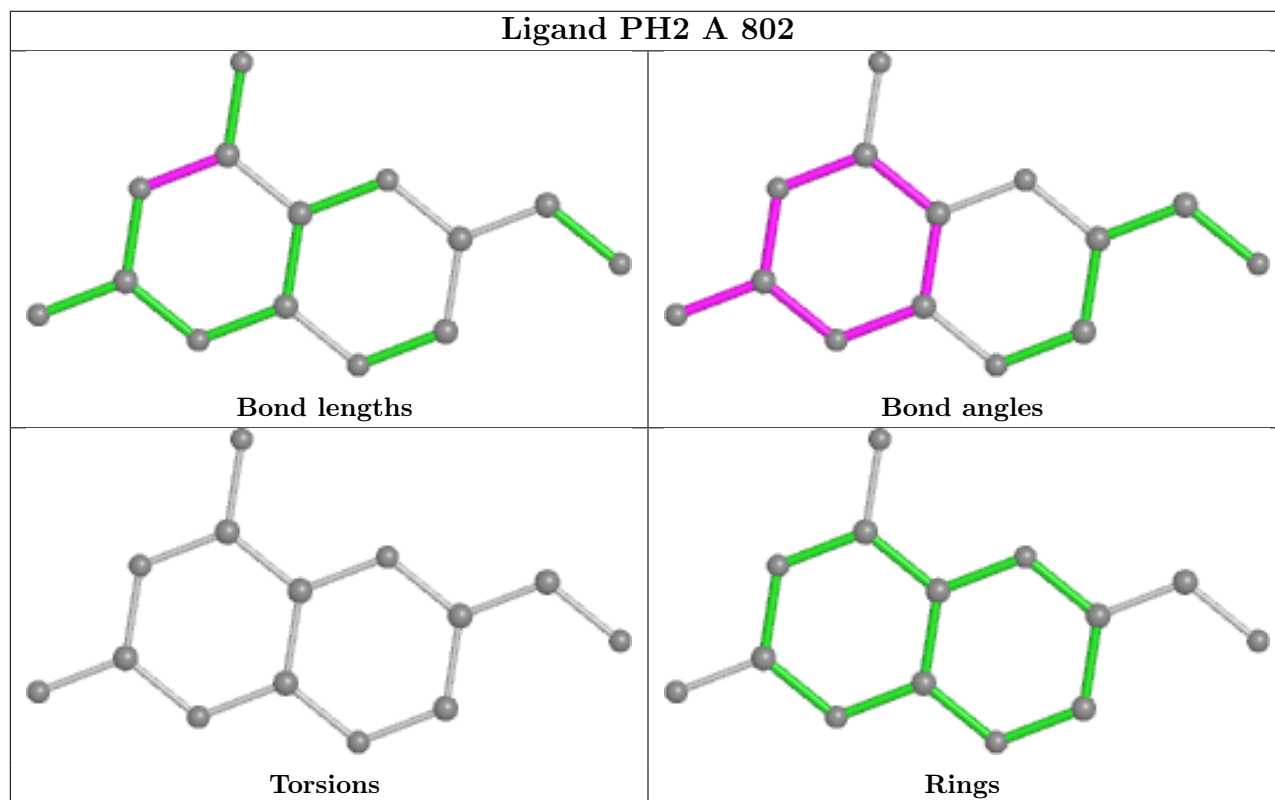
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	802	ATP	3	0
2	A	801	CKL	2	0

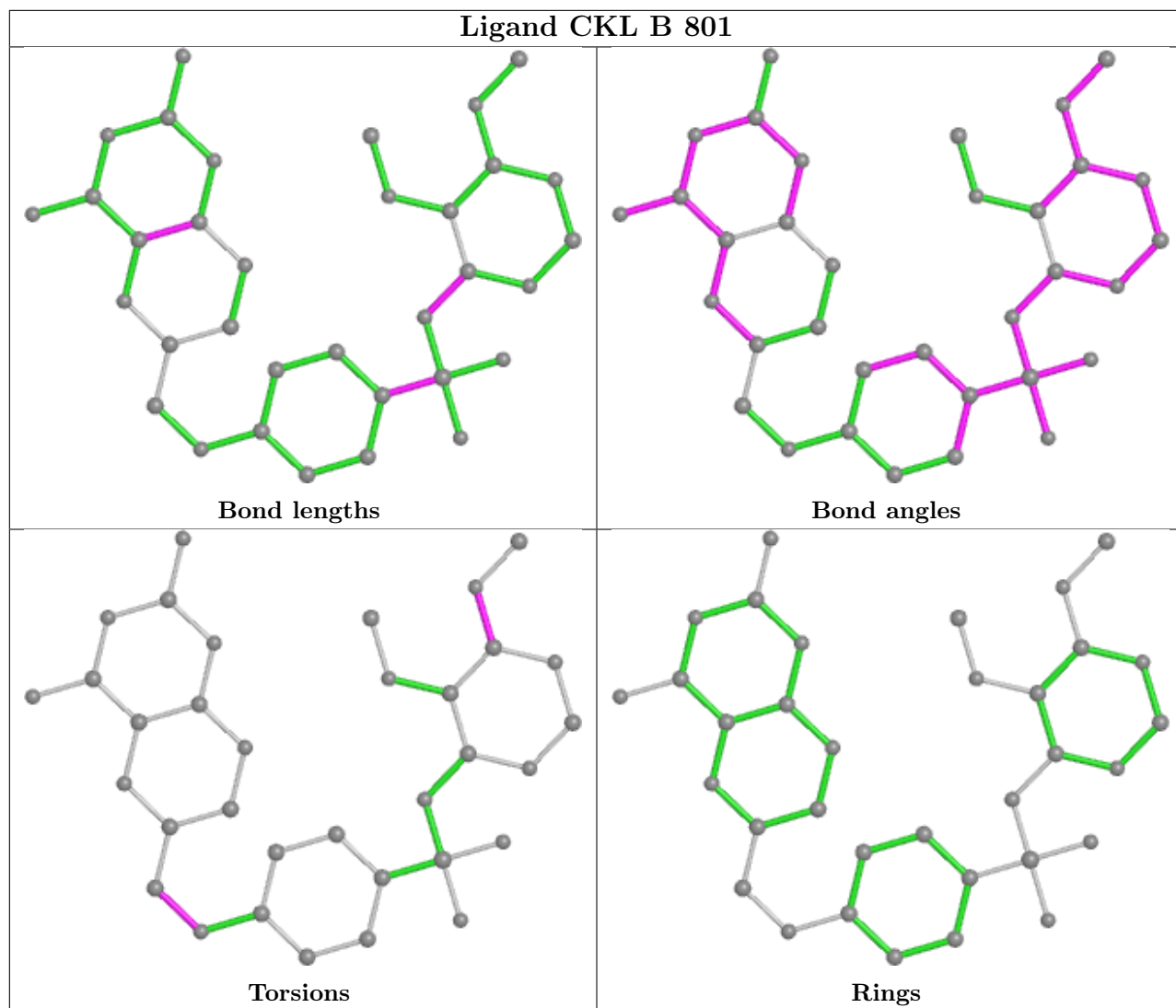
Continued on next page...

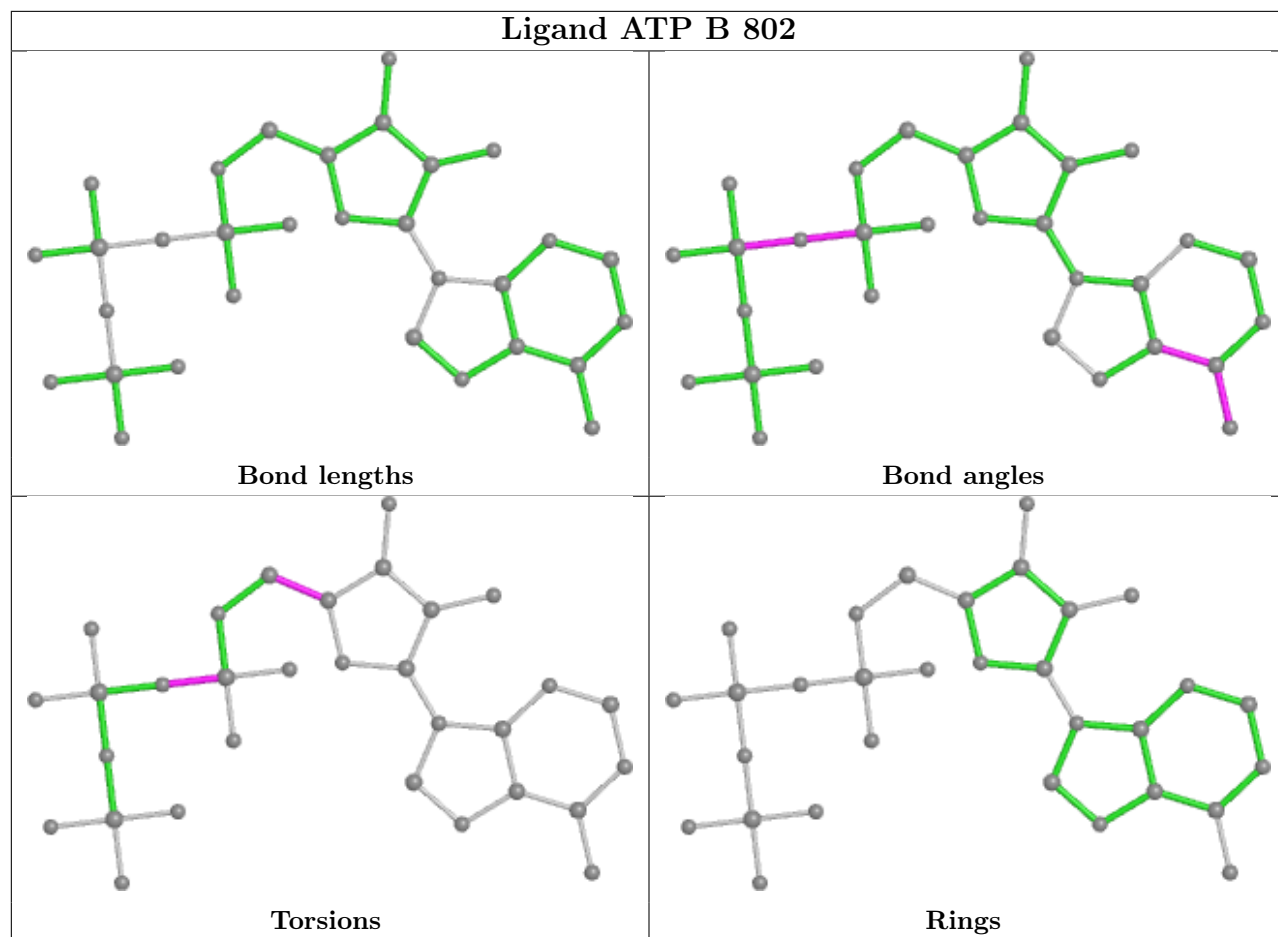
Continued from previous page...

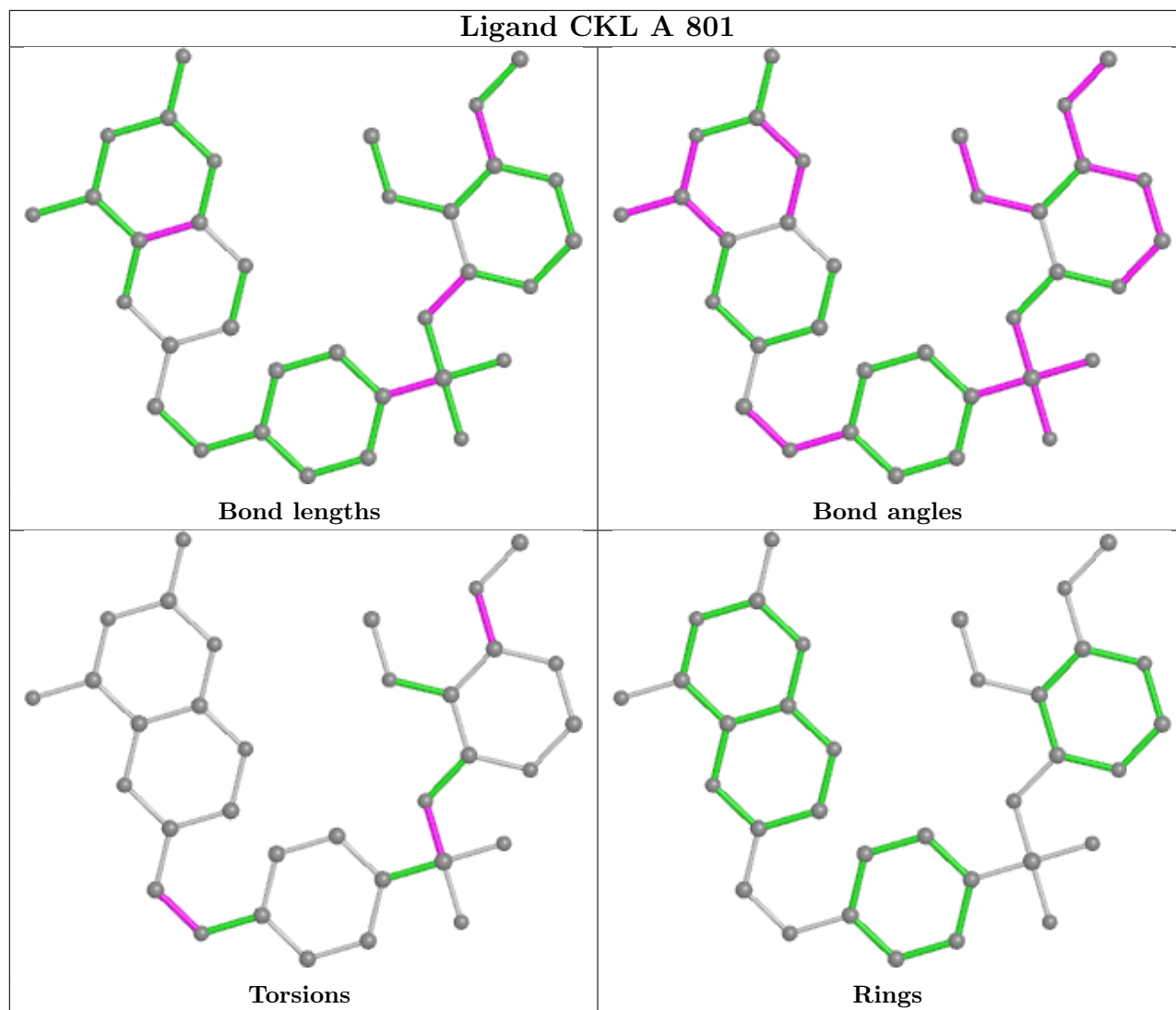
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	ATP	2	0
7	A	808	ACT	1	0

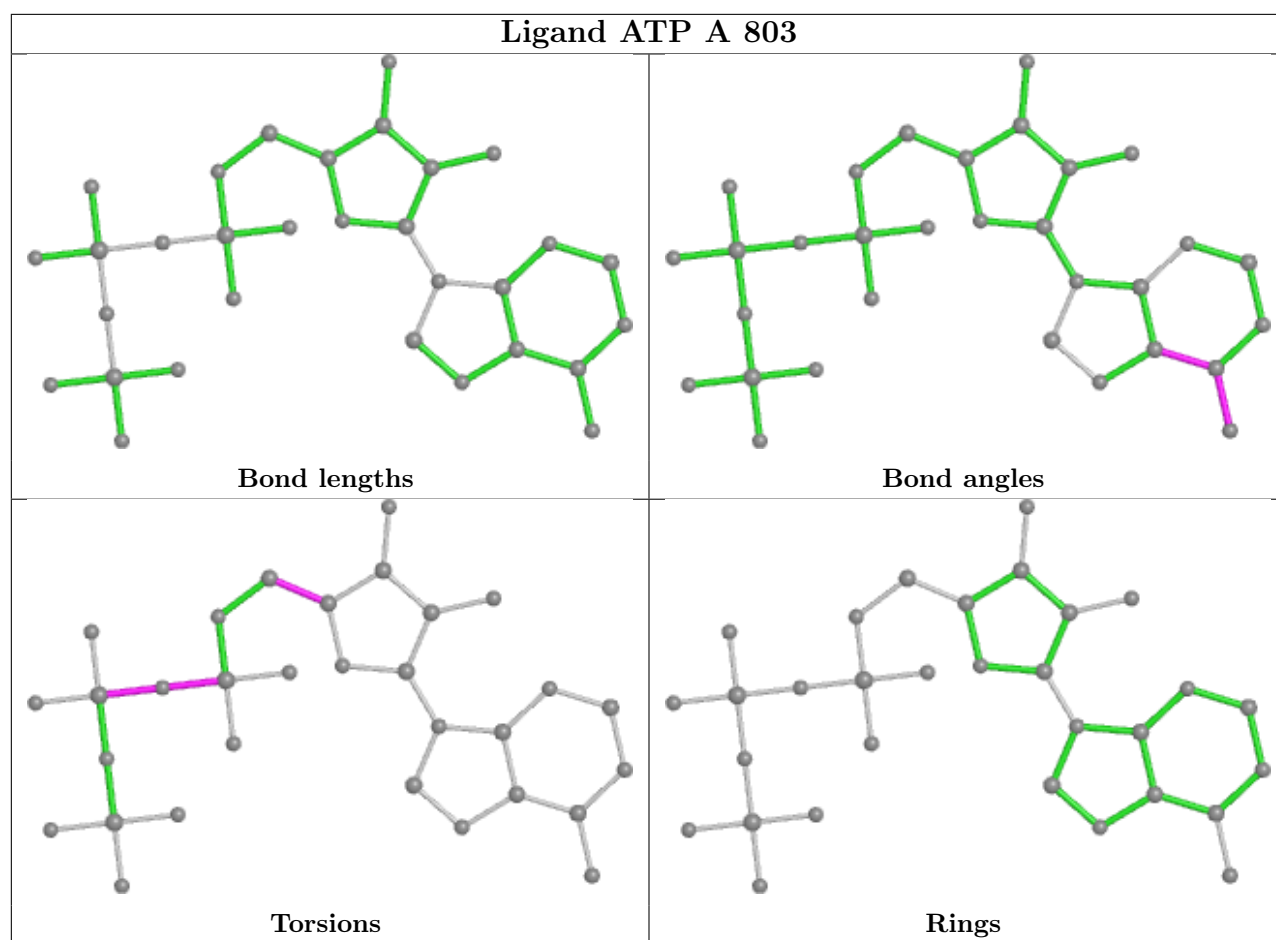
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	538/728 (73%)	-0.06	31 (5%) 23 24	10, 31, 93, 120	0
1	B	529/728 (72%)	0.54	78 (14%) 2 2	12, 61, 119, 120	0
All	All	1067/1456 (73%)	0.24	109 (10%) 6 6	10, 41, 114, 120	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	TYR	6.3
1	B	306	ILE	5.8
1	B	133	LEU	5.6
1	B	366	ILE	5.5
1	B	134	LEU	5.4
1	B	161	SER	5.2
1	B	231	ILE	5.2
1	B	229	ASN	5.2
1	B	660	GLN	4.9
1	B	129	VAL	4.9
1	B	137	ASN	4.7
1	B	312	ASN	4.7
1	B	130	GLU	4.7
1	B	307	ASN	4.6
1	B	142	LYS	4.6
1	B	140	ILE	4.6
1	A	473	CYS	4.5
1	B	138	ASN	4.5
1	B	305	ILE	4.4
1	B	474	ASP	4.4
1	A	145	GLU	4.4
1	B	20	LEU	4.3
1	A	62	ILE	4.3
1	A	147	MET	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	211	ILE	4.2
1	B	228	LYS	4.2
1	B	367	ASN	4.2
1	A	150	ASN	4.1
1	B	90	GLN	4.1
1	A	303	GLN	4.1
1	B	87	GLU	4.1
1	A	708	ASP	4.1
1	B	141	VAL	4.0
1	B	89	MET	3.9
1	A	707	LYS	3.7
1	B	97	TYR	3.6
1	B	227	GLU	3.6
1	A	193	ARG	3.6
1	A	149	ASN	3.5
1	B	22	LEU	3.5
1	B	58	VAL	3.4
1	A	662	LEU	3.3
1	B	661	LEU	3.3
1	B	223	ASN	3.2
1	B	233	LYS	3.2
1	A	536	HIS	3.2
1	B	365	ASN	3.2
1	B	117	GLY	3.2
1	A	146	ILE	3.1
1	B	98	GLU	3.1
1	A	148	LYS	3.1
1	B	226	LEU	3.1
1	A	661	LEU	3.0
1	B	225	LYS	2.9
1	B	118	LYS	2.9
1	A	659	ASP	2.9
1	B	220	PHE	2.9
1	B	344	VAL	2.8
1	A	118	LYS	2.8
1	B	222	LYS	2.8
1	B	536	HIS	2.8
1	B	85	ILE	2.7
1	B	466	ILE	2.7
1	B	706	VAL	2.7
1	A	366	ILE	2.7
1	B	419	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	315	PHE	2.6
1	B	445	LYS	2.6
1	B	191	MET	2.6
1	B	209	ILE	2.6
1	B	27	ARG	2.6
1	A	362	GLU	2.5
1	A	359	ARG	2.5
1	A	228	LYS	2.5
1	B	166	LEU	2.5
1	A	472	LYS	2.5
1	B	25	ASN	2.5
1	B	357	VAL	2.5
1	B	144	ASP	2.4
1	B	168	VAL	2.4
1	B	343	ASN	2.4
1	A	7	LEU	2.4
1	A	61	TYR	2.4
1	B	723	HIS	2.4
1	A	87	GLU	2.4
1	B	21	ASN	2.4
1	A	410	GLU	2.4
1	B	465	ASP	2.3
1	B	125	LYS	2.3
1	B	145	GLU	2.3
1	B	143	ASN	2.3
1	A	205	ARG	2.3
1	A	539	ASP	2.3
1	B	84	TYR	2.2
1	B	322	TYR	2.2
1	A	446	ILE	2.2
1	B	136	CYS	2.2
1	A	399	TYR	2.1
1	B	186	TYR	2.1
1	B	131	ASN	2.1
1	B	240	HIS	2.1
1	B	132	TYR	2.1
1	B	184	ILE	2.1
1	B	311	ASP	2.1
1	B	364	TYR	2.1
1	B	120	ASP	2.1
1	A	413	ARG	2.0
1	B	361	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	86	ASN	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](#)

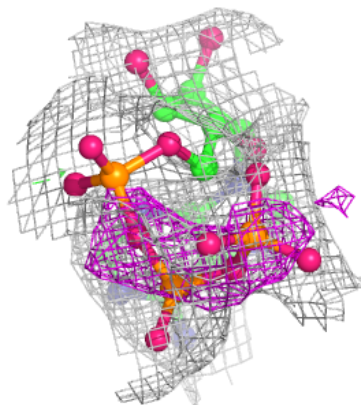
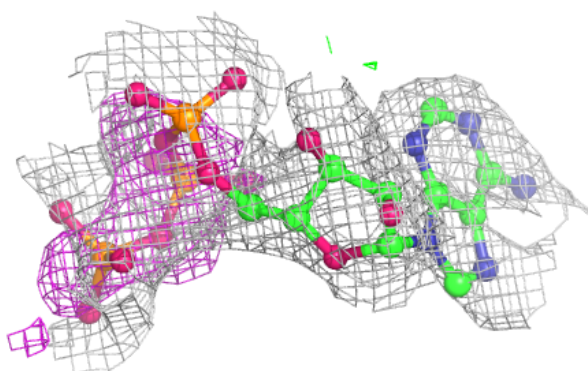
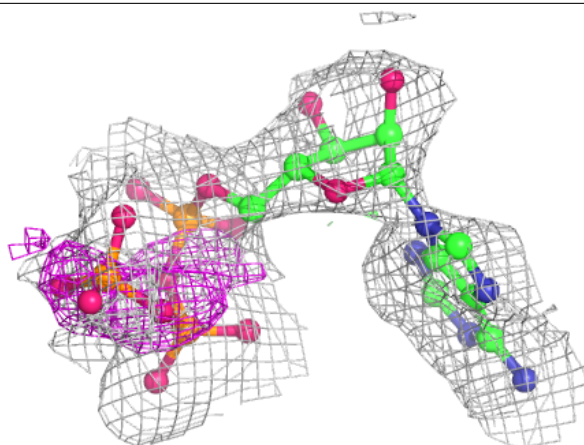
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ATP	B	802	31/31	0.58	0.25	87,116,120,120	0
3	PH2	A	802	14/14	0.90	0.15	57,62,77,82	0
2	CKL	A	801	34/34	0.90	0.19	9,26,96,104	0
4	ATP	A	803	31/31	0.93	0.15	30,60,120,120	0
5	MG	A	804	1/1	0.94	0.29	79,79,79,79	0
2	CKL	B	801	34/34	0.95	0.15	12,26,97,104	0
5	MG	B	803	1/1	0.95	0.11	80,80,80,80	0
7	ACT	A	807	4/4	0.96	0.11	27,29,29,29	0
7	ACT	A	808	4/4	0.96	0.15	31,31,35,37	0
7	ACT	B	806	4/4	0.96	0.20	40,41,43,47	0
6	CA	A	806	1/1	0.97	0.12	25,25,25,25	0
7	ACT	B	805	4/4	0.98	0.09	31,35,36,38	0
5	MG	A	805	1/1	0.99	0.12	27,27,27,27	0
7	ACT	B	804	4/4	0.99	0.15	19,20,20,20	0

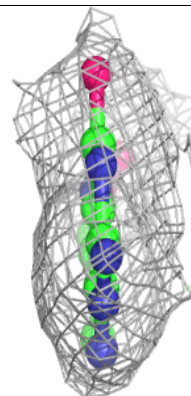
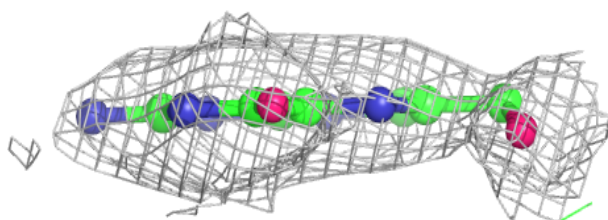
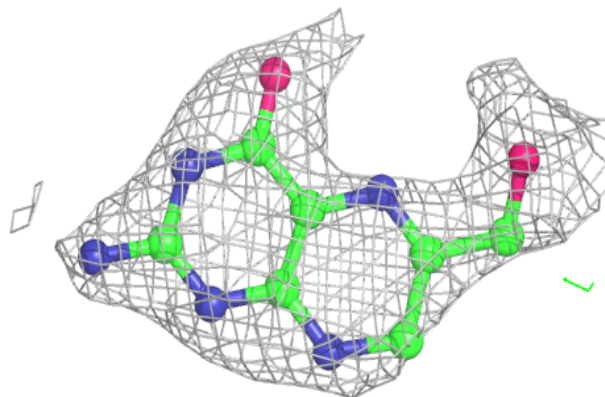
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

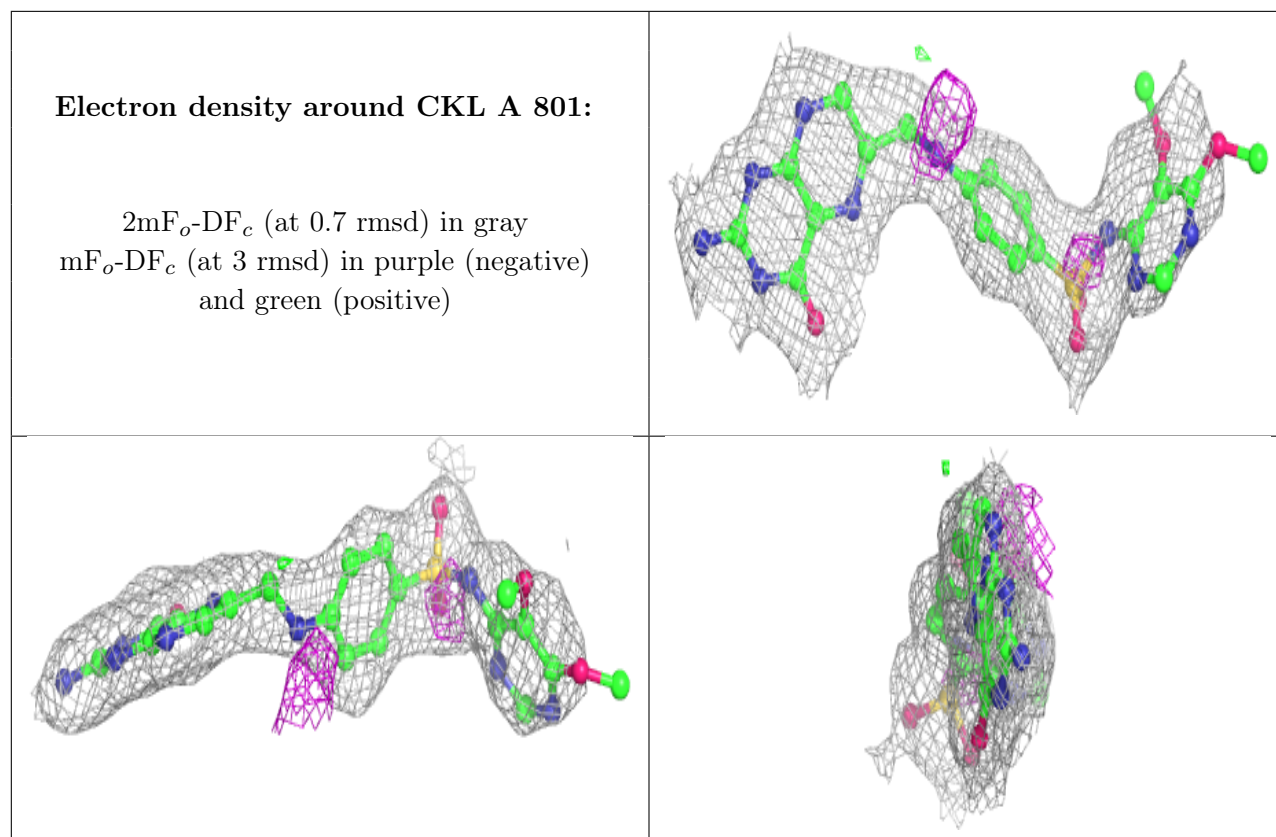
Electron density around ATP B 802:

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

**Electron density around PH2 A 802:**

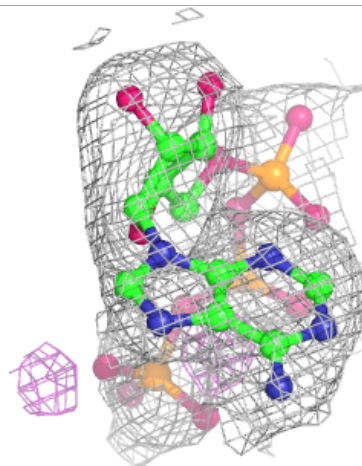
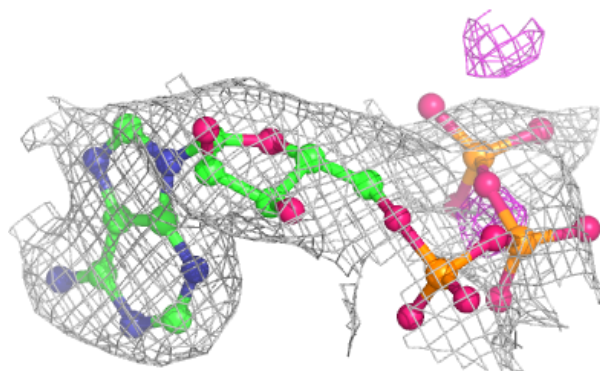
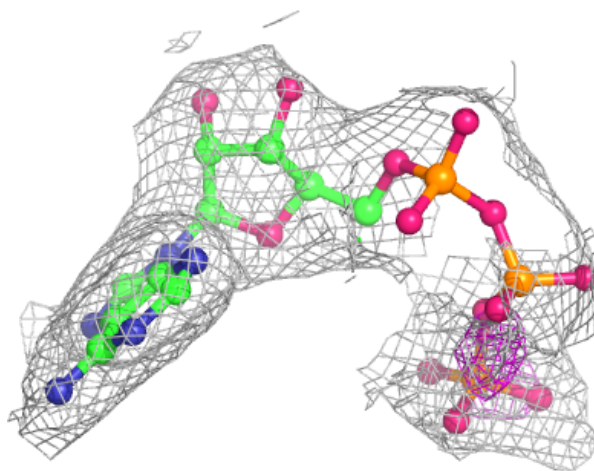
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

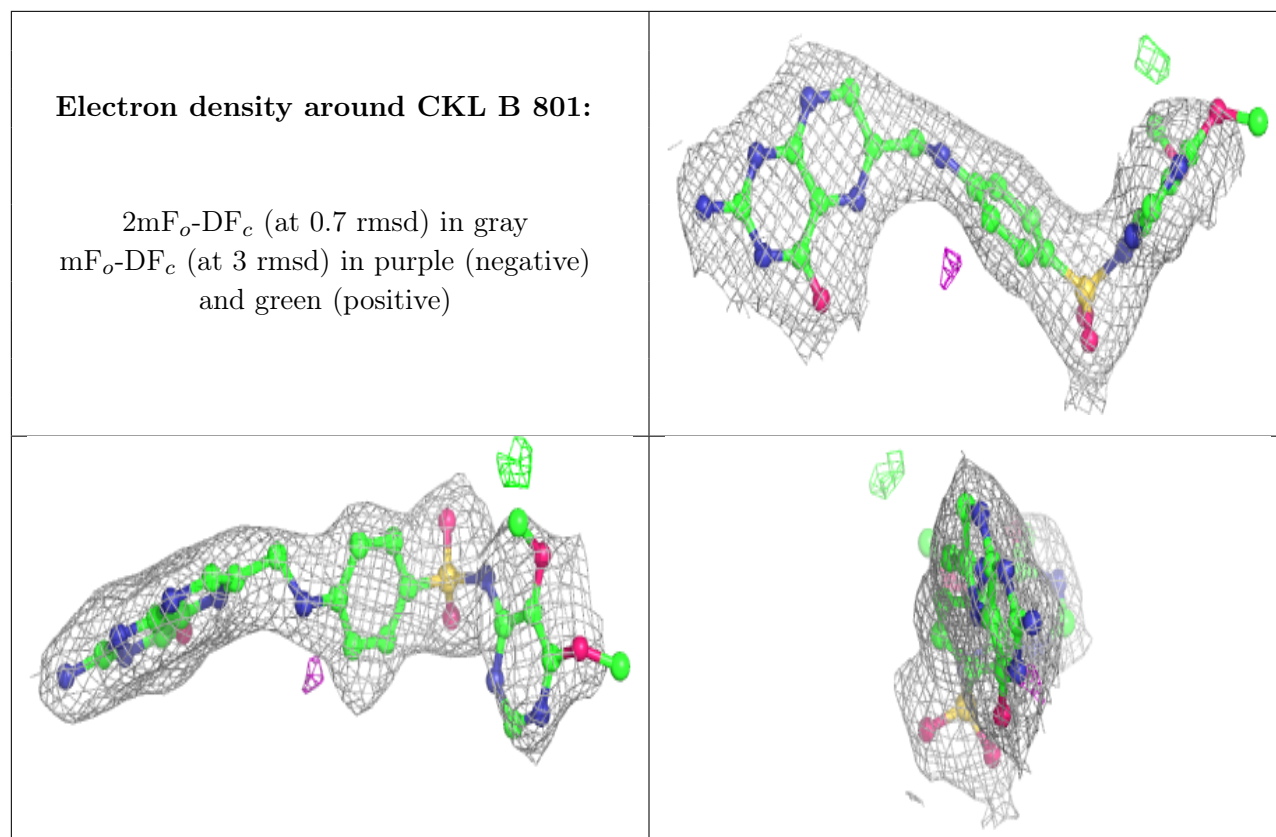




Electron density around ATP A 803:

$2mF_o-DF_c$ (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.