



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:04 PM UTC

PDB ID : 2D32 / pdb_00002d32
Title : Crystal Structure of Michaelis Complex of gamma-Glutamylcysteine Synthetase
Authors : Hibi, T.; Nakayama, M.; Nii, H.; Kurokawa, Y.; Katano, H.; Oda, J.
Deposited on : 2005-09-25
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

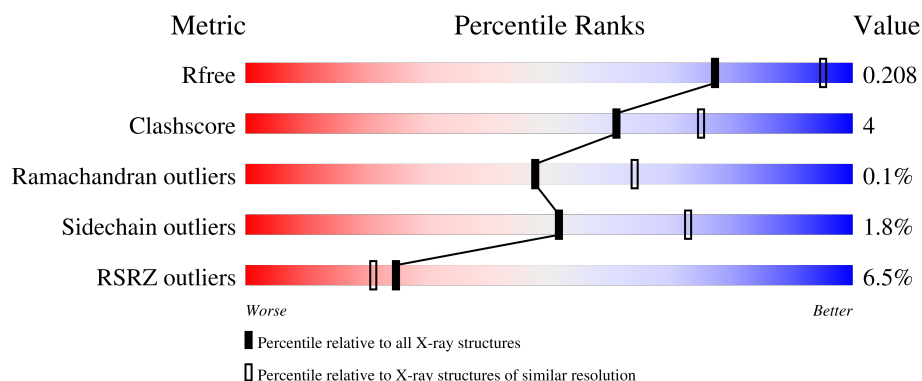
1 Overall quality at a glance

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	518	3% 89% 8% ..
1	B	518	5% 86% 11% .
1	C	518	10% 83% 13% .
1	D	518	7% 88% 9% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16833 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 Glutamate–cysteine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4030	2558	689	765	18			
1	B	499	Total	C	N	O	S	0	0	0
			3937	2507	670	742	18			
1	C	499	Total	C	N	O	S	0	0	0
			3906	2489	665	734	18			
1	D	504	Total	C	N	O	S	0	0	0
			3955	2517	678	742	18			

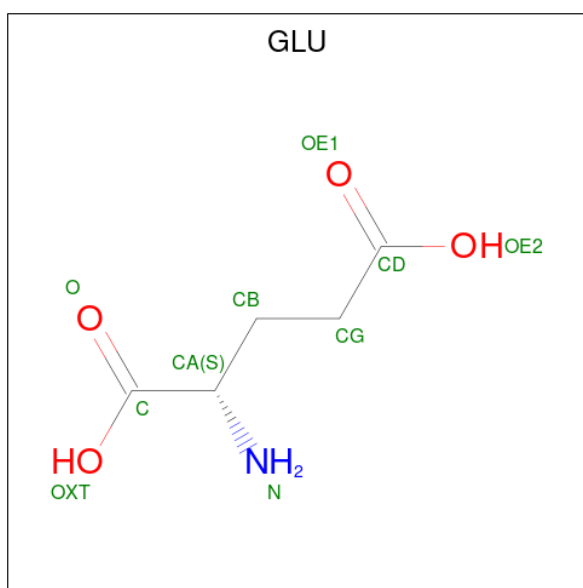
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	SER	CYS	engineered mutation	UNP P0A6W9
A	164	SER	CYS	engineered mutation	UNP P0A6W9
A	205	SER	CYS	engineered mutation	UNP P0A6W9
A	223	SER	CYS	engineered mutation	UNP P0A6W9
B	106	SER	CYS	engineered mutation	UNP P0A6W9
B	164	SER	CYS	engineered mutation	UNP P0A6W9
B	205	SER	CYS	engineered mutation	UNP P0A6W9
B	223	SER	CYS	engineered mutation	UNP P0A6W9
C	106	SER	CYS	engineered mutation	UNP P0A6W9
C	164	SER	CYS	engineered mutation	UNP P0A6W9
C	205	SER	CYS	engineered mutation	UNP P0A6W9
C	223	SER	CYS	engineered mutation	UNP P0A6W9
D	106	SER	CYS	engineered mutation	UNP P0A6W9
D	164	SER	CYS	engineered mutation	UNP P0A6W9
D	205	SER	CYS	engineered mutation	UNP P0A6W9
D	223	SER	CYS	engineered mutation	UNP P0A6W9

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

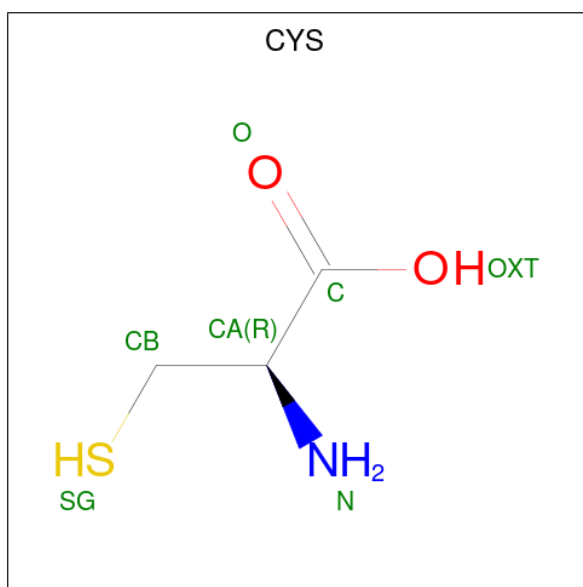
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Mg 4 4	0	0
2	B	3	Total Mg 3 3	0	0
2	C	3	Total Mg 3 3	0	0
2	D	3	Total Mg 3 3	0	0

- Molecule 3 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



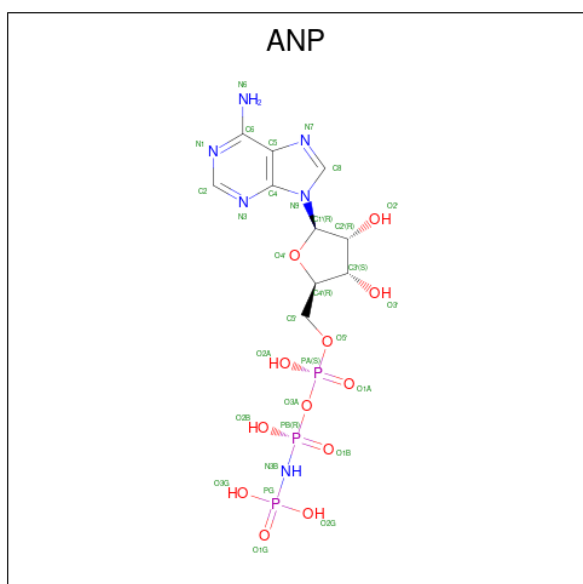
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 10 5 1 4	0	0
3	B	1	Total C N O 10 5 1 4	0	0
3	C	1	Total C N O 10 5 1 4	0	0
3	D	1	Total C N O 10 5 1 4	0	0

- Molecule 4 is CYSTEINE (CCD ID: CYS) (formula: C₃H₇NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 7	C 3	N 1	O 2	S 1	0	0
4	B	1	Total 7	C 3	N 1	O 2	S 1	0	0
4	C	1	Total 7	C 3	N 1	O 2	S 1	0	0
4	D	1	Total 7	C 3	N 1	O 2	S 1	0	0

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$).



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

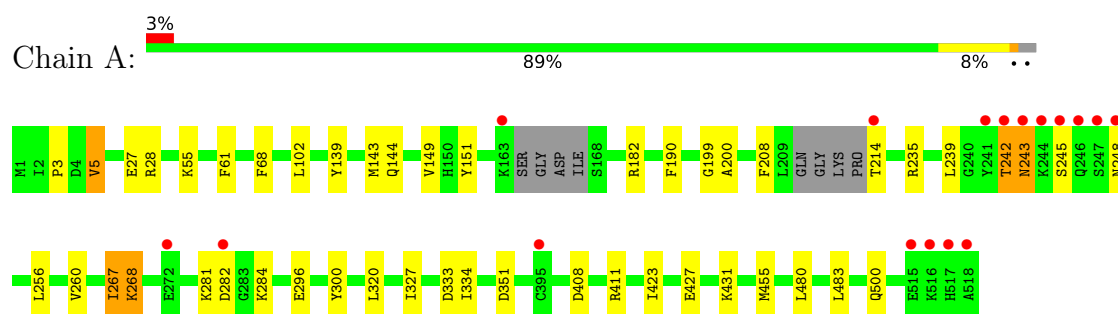
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	363	Total	O	0	0
			363	363		
6	B	163	Total	O	0	0
			163	163		
6	C	87	Total	O	0	0
			87	87		
6	D	187	Total	O	0	0
			187	187		

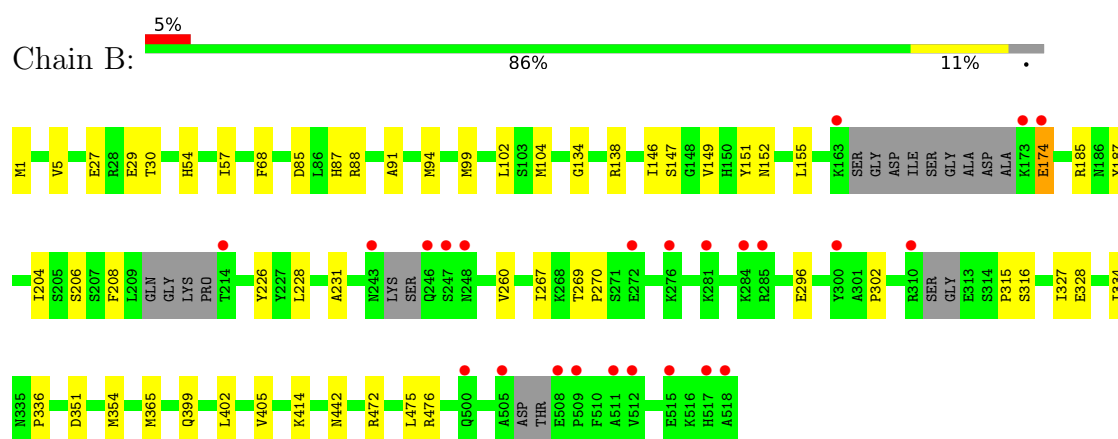
3 Residue-property plots [i](#)

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.

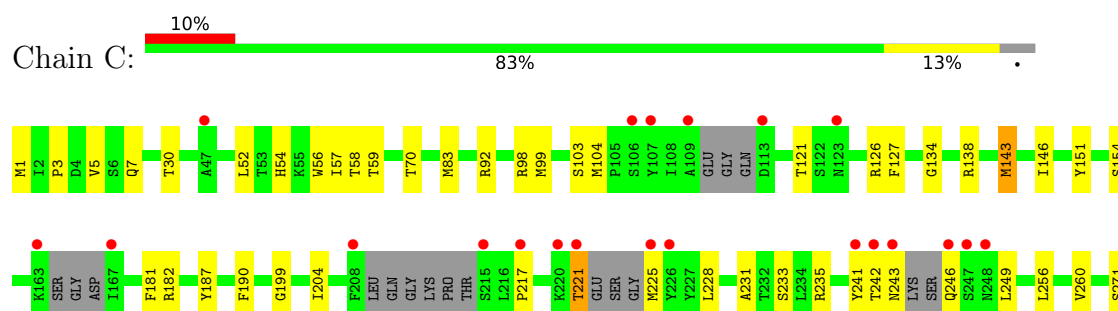
• Molecule 1: Glutamate–cysteine ligase

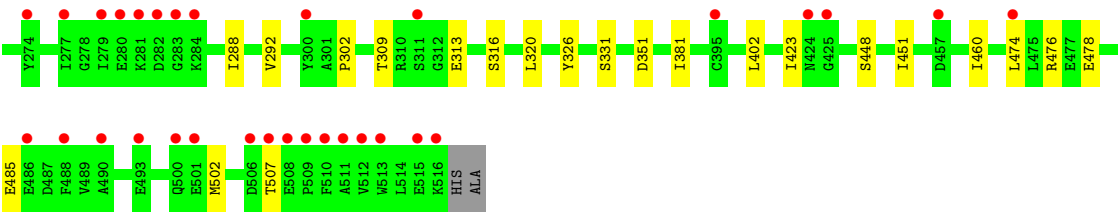


• Molecule 1: Glutamate–cysteine ligase

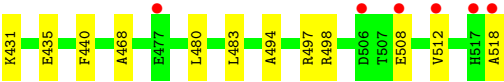
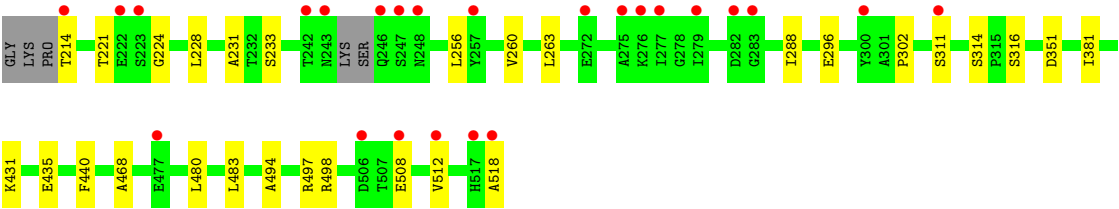
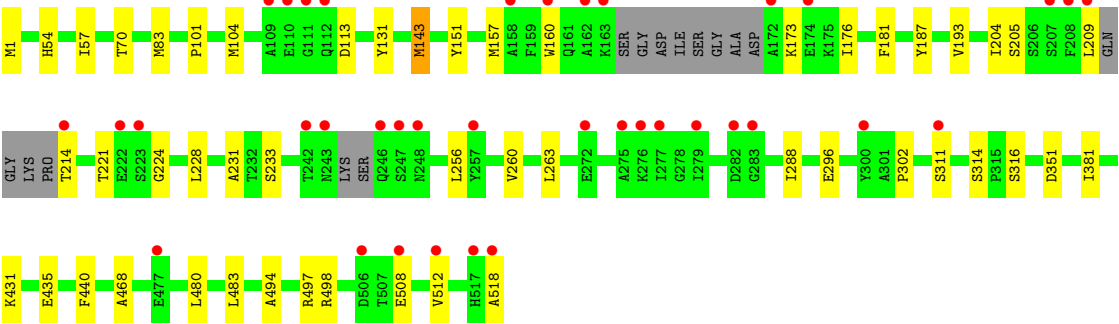
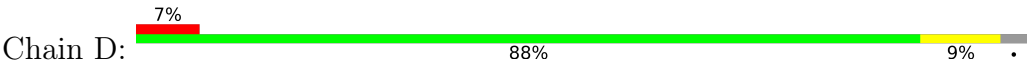


• Molecule 1: Glutamate–cysteine ligase





● Molecule 1: Glutamate-cysteine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	325.53Å 325.53Å 105.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.40 40.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.40) 100.0 (40.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.168 , 0.198 0.179 , 0.208	Depositor DCC
R_{free} test set	8122 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16833	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, MG

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	0.94	2/4117 (0.0%)	0.95	2/5572 (0.0%)
1	B	0.74	0/4021	0.88	2/5443 (0.0%)
1	C	0.72	0/3989	0.86	2/5403 (0.0%)
1	D	0.79	0/4041	0.90	0/5476
All	All	0.80	2/16168 (0.0%)	0.90	6/21894 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	VAL	CA-CB	5.25	1.60	1.54
1	A	200	ALA	CA-CB	5.02	1.58	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	GLY	N-CA-C	-5.25	105.22	111.36
1	B	155	LEU	CA-C-N	-5.20	115.38	120.52
1	B	155	LEU	C-N-CA	-5.20	115.38	120.52
1	A	199	GLY	N-CA-C	-5.14	105.34	111.36
1	A	256	LEU	N-CA-C	5.01	116.43	111.07
1	C	331	SER	N-CA-C	5.01	119.02	113.01

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	4030	0	3944	27	0
1	B	3937	0	3835	39	0
1	C	3906	0	3785	42	0
1	D	3955	0	3845	25	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	10	0	5	0	0
3	B	10	0	5	0	0
3	C	10	0	5	0	0
3	D	10	0	5	1	0
4	A	7	0	4	0	0
4	B	7	0	4	0	0
4	C	7	0	4	0	0
4	D	7	0	4	1	0
5	A	31	0	13	0	0
5	B	31	0	13	0	0
5	C	31	0	13	0	0
5	D	31	0	13	0	0
6	A	363	0	0	1	0
6	B	163	0	0	2	0
6	C	87	0	0	1	0
6	D	187	0	0	1	0
All	All	16833	0	15497	133	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 4.

All (133) 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:139:TYR:HB3	1:A:242:THR:HB	1.52	0.90
1:D:104:MET:HE2	1:D:204:ILE:HG13	1.58	0.85
1:C:54:HIS:HD2	1:C:56:TRP:H	1.30	0.80
1:D:508:GLU:CD	1:D:508:GLU:H	1.92	0.78
1:B:91:ALA:HA	1:B:94:MET:HE2	1.69	0.74
1:A:143:MET:HG3	1:A:242:THR:HG23	1.70	0.73
1:B:472:ARG:O	1:B:476:ARG:HG3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:LEU:HD21	1:D:296:GLU:HG2	1.73	0.68
1:B:104:MET:HE2	1:B:204:ILE:HG13	1.77	0.67
1:C:70:THR:HG23	1:C:83:MET:HE2	1.76	0.67
1:B:260:VAL:HG13	1:B:316:SER:HB2	1.77	0.66
1:C:121:THR:O	1:C:126:ARG:HD2	1.96	0.65
1:D:157:MET:HA	1:D:157:MET:HE2	1.80	0.63
1:B:91:ALA:HA	1:B:94:MET:CE	2.30	0.61
1:D:1:MET:HE3	6:D:4709:HOH:O	2.00	0.61
1:D:314:SER:HB3	1:D:518:ALA:HA	1.85	0.58
1:C:54:HIS:CD2	1:C:57:ILE:H	2.22	0.58
1:B:327:ILE:CD1	1:B:354:MET:HE2	2.34	0.57
1:D:260:VAL:HG13	1:D:316:SER:HB2	1.86	0.57
1:C:5:VAL:HG12	1:C:5:VAL:O	2.05	0.57
1:C:260:VAL:HG11	1:C:320:LEU:HG	1.87	0.55
1:A:102:LEU:HD13	1:A:455:MET:CE	2.37	0.55
1:B:327:ILE:HD13	1:B:354:MET:HE2	1.87	0.55
1:C:104:MET:HE1	1:C:146:ILE:HD13	1.89	0.54
1:B:152:ASN:OD1	1:B:328:GLU:HG3	2.07	0.54
1:A:102:LEU:HD13	1:A:455:MET:HE2	1.89	0.54
1:B:402:LEU:C	1:B:402:LEU:HD23	2.34	0.53
1:B:206:SER:HB3	1:B:226:TYR:HE1	1.74	0.53
1:D:494:ALA:O	1:D:498:ARG:HG3	2.07	0.53
1:C:181:PHE:CE2	1:C:256:LEU:HA	2.44	0.53
1:C:243:ASN:C	1:C:246:GLN:HB2	2.34	0.53
1:D:187:TYR:HE1	1:D:302:PRO:HB2	1.74	0.53
1:B:1:MET:HE2	1:B:405:VAL:HG11	1.92	0.52
1:B:149:VAL:HG23	1:B:334:ILE:HD13	1.91	0.51
1:A:427:GLU:O	1:A:431:LYS:HG2	2.11	0.51
1:B:94:MET:HE1	1:B:99:MET:HG3	1.92	0.51
1:A:408:ASP:OD1	1:A:411:ARG:NH2	2.43	0.51
1:B:185:ARG:HB3	1:B:365:MET:CE	2.41	0.51
1:C:143:MET:HE3	1:C:242:THR:H	1.76	0.51
1:D:263:LEU:CD2	1:D:296:GLU:HG2	2.41	0.51
1:C:225:MET:SD	1:C:460:ILE:HG13	2.51	0.50
1:C:70:THR:CG2	1:C:83:MET:HE2	2.41	0.50
1:A:139:TYR:CB	1:A:242:THR:HB	2.33	0.50
1:D:431:LYS:HE3	1:D:435:GLU:OE2	2.12	0.50
1:A:139:TYR:HB3	1:A:242:THR:CB	2.32	0.49
1:D:228:LEU:HB2	1:D:231:ALA:HB2	1.94	0.49
1:A:214:THR:HG21	1:A:239:LEU:HD21	1.94	0.49
1:B:187:TYR:HE1	1:B:302:PRO:HB2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:TYR:HB2	1:D:288:ILE:HD11	1.93	0.49
1:B:1:MET:HE3	6:B:2674:HOH:O	2.11	0.49
1:A:260:VAL:HG11	1:A:320:LEU:HG	1.93	0.49
1:C:151:TYR:OH	1:C:351:ASP:OD1	2.30	0.49
1:C:104:MET:SD	1:C:204:ILE:HG22	2.53	0.49
1:C:309:THR:HB	1:C:313:GLU:HB3	1.95	0.49
1:D:480:LEU:HB3	1:D:483:LEU:O	2.13	0.49
1:A:267:ILE:HD11	1:A:296:GLU:N	2.27	0.48
1:B:365:MET:HE2	6:B:2659:HOH:O	2.13	0.48
1:A:5:VAL:O	1:A:5:VAL:HG12	2.13	0.48
1:B:228:LEU:HB2	1:B:231:ALA:HB2	1.95	0.48
1:D:151:TYR:OH	1:D:351:ASP:OD1	2.32	0.48
1:A:245:SER:HB2	1:A:248:ASN:H	1.77	0.48
1:B:146:ILE:HD11	1:B:208:PHE:CE2	2.49	0.48
1:B:267:ILE:O	1:B:267:ILE:HG22	2.14	0.47
1:A:55:LYS:HE3	6:A:1757:HOH:O	2.13	0.47
1:B:134:GLY:O	1:B:138:ARG:HG3	2.14	0.47
1:A:151:TYR:OH	1:A:351:ASP:OD1	2.33	0.47
1:C:54:HIS:CD2	1:C:56:TRP:H	2.21	0.46
1:B:5:VAL:HG12	1:B:5:VAL:O	2.16	0.46
1:D:101:PRO:HD3	1:D:468:ALA:HB2	1.97	0.46
1:C:134:GLY:O	1:C:138:ARG:HG3	2.15	0.46
1:C:228:LEU:HB2	1:C:231:ALA:HB2	1.95	0.46
1:B:54:HIS:HB3	1:B:57:ILE:O	2.16	0.46
1:B:296:GLU:OE1	1:B:315:PRO:HD2	2.16	0.46
1:D:233:SER:O	1:D:381:ILE:HG23	2.17	0.45
1:C:402:LEU:C	1:C:402:LEU:HD23	2.42	0.45
1:B:174:GLU:OE1	1:B:174:GLU:HA	2.16	0.45
1:B:296:GLU:OE2	1:B:316:SER:OG	2.35	0.45
1:B:327:ILE:C	1:B:327:ILE:HD12	2.42	0.44
1:B:204:ILE:HG12	1:B:208:PHE:HB2	1.99	0.44
1:A:61:PHE:CD2	1:A:144:GLN:HB2	2.53	0.44
1:C:260:VAL:HG13	1:C:316:SER:HB2	1.98	0.44
1:D:193:VAL:HG23	1:D:440:PHE:HZ	1.82	0.44
1:A:143:MET:HE1	1:A:208:PHE:HB3	1.99	0.44
1:C:249:LEU:HD21	1:C:292:VAL:HG11	1.99	0.44
1:C:181:PHE:HE2	1:C:256:LEU:HA	1.83	0.43
1:C:474:LEU:O	1:C:478:GLU:HG3	2.18	0.43
3:D:4519:GLU:CD	4:D:4520:CYS:HA	2.42	0.43
1:A:268:LYS:O	1:A:268:LYS:HG2	2.16	0.43
1:C:30:THR:OG1	1:C:99:MET:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LEU:HD21	1:C:502:MET:HE1	2.00	0.43
1:C:104:MET:CE	1:C:235:ARG:HA	2.49	0.43
1:C:221:THR:CG2	1:C:225:MET:HB3	2.48	0.43
1:A:268:LYS:HE3	1:B:442:ASN:HA	1.99	0.43
1:B:151:TYR:OH	1:B:351:ASP:OD1	2.35	0.43
1:B:87:HIS:HB3	1:B:475:LEU:HD13	2.01	0.43
1:B:27:GLU:HA	1:B:68:PHE:O	2.18	0.42
1:D:54:HIS:HB3	1:D:57:ILE:O	2.18	0.42
1:C:92:ARG:HG2	1:C:476:ARG:HG2	2.02	0.42
1:D:160:TRP:CD1	1:D:176:ILE:HG12	2.55	0.42
1:A:235:ARG:HD3	1:A:333:ASP:OD1	2.18	0.42
1:A:281:LYS:O	1:A:282:ASP:HB2	2.19	0.42
1:C:320:LEU:HD23	1:C:320:LEU:HA	1.92	0.42
1:D:143:MET:O	1:D:143:MET:HG2	2.18	0.42
1:C:187:TYR:HE1	1:C:302:PRO:HB2	1.84	0.42
1:A:27:GLU:HA	1:A:68:PHE:O	2.20	0.42
1:B:29:GLU:HB2	1:B:147:SER:HB2	2.01	0.42
1:A:243:ASN:HB2	1:A:300:TYR:HB2	2.00	0.41
1:B:102:LEU:HD23	1:B:336:PRO:HB3	2.02	0.41
1:C:127:PHE:CZ	1:C:288:ILE:HD13	2.55	0.41
1:C:143:MET:HE3	1:C:241:TYR:HA	2.03	0.41
1:D:181:PHE:CE2	1:D:256:LEU:HA	2.55	0.41
1:A:3:PRO:HD3	1:A:190:PHE:CZ	2.55	0.41
1:B:269:THR:HA	1:B:270:PRO:HD3	1.96	0.41
1:C:58:THR:OG1	1:C:59:THR:N	2.54	0.41
1:C:154:SER:HB3	1:C:326:TYR:HB3	2.03	0.41
1:C:233:SER:O	1:C:381:ILE:HG23	2.20	0.41
1:B:30:THR:OG1	1:B:99:MET:HB3	2.20	0.41
1:C:98:ARG:H	1:C:98:ARG:HD2	1.86	0.41
1:C:143:MET:O	1:C:143:MET:HG2	2.21	0.41
1:C:241:TYR:O	1:C:242:THR:HG23	2.21	0.41
1:C:448:SER:HA	1:C:451:ILE:HG22	2.03	0.41
1:D:70:THR:HG23	1:D:83:MET:HE2	2.03	0.41
1:C:3:PRO:HD3	1:C:190:PHE:CZ	2.56	0.41
1:D:221:THR:O	1:D:224:GLY:N	2.52	0.41
1:A:480:LEU:HB3	1:A:483:LEU:O	2.21	0.40
1:B:94:MET:CE	1:B:99:MET:HE2	2.51	0.40
1:B:94:MET:HE1	1:B:99:MET:HE2	2.02	0.40
1:D:104:MET:HE2	1:D:204:ILE:CG1	2.39	0.40
1:A:214:THR:CG2	1:A:239:LEU:HD21	2.52	0.40
1:C:1:MET:HE3	6:C:3599:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:HIS:HB3	1:C:57:ILE:O	2.22	0.40
1:A:149:VAL:HG23	1:A:334:ILE:HD13	2.03	0.40
1:B:85:ASP:HA	1:B:88:ARG:HD2	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	504/518 (97%)	491 (97%)	13 (3%)	0	100	100
1	B	487/518 (94%)	473 (97%)	14 (3%)	0	100	100
1	C	487/518 (94%)	471 (97%)	14 (3%)	2 (0%)	30	43
1	D	496/518 (96%)	484 (98%)	12 (2%)	0	100	100
All	All	1974/2072 (95%)	1919 (97%)	53 (3%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	507	THR
1	C	217	PRO

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	422/434 (97%)	412 (98%)	10 (2%)	43	65
1	B	409/434 (94%)	406 (99%)	3 (1%)	76	88
1	C	400/434 (92%)	392 (98%)	8 (2%)	48	70
1	D	407/434 (94%)	398 (98%)	9 (2%)	45	67
All	All	1638/1736 (94%)	1608 (98%)	30 (2%)	51	73

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	182	ARG
1	A	242	THR
1	A	243	ASN
1	A	267	ILE
1	A	268	LYS
1	A	284	LYS
1	A	327	ILE
1	A	423	ILE
1	A	500	GLN
1	B	174	GLU
1	B	399	GLN
1	B	414	LYS
1	C	7	GLN
1	C	103	SER
1	C	143	MET
1	C	182	ARG
1	C	221	THR
1	C	271	SER
1	C	423	ILE
1	C	485	GLU
1	D	113	ASP
1	D	143	MET
1	D	173	LYS
1	D	205	SER
1	D	209	LEU
1	D	214	THR
1	D	311	SER
1	D	497	ARG
1	D	512	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	265	GLN
1	A	418	GLN
1	A	499	GLN
1	A	517	HIS
1	B	123	ASN
1	B	144	GLN
1	C	34	ASN
1	C	54	HIS
1	C	378	ASN
1	C	399	GLN
1	D	34	ASN
1	D	297	ASN
1	D	500	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 13 are monoatomic - leaving 12 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	B	2521	2	33,33,33	2.37	10 (30%)	45,52,52	2.04	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLU	D	4519	2	8,9,9	1.03	0	8,11,11	1.46	1 (12%)
5	ANP	C	3521	2	33,33,33	2.40	10 (30%)	45,52,52	2.10	15 (33%)
4	CYS	D	4520	-	5,6,6	1.24	0	3,7,7	1.27	0
3	GLU	A	1519	2	8,9,9	1.05	0	8,11,11	1.01	0
4	CYS	C	3520	-	5,6,6	1.05	1 (20%)	3,7,7	1.42	1 (33%)
5	ANP	D	4521	2	33,33,33	2.47	9 (27%)	45,52,52	2.08	14 (31%)
5	ANP	A	1521	2	33,33,33	2.40	10 (30%)	45,52,52	2.05	14 (31%)
4	CYS	A	1520	-	5,6,6	1.25	1 (20%)	3,7,7	1.68	1 (33%)
3	GLU	B	2519	2	8,9,9	0.92	0	8,11,11	1.30	1 (12%)
4	CYS	B	2520	-	5,6,6	0.99	0	3,7,7	1.47	1 (33%)
3	GLU	C	3519	2	8,9,9	1.03	0	8,11,11	1.25	1 (12%)

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	B	2521	2	-	4/18/38/38	0/3/3/3
3	GLU	D	4519	2	-	4/9/9/9	-
5	ANP	C	3521	2	-	3/18/38/38	0/3/3/3
4	CYS	D	4520	-	-	2/6/6/6	-
3	GLU	A	1519	2	-	6/9/9/9	-
4	CYS	C	3520	-	-	3/6/6/6	-
5	ANP	D	4521	2	-	3/18/38/38	0/3/3/3
5	ANP	A	1521	2	-	3/18/38/38	0/3/3/3
4	CYS	A	1520	-	-	1/6/6/6	-
3	GLU	B	2519	2	-	5/9/9/9	-
4	CYS	B	2520	-	-	1/6/6/6	-
3	GLU	C	3519	2	-	6/9/9/9	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	4521	ANP	PG-O1G	6.67	1.56	1.46
5	A	1521	ANP	PG-O1G	6.22	1.55	1.46
5	B	2521	ANP	PG-O1G	5.27	1.54	1.46
5	A	1521	ANP	PB-O1B	5.17	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2521	ANP	PB-O1B	5.15	1.54	1.46
5	C	3521	ANP	PA-O3A	5.10	1.65	1.59
5	B	2521	ANP	C5-C4	4.98	1.48	1.39
5	D	4521	ANP	PB-O1B	4.96	1.53	1.46
5	A	1521	ANP	PB-N3B	4.94	1.76	1.63
5	B	2521	ANP	PG-N3B	4.76	1.75	1.63
5	C	3521	ANP	PB-O3A	4.75	1.65	1.59
5	C	3521	ANP	PG-O1G	4.74	1.53	1.46
5	C	3521	ANP	PB-N3B	4.71	1.75	1.63
5	D	4521	ANP	C5-C4	4.71	1.47	1.39
5	A	1521	ANP	C5-C4	4.66	1.47	1.39
5	C	3521	ANP	PG-N3B	4.65	1.75	1.63
5	D	4521	ANP	PB-O3A	4.62	1.64	1.59
5	D	4521	ANP	PG-N3B	4.60	1.75	1.63
5	D	4521	ANP	PB-N3B	4.53	1.75	1.63
5	C	3521	ANP	C5-C4	4.47	1.47	1.39
5	A	1521	ANP	PG-N3B	4.43	1.74	1.63
5	B	2521	ANP	PB-N3B	4.38	1.74	1.63
5	B	2521	ANP	PA-O3A	4.37	1.64	1.59
5	C	3521	ANP	PB-O1B	4.34	1.52	1.46
5	D	4521	ANP	PA-O3A	4.09	1.63	1.59
5	A	1521	ANP	PA-O3A	3.82	1.63	1.59
5	B	2521	ANP	PB-O3A	3.38	1.63	1.59
5	A	1521	ANP	PB-O3A	3.36	1.63	1.59
5	B	2521	ANP	C5-C6	2.90	1.49	1.41
5	D	4521	ANP	C8-N7	2.62	1.36	1.31
5	C	3521	ANP	C8-N7	2.58	1.36	1.31
5	A	1521	ANP	C8-N7	2.54	1.36	1.31
5	C	3521	ANP	C5-C6	2.50	1.48	1.41
5	A	1521	ANP	C5-C6	2.48	1.47	1.41
5	A	1521	ANP	C4-N9	-2.42	1.32	1.37
5	C	3521	ANP	C5-N7	-2.35	1.34	1.39
5	D	4521	ANP	C5-C6	2.27	1.47	1.41
4	A	1520	CYS	CB-CA	2.17	1.55	1.53
5	B	2521	ANP	C5-N7	-2.12	1.35	1.39
5	B	2521	ANP	C8-N7	2.07	1.35	1.31
4	C	3520	CYS	OXT-C	-2.02	1.24	1.30

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2521	ANP	C5-C4-N3	-6.39	117.92	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	3521	ANP	C5-C4-N3	-5.56	119.06	126.72
5	B	2521	ANP	N3-C4-N9	5.21	136.02	127.17
5	A	1521	ANP	C5-C4-N3	-4.99	119.85	126.72
5	D	4521	ANP	C5-C4-N3	-4.80	120.10	126.72
5	D	4521	ANP	N3-C4-N9	4.63	135.04	127.17
5	A	1521	ANP	N3-C2-N1	-4.45	121.85	128.58
5	B	2521	ANP	C2-N3-C4	4.37	122.51	111.83
5	C	3521	ANP	N3-C4-N9	4.30	134.48	127.17
5	D	4521	ANP	O2B-PB-O1B	4.23	118.95	109.87
5	C	3521	ANP	C2-N3-C4	4.18	122.03	111.83
5	A	1521	ANP	O2B-PB-O1B	4.16	118.80	109.87
5	D	4521	ANP	C4-N9-C8	4.14	110.09	105.74
5	A	1521	ANP	C2-N3-C4	4.14	121.93	111.83
5	D	4521	ANP	N3-C2-N1	-4.01	122.52	128.58
5	A	1521	ANP	N3-C4-N9	3.98	133.93	127.17
5	C	3521	ANP	N3-C2-N1	-3.94	122.62	128.58
5	D	4521	ANP	C2-N3-C4	3.83	121.19	111.83
5	C	3521	ANP	C4-C5-N7	-3.66	106.40	110.58
5	B	2521	ANP	C4-C5-N7	-3.50	106.58	110.58
5	B	2521	ANP	N3-C2-N1	-3.43	123.39	128.58
5	C	3521	ANP	O2B-PB-O1B	3.43	117.22	109.87
5	A	1521	ANP	C4-N9-C8	3.35	109.26	105.74
5	B	2521	ANP	O2B-PB-O1B	3.27	116.87	109.87
5	C	3521	ANP	C5-N7-C8	3.12	108.35	103.45
5	D	4521	ANP	O2B-PB-O3A	-3.09	94.33	104.64
5	C	3521	ANP	C4-N9-C8	3.04	108.93	105.74
5	C	3521	ANP	O1B-PB-N3B	-3.02	107.32	111.77
5	A	1521	ANP	O2B-PB-O3A	-3.00	94.62	104.64
5	B	2521	ANP	O1B-PB-N3B	-2.95	107.43	111.77
5	A	1521	ANP	C4-C5-N7	-2.94	107.22	110.58
5	B	2521	ANP	C5-N7-C8	2.92	108.05	103.45
5	A	1521	ANP	C6-C5-N7	2.89	137.67	132.09
5	C	3521	ANP	N9-C8-N7	-2.86	109.87	113.94
5	D	4521	ANP	O1B-PB-N3B	-2.85	107.57	111.77
5	C	3521	ANP	C6-C5-N7	2.83	137.54	132.09
5	A	1521	ANP	O2G-PG-O3G	2.83	115.19	107.59
5	D	4521	ANP	O1G-PG-N3B	-2.77	107.69	111.77
5	D	4521	ANP	N9-C8-N7	-2.74	110.05	113.94
5	B	2521	ANP	O1G-PG-N3B	-2.74	107.74	111.77
5	C	3521	ANP	O1G-PG-N3B	-2.68	107.82	111.77
5	C	3521	ANP	O2G-PG-O3G	2.65	114.71	107.59
3	C	3519	GLU	OXT-C-O	-2.65	118.08	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2521	ANP	C4-N9-C8	2.60	108.47	105.74
3	B	2519	GLU	OXT-C-O	-2.58	118.23	124.08
3	D	4519	GLU	OXT-C-O	-2.50	118.42	124.08
5	D	4521	ANP	C6-C5-N7	2.49	136.90	132.09
5	B	2521	ANP	C6-C5-N7	2.43	136.77	132.09
5	D	4521	ANP	C4-C5-N7	-2.31	107.94	110.58
4	C	3520	CYS	OXT-C-O	-2.29	118.88	124.08
5	D	4521	ANP	C5-N7-C8	2.29	107.04	103.45
4	B	2520	CYS	OXT-C-O	-2.22	119.03	124.08
5	C	3521	ANP	O5'-C5'-C4'	-2.21	101.46	108.99
4	A	1520	CYS	OXT-C-O	-2.18	119.14	124.08
5	B	2521	ANP	N9-C8-N7	-2.17	110.85	113.94
5	A	1521	ANP	N9-C8-N7	-2.15	110.89	113.94
5	A	1521	ANP	O4'-C1'-N9	2.14	112.20	108.09
5	A	1521	ANP	C2-N1-C6	2.13	122.23	118.73
5	D	4521	ANP	C2-N1-C6	2.11	122.20	118.73
5	A	1521	ANP	O1B-PB-N3B	-2.07	108.72	111.77
5	C	3521	ANP	C5'-C4'-C3'	-2.00	108.01	115.21

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1521	ANP	PB-N3B-PG-O1G
5	B	2521	ANP	PB-N3B-PG-O1G
5	C	3521	ANP	PB-N3B-PG-O1G
5	D	4521	ANP	PB-N3B-PG-O1G
3	C	3519	GLU	OXT-C-CA-CB
4	B	2520	CYS	C-CA-CB-SG
3	C	3519	GLU	O-C-CA-CB
3	A	1519	GLU	OXT-C-CA-CB
5	D	4521	ANP	O4'-C4'-C5'-O5'
3	C	3519	GLU	OXT-C-CA-N
3	A	1519	GLU	O-C-CA-CB
3	D	4519	GLU	O-C-CA-CB
5	A	1521	ANP	C3'-C4'-C5'-O5'
5	D	4521	ANP	C3'-C4'-C5'-O5'
3	C	3519	GLU	O-C-CA-N
3	B	2519	GLU	O-C-CA-CB
3	B	2519	GLU	OXT-C-CA-CB
4	C	3520	CYS	C-CA-CB-SG
3	D	4519	GLU	OXT-C-CA-CB

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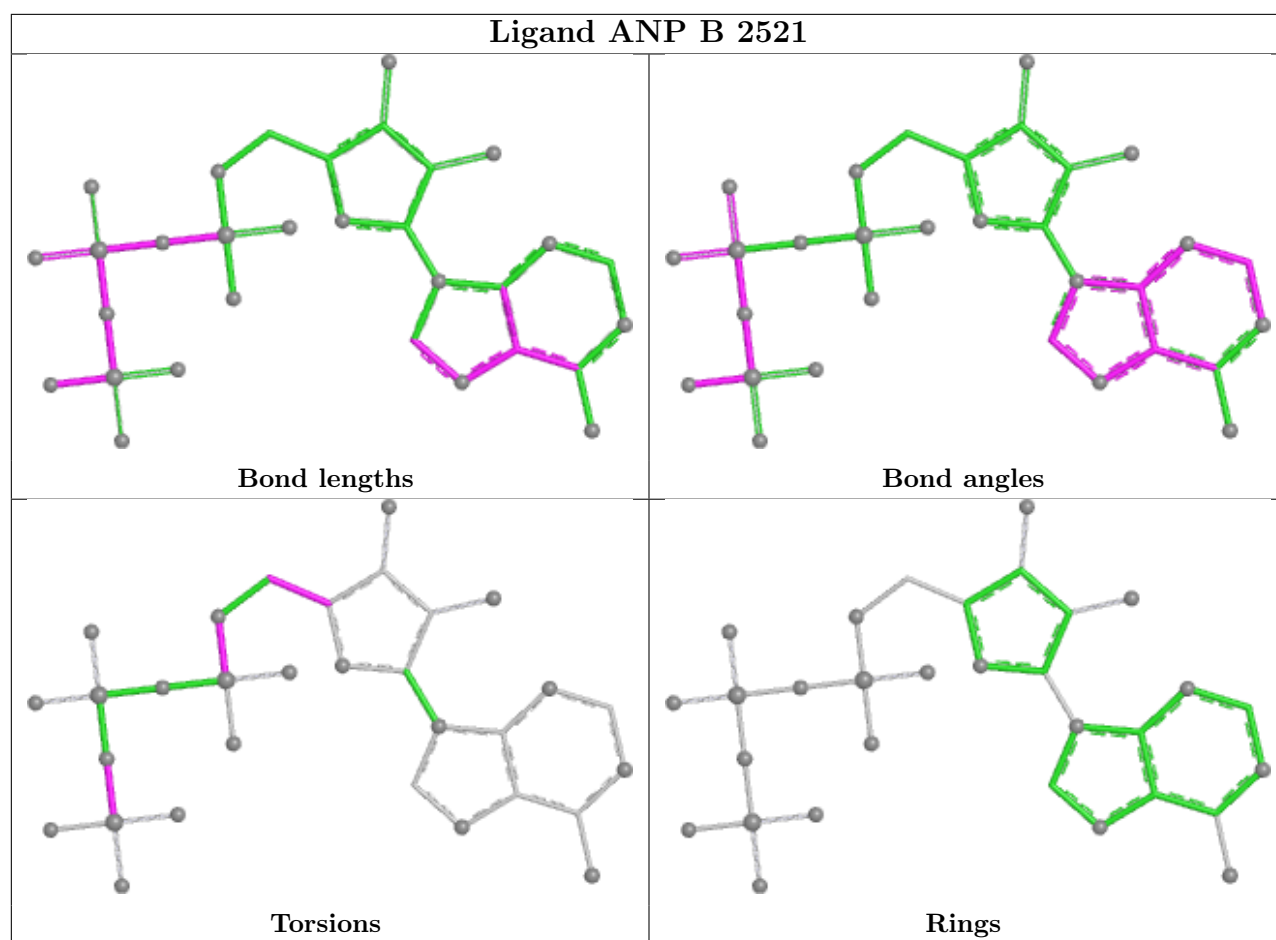
Mol	Chain	Res	Type	Atoms
5	A	1521	ANP	O4'-C4'-C5'-O5'
5	B	2521	ANP	O4'-C4'-C5'-O5'
5	B	2521	ANP	C5'-O5'-PA-O1A
5	C	3521	ANP	C5'-O5'-PA-O1A
3	A	1519	GLU	OXT-C-CA-N
3	B	2519	GLU	OE2-CD-CG-CB
4	C	3520	CYS	O-C-CA-CB
4	C	3520	CYS	OXT-C-CA-CB
4	D	4520	CYS	O-C-CA-CB
4	D	4520	CYS	OXT-C-CA-CB
3	A	1519	GLU	O-C-CA-N
4	A	1520	CYS	O-C-CA-N
3	B	2519	GLU	OE1-CD-CG-CB
3	D	4519	GLU	OE1-CD-CG-CB
3	A	1519	GLU	OE2-CD-CG-CB
3	D	4519	GLU	OE2-CD-CG-CB
3	A	1519	GLU	OE1-CD-CG-CB
3	C	3519	GLU	OE2-CD-CG-CB
5	B	2521	ANP	C3'-C4'-C5'-O5'
3	C	3519	GLU	OE1-CD-CG-CB
3	B	2519	GLU	OXT-C-CA-N
5	C	3521	ANP	O4'-C4'-C5'-O5'

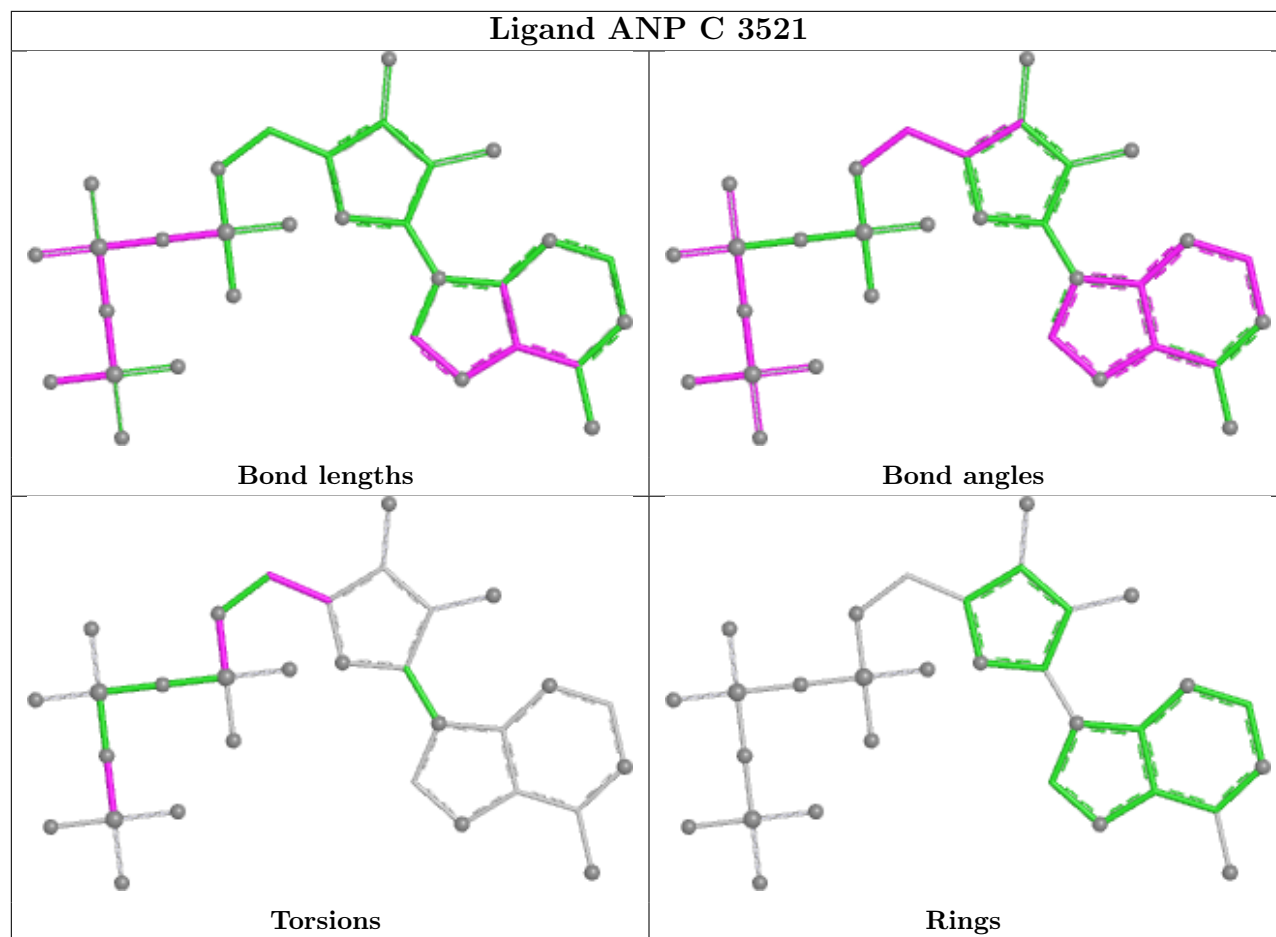
There are no ring outliers.

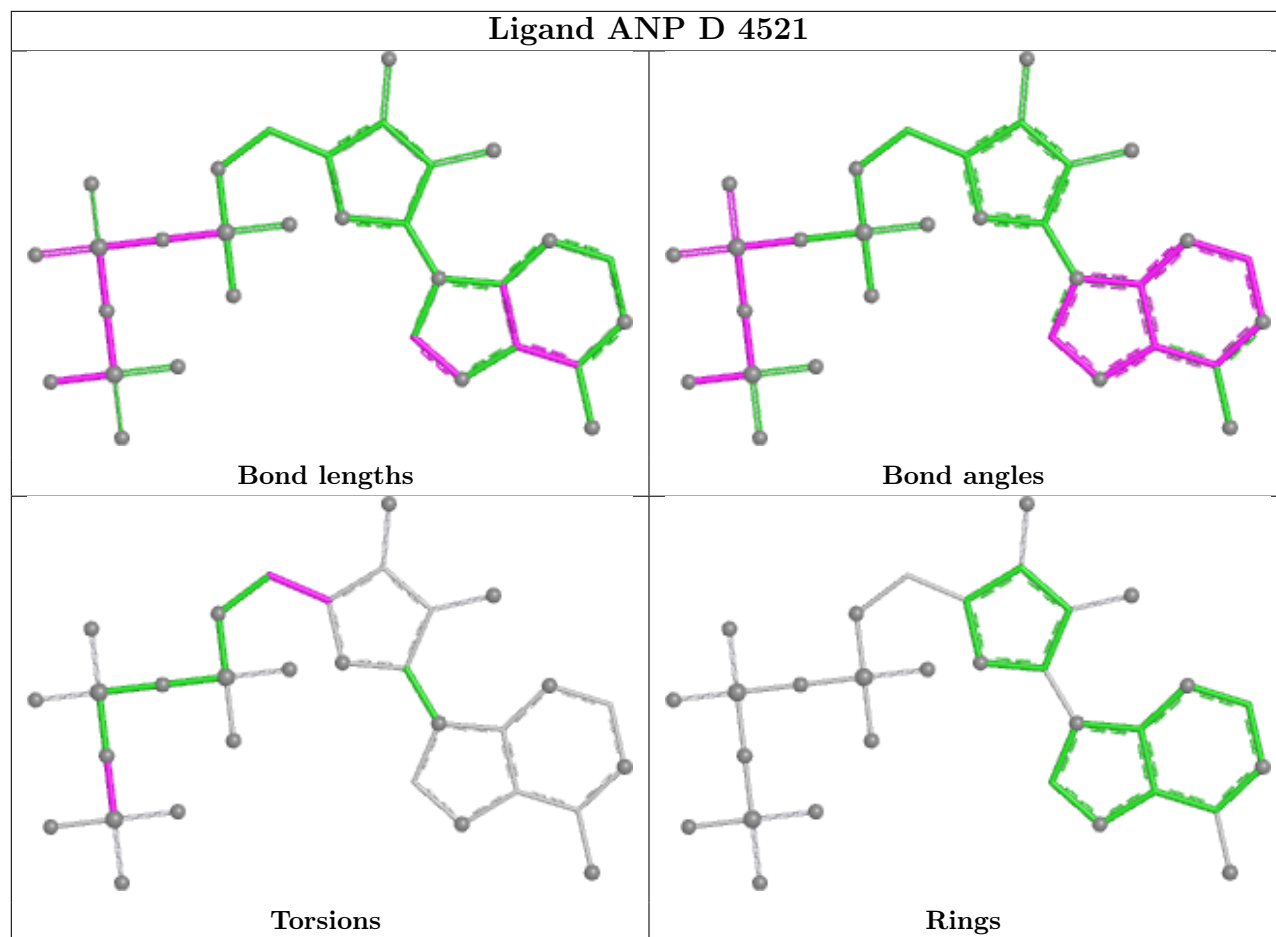
2 monomers are involved in 1 short contact:

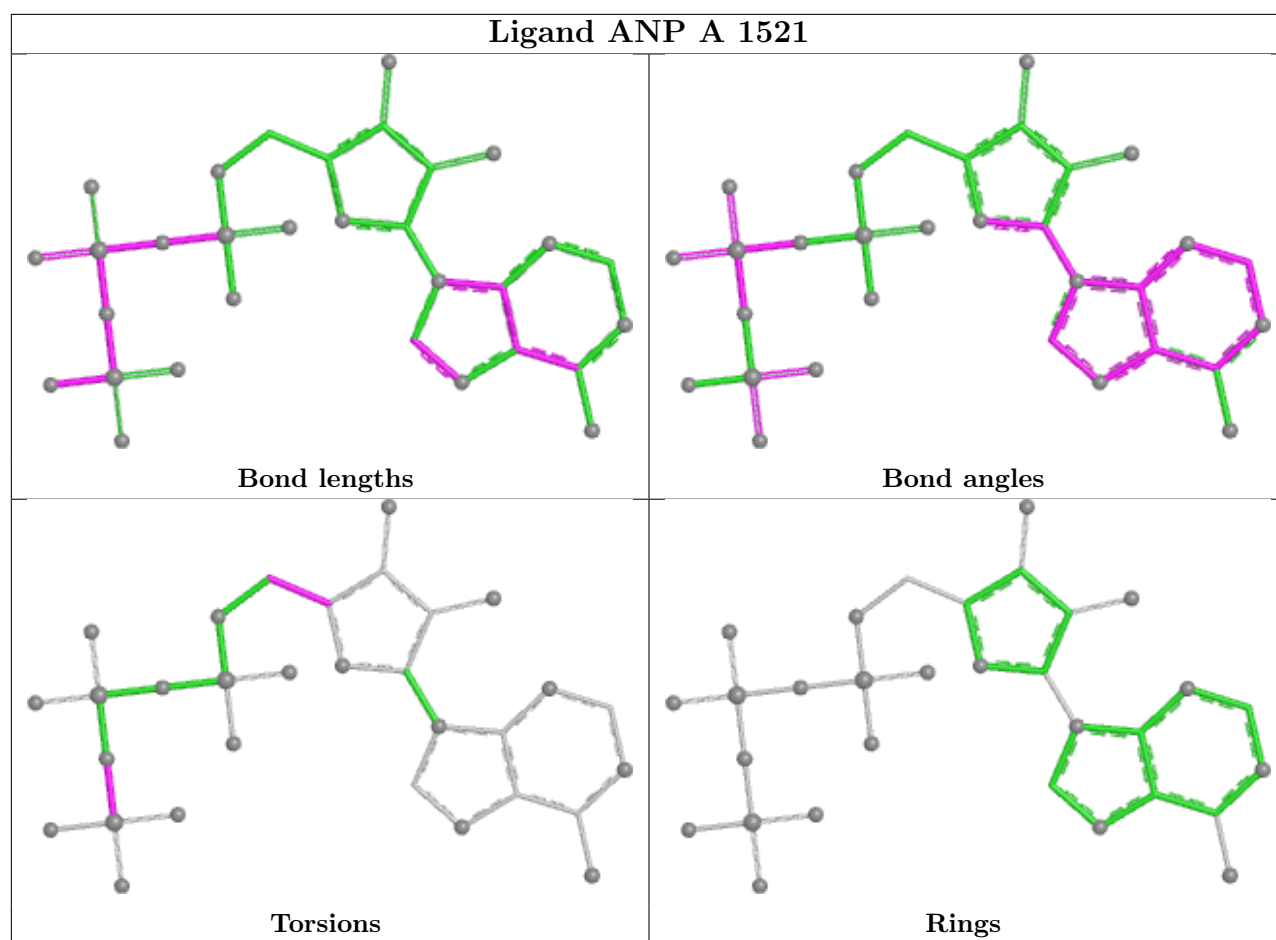
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	4519	GLU	1	0
4	D	4520	CYS	1	0

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	510/518 (98%)	-0.37	17 (3%)	49	45	20, 33, 58, 85	0
1	B	499/518 (96%)	0.20	24 (4%)	35	32	27, 46, 73, 100	0
1	C	499/518 (96%)	0.61	52 (10%)	11	9	35, 53, 85, 95	0
1	D	504/518 (97%)	0.16	37 (7%)	21	17	28, 44, 75, 94	0
All	All	2012/2072 (97%)	0.15	130 (6%)	25	21	20, 45, 76, 100	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	ASN	8.2
1	A	244	LYS	6.6
1	C	109	ALA	6.5
1	D	109	ALA	5.5
1	C	243	ASN	5.3
1	D	163	LYS	5.2
1	D	110	GLU	5.2
1	C	167	ILE	5.2
1	B	508	GLU	5.0
1	D	518	ALA	4.9
1	C	282	ASP	4.8
1	D	111	GLY	4.7
1	B	173	LYS	4.5
1	C	221	THR	4.4
1	D	172	ALA	4.4
1	C	247	SER	4.3
1	C	501	GLU	4.3
1	D	282	ASP	4.3
1	A	246	GLN	4.3
1	C	507	THR	4.2
1	B	248	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	310	ARG	4.2
1	C	511	ALA	4.1
1	B	512	VAL	4.0
1	A	518	ALA	3.9
1	C	248	ASN	3.9
1	C	500	GLN	3.9
1	C	510	PHE	3.9
1	D	243	ASN	3.8
1	C	281	LYS	3.8
1	C	311	SER	3.8
1	D	209	LEU	3.8
1	A	242	THR	3.7
1	D	223	SER	3.7
1	B	518	ALA	3.6
1	C	508	GLU	3.6
1	B	515	GLU	3.5
1	A	245	SER	3.5
1	C	516	LYS	3.5
1	B	505	ALA	3.4
1	A	247	SER	3.4
1	D	283	GLY	3.4
1	C	215	SER	3.3
1	C	113	ASP	3.2
1	B	509	PRO	3.1
1	B	281	LYS	3.1
1	B	246	GLN	3.1
1	D	158	ALA	3.1
1	B	300	TYR	3.0
1	D	300	TYR	3.0
1	D	247	SER	3.0
1	C	283	GLY	3.0
1	C	226	TYR	2.9
1	D	214	THR	2.9
1	B	174	GLU	2.9
1	C	279	ILE	2.8
1	C	512	VAL	2.8
1	A	241	TYR	2.8
1	B	517	HIS	2.8
1	D	279	ILE	2.8
1	D	222	GLU	2.8
1	C	106	SER	2.7
1	C	242	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	163	LYS	2.7
1	B	247	SER	2.7
1	D	517	HIS	2.6
1	C	486	GLU	2.6
1	A	272	GLU	2.6
1	D	207	SER	2.6
1	D	162	ALA	2.6
1	C	107	TYR	2.6
1	C	284	LYS	2.6
1	B	272	GLU	2.6
1	C	280	GLU	2.6
1	A	243	ASN	2.6
1	C	123	ASN	2.6
1	D	248	ASN	2.6
1	B	511	ALA	2.6
1	B	163	LYS	2.6
1	C	506	ASP	2.5
1	A	248	ASN	2.5
1	A	516	LYS	2.5
1	A	517	HIS	2.5
1	D	242	THR	2.5
1	D	277	ILE	2.5
1	C	474	LEU	2.5
1	B	500	GLN	2.5
1	C	277	ILE	2.4
1	A	163	LYS	2.4
1	D	257	TYR	2.4
1	D	272	GLU	2.4
1	C	47	ALA	2.4
1	A	214	THR	2.3
1	D	506	ASP	2.3
1	D	208	PHE	2.3
1	C	246	GLN	2.3
1	C	457	ASP	2.3
1	C	300	TYR	2.3
1	D	512	VAL	2.3
1	A	515	GLU	2.3
1	A	282	ASP	2.3
1	C	225	MET	2.3
1	C	395	CYS	2.3
1	C	515	GLU	2.3
1	C	208	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	214	THR	2.2
1	C	274	TYR	2.2
1	D	275	ALA	2.2
1	B	284	LYS	2.2
1	D	174	GLU	2.2
1	D	477	GLU	2.2
1	C	217	PRO	2.2
1	C	424	ASN	2.2
1	C	220	LYS	2.2
1	D	276	LYS	2.2
1	C	490	ALA	2.1
1	C	509	PRO	2.1
1	D	112	GLN	2.1
1	A	395	CYS	2.1
1	D	160	TRP	2.1
1	C	241	TYR	2.1
1	C	425	GLY	2.1
1	D	508	GLU	2.1
1	B	276	LYS	2.1
1	D	246	GLN	2.0
1	B	285	ARG	2.0
1	C	488	PHE	2.0
1	C	493	GLU	2.0
1	C	513	TRP	2.0
1	D	311	SER	2.0

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

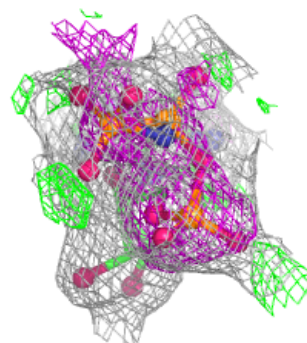
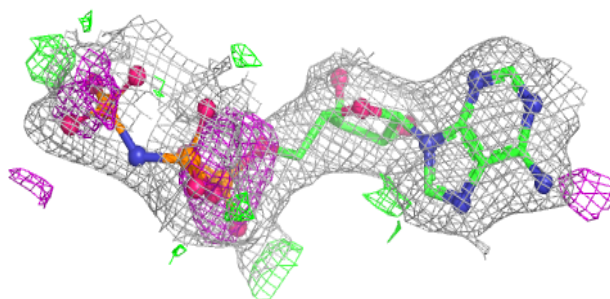
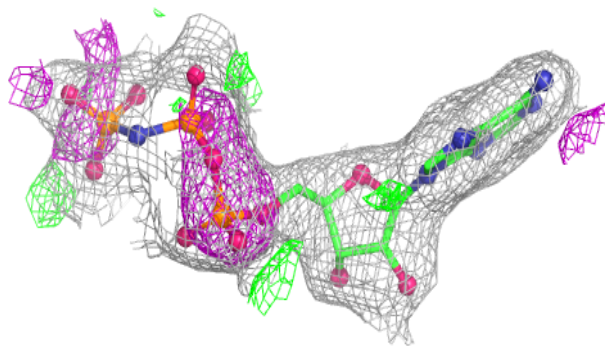
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	MG	B	2524	1/1	0.83	0.27	76,76,76,76	0
3	GLU	A	1519	10/10	0.86	0.16	44,46,49,50	0
5	ANP	C	3521	31/31	0.90	0.10	37,52,72,72	0
2	MG	C	3522	1/1	0.91	0.06	52,52,52,52	0
5	ANP	B	2521	31/31	0.91	0.11	39,44,64,65	0
2	MG	C	3524	1/1	0.91	0.13	67,67,67,67	0
5	ANP	D	4521	31/31	0.91	0.10	30,38,62,63	0
3	GLU	B	2519	10/10	0.92	0.11	45,48,49,51	0
3	GLU	C	3519	10/10	0.92	0.11	56,57,59,59	0
4	CYS	D	4520	7/7	0.92	0.18	42,52,54,55	0
5	ANP	A	1521	31/31	0.93	0.10	25,34,58,58	0
2	MG	B	2522	1/1	0.93	0.09	45,45,45,45	0
2	MG	B	2523	1/1	0.94	0.10	49,49,49,49	0
2	MG	D	4522	1/1	0.94	0.04	33,33,33,33	0
2	MG	D	4523	1/1	0.94	0.12	45,45,45,45	0
3	GLU	D	4519	10/10	0.94	0.13	36,38,39,39	0
4	CYS	C	3520	7/7	0.94	0.13	58,59,60,60	0
2	MG	A	1522	1/1	0.95	0.09	38,38,38,38	0
2	MG	C	3523	1/1	0.96	0.08	58,58,58,58	0
4	CYS	B	2520	7/7	0.96	0.14	50,53,54,54	0
2	MG	A	1524	1/1	0.97	0.14	42,42,42,42	0
2	MG	A	1523	1/1	0.97	0.06	49,49,49,49	0
2	MG	D	4524	1/1	0.98	0.14	48,48,48,48	0
4	CYS	A	1520	7/7	0.98	0.12	31,36,39,40	0
2	MG	A	1525	1/1	0.98	0.12	40,40,40,40	0

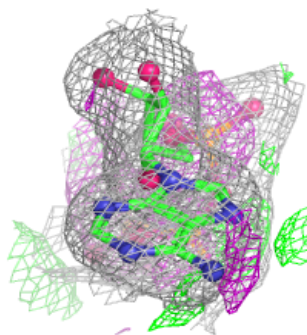
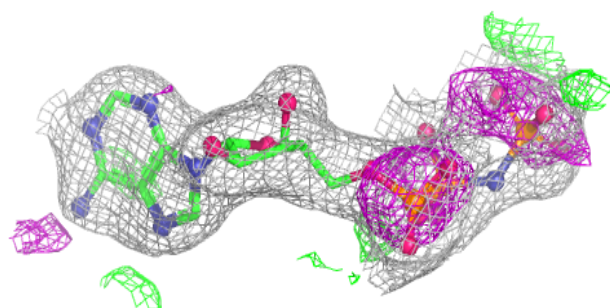
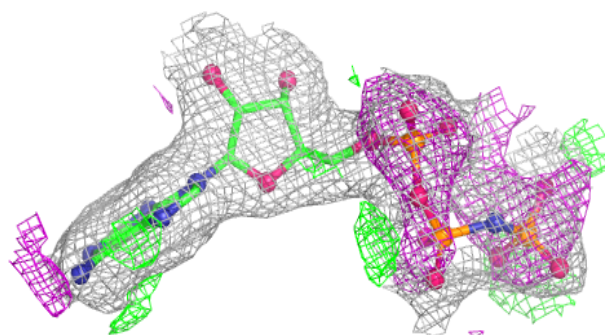
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP C 3521:

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

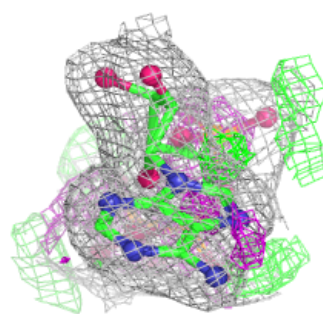
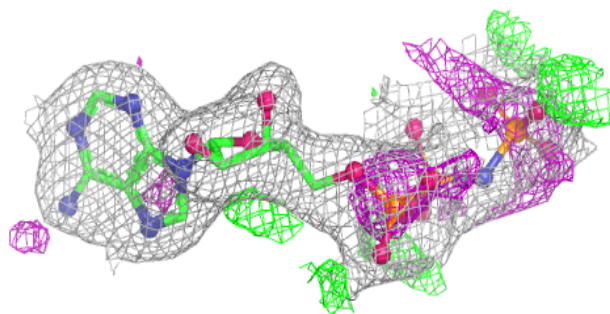
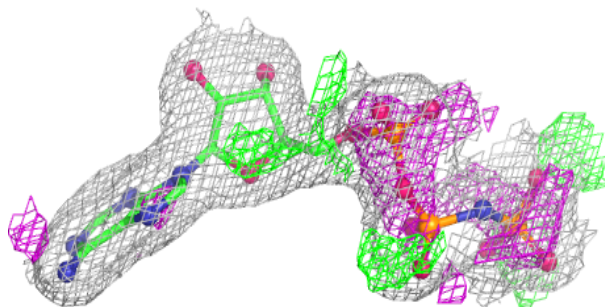
**Electron density around ANP B 2521:**

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

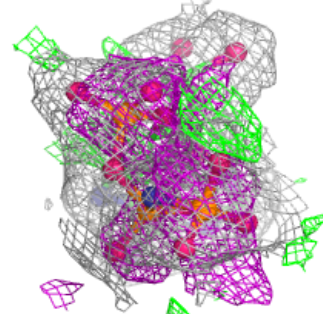
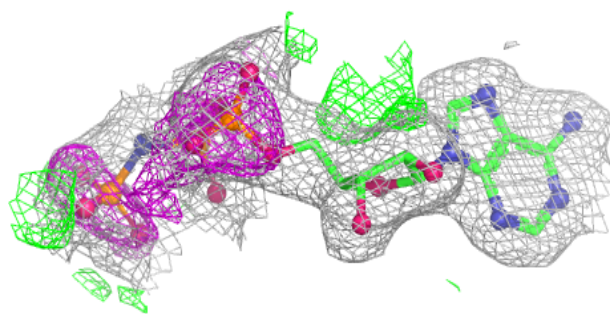
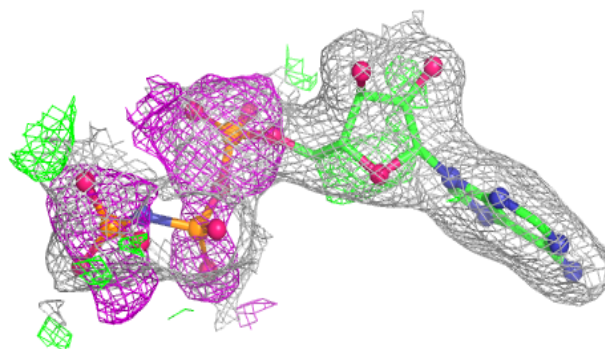


Electron density around ANP D 4521:

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

**Electron density around ANP A 1521:**

$2mF_o-DF_c$ (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.