Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 10:08 AM EDT

PDB ID	:	2AJ4
Title	:	Crystal structure of Saccharomyces cerevisiae Galactokinase in complex with galactose and Mg:AMPPNP
Authors	:	Thoden, J.B.; Sellick, C.A.; Timson, D.J.; Reece, R.J.; Holden, H.M.
Deposited on	:	2005-08-01
Resolution	:	2.40 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:

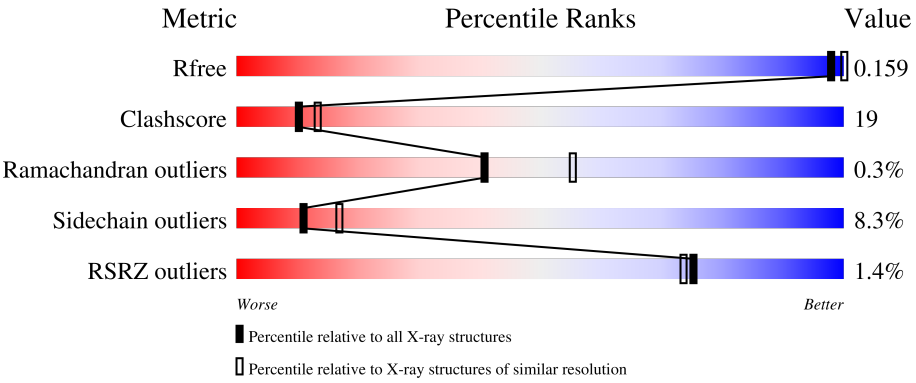
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

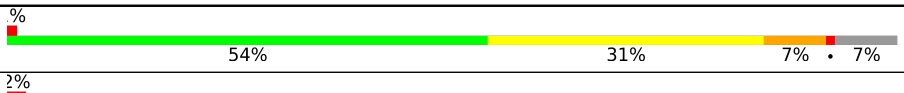
The reported resolution of this entry is 2.40 Å.

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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	548	
1	B	548	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8129 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 Galactokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			3938	2517	656	742	23			
1	B	505	Total	C	N	O	S	0	0	0
			3910	2498	652	737	23			

There are 42 discrepancies between the modelled and reference sequences:

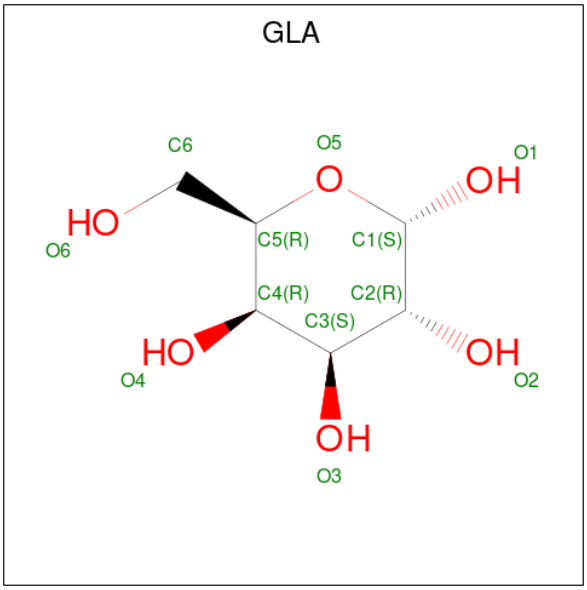
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	cloning artifact	UNP P04385
A	-18	GLY	-	cloning artifact	UNP P04385
A	-17	SER	-	cloning artifact	UNP P04385
A	-16	SER	-	cloning artifact	UNP P04385
A	-15	HIS	-	expression tag	UNP P04385
A	-14	HIS	-	expression tag	UNP P04385
A	-13	HIS	-	expression tag	UNP P04385
A	-12	HIS	-	expression tag	UNP P04385
A	-11	HIS	-	expression tag	UNP P04385
A	-10	HIS	-	expression tag	UNP P04385
A	-9	SER	-	cloning artifact	UNP P04385
A	-8	SER	-	cloning artifact	UNP P04385
A	-7	GLU	-	cloning artifact	UNP P04385
A	-6	ASN	-	cloning artifact	UNP P04385
A	-5	LEU	-	cloning artifact	UNP P04385
A	-4	TYR	-	cloning artifact	UNP P04385
A	-3	PHE	-	cloning artifact	UNP P04385
A	-2	GLN	-	cloning artifact	UNP P04385
A	-1	GLY	-	cloning artifact	UNP P04385
A	0	HIS	-	cloning artifact	UNP P04385
A	1	MET	-	cloning artifact	UNP P04385
B	-19	MET	-	cloning artifact	UNP P04385
B	-18	GLY	-	cloning artifact	UNP P04385
B	-17	SER	-	cloning artifact	UNP P04385
B	-16	SER	-	cloning artifact	UNP P04385

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP P04385
B	-14	HIS	-	expression tag	UNP P04385
B	-13	HIS	-	expression tag	UNP P04385
B	-12	HIS	-	expression tag	UNP P04385
B	-11	HIS	-	expression tag	UNP P04385
B	-10	HIS	-	expression tag	UNP P04385
B	-9	SER	-	cloning artifact	UNP P04385
B	-8	SER	-	cloning artifact	UNP P04385
B	-7	GLU	-	cloning artifact	UNP P04385
B	-6	ASN	-	cloning artifact	UNP P04385
B	-5	LEU	-	cloning artifact	UNP P04385
B	-4	TYR	-	cloning artifact	UNP P04385
B	-3	PHE	-	cloning artifact	UNP P04385
B	-2	GLN	-	cloning artifact	UNP P04385
B	-1	GLY	-	cloning artifact	UNP P04385
B	0	HIS	-	cloning artifact	UNP P04385
B	1	MET	-	cloning artifact	UNP P04385

- Molecule 2 is alpha-D-galactopyranose (three-letter code: GLA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0

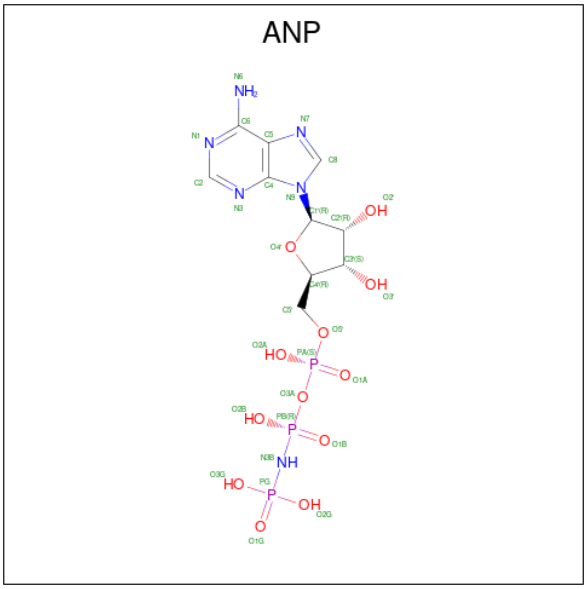
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 31 10 6 12 3	0	0
5	B	1	Total C N O P 31 10 6 12 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	106	Total O 106 106	0	0

Continued on next page...

Continued from previous page...

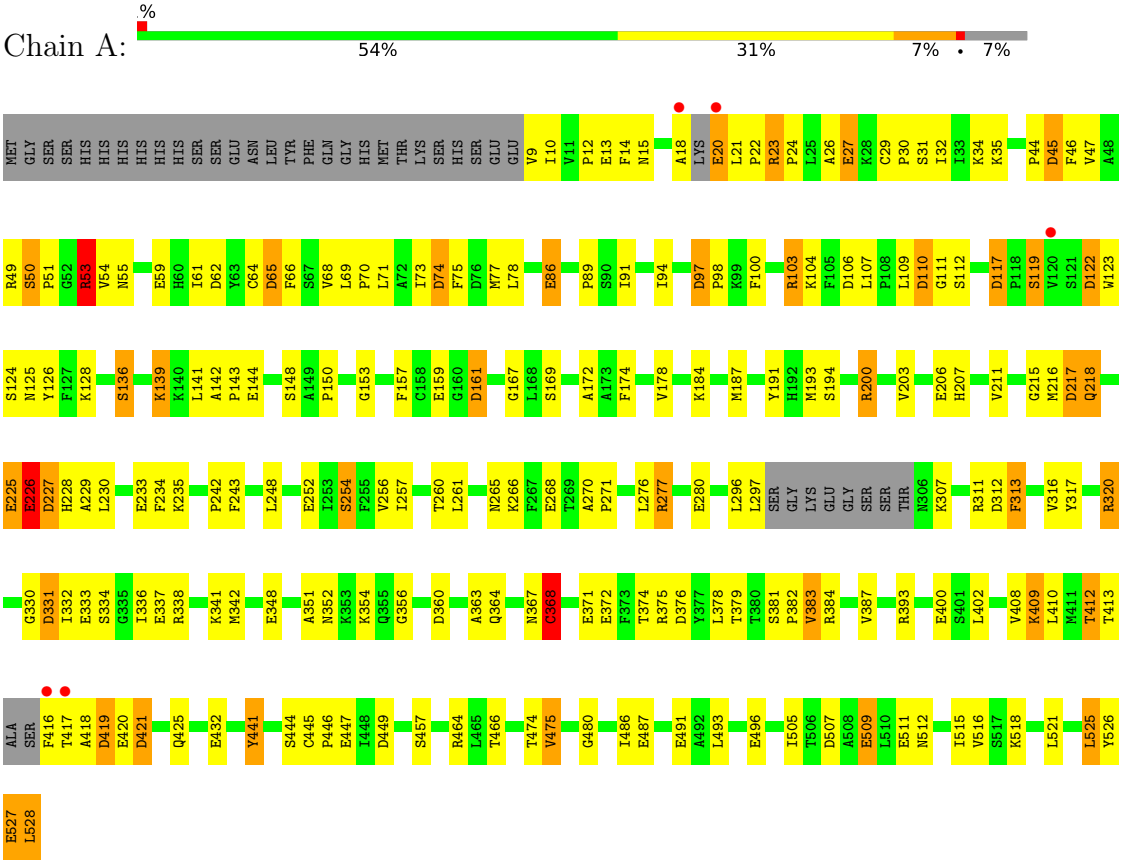
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	B	85	85	85	0	0

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.

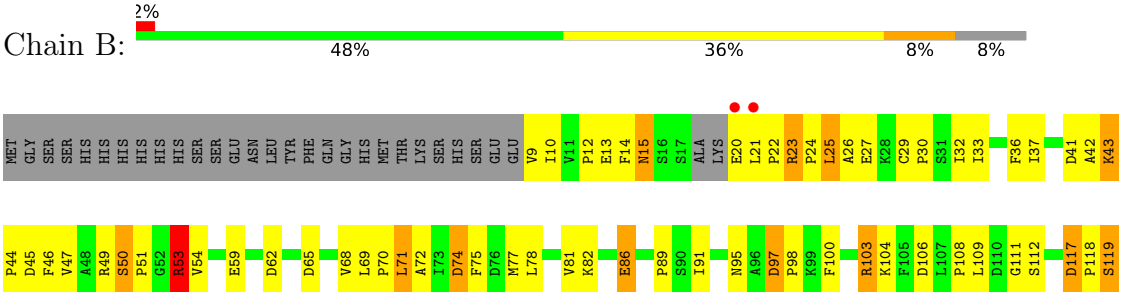
- Molecule 1: Galactokinase

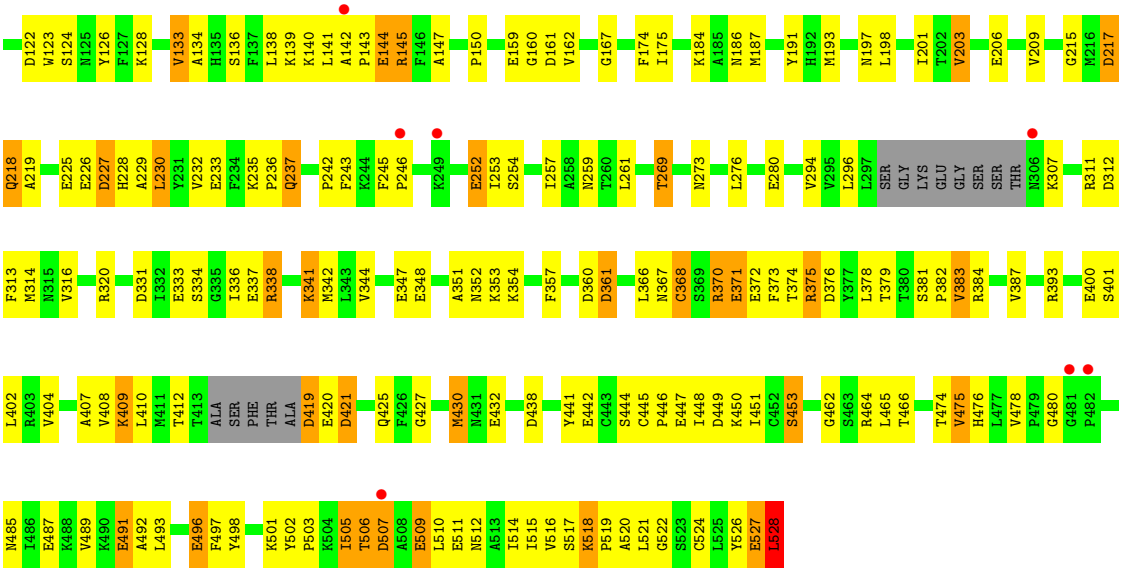
Chain A:



- Molecule 1: Galactokinase

Chain B:




D122 W123 S124 N125 Y126 F127 K128 V133 A134 H135 S136 F137 L138 K139 K140 L141 A142 P143 E144 R145 F146 A147 P150 E159 G160 D161 V162 G167 F174 I175 K184 A185 N186 M187 Y191 H192 M193 N197 L198 I201 T202 V203 E206 V209 G215 M216 D217
Q218 A219 E225 E226 D227 H228 A229 L230 Y231 V232 E233 F234 K235 P236 Q237 P242 F243 K244 F245 P246 K249 E252 I253 S254 I257 A258 N259 T260 L261 T269 N273 L276 E280 V294 V295 L296 L297 SER GLY LYS GLU GLY SER SER THR N306 K307 R311 D312
F313 M314 N315 V316 R320 D331 I332 E333 S334 G335 I336 E337 R338 K341 M342 L343 V344 E347 E348 A351 N352 K353 K354 F357 D360 D361 L366 N367 C368 S369 R370 E371 E372 F373 T374 R375 D376 Y377 L378 T379 T380 S381 P382 V383 R384 V387 R393 E400 S401
L402 R403 V404 A407 V408 K409 L410 M411 T412 T413 ALA SER PHE THR ALA D419 E420 D421 Q425 F426 G427 M430 N431 E432 D438 Y441 E442 G443 S444 C445 P446 E447 I448 D449 K450 I451 G452 S453 G462 S463 R464 L465 T466 T474 V475 H476 L477 V478 P479 G480 G481 P482
N485 I486 E487 K488 V489 K490 E491 A492 L493 E496 F497 Y498 K501 Y502 P503 K504 I505 T506 D507 A508 E509 L510 E511 N512 A513 I514 I515 V516 S517 K518 P519 A520 L521 G522 S523 C524 L525 Y526 E527 I528

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.30Å 85.00Å 112.30Å 90.00° 96.70° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.5 (30.00-2.40) 95.5 (29.48-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	0.75 (at 2.39Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.172 , 0.205 0.164 , 0.159	Depositor DCC
R_{free} test set	4490 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 103.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8129	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 6.44% 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: MG, CL, ANP, GLA

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	0.99	29/4022 (0.7%)	1.41	48/5451 (0.9%)
1	B	1.02	31/3993 (0.8%)	1.39	49/5411 (0.9%)
All	All	1.00	60/8015 (0.7%)	1.40	97/10862 (0.9%)

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	528	LEU	C-OXT	16.33	1.54	1.23
1	A	528	LEU	C-OXT	9.71	1.41	1.23
1	B	528	LEU	C-O	-8.77	1.06	1.23
1	A	333	GLU	CD-OE2	7.24	1.33	1.25
1	B	491	GLU	CD-OE2	7.23	1.33	1.25
1	A	144	GLU	CD-OE2	7.06	1.33	1.25
1	B	252	GLU	CD-OE2	6.85	1.33	1.25
1	A	20	GLU	CD-OE2	6.82	1.33	1.25
1	A	400	GLU	CD-OE2	6.71	1.33	1.25
1	A	159	GLU	CD-OE2	6.64	1.32	1.25
1	A	280	GLU	CD-OE2	6.57	1.32	1.25
1	A	527	GLU	CD-OE2	6.55	1.32	1.25
1	A	511	GLU	CD-OE2	6.53	1.32	1.25
1	B	206	GLU	CD-OE2	6.50	1.32	1.25
1	B	447	GLU	CD-OE2	6.47	1.32	1.25
1	A	27	GLU	CD-OE2	6.45	1.32	1.25
1	B	348	GLU	CD-OE2	6.45	1.32	1.25
1	A	372	GLU	CD-OE2	6.43	1.32	1.25
1	B	511	GLU	CD-OE2	6.43	1.32	1.25
1	B	337	GLU	CD-OE2	6.24	1.32	1.25
1	A	252	GLU	CD-OE2	6.23	1.32	1.25
1	A	13	GLU	CD-OE2	6.21	1.32	1.25
1	A	226	GLU	CD-OE2	6.20	1.32	1.25
1	B	159	GLU	CD-OE2	6.19	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	527	GLU	CD-OE2	6.19	1.32	1.25
1	B	400	GLU	CD-OE2	6.18	1.32	1.25
1	B	487	GLU	CD-OE2	6.17	1.32	1.25
1	B	333	GLU	CD-OE2	6.14	1.32	1.25
1	B	13	GLU	CD-OE2	6.12	1.32	1.25
1	B	20	GLU	CD-OE2	6.12	1.32	1.25
1	B	432	GLU	CD-OE2	6.12	1.32	1.25
1	A	206	GLU	CD-OE2	6.11	1.32	1.25
1	B	27	GLU	CD-OE2	6.08	1.32	1.25
1	A	432	GLU	CD-OE2	6.00	1.32	1.25
1	B	144	GLU	CD-OE2	5.90	1.32	1.25
1	A	348	GLU	CD-OE2	5.88	1.32	1.25
1	B	371	GLU	CD-OE2	5.88	1.32	1.25
1	A	233	GLU	CD-OE2	5.87	1.32	1.25
1	A	447	GLU	CD-OE2	5.85	1.32	1.25
1	A	420	GLU	CD-OE2	5.85	1.32	1.25
1	B	86	GLU	CD-OE2	5.84	1.32	1.25
1	A	225	GLU	CD-OE2	5.83	1.32	1.25
1	B	496	GLU	CD-OE2	5.82	1.32	1.25
1	B	420	GLU	CD-OE2	5.81	1.32	1.25
1	A	491	GLU	CD-OE2	5.78	1.32	1.25
1	B	225	GLU	CD-OE2	5.78	1.32	1.25
1	A	337	GLU	CD-OE2	5.78	1.32	1.25
1	B	226	GLU	CD-OE2	5.71	1.31	1.25
1	A	371	GLU	CD-OE2	5.69	1.31	1.25
1	B	528	LEU	CA-C	5.59	1.67	1.52
1	A	487	GLU	CD-OE2	5.56	1.31	1.25
1	A	86	GLU	CD-OE2	5.52	1.31	1.25
1	B	509	GLU	CD-OE2	5.39	1.31	1.25
1	B	372	GLU	CD-OE2	5.37	1.31	1.25
1	B	233	GLU	CD-OE2	5.30	1.31	1.25
1	A	496	GLU	CD-OE2	5.29	1.31	1.25
1	B	442	GLU	CD-OE2	5.14	1.31	1.25
1	A	268	GLU	CD-OE2	5.12	1.31	1.25
1	A	509	GLU	CD-OE2	5.03	1.31	1.25
1	B	280	GLU	CD-OE2	5.00	1.31	1.25

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	ARG	NE-CZ-NH1	14.32	127.46	120.30
1	A	528	LEU	CB-CA-C	-11.15	89.02	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	393	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	B	53	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	B	117	ASP	CB-CG-OD1	9.12	126.50	118.30
1	A	62	ASP	CB-CG-OD1	8.52	125.96	118.30
1	B	62	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	B	103	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	B	528	LEU	CA-C-O	8.43	137.80	120.10
1	A	122	ASP	CB-CG-OD2	-8.36	110.78	118.30
1	B	117	ASP	CB-CG-OD2	-8.33	110.80	118.30
1	B	161	ASP	CB-CG-OD2	-8.17	110.95	118.30
1	A	62	ASP	CB-CG-OD2	-8.05	111.05	118.30
1	B	528	LEU	CB-CA-C	-8.03	94.95	110.20
1	A	53	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	A	277	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	B	62	ASP	CB-CG-OD1	7.83	125.35	118.30
1	A	376	ASP	CB-CG-OD2	-7.82	111.26	118.30
1	B	122	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	B	161	ASP	CB-CG-OD1	7.54	125.08	118.30
1	B	65	ASP	CB-CG-OD1	7.33	124.90	118.30
1	A	103	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	393	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	B	65	ASP	CB-CG-OD2	-7.17	111.84	118.30
1	A	331	ASP	CB-CG-OD1	7.15	124.73	118.30
1	A	376	ASP	CB-CG-OD1	7.14	124.73	118.30
1	B	368	CYS	N-CA-CB	-7.10	97.82	110.60
1	A	122	ASP	CB-CG-OD1	6.87	124.48	118.30
1	B	97	ASP	CB-CG-OD1	6.86	124.47	118.30
1	B	122	ASP	CB-CG-OD1	6.85	124.46	118.30
1	B	312	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	B	376	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	A	117	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	B	421	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	A	313	PHE	CB-CG-CD1	6.55	125.38	120.80
1	A	419	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	B	421	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	97	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	B	106	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	A	421	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	A	227	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	B	438	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	B	227	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	A	106	ASP	CB-CG-OD2	-6.23	112.69	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	360	ASP	CB-CG-OD2	-6.23	112.70	118.30
1	A	384	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	368	CYS	N-CA-CB	-6.18	99.48	110.60
1	A	507	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	B	528	LEU	N-CA-CB	6.01	122.42	110.40
1	B	117	ASP	N-CA-CB	5.99	121.39	110.60
1	B	384	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	312	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	45	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	449	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	B	331	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	331	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	A	227	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	361	ASP	CB-CG-OD2	-5.79	113.08	118.30
1	A	117	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	161	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	B	97	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	B	45	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	B	106	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	320	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	449	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	217	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	320	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	103	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	B	419	ASP	CB-CG-OD1	5.55	123.30	118.30
1	B	419	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	512	ASN	CB-CA-C	5.48	121.37	110.40
1	A	528	LEU	N-CA-C	5.47	125.76	111.00
1	B	269	THR	CA-CB-CG2	-5.46	104.76	112.40
1	A	71	LEU	N-CA-CB	-5.44	99.52	110.40
1	A	507	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	419	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	311	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	277	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	B	74	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	B	507	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	B	449	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	A	217	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	B	449	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	393	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	B	311	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	376	ASP	CB-CG-OD1	5.17	122.96	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	110	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	515	ILE	CB-CA-C	-5.11	101.38	111.60
1	B	375	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	438	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	65	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	B	312	ASP	CB-CG-OD1	5.08	122.87	118.30
1	B	338	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	74	ASP	CB-CG-OD1	5.04	122.83	118.30
1	B	370	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	65	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	384	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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	3938	0	3924	130	0
1	B	3910	0	3898	166	0
2	A	12	0	12	1	0
2	B	12	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	31	0	13	2	0
5	B	31	0	13	3	0
6	A	106	0	0	2	0
6	B	85	0	0	1	0
All	All	8129	0	7872	297	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 19.

All (297) 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:203:VAL:HG22	1:B:215:GLY:HA3	1.42	0.98
1:B:218:GLN:HE21	1:B:218:GLN:H	1.11	0.95
1:A:218:GLN:NE2	1:A:218:GLN:H	1.67	0.93
1:B:218:GLN:H	1:B:218:GLN:NE2	1.66	0.92
1:B:505:ILE:HD13	1:B:510:LEU:HD12	1.53	0.89
1:B:353:LYS:NZ	1:B:361:ASP:HB3	1.89	0.88
1:A:218:GLN:H	1:A:218:GLN:HE21	1.13	0.88
1:A:480:GLY:HA2	1:A:486:ILE:HD12	1.60	0.82
1:B:353:LYS:HZ2	1:B:361:ASP:HB3	1.45	0.80
1:B:404:VAL:O	1:B:408:VAL:HG23	1.82	0.79
1:A:49:ARG:HB2	1:A:78:LEU:CD2	2.13	0.78
1:B:334:SER:O	1:B:338:ARG:HG3	1.84	0.77
1:B:245:PHE:HB3	1:B:246:PRO:HD2	1.66	0.77
1:A:21:LEU:HD22	1:A:22:PRO:HD2	1.67	0.75
1:B:506:THR:HG23	1:B:509:GLU:OE1	1.87	0.75
1:B:374:THR:O	1:B:379:THR:HG23	1.87	0.74
1:B:36:PHE:CZ	1:B:82:LYS:HB2	2.23	0.74
1:A:117:ASP:OD1	1:A:119:SER:HB3	1.88	0.73
1:B:29:CYS:O	1:B:33:ILE:HD12	1.88	0.73
1:A:412:THR:HG22	1:A:413:THR:HG23	1.70	0.72
1:B:445:CYS:HB2	1:B:446:PRO:HD2	1.71	0.71
1:B:193:MET:HE3	1:B:198:LEU:HD13	1.72	0.71
1:A:296:LEU:O	1:A:297:LEU:HD23	1.90	0.71
1:B:12:PRO:HB2	1:B:14:PHE:CE1	2.26	0.71
1:B:276:LEU:HD13	1:B:383:VAL:HG13	1.72	0.71
1:B:49:ARG:HG2	1:B:50:SER:N	2.05	0.71
1:B:43:LYS:O	1:B:82:LYS:HE3	1.91	0.70
1:B:49:ARG:HB2	1:B:78:LEU:CD2	2.20	0.70
1:A:332:ILE:HD11	1:A:408:VAL:HG11	1.72	0.70
1:A:23:ARG:HB3	1:A:24:PRO:HD3	1.72	0.69
1:B:505:ILE:HD13	1:B:510:LEU:CD1	2.21	0.69
1:B:108:PRO:HG2	1:B:112:SER:O	1.93	0.69
1:B:485:ASN:O	1:B:489:VAL:HG23	1.91	0.68
1:A:408:VAL:O	1:A:412:THR:HB	1.92	0.68
1:A:54:VAL:CG2	1:A:73:ILE:HG21	2.24	0.67
1:B:10:ILE:O	1:B:10:ILE:HD12	1.95	0.67
1:A:330:GLY:O	1:A:331:ASP:C	2.32	0.66
1:A:466:THR:HB	1:A:475:VAL:HG22	1.78	0.66
1:A:49:ARG:HB2	1:A:78:LEU:HD21	1.78	0.66
1:B:111:GLY:O	1:B:139:LYS:NZ	2.29	0.65
1:B:421:ASP:O	1:B:425:GLN:HG3	1.96	0.65
1:B:36:PHE:HZ	1:B:82:LYS:HB2	1.59	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ARG:NH2	1:B:167:GLY:O	2.30	0.65
1:B:502:TYR:O	1:B:505:ILE:HB	1.97	0.65
1:A:53:ARG:NH2	1:A:167:GLY:O	2.30	0.64
1:A:45:ASP:O	1:A:528:LEU:HB2	1.98	0.64
1:A:466:THR:HB	1:A:475:VAL:CG2	2.27	0.64
1:B:448:ILE:HD13	1:B:465:LEU:HB3	1.79	0.64
1:B:498:TYR:CE1	1:B:514:ILE:HD11	2.32	0.64
1:B:184:LYS:NZ	1:B:527:GLU:HG2	2.12	0.64
1:A:110:ASP:OD1	1:A:112:SER:N	2.30	0.64
1:A:21:LEU:CD2	1:A:22:PRO:HD2	2.28	0.63
1:A:184:LYS:NZ	1:A:191:TYR:O	2.31	0.63
1:A:187:MET:HB3	1:A:191:TYR:CB	2.27	0.63
1:B:126:TYR:CE2	5:B:532:ANP:H4'	2.34	0.63
1:B:22:PRO:O	1:B:25:LEU:HB2	1.99	0.62
1:B:493:LEU:O	1:B:497:PHE:N	2.30	0.62
1:B:498:TYR:HE1	1:B:514:ILE:HD11	1.65	0.62
1:A:336:ILE:HG23	1:A:402:LEU:HD11	1.82	0.62
1:B:197:ASN:O	1:B:201:ILE:HG12	1.98	0.62
1:B:86:GLU:OE1	1:B:89:PRO:HA	2.00	0.62
1:A:111:GLY:O	1:A:139:LYS:NZ	2.33	0.61
1:B:336:ILE:HG23	1:B:402:LEU:HD11	1.83	0.60
1:B:109:LEU:O	1:B:150:PRO:HD3	2.01	0.60
1:A:12:PRO:HB2	1:A:14:PHE:CE1	2.37	0.60
1:A:480:GLY:HA2	1:A:486:ILE:CD1	2.30	0.60
1:A:109:LEU:HA	1:A:150:PRO:HG3	1.82	0.59
1:B:29:CYS:C	1:B:33:ILE:HD12	2.23	0.59
1:B:51:PRO:HG3	1:B:521:LEU:O	2.02	0.59
1:B:341:LYS:O	1:B:344:VAL:HB	2.01	0.59
1:B:184:LYS:HZ3	1:B:527:GLU:HG2	1.65	0.59
1:A:31:SER:O	1:A:35:LYS:HG3	2.01	0.59
1:A:54:VAL:HG21	1:A:73:ILE:HG21	1.85	0.58
1:A:30:PRO:O	1:A:34:LYS:HG3	2.02	0.58
1:B:506:THR:O	1:B:509:GLU:HB2	2.04	0.58
1:A:218:GLN:HE21	1:A:218:GLN:N	1.95	0.57
1:B:501:LYS:C	1:B:503:PRO:HD3	2.24	0.57
1:B:466:THR:HB	1:B:475:VAL:HG22	1.86	0.57
1:B:526:TYR:CE2	1:B:528:LEU:HD23	2.39	0.57
1:B:218:GLN:HE21	1:B:218:GLN:N	1.94	0.56
1:A:44:PRO:HG2	1:A:528:LEU:HD12	1.87	0.56
1:A:332:ILE:HD11	1:A:408:VAL:CG1	2.36	0.56
1:A:44:PRO:HG2	1:A:528:LEU:CD1	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PHE:CD1	1:A:525:LEU:HD21	2.40	0.56
1:B:97:ASP:OD2	1:B:98:PRO:HD2	2.06	0.56
1:A:123:TRP:CE3	5:A:532:ANP:H2	2.41	0.56
1:B:218:GLN:NE2	1:B:218:GLN:N	2.47	0.56
1:B:314:MET:HA	1:B:342:MET:CE	2.36	0.55
1:B:53:ARG:NH1	1:B:217:ASP:OD1	2.38	0.55
1:B:140:LYS:O	1:B:143:PRO:HD3	2.06	0.55
1:B:126:TYR:HD1	1:B:175:ILE:HD11	1.71	0.55
1:A:410:LEU:HD22	1:A:416:PHE:CZ	2.42	0.55
1:B:123:TRP:CE3	5:B:532:ANP:H2	2.42	0.55
1:B:139:LYS:HE3	1:B:147:ALA:HA	1.89	0.55
1:A:77:MET:HG2	1:A:174:PHE:HA	1.89	0.55
1:A:338:ARG:O	1:A:341:LYS:HB3	2.07	0.55
1:A:51:PRO:HG3	1:A:521:LEU:O	2.06	0.55
1:A:122:ASP:O	1:A:125:ASN:HB2	2.07	0.55
1:B:59:GLU:HB2	1:B:464:ARG:NH2	2.22	0.55
1:A:49:ARG:HG2	1:A:50:SER:N	2.22	0.54
1:B:237:GLN:OE1	1:B:237:GLN:HA	2.07	0.54
1:A:54:VAL:HG23	1:A:73:ILE:HG21	1.87	0.54
1:B:68:VAL:HG23	1:B:232:VAL:HB	1.89	0.54
1:A:49:ARG:HB2	1:A:78:LEU:HD23	1.90	0.54
1:B:75:PHE:HB3	1:B:162:VAL:HG22	1.90	0.54
1:B:371:GLU:O	1:B:375:ARG:HG3	2.07	0.54
1:B:9:VAL:HG12	1:B:10:ILE:N	2.23	0.54
1:A:412:THR:CG2	1:A:413:THR:HG23	2.37	0.53
1:B:141:LEU:C	1:B:143:PRO:HD3	2.29	0.53
1:A:29:CYS:HB2	1:A:30:PRO:HD3	1.88	0.53
1:B:117:ASP:OD1	1:B:119:SER:N	2.33	0.53
1:B:68:VAL:C	1:B:70:PRO:HD3	2.29	0.53
1:B:91:ILE:O	1:B:104:LYS:HA	2.07	0.53
1:A:97:ASP:OD2	1:A:98:PRO:HD2	2.09	0.53
1:B:23:ARG:O	1:B:24:PRO:C	2.46	0.53
1:B:276:LEU:HD13	1:B:383:VAL:CG1	2.38	0.53
1:B:444:SER:HB3	6:B:570:HOH:O	2.08	0.53
1:A:69:LEU:HD12	1:A:230:LEU:O	2.09	0.52
1:B:44:PRO:O	1:B:528:LEU:HD12	2.08	0.52
1:B:54:VAL:HG21	1:B:257:ILE:CD1	2.40	0.52
1:B:466:THR:HB	1:B:475:VAL:CG2	2.38	0.52
1:A:234:PHE:O	1:A:235:LYS:HG2	2.08	0.52
1:B:12:PRO:O	1:B:524:CYS:HB2	2.09	0.52
1:B:95:ASN:HB2	1:B:123:TRP:CH2	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:TYR:HE2	1:B:528:LEU:CD2	2.23	0.52
1:A:18:ALA:O	1:A:20:GLU:N	2.43	0.51
1:A:54:VAL:HG23	1:A:73:ILE:CG2	2.41	0.51
1:A:203:VAL:HB	1:A:215:GLY:HA3	1.92	0.51
1:B:313:PHE:CD2	1:B:342:MET:HE3	2.46	0.51
1:B:526:TYR:HE2	1:B:528:LEU:HD23	1.76	0.51
1:A:86:GLU:OE1	1:A:89:PRO:HA	2.11	0.51
1:A:351:ALA:O	1:A:354:LYS:HG3	2.11	0.51
1:B:259:ASN:OD1	1:B:261:LEU:N	2.30	0.51
1:A:277:ARG:HD2	1:A:441:TYR:CE2	2.47	0.50
1:A:229:ALA:O	1:A:242:PRO:HA	2.12	0.50
1:A:86:GLU:OE1	1:A:153:GLY:HA3	2.11	0.50
1:A:254:SER:OG	1:A:480:GLY:HA3	2.11	0.50
1:A:29:CYS:N	1:A:30:PRO:HD2	2.26	0.50
1:B:54:VAL:HG21	1:B:257:ILE:HD11	1.94	0.50
1:A:200:ARG:HG2	1:A:200:ARG:HH11	1.77	0.50
1:A:410:LEU:HD22	1:A:416:PHE:HZ	1.76	0.50
1:B:29:CYS:N	1:B:30:PRO:HD2	2.27	0.50
1:A:356:GLY:HA3	1:A:387:VAL:HG21	1.94	0.50
1:B:353:LYS:HZ3	1:B:361:ASP:HB3	1.75	0.50
1:A:91:ILE:HD12	1:A:107:LEU:HD21	1.94	0.49
1:A:124:SER:O	1:A:128:LYS:HG3	2.12	0.49
1:B:72:ALA:HB3	1:B:520:ALA:O	2.12	0.49
1:A:61:ILE:HB	1:A:66:PHE:HB2	1.94	0.49
1:A:69:LEU:N	1:A:70:PRO:HD3	2.26	0.49
1:B:81:VAL:HG12	1:B:82:LYS:N	2.27	0.49
1:B:294:VAL:HB	1:B:316:VAL:HG11	1.95	0.49
1:B:44:PRO:HG2	1:B:528:LEU:HD11	1.95	0.49
1:B:124:SER:O	1:B:128:LYS:HG3	2.12	0.49
1:B:187:MET:HB3	1:B:191:TYR:HB2	1.94	0.49
1:B:410:LEU:HA	1:B:410:LEU:HD23	1.60	0.49
1:A:363:ALA:HB1	1:A:368:CYS:HB3	1.94	0.48
1:B:100:PHE:HB3	1:B:123:TRP:CE2	2.48	0.48
1:B:526:TYR:CE2	1:B:528:LEU:CD2	2.97	0.48
1:A:374:THR:HG23	1:A:378:LEU:HB2	1.95	0.48
1:B:193:MET:CE	1:B:198:LEU:HD13	2.43	0.48
1:A:313:PHE:CD2	1:A:342:MET:HE1	2.49	0.48
1:A:417:THR:HG22	1:A:418:ALA:N	2.28	0.48
1:A:64:CYS:O	1:A:65:ASP:HB2	2.12	0.48
1:A:276:LEU:HA	1:A:383:VAL:HG21	1.95	0.48
1:B:245:PHE:HB3	1:B:253:ILE:CD1	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:SER:HB3	6:A:635:HOH:O	2.14	0.48
1:A:445:CYS:HB2	1:A:446:PRO:CD	2.44	0.47
1:B:23:ARG:HB3	1:B:24:PRO:HD3	1.96	0.47
1:A:59:GLU:HB2	1:A:464:ARG:NH2	2.29	0.47
1:B:445:CYS:HB2	1:B:446:PRO:CD	2.40	0.47
1:A:248:LEU:HB3	1:A:419:ASP:CG	2.34	0.47
1:B:47:VAL:HB	1:B:526:TYR:HB3	1.96	0.47
1:B:49:ARG:HB2	1:B:78:LEU:HD23	1.95	0.47
1:A:444:SER:OG	1:A:445:CYS:N	2.47	0.47
1:B:70:PRO:HD2	1:B:230:LEU:O	2.15	0.47
1:A:23:ARG:HB3	1:A:24:PRO:CD	2.41	0.47
1:A:109:LEU:O	1:A:150:PRO:HD3	2.15	0.47
1:A:296:LEU:HA	1:A:296:LEU:HD23	1.55	0.47
1:B:235:LYS:HA	1:B:236:PRO:C	2.35	0.47
1:B:462:GLY:O	1:B:476:HIS:HA	2.14	0.47
1:B:515:ILE:HG22	1:B:516:VAL:N	2.30	0.47
1:B:77:MET:HG2	1:B:174:PHE:HA	1.95	0.47
1:B:142:ALA:HB1	1:B:145:ARG:HB2	1.96	0.47
1:A:55:ASN:HA	1:A:70:PRO:HA	1.97	0.47
1:B:229:ALA:HB3	1:B:243:PHE:CZ	2.50	0.47
1:A:218:GLN:NE2	1:A:218:GLN:N	2.49	0.46
1:A:505:ILE:HA	1:A:509:GLU:OE1	2.14	0.46
1:A:23:ARG:O	1:A:26:ALA:HB3	2.16	0.46
1:A:29:CYS:O	1:A:32:ILE:HG22	2.15	0.46
1:A:332:ILE:HG21	1:A:409:LYS:HD2	1.97	0.46
1:A:381:SER:HA	1:A:382:PRO:HD3	1.70	0.46
1:B:252:GLU:HB2	1:B:480:GLY:C	2.36	0.46
1:B:109:LEU:HA	1:B:150:PRO:HG3	1.97	0.46
1:B:228:HIS:O	1:B:519:PRO:HB3	2.16	0.46
1:B:296:LEU:HD23	1:B:296:LEU:HA	1.76	0.46
1:A:226:GLU:O	1:A:227:ASP:HB2	2.14	0.46
1:B:69:LEU:N	1:B:70:PRO:HD3	2.31	0.46
1:B:228:HIS:H	1:B:519:PRO:HB2	1.81	0.46
1:A:23:ARG:HG2	1:A:27:GLU:OE2	2.16	0.45
1:A:142:ALA:N	1:A:143:PRO:HD3	2.31	0.45
1:A:316:VAL:O	1:A:317:TYR:C	2.55	0.45
1:B:351:ALA:O	1:B:354:LYS:HG3	2.16	0.45
1:A:187:MET:HB3	1:A:191:TYR:HB2	1.98	0.45
1:A:256:VAL:HG22	1:A:516:VAL:HG22	1.96	0.45
1:B:313:PHE:CD2	1:B:342:MET:CE	3.00	0.45
1:B:506:THR:N	1:B:509:GLU:OE1	2.43	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:ILE:CG2	1:B:516:VAL:N	2.80	0.45
1:A:29:CYS:N	1:A:30:PRO:CD	2.80	0.45
1:A:229:ALA:HB3	1:A:243:PHE:CZ	2.52	0.45
1:A:270:ALA:N	1:A:271:PRO:CD	2.80	0.45
1:A:313:PHE:CD2	1:A:342:MET:CE	3.00	0.45
1:B:307:LYS:HD2	1:B:307:LYS:HA	1.65	0.45
1:A:260:THR:O	1:A:261:LEU:HB2	2.17	0.45
1:A:271:PRO:O	1:A:383:VAL:HG22	2.16	0.45
1:B:254:SER:HB2	1:B:478:VAL:O	2.17	0.45
1:A:75:PHE:HD2	1:A:161:ASP:O	2.00	0.44
1:B:77:MET:HA	1:B:160:GLY:HA2	1.99	0.44
1:B:37:ILE:O	1:B:41:ASP:N	2.43	0.44
1:B:141:LEU:O	1:B:143:PRO:HD3	2.18	0.44
1:B:252:GLU:HB2	1:B:480:GLY:O	2.18	0.44
1:A:53:ARG:NH1	1:A:217:ASP:OD1	2.48	0.44
1:A:126:TYR:CE2	5:A:532:ANP:H4'	2.52	0.44
1:B:15:ASN:HD22	1:B:15:ASN:HA	1.53	0.44
1:B:41:ASP:O	1:B:42:ALA:HB2	2.16	0.44
1:B:138:LEU:HD11	1:B:186:ASN:HB2	2.00	0.44
1:B:21:LEU:HD23	1:B:26:ALA:HA	2.00	0.44
1:B:44:PRO:HG2	1:B:528:LEU:CD1	2.48	0.44
1:B:117:ASP:OD1	1:B:118:PRO:N	2.50	0.44
1:A:225:GLU:O	1:A:228:HIS:HB2	2.18	0.44
1:B:518:LYS:O	1:B:519:PRO:C	2.55	0.44
1:A:313:PHE:HD2	1:A:342:MET:CE	2.32	0.43
1:B:184:LYS:NZ	1:B:527:GLU:CG	2.80	0.43
1:B:43:LYS:O	1:B:82:LYS:HG3	2.18	0.43
1:B:269:THR:O	1:B:273:ASN:N	2.46	0.43
1:B:9:VAL:CG1	1:B:10:ILE:N	2.81	0.43
1:A:207:HIS:HD2	1:A:211:VAL:O	2.02	0.43
1:B:46:PHE:CB	1:B:184:LYS:HZ2	2.31	0.43
1:B:227:ASP:HA	1:B:519:PRO:HG2	1.99	0.43
1:B:229:ALA:O	1:B:242:PRO:HA	2.18	0.43
1:B:512:ASN:O	1:B:515:ILE:HD11	2.18	0.43
1:B:23:ARG:O	1:B:26:ALA:N	2.52	0.43
1:B:133:VAL:HG12	1:B:134:ALA:N	2.34	0.43
1:B:54:VAL:O	1:B:71:LEU:N	2.50	0.43
1:B:75:PHE:CB	1:B:162:VAL:HG22	2.49	0.43
1:A:265:ASN:HB2	6:A:563:HOH:O	2.19	0.42
1:B:492:ALA:O	1:B:496:GLU:HB2	2.20	0.42
1:A:418:ALA:O	1:A:421:ASP:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:LEU:HB2	1:B:368:CYS:HB2	2.02	0.42
1:B:408:VAL:O	1:B:409:LYS:C	2.58	0.42
1:A:276:LEU:HD13	1:A:383:VAL:HG13	2.02	0.42
1:A:320:ARG:O	1:A:320:ARG:HG3	2.19	0.42
1:A:505:ILE:HG13	1:A:509:GLU:OE1	2.19	0.42
1:B:53:ARG:HH11	1:B:217:ASP:CG	2.21	0.42
1:B:69:LEU:HD12	1:B:230:LEU:O	2.19	0.42
1:B:50:SER:HA	1:B:51:PRO:HD3	1.90	0.42
1:A:257:ILE:HA	1:A:474:THR:O	2.20	0.41
5:B:532:ANP:O1A	5:B:532:ANP:O3G	2.37	0.41
1:A:10:ILE:HA	1:A:194:SER:HA	2.01	0.41
1:A:59:GLU:HB2	1:A:464:ARG:HH22	1.83	0.41
1:B:314:MET:HA	1:B:342:MET:HE1	2.01	0.41
1:B:450:LYS:O	1:B:451:ILE:C	2.56	0.41
1:B:493:LEU:HD23	1:B:493:LEU:HA	1.88	0.41
1:A:47:VAL:HB	1:A:526:TYR:HB3	2.02	0.41
1:B:374:THR:O	1:B:375:ARG:C	2.57	0.41
1:B:381:SER:HA	1:B:382:PRO:HD3	1.85	0.41
1:A:410:LEU:HD11	1:A:425:GLN:HB3	2.02	0.41
1:B:521:LEU:HG	1:B:522:GLY:N	2.34	0.41
1:A:21:LEU:HD23	1:A:21:LEU:HA	1.68	0.41
1:A:266:LYS:HE3	2:A:529:GLA:O2	2.20	0.41
1:A:374:THR:O	1:A:379:THR:HG23	2.21	0.41
1:B:117:ASP:HA	1:B:118:PRO:HD2	1.90	0.41
1:A:94:ILE:HG22	1:A:157:PHE:CE1	2.55	0.41
1:A:141:LEU:HD12	1:A:141:LEU:HA	1.79	0.41
1:A:215:GLY:O	1:A:216:MET:C	2.58	0.41
1:A:68:VAL:C	1:A:70:PRO:HD3	2.41	0.41
1:A:174:PHE:O	1:A:178:VAL:HG23	2.21	0.41
1:A:141:LEU:C	1:A:143:PRO:HD3	2.41	0.41
1:A:493:LEU:HD23	1:A:493:LEU:HA	1.85	0.41
1:B:245:PHE:HB3	1:B:253:ILE:HD13	2.03	0.41
1:B:404:VAL:O	1:B:407:ALA:HB3	2.20	0.41
1:B:408:VAL:HG23	1:B:408:VAL:H	1.56	0.41
1:B:491:GLU:O	1:B:492:ALA:C	2.60	0.41
1:A:169:SER:OG	1:A:172:ALA:HB3	2.22	0.41
1:B:126:TYR:CD1	1:B:175:ILE:HD11	2.53	0.40
1:B:218:GLN:O	1:B:219:ALA:C	2.58	0.40
1:B:373:PHE:CE2	1:B:378:LEU:HD21	2.55	0.40
1:A:141:LEU:HG	1:A:187:MET:HE1	2.03	0.40
1:B:187:MET:HB3	1:B:191:TYR:CB	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:ASP:OD1	1:B:370:ARG:HD2	2.21	0.40
1:B:257:ILE:HG23	1:B:474:THR:O	2.21	0.40
1:A:14:PHE:HB3	1:A:21:LEU:HD21	2.03	0.40
1:A:331:ASP:HB3	1:A:334:SER:HG	1.85	0.40
1:B:10:ILE:HD12	1:B:10:ILE:C	2.41	0.40
1:B:245:PHE:HB3	1:B:246:PRO:CD	2.45	0.40
1:A:97:ASP:HB3	1:A:100:PHE:HD1	1.87	0.40
1:B:276:LEU:CD1	1:B:383:VAL:CG1	2.99	0.40
1:B:427:GLY:HA2	1:B:430:MET:HG3	2.02	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	501/548 (91%)	483 (96%)	17 (3%)	1 (0%)	47	62
1	B	497/548 (91%)	460 (93%)	35 (7%)	2 (0%)	34	48
All	All	998/1096 (91%)	943 (94%)	52 (5%)	3 (0%)	41	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	ASP
1	B	23	ARG
1	B	453	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	433/467 (93%)	401 (93%)	32 (7%)	13 22
1	B	431/467 (92%)	391 (91%)	40 (9%)	9 13
All	All	864/934 (92%)	792 (92%)	72 (8%)	11 17

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	15	ASN
1	A	23	ARG
1	A	50	SER
1	A	53	ARG
1	A	74	ASP
1	A	103	ARG
1	A	104	LYS
1	A	119	SER
1	A	136	SER
1	A	139	LYS
1	A	148	SER
1	A	193	MET
1	A	200	ARG
1	A	218	GLN
1	A	226	GLU
1	A	254	SER
1	A	307	LYS
1	A	352	ASN
1	A	364	GLN
1	A	367	ASN
1	A	368	CYS
1	A	375	ARG
1	A	383	VAL
1	A	409	LYS
1	A	412	THR
1	A	441	TYR
1	A	457	SER
1	A	475	VAL
1	A	518	LYS
1	A	525	LEU
1	A	527	GLU
1	B	15	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	25	LEU
1	B	32	ILE
1	B	43	LYS
1	B	50	SER
1	B	53	ARG
1	B	71	LEU
1	B	74	ASP
1	B	103	ARG
1	B	119	SER
1	B	133	VAL
1	B	136	SER
1	B	144	GLU
1	B	145	ARG
1	B	203	VAL
1	B	209	VAL
1	B	218	GLN
1	B	230	LEU
1	B	237	GLN
1	B	341	LYS
1	B	347	GLU
1	B	352	ASN
1	B	357	PHE
1	B	367	ASN
1	B	383	VAL
1	B	387	VAL
1	B	401	SER
1	B	409	LYS
1	B	412	THR
1	B	419	ASP
1	B	430	MET
1	B	441	TYR
1	B	453	SER
1	B	475	VAL
1	B	505	ILE
1	B	506	THR
1	B	507	ASP
1	B	517	SER
1	B	518	LYS
1	B	528	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	155	GLN
1	A	218	GLN
1	A	251	HIS
1	A	273	ASN
1	A	364	GLN
1	B	15	ASN
1	B	102	GLN
1	B	155	GLN
1	B	192	HIS
1	B	197	ASN
1	B	218	GLN
1	B	273	ASN
1	B	364	GLN
1	B	425	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)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\|>2$
5	ANP	A	532	3	29,33,33	1.34	4 (13%)	31,52,52	1.73	6 (19%)
2	GLA	A	529	-	12,12,12	0.70	0	17,17,17	1.27	1 (5%)
2	GLA	B	529	-	12,12,12	0.61	0	17,17,17	0.92	1 (5%)
5	ANP	B	532	3	29,33,33	1.48	5 (17%)	31,52,52	1.84	8 (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
5	ANP	A	532	3	-	4/14/38/38	0/3/3/3
2	GLA	A	529	-	-	1/2/22/22	0/1/1/1
2	GLA	B	529	-	-	1/2/22/22	0/1/1/1
5	ANP	B	532	3	-	3/14/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	532	ANP	PB-O1B	3.93	1.52	1.46
5	A	532	ANP	PB-O1B	3.52	1.51	1.46
5	A	532	ANP	PG-O1G	3.15	1.51	1.46
5	B	532	ANP	PG-O1G	2.69	1.50	1.46
5	A	532	ANP	C6-N6	-2.59	1.24	1.34
5	B	532	ANP	C6-N6	-2.54	1.24	1.34
5	B	532	ANP	PG-O2G	-2.45	1.50	1.56
5	A	532	ANP	C2-N1	2.36	1.38	1.33
5	B	532	ANP	C2-N1	2.02	1.37	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	532	ANP	C5-C6-N6	5.59	128.85	120.35
5	A	532	ANP	C5-C6-N6	4.23	126.77	120.35
5	A	532	ANP	O1B-PB-N3B	-3.67	106.37	111.77
5	B	532	ANP	C2-N1-C6	3.60	124.92	118.75
5	A	532	ANP	C2-N1-C6	3.47	124.70	118.75
5	B	532	ANP	N3-C2-N1	-3.41	123.35	128.68
5	A	532	ANP	C5-C6-N1	-3.31	112.84	120.35
5	A	532	ANP	N3-C2-N1	-3.27	123.57	128.68
2	A	529	GLA	O4-C4-C3	3.17	117.67	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	532	ANP	C5-C6-N1	-3.10	113.33	120.35
5	A	532	ANP	O1G-PG-N3B	-2.85	107.58	111.77
5	B	532	ANP	O1G-PG-N3B	-2.54	108.03	111.77
2	B	529	GLA	O4-C4-C3	2.44	115.98	110.35
5	B	532	ANP	O3'-C3'-C2'	2.25	119.10	111.82
5	B	532	ANP	O2G-PG-O1G	-2.17	107.99	113.45
5	B	532	ANP	PA-O5'-C5'	-2.15	109.08	121.68

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	532	ANP	PB-N3B-PG-O1G
5	A	532	ANP	PG-N3B-PB-O1B
5	A	532	ANP	PA-O3A-PB-O1B
5	B	532	ANP	PB-N3B-PG-O1G
5	B	532	ANP	PG-N3B-PB-O1B
5	B	532	ANP	PA-O3A-PB-O1B
2	A	529	GLA	O5-C5-C6-O6
2	B	529	GLA	O5-C5-C6-O6
5	A	532	ANP	C4'-C5'-O5'-PA

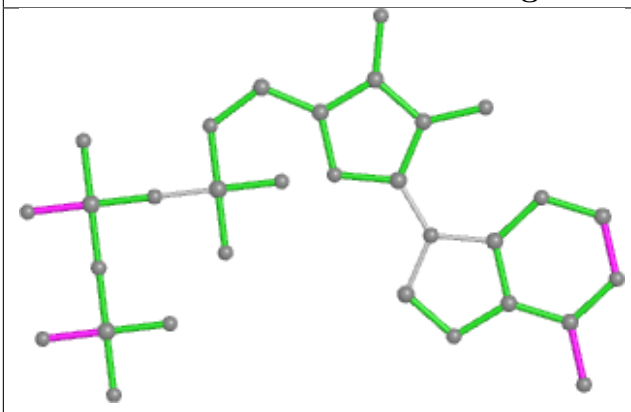
There are no ring outliers.

3 monomers are involved in 6 short contacts:

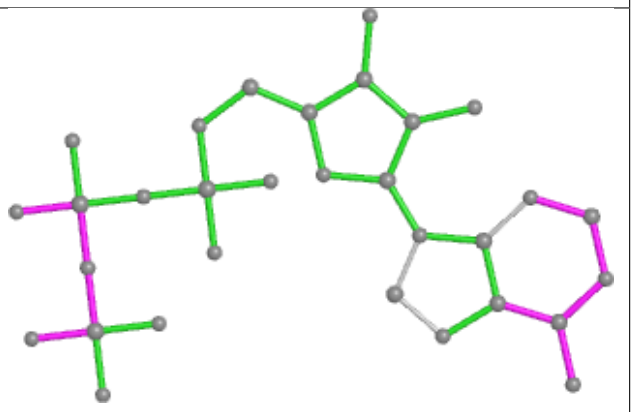
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	532	ANP	2	0
2	A	529	GLA	1	0
5	B	532	ANP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

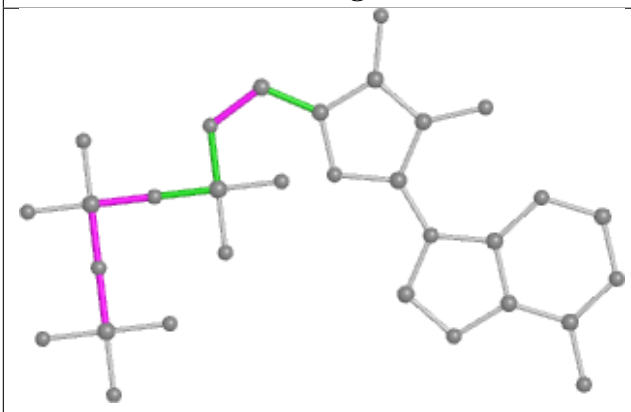
Ligand ANP A 532



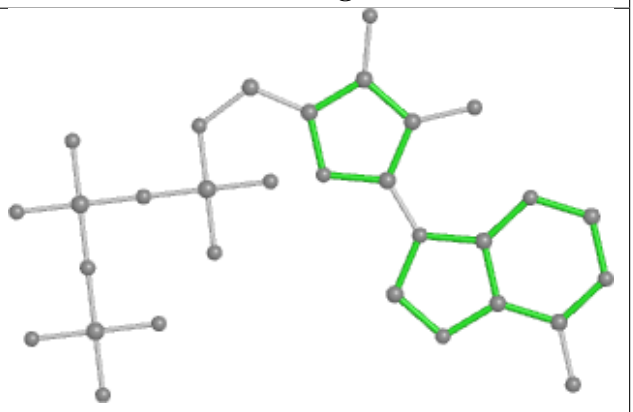
Bond lengths



Bond angles

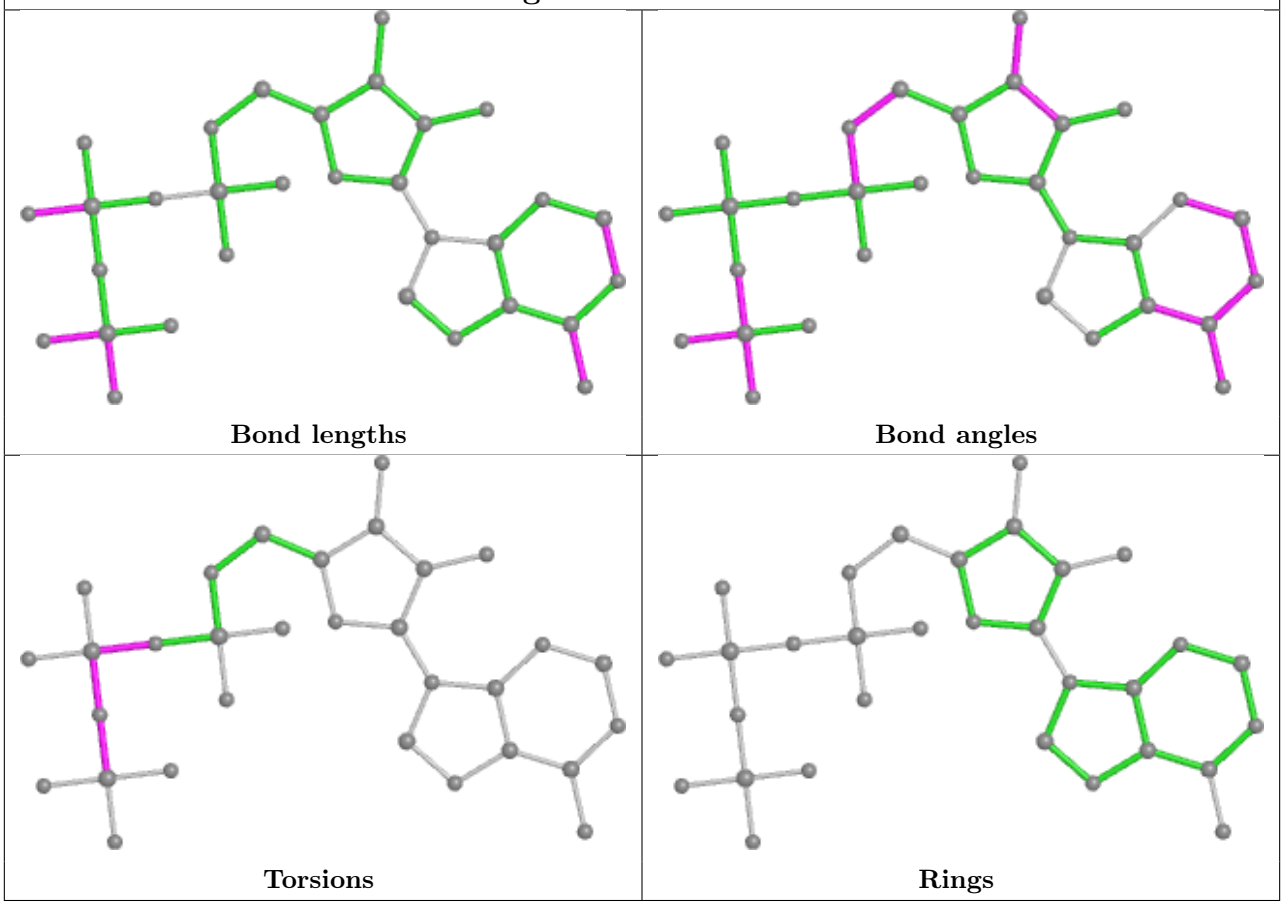


Torsions



Rings

Ligand ANP B 532



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, 95^{th} 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	509/548 (92%)	-0.63	5 (0%)	82	80	12, 28, 67, 96	0
1	B	505/548 (92%)	-0.31	9 (1%)	68	66	13, 39, 85, 98	0
All	All	1014/1096 (92%)	-0.47	14 (1%)	75	73	12, 33, 80, 98	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	ALA	3.5
1	A	120	VAL	3.4
1	B	249	LYS	3.2
1	B	142	ALA	2.9
1	B	306	ASN	2.7
1	A	416	PHE	2.7
1	A	20	GLU	2.7
1	B	482	PRO	2.6
1	A	417	THR	2.5
1	B	20	GLU	2.5
1	B	481	GLY	2.5
1	B	246	PRO	2.4
1	B	507	ASP	2.4
1	B	21	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

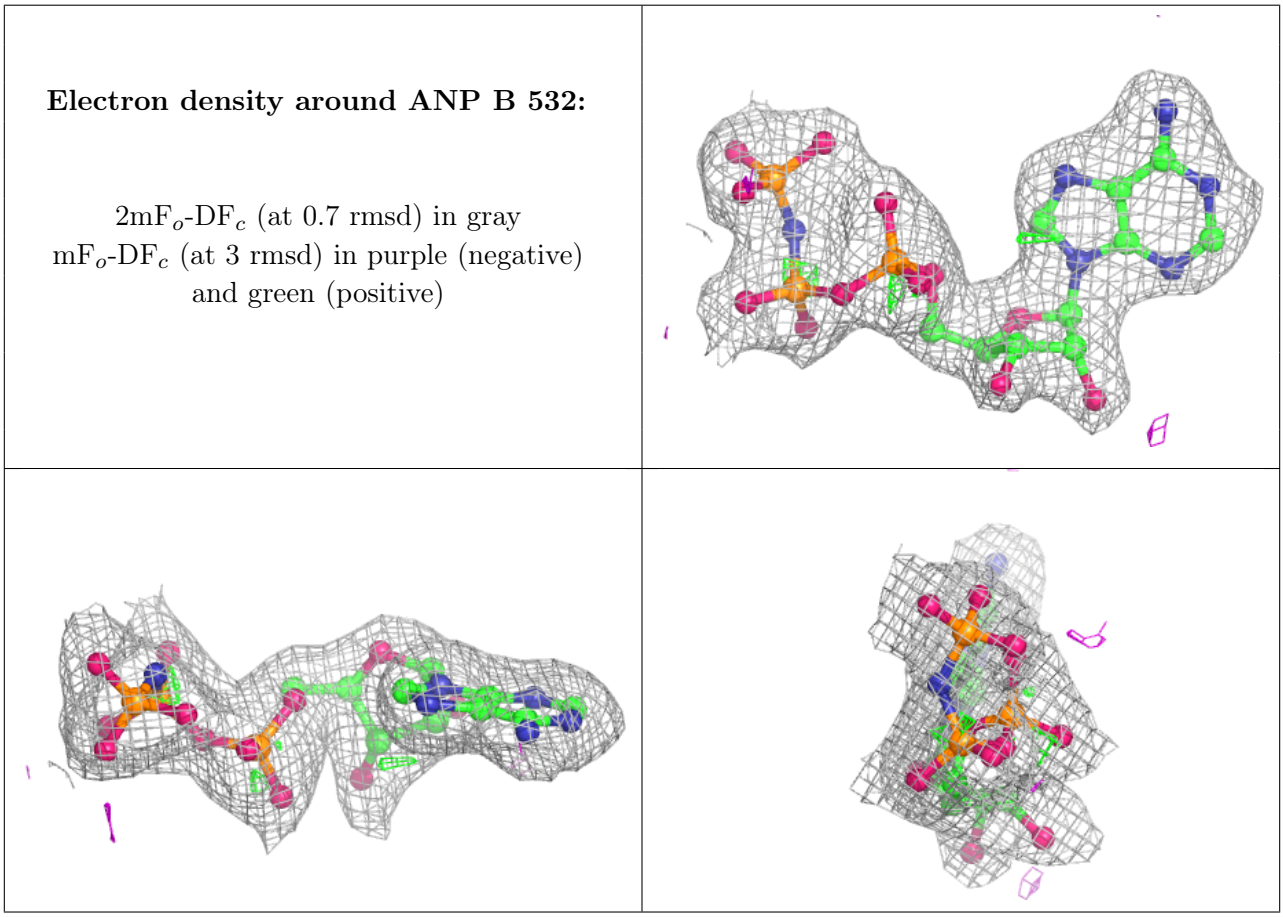
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	MG	B	530	1/1	0.91	0.22	44,44,44,44	0
3	MG	A	530	1/1	0.93	0.22	34,34,34,34	0
4	CL	A	531	1/1	0.97	0.06	33,33,33,33	0
4	CL	B	531	1/1	0.97	0.08	48,48,48,48	0
2	GLA	A	529	12/12	0.98	0.15	5,14,22,27	0
2	GLA	B	529	12/12	0.98	0.15	11,17,30,33	0
5	ANP	B	532	31/31	0.98	0.10	9,28,51,95	0
5	ANP	A	532	31/31	0.99	0.11	10,22,36,51	0

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

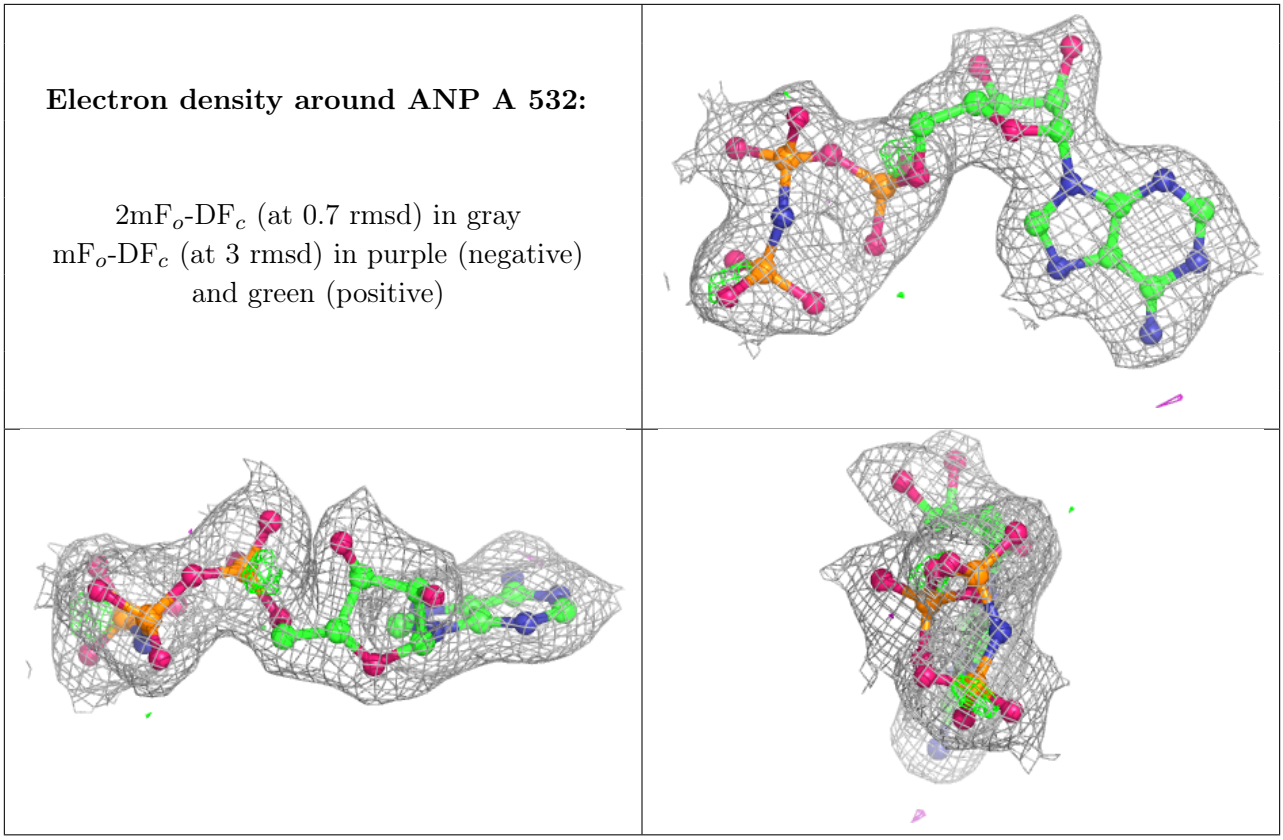
Electron density around ANP B 532:

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



Electron density around ANP A 532:

$2mF_o$-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.