



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:56 PM UTC

PDB ID : 2AJ4 / pdb_00002aj4
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

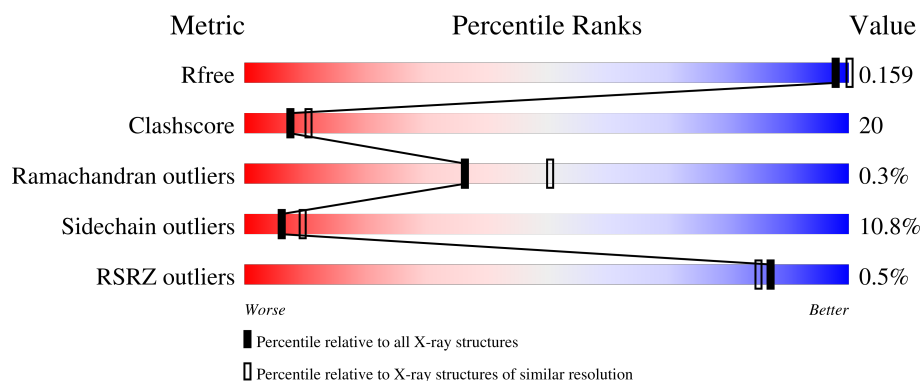
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	548	
1	B	548	

2 Entry composition

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:

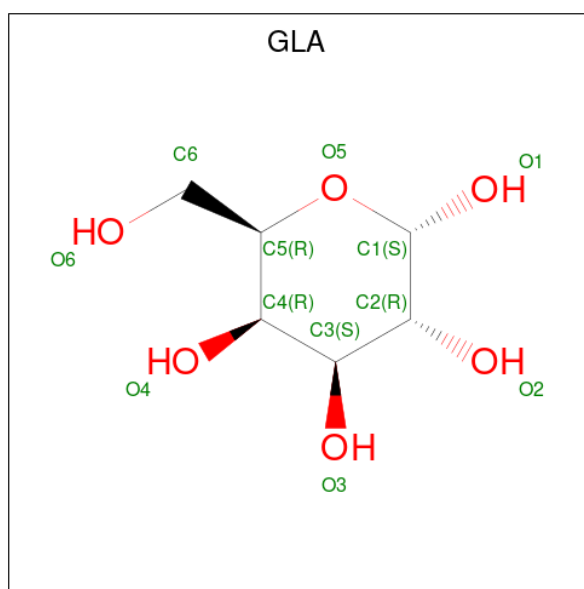
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	cloning artifact	UNP P04385
A	-18	GLY	-	cloning artifact	UNP P04385
A	-17	SER	-	cloning artifact	UNP P04385
A	-16	SER	-	cloning artifact	UNP P04385
A	-15	HIS	-	expression tag	UNP P04385
A	-14	HIS	-	expression tag	UNP P04385
A	-13	HIS	-	expression 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

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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 (CCD ID: GLA) (formula: C₆H₁₂O₆).



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

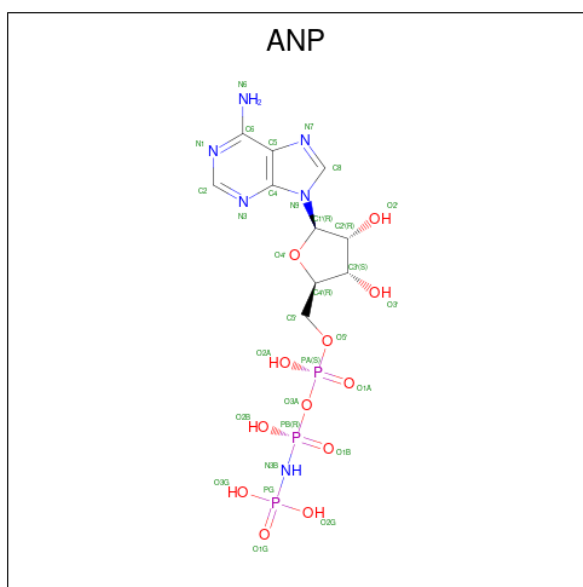
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 (CCD ID: 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 (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

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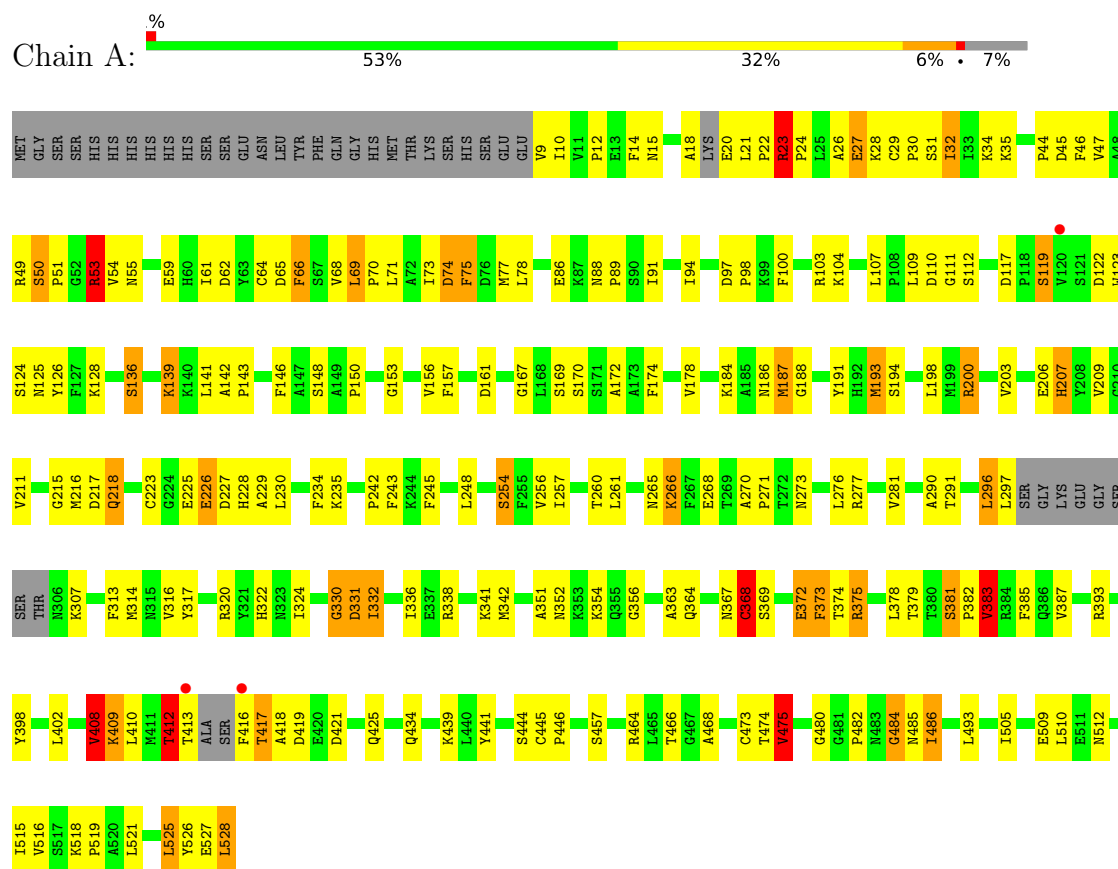
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	85	Total	O	0	0
			85	85		

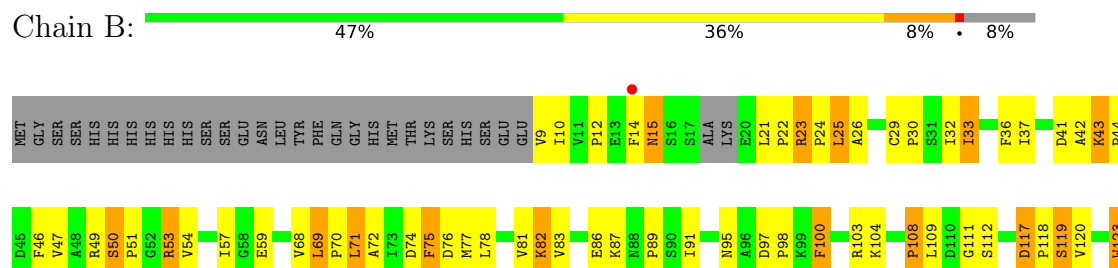
3 Residue-property plots

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



• Molecule 1: Galactokinase



A488	G215	LYS	R384	S124
T474	M216	GLU	F385	R125
V475	M217	GLY	Q386	Y126
H476	Q218	SER	V387	F127
L477	A219	SER	Q392	K128
V478	C223	THR	V397	H132
P479	D227	N306	S401	V133
G480	H228	K307	L402	A134
N483	A229	F313	R403	H135
G484	L230	M314	V404	S136
N485	Y231	N315	G404	F137
V489	V232	V316	A407	L138
K490	K235	Y317	V408	K139
E491	P236	D331	V409	K140
A492	Q237	S334	K409	L141
L493	T241	I336	L410	A142
E496	P242	I337	M411	P143
F497	F243	E337	T412	E144
Y498	F244	R338	T413	R145
K501	K245	ALA	ALA	F146
Y502	F246	SER	PHE	A147
P503	P246	THR	THR	P150
K504	H251	ALA	D419	G153
T505	E252	E420	E420	V156
T506	I253	D421	D421	G160
D507	S254	F422	F422	D161
A508	I257	Q425	Q425	V162
E509	A258	F426	F426	G167
L510	N259	G427	G427	F174
P511	T260	M430	M430	I175
N512	L261	K439	K439	K184
A513	V262	L440	L440	A185
I514	V263	Y441	Y441	N186
I515	K266	S444	S444	M187
V516	T269	C445	C445	Y191
S517	N272	P446	P446	H192
K518	N273	E447	E447	M193
P519	Y274	I448	I448	N197
A520	L276	D449	D449	L198
L521	A290	K450	K450	M199
G522	T291	I451	I451	R200
S523	Y292	C452	C452	I201
C524	G293	S453	S453	V203
L525	V294	I454	I454	E206
Y526	V295	A455	A455	V209
E527	L296	G462	G462	N212
L528	L297	S463	S463	
	SER	R464	R464	
	GLY	L465	L465	
		T466	T466	
		G467	G467	

4 Data and refinement statistics

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 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.5 (30.00-2.40) 95.5 (30.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.33 , 111.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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: MG, CL, GLA, ANP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.15	1/4022 (0.0%)	1.69	57/5451 (1.0%)
1	B	1.17	3/3993 (0.1%)	1.68	57/5411 (1.1%)
All	All	1.16	4/8015 (0.0%)	1.69	114/10862 (1.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	528	LEU	C-OXT	15.41	1.54	1.23
1	A	528	LEU	C-OXT	9.12	1.41	1.23
1	B	528	LEU	C-O	-8.43	1.06	1.23
1	B	528	LEU	CA-C	6.92	1.67	1.52

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	528	LEU	CB-CA-C	-11.10	89.02	110.10
1	B	217	ASP	CA-CB-CG	-9.65	102.95	112.60
1	B	87	LYS	N-CA-C	-9.27	100.74	111.03
1	A	188	GLY	CA-C-N	9.17	129.23	119.05
1	A	188	GLY	C-N-CA	9.17	129.23	119.05
1	B	368	CYS	N-CA-CB	-8.29	97.82	111.66
1	A	146	PHE	CA-CB-CG	-8.16	105.64	113.80
1	B	528	LEU	CB-CA-C	-7.97	94.95	110.10
1	B	223	CYS	N-CA-C	7.64	122.29	113.19
1	B	367	ASN	N-CA-C	-7.58	102.05	110.91
1	A	368	CYS	N-CA-CB	-7.49	99.48	111.62
1	B	132	HIS	CA-CB-CG	-7.26	106.54	113.80
1	B	439	LYS	N-CA-C	7.23	119.25	111.36
1	B	528	LEU	N-CA-CB	7.01	122.42	110.50
1	B	307	LYS	N-CA-C	-7.01	97.98	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	PHE	CA-CB-CG	-6.95	106.85	113.80
1	A	62	ASP	CA-CB-CG	6.80	119.40	112.60
1	A	170	SER	N-CA-C	-6.78	103.95	111.82
1	A	223	CYS	N-CA-C	6.65	121.41	113.16
1	B	296	LEU	N-CA-C	6.63	118.17	111.07
1	A	273	ASN	CA-C-O	6.58	123.56	119.55
1	B	153	GLY	N-CA-C	-6.57	103.66	112.14
1	A	71	LEU	N-CA-CB	-6.48	99.52	110.99
1	B	146	PHE	N-CA-C	6.45	122.23	113.97
1	A	296	LEU	N-CA-C	6.34	117.86	111.07
1	A	75	PHE	CA-CB-CG	-6.33	107.47	113.80
1	B	468	ALA	N-CA-C	6.33	118.99	111.71
1	B	100	PHE	CA-CB-CG	-6.32	107.48	113.80
1	A	519	PRO	N-CA-CB	6.28	108.92	103.27
1	A	485	ASN	CB-CA-C	-6.24	100.91	111.02
1	A	266	LYS	N-CA-C	6.12	118.75	111.71
1	B	307	LYS	CA-C-N	-6.12	113.11	121.06
1	B	307	LYS	C-N-CA	-6.12	113.11	121.06
1	A	381	SER	CA-C-N	6.09	126.30	119.90
1	A	381	SER	C-N-CA	6.09	126.30	119.90
1	A	324	ILE	CA-C-N	6.06	128.32	120.44
1	A	324	ILE	C-N-CA	6.06	128.32	120.44
1	B	146	PHE	CA-CB-CG	-6.06	107.74	113.80
1	B	117	ASP	N-CA-CB	6.03	121.39	110.17
1	A	322	HIS	CA-CB-CG	-6.02	107.78	113.80
1	B	75	PHE	CA-CB-CG	-6.01	107.79	113.80
1	A	53	ARG	NE-CZ-NH1	5.96	127.46	121.50
1	A	515	ILE	CB-CA-C	-5.92	101.38	110.50
1	B	272	THR	N-CA-C	-5.88	106.72	114.31
1	A	512	ASN	CA-CB-CG	-5.87	106.73	112.60
1	A	146	PHE	N-CA-C	5.85	120.54	113.17
1	B	274	TYR	N-CA-C	5.80	118.09	111.02
1	B	349	SER	N-CA-C	5.77	120.33	113.12
1	B	262	VAL	N-CA-CB	5.75	117.94	111.21
1	A	245	PHE	CA-CB-CG	-5.75	108.06	113.80
1	A	88	ASN	CA-C-N	5.74	125.76	119.90
1	A	88	ASN	C-N-CA	5.74	125.76	119.90
1	A	475	VAL	CB-CA-C	-5.73	102.08	110.62
1	B	392	GLN	N-CA-C	5.72	117.97	111.11
1	B	376	ASP	N-CA-C	5.71	117.50	111.28
1	B	147	ALA	N-CA-C	5.70	118.23	111.33
1	A	373	PHE	CA-CB-CG	-5.69	108.11	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	GLU	N-CA-C	5.66	118.66	111.69
1	B	397	VAL	N-CA-C	5.65	116.11	110.23
1	A	383	VAL	CA-C-N	-5.64	115.04	122.99
1	A	383	VAL	C-N-CA	-5.64	115.04	122.99
1	B	528	LEU	CA-C-O	5.60	137.80	121.00
1	A	369	SER	N-CA-C	-5.57	101.09	109.95
1	B	209	VAL	CB-CA-C	5.54	118.89	111.85
1	B	156	VAL	N-CA-C	5.51	116.42	108.48
1	B	485	ASN	CB-CA-C	-5.51	102.15	111.02
1	A	332	ILE	N-CA-C	5.47	115.60	110.30
1	B	483	ASN	CA-C-N	5.46	127.53	120.64
1	B	483	ASN	C-N-CA	5.46	127.53	120.64
1	A	512	ASN	CB-CA-C	5.44	121.37	109.99
1	A	268	GLU	N-CA-C	5.44	117.92	111.33
1	A	439	LYS	N-CA-CB	5.41	118.17	110.16
1	B	266	LYS	N-CA-C	5.40	117.87	111.33
1	A	156	VAL	N-CA-C	5.39	116.24	108.48
1	A	434	GLN	CA-C-O	5.37	126.25	120.55
1	A	412	THR	N-CA-CB	-5.37	102.86	110.81
1	B	241	THR	CA-C-O	5.35	125.00	119.49
1	A	468	ALA	N-CA-C	5.34	117.85	111.71
1	B	167	GLY	N-CA-C	-5.33	107.91	115.43
1	B	306	ASN	CA-CB-CG	5.33	117.93	112.60
1	B	479	PRO	N-CA-CB	5.30	107.54	103.30
1	B	251	HIS	N-CA-C	5.29	117.45	109.41
1	A	408	VAL	N-CA-CB	-5.28	103.36	110.54
1	A	528	LEU	N-CA-C	5.27	125.76	111.00
1	B	331	ASP	N-CA-CB	5.26	117.91	109.28
1	B	123	TRP	N-CA-C	5.26	117.76	111.71
1	B	76	ASP	N-CA-C	5.24	115.05	108.45
1	B	292	TYR	N-CA-CB	5.24	118.45	110.44
1	A	330	GLY	N-CA-C	-5.23	108.12	114.92
1	B	373	PHE	CA-CB-CG	-5.23	108.57	113.80
1	B	361	ASP	CA-CB-CG	-5.17	107.43	112.60
1	A	186	ASN	CA-CB-CG	-5.17	107.43	112.60
1	B	455	ALA	N-CA-C	5.16	116.59	111.07
1	A	281	VAL	N-CA-CB	5.14	117.53	110.54
1	A	88	ASN	O-C-N	5.14	126.08	121.04
1	A	23	ARG	CA-C-N	5.13	124.57	119.24
1	A	23	ARG	C-N-CA	5.13	124.57	119.24
1	A	207	HIS	N-CA-C	-5.13	105.81	111.71
1	B	351	ALA	N-CA-C	5.12	118.31	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	PRO	CA-C-N	5.08	127.40	120.54
1	B	108	PRO	C-N-CA	5.08	127.40	120.54
1	B	382	PRO	CB-CA-C	-5.08	105.24	111.64
1	B	263	VAL	CB-CA-C	-5.07	105.14	111.08
1	B	203	VAL	N-CA-CB	-5.07	102.86	111.23
1	A	330	GLY	CA-C-N	-5.06	113.82	121.05
1	A	330	GLY	C-N-CA	-5.06	113.82	121.05
1	A	484	GLY	N-CA-C	5.05	120.33	112.60
1	A	331	ASP	N-CA-CB	5.05	117.30	109.48
1	A	473	CYS	N-CA-C	5.04	117.92	110.46
1	B	212	ASN	N-CA-C	5.02	117.66	110.68
1	B	385	PHE	CA-CB-CG	-5.01	108.78	113.80
1	B	381	SER	CA-C-N	5.00	125.23	119.83
1	B	381	SER	C-N-CA	5.00	125.23	119.83
1	A	385	PHE	CA-CB-CG	-5.00	108.80	113.80

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	140	0
1	B	3910	0	3898	179	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	320	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 20.

All (320) 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:313:PHE:CD2	1:A:342:MET:HE1	2.11	0.86
1:A:480:GLY:HA2	1:A:486:ILE:HD12	1.60	0.82
1:B:404:VAL:O	1:B:408:VAL:HG23	1.82	0.79
1:B:411:MET:HE2	1:B:422:PHE:HZ	1.49	0.78
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:B:353:LYS:HZ2	1:B:361:ASP:HB3	1.47	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:B:193:MET:HE3	1:B:198:LEU:HD13	1.71	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: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:A:330:GLY:O	1:A:331:ASP:C	2.32	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:A:313:PHE:HD2	1:A:342:MET:HE1	1.57	0.68
1:B:485:ASN:O	1:B:489:VAL:HG23	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:314:MET:HA	1:B:342:MET:HE2	1.79	0.64
1:A:53:ARG:NH2	1:A:167:GLY:O	2.30	0.64
1:B:29:CYS:C	1:B:33:ILE:HD12	2.23	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:501:LYS:C	1:B:503:PRO:HD3	2.24	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:141:LEU:CD2	1:A:187:MET:HE2	2.29	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: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:B:314:MET:CA	1:B:342:MET:HE2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:141:LEU:C	1:B:143:PRO:HD3	2.29	0.58
1:B:68:VAL:C	1:B:70:PRO:HD3	2.29	0.58
1:A:218:GLN:HE21	1:A:218:GLN:N	1.95	0.57
1:B:23:ARG:O	1:B:24:PRO:C	2.46	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:141:LEU:HD23	1:A:187:MET:HE2	1.90	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:A:248:LEU:HB3	1:A:419:ASP:CG	2.34	0.52
1:A:342:MET:HE3	1:A:398:TYR:CZ	2.45	0.52
1:B:95:ASN:HB2	1:B:123:TRP:CH2	2.45	0.52
1:B:235:LYS:HA	1:B:236:PRO:C	2.35	0.52
1:B:313:PHE:CD2	1:B:342:MET:HE1	2.45	0.52
1:B:353:LYS:HZ3	1:B:361:ASP:HB3	1.73	0.52
1:B:430:MET:HE2	1:B:462:GLY:C	2.35	0.52
1:B:526:TYR:HE2	1:B:528:LEU:CD2	2.23	0.52
1:B:430:MET:HE2	1:B:462:GLY:O	2.10	0.51
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: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:B:252:GLU:HB2	1:B:480:GLY:C	2.36	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:A:316:VAL:O	1:A:317:TYR:C	2.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:314:MET:HB2	1:A:342:MET:HE2	1.95	0.48
1:B:518:LYS:O	1:B:519:PRO:C	2.55	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: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
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: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: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:408:VAL:O	1:B:409:LYS:C	2.58	0.47
1:B:462:GLY:O	1:B:476:HIS:HA	2.14	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:B:53:ARG:HH11	1:B:217:ASP:CG	2.21	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:450:LYS:O	1:B:451:ILE:C	2.56	0.46
1:B:374:THR:O	1:B:375:ARG:C	2.57	0.46
1:B:515:ILE:HG22	1:B:516:VAL:N	2.30	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:215:GLY:O	1:A:216:MET:C	2.58	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:68:VAL:C	1:A:70:PRO:HD3	2.41	0.45
1:A:142:ALA:N	1:A:143:PRO:HD3	2.31	0.45
1:B:491:GLU:O	1:B:492:ALA:C	2.60	0.45
1:B:351:ALA:O	1:B:354:LYS:HG3	2.16	0.45
1:A:141:LEU:C	1:A:143:PRO:HD3	2.41	0.45
1:B:218:GLN:O	1:B:219:ALA:C	2.58	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
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:444:SER:OG	1:A:445:CYS:N	2.47	0.45
1:B:10:ILE:HD12	1:B:10:ILE:C	2.41	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:A:193:MET:HE3	1:A:198:LEU:HD13	1.98	0.44
1:B:77:MET:HA	1:B:160:GLY:HA2	1.99	0.44
1:B:453:SER:O	1:B:454:ILE:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:316:VAL:O	1:B:317:TYR:C	2.55	0.44
1:A:225:GLU:O	1:A:228:HIS:HB2	2.18	0.44
1:B:184:LYS:NZ	1:B:527:GLU:CG	2.80	0.43
1:B:193:MET:CE	1:B:198:LEU:HD13	2.43	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:A:314:MET:HE2	1:A:314:MET:HB3	1.93	0.43
1:A:372:GLU:O	1:A:373:PHE:C	2.61	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:A:482:PRO:C	1:A:484:GLY:H	2.27	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:28:LYS:O	1:A:29:CYS:C	2.61	0.42
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
1:B:366:LEU:HB2	1:B:368:CYS:HB2	2.02	0.42
1:A:276:LEU:HD13	1:A:383:VAL:HG13	2.02	0.42
1:B:25:LEU:O	1:B:26:ALA:C	2.62	0.42
1:B:290:ALA:O	1:B:291:THR:C	2.59	0.42
1:A:22:PRO:O	1:A:23:ARG:C	2.62	0.42
1:A:320:ARG:O	1:A:320:ARG:HG3	2.19	0.42
1:A:374:THR:O	1:A:375:ARG:C	2.59	0.42
1:A:505:ILE:HG13	1:A:509:GLU:OE1	2.19	0.42
1:B:22:PRO:O	1:B:23:ARG:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:199:MET:O	1:B:200:ARG:C	2.61	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: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:174:PHE:O	1:A:178:VAL:HG23	2.21	0.41
1:A:493:LEU:HD23	1:A:493:LEU:HA	1.85	0.41
1:A:509:GLU:O	1:A:510:LEU:C	2.63	0.41
1:B:245:PHE:HB3	1:B:253:ILE:HD13	2.03	0.41
1:B:379:THR:O	1:B:380:THR:C	2.61	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:A:169:SER:OG	1:A:172:ALA:HB3	2.22	0.41
1:A:290:ALA:O	1:A:291:THR:C	2.62	0.41
1:B:126:TYR:CD1	1:B:175:ILE:HD11	2.53	0.40
1:B:373:PHE:CE2	1:B:378:LEU:HD21	2.55	0.40
1:B:187:MET:HB3	1:B:191:TYR:CB	2.51	0.40
1:B:360:ASP:OD1	1:B:370:ARG:HD2	2.21	0.40
1:B:187:MET:CA	1:B:187:MET:HE3	2.51	0.40
1:B:257:ILE:HG23	1:B:474:THR:O	2.21	0.40
1:B:449:ASP:O	1:B:450:LYS:C	2.62	0.40
1:A:14:PHE:HB3	1:A:21:LEU:HD21	2.03	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	43	58
1	B	497/548 (91%)	460 (93%)	35 (7%)	2 (0%)	30	43
All	All	998/1096 (91%)	943 (94%)	52 (5%)	3 (0%)	36	50

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 ⓘ

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%)	392 (90%)	41 (10%)	8	13
1	B	431/467 (92%)	379 (88%)	52 (12%)	5	7
All	All	864/934 (92%)	771 (89%)	93 (11%)	6	9

All (93) 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

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Mol	Chain	Res	Type
1	A	32	ILE
1	A	50	SER
1	A	53	ARG
1	A	69	LEU
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	187	MET
1	A	193	MET
1	A	200	ARG
1	A	206	GLU
1	A	209	VAL
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	372	GLU
1	A	375	ARG
1	A	383	VAL
1	A	393	ARG
1	A	408	VAL
1	A	409	LYS
1	A	412	THR
1	A	417	THR
1	A	457	SER
1	A	475	VAL
1	A	486	ILE
1	A	518	LYS
1	A	525	LEU
1	A	527	GLU
1	B	15	ASN
1	B	25	LEU
1	B	32	ILE
1	B	33	ILE

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Mol	Chain	Res	Type
1	B	43	LYS
1	B	50	SER
1	B	53	ARG
1	B	57	ILE
1	B	69	LEU
1	B	71	LEU
1	B	74	ASP
1	B	82	LYS
1	B	83	VAL
1	B	103	ARG
1	B	119	SER
1	B	120	VAL
1	B	133	VAL
1	B	136	SER
1	B	139	LYS
1	B	144	GLU
1	B	145	ARG
1	B	193	MET
1	B	203	VAL
1	B	206	GLU
1	B	209	VAL
1	B	218	GLN
1	B	230	LEU
1	B	237	GLN
1	B	307	LYS
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	451	ILE
1	B	453	SER
1	B	475	VAL
1	B	489	VAL

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Mol	Chain	Res	Type
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 (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	218	GLN
1	A	251	HIS
1	A	273	ASN
1	A	364	GLN
1	A	425	GLN
1	B	15	ASN
1	B	88	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
1	B	495	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	33,33,33	1.42	6 (18%)	45,52,52	1.31	4 (8%)
2	GLA	A	529	-	12,12,12	0.70	0	17,17,17	1.25	1 (5%)
5	ANP	B	532	3	33,33,33	1.52	6 (18%)	45,52,52	1.37	8 (17%)
2	GLA	B	529	-	12,12,12	0.61	0	17,17,17	0.91	1 (5%)

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	-	4/18/38/38	0/3/3/3
2	GLA	A	529	-	-	1/2/22/22	0/1/1/1
5	ANP	B	532	3	-	3/18/38/38	0/3/3/3
2	GLA	B	529	-	-	1/2/22/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	532	ANP	PB-O1B	4.10	1.52	1.46
5	A	532	ANP	C6-N6	-3.83	1.24	1.34
5	B	532	ANP	C6-N6	-3.76	1.24	1.34
5	A	532	ANP	PB-O1B	3.67	1.51	1.46
5	A	532	ANP	PG-O1G	3.29	1.51	1.46
5	B	532	ANP	PG-O1G	2.80	1.50	1.46
5	B	532	ANP	PG-O2G	-2.51	1.50	1.56
5	A	532	ANP	C2-N1	2.46	1.38	1.33
5	B	532	ANP	C2-N1	2.10	1.37	1.33
5	A	532	ANP	PG-O2G	-2.05	1.51	1.56
5	A	532	ANP	PB-O2B	-2.02	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	532	ANP	C2-N3	-2.00	1.30	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	532	ANP	C2-N1-C6	3.77	124.92	118.73
5	A	532	ANP	O1B-PB-N3B	-3.67	106.37	111.77
5	A	532	ANP	C2-N1-C6	3.63	124.70	118.73
5	B	532	ANP	N3-C2-N1	-3.46	123.35	128.58
5	A	532	ANP	N3-C2-N1	-3.31	123.57	128.58
2	A	529	GLA	O4-C4-C3	3.10	117.67	110.38
5	A	532	ANP	O1G-PG-N3B	-2.85	107.58	111.77
5	B	532	ANP	C2'-C1'-N9	-2.71	106.56	113.30
5	B	532	ANP	O1G-PG-N3B	-2.54	108.03	111.77
2	B	529	GLA	O4-C4-C3	2.38	115.98	110.38
5	B	532	ANP	O3'-C3'-C2'	2.27	119.10	111.82
5	B	532	ANP	C5-C6-N6	2.25	128.85	123.29
5	B	532	ANP	O2G-PG-O1G	-2.18	107.99	113.45
5	B	532	ANP	PA-O5'-C5'	-2.14	109.08	121.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

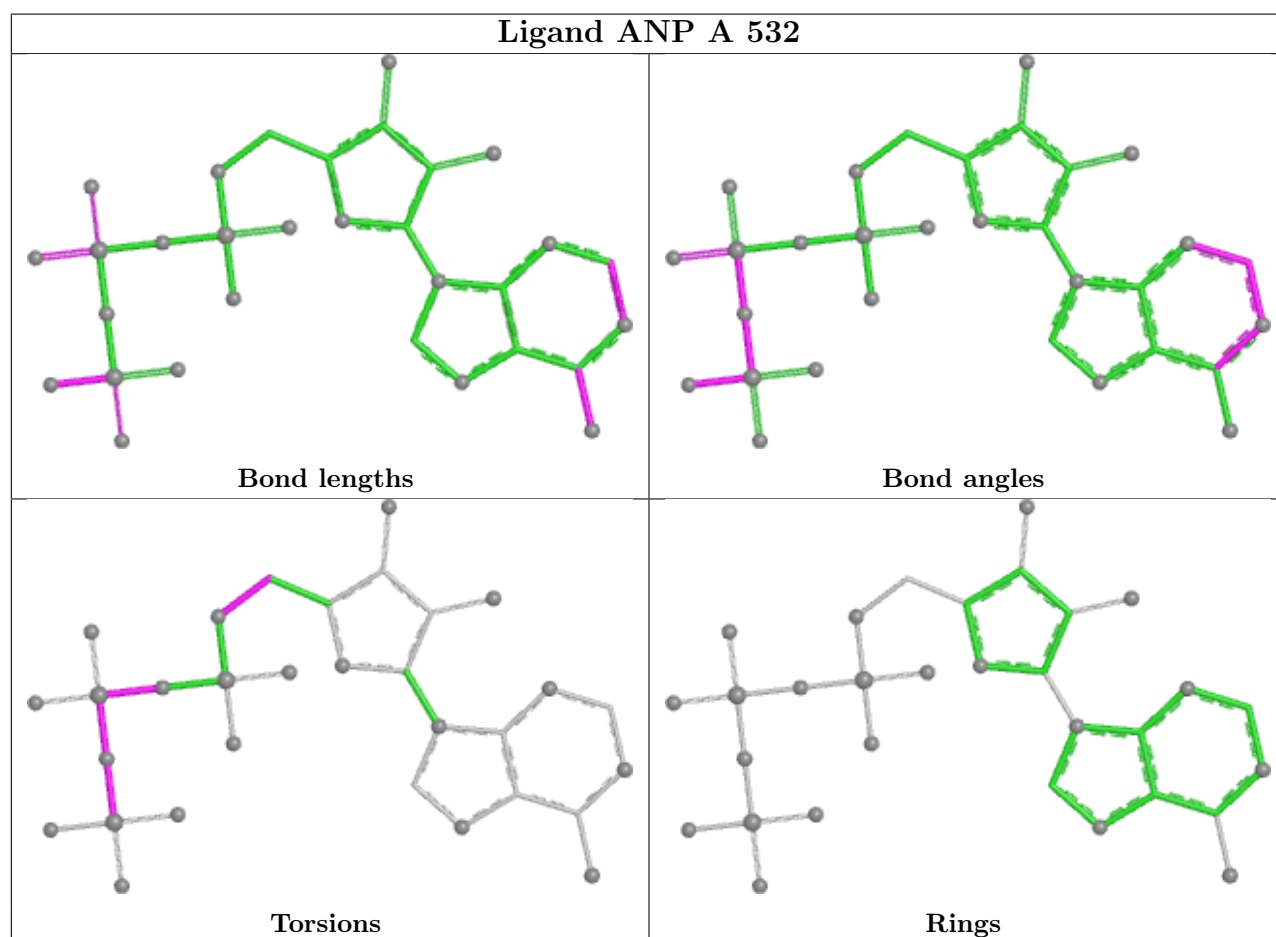
Mol	Chain	Res	Type	Atoms
5	A	532	ANP	PB-N3B-PG-O1G
5	A	532	ANP	PG-N3B-PB-O1B
5	B	532	ANP	PB-N3B-PG-O1G
5	B	532	ANP	PG-N3B-PB-O1B
2	A	529	GLA	O5-C5-C6-O6
2	B	529	GLA	O5-C5-C6-O6
5	A	532	ANP	C4'-C5'-O5'-PA
5	A	532	ANP	PA-O3A-PB-O1B
5	B	532	ANP	PA-O3A-PB-O1B

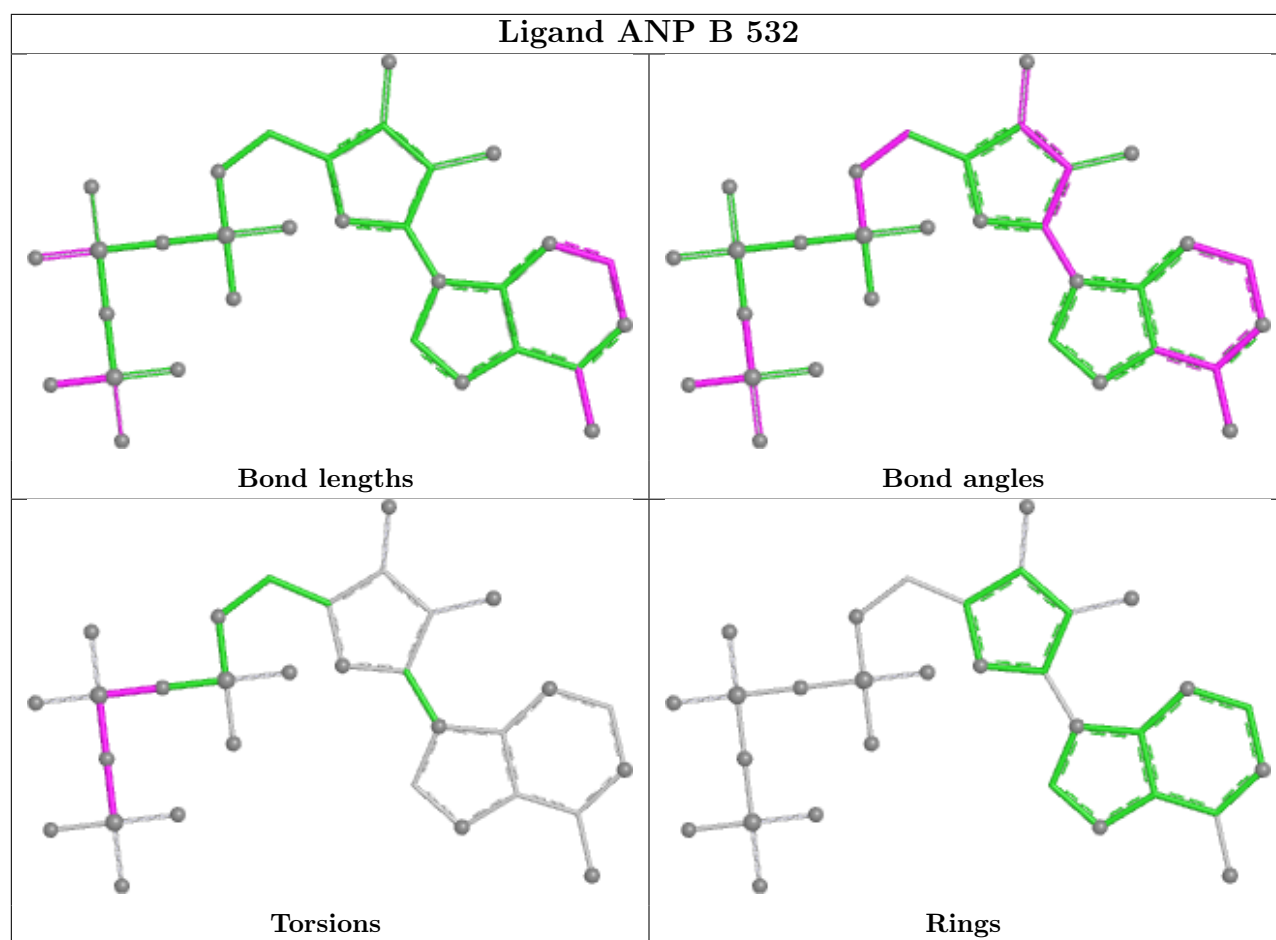
There are no ring outliers.

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 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 [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	509/548 (92%)	-0.55	3 (0%) 85 83	12, 28, 67, 96	0
1	B	505/548 (92%)	-0.18	2 (0%) 88 86	13, 39, 85, 98	0
All	All	1014/1096 (92%)	-0.37	5 (0%) 87 85	12, 33, 80, 98	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	416	PHE	4.4
1	B	528	LEU	3.2
1	A	120	VAL	2.9
1	B	14	PHE	2.4
1	A	413	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

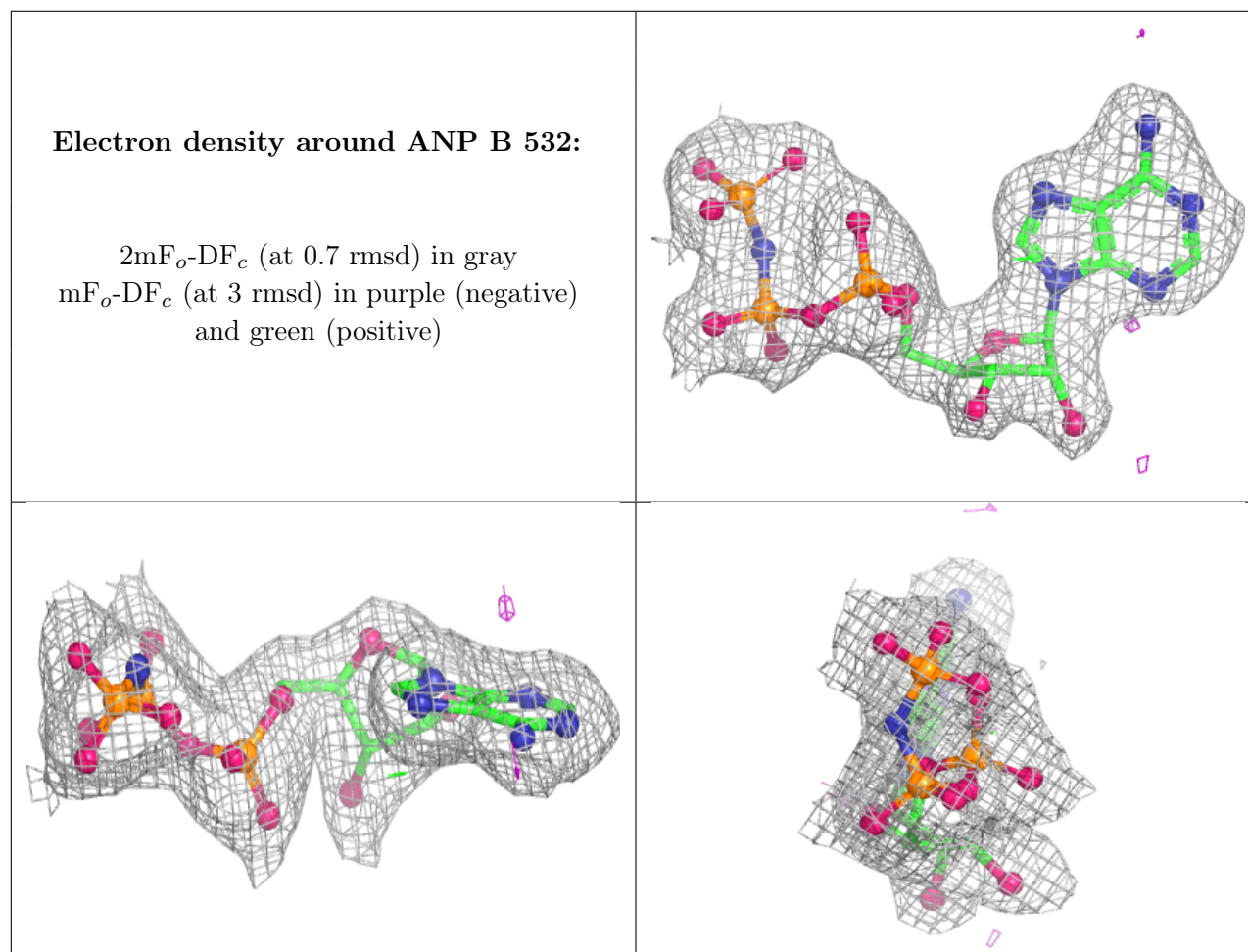
There are no oligosaccharides in this entry.

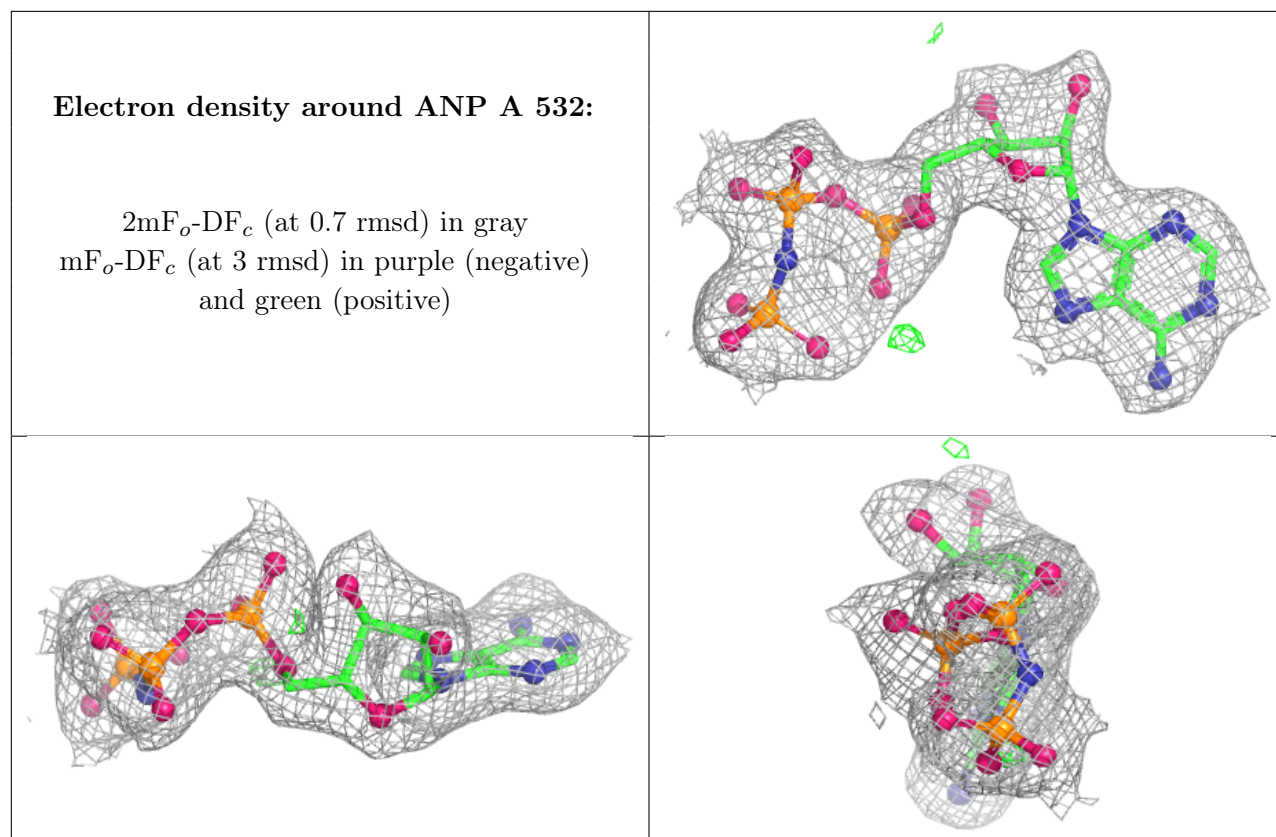
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
3	MG	B	530	1/1	0.95	0.10	44,44,44,44	0
4	CL	B	531	1/1	0.96	0.07	48,48,48,48	0
3	MG	A	530	1/1	0.97	0.07	34,34,34,34	0
2	GLA	B	529	12/12	0.98	0.05	11,17,30,33	0
4	CL	A	531	1/1	0.98	0.03	33,33,33,33	0
2	GLA	A	529	12/12	0.98	0.05	5,14,22,27	0
5	ANP	B	532	31/31	0.98	0.05	9,28,51,95	0
5	ANP	A	532	31/31	0.99	0.05	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.