



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:07 PM UTC

PDB ID : 2D33 / pdb_00002d33
Title : Crystal Structure of gamma-Glutamylcysteine Synthetase Complexed with Aluminum Fluoride
Authors : Hibi, T.; Nakayama, M.; Nii, H.; Kurokawa, Y.; Katano, H.; Oda, J.
Deposited on : 2005-09-25
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

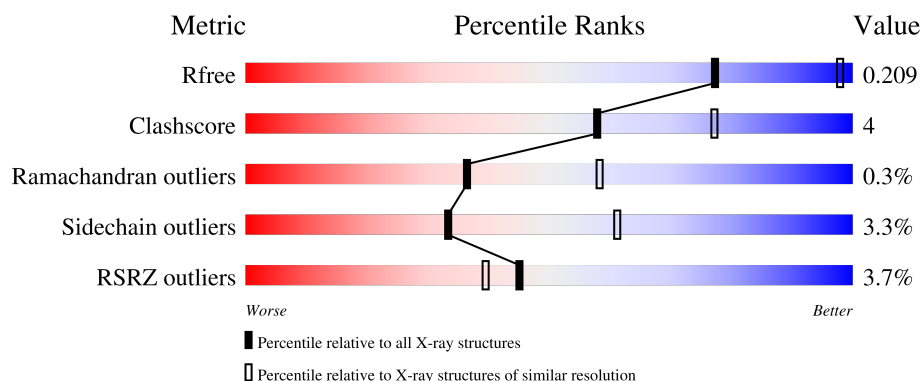
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	2% 87% 10% ..
1	B	518	4% 85% 12% ..
1	C	518	5% 85% 10% ..
1	D	518	4% 85% 11% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16327 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
			4009	2546	685	760	18			
1	B	503	Total	C	N	O	S	0	0	0
			3933	2508	669	738	18			
1	C	504	Total	C	N	O	S	0	0	0
			3925	2508	662	737	18			
1	D	499	Total	C	N	O	S	0	0	0
			3909	2490	666	735	18			

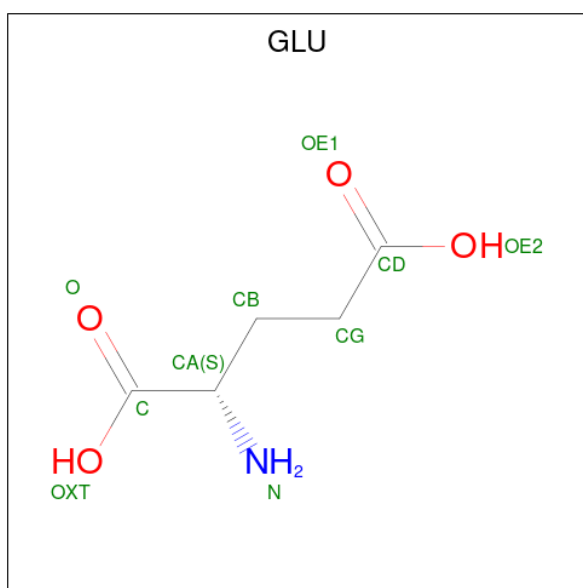
There are 16 discrepancies between the modelled and reference sequences:

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).

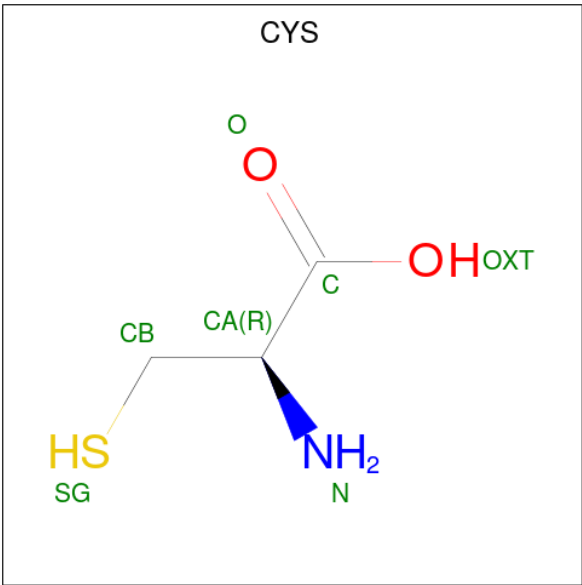
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total 4 Mg 4	0	0
2	B	3	Total 3 Mg 3	0	0
2	C	3	Total 3 Mg 3	0	0
2	D	3	Total 3 Mg 3	0	0

- Molecule 3 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$).



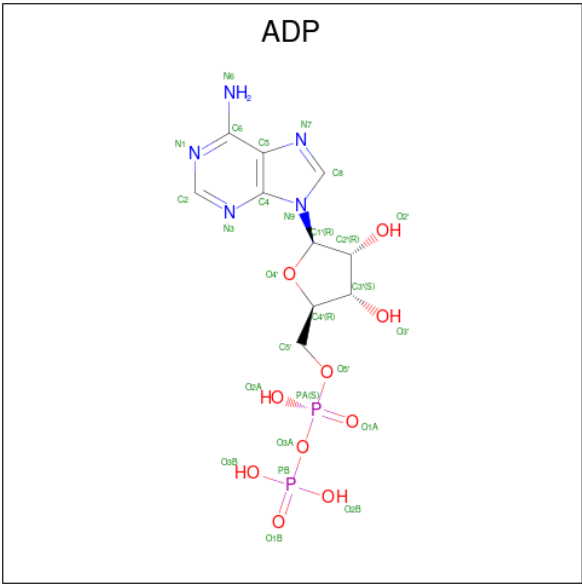
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total 10 C 5 N 1 O 4	0	0
3	B	1	Total 10 C 5 N 1 O 4	0	0
3	C	1	Total 10 C 5 N 1 O 4	0	0
3	D	1	Total 10 C 5 N 1 O 4	0	0

- Molecule 4 is CYSTEINE (CCD ID: CYS) (formula: $C_3H_7NO_2S$).



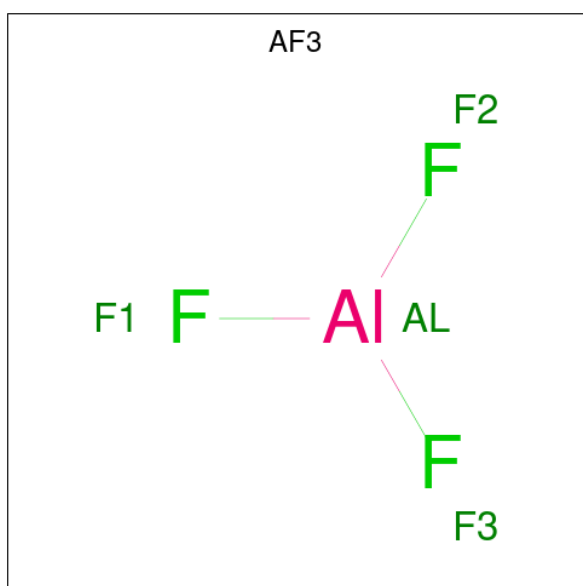
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
4	B	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
4	C	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
4	D	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Al	F	0	0
			4	1	3		
6	B	1	Total	Al	F	0	0
			4	1	3		
6	C	1	Total	Al	F	0	0
			4	1	3		
6	D	1	Total	Al	F	0	0
			4	1	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	174	Total	O	0	0
			174	174		
7	B	66	Total	O	0	0
			66	66		

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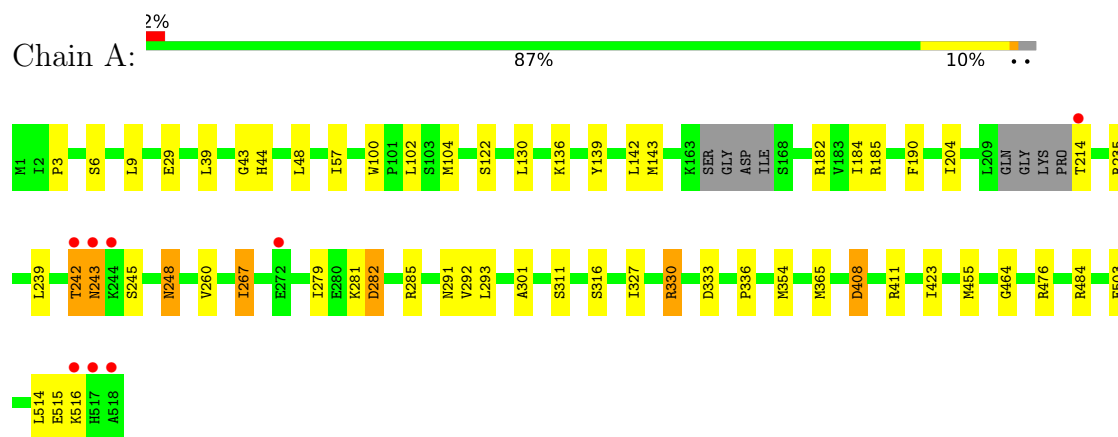
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	27	Total	O	0	0
			27	27		
7	D	79	Total	O	0	0
			79	79		

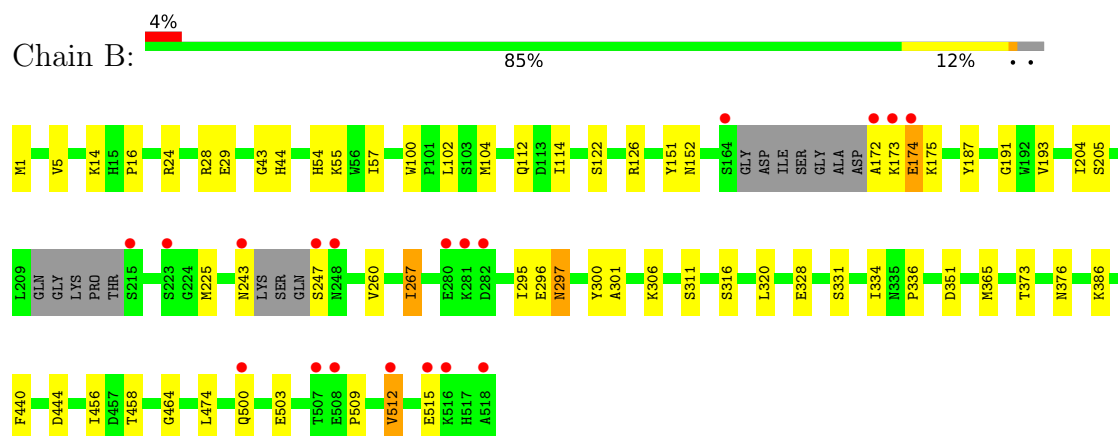
3 Residue-property plots

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.

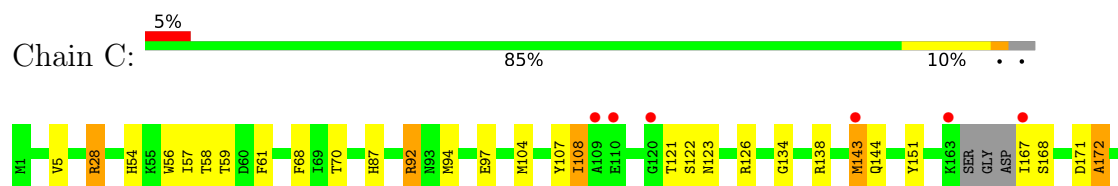
- Molecule 1: Glutamate–cysteine ligase

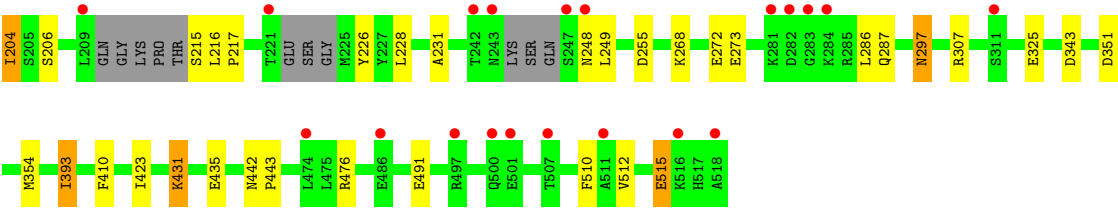


- Molecule 1: Glutamate–cysteine ligase

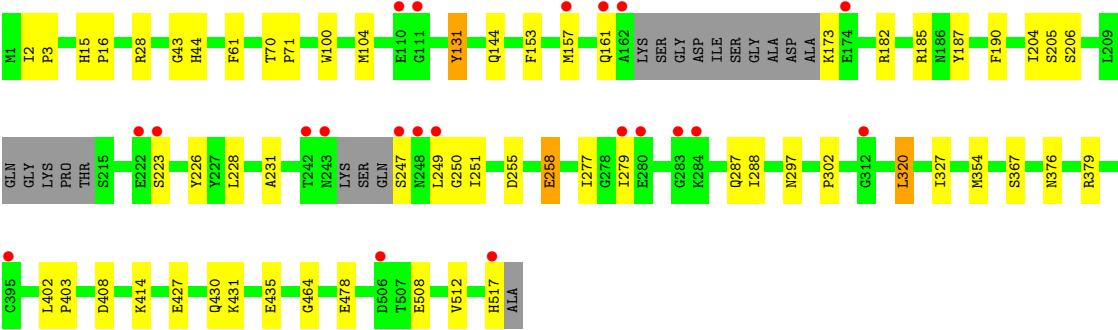
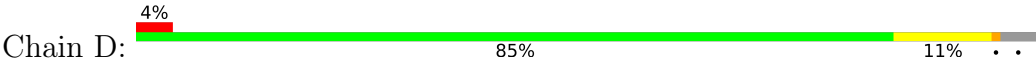


- Molecule 1: Glutamate–cysteine ligase





● 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	325.23Å 325.23Å 105.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.60 40.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.60) 99.9 (40.00-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.18 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.162 , 0.191 0.182 , 0.209	Depositor DCC
R_{free} test set	6408 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16327	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: AF3, ADP, 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	0.96	0/4096	1.02	3/5547 (0.1%)
1	B	0.81	0/4019	0.96	4/5447 (0.1%)
1	C	0.76	0/4010	0.92	2/5431 (0.0%)
1	D	0.83	0/3993	0.98	7/5414 (0.1%)
All	All	0.85	0/16118	0.97	16/21839 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ASN	N-CA-C	6.78	118.75	111.36
1	D	279	ILE	N-CA-C	-5.95	107.08	111.90
1	D	2	ILE	CA-C-N	-5.93	114.16	120.03
1	D	2	ILE	C-N-CA	-5.93	114.16	120.03
1	A	267	ILE	CB-CA-C	-5.82	103.55	112.05
1	B	301	ALA	CA-C-N	5.81	125.67	119.28
1	B	301	ALA	C-N-CA	5.81	125.67	119.28
1	C	410	PHE	N-CA-C	5.62	118.33	111.82
1	A	184	ILE	N-CA-C	5.60	115.80	110.42
1	C	393	ILE	CB-CA-C	-5.38	104.78	111.08
1	D	182	ARG	N-CA-C	-5.22	105.59	111.28
1	B	311	SER	N-CA-C	5.21	118.32	111.28
1	B	444	ASP	N-CA-C	5.08	118.96	112.87
1	D	131	TYR	N-CA-C	-5.05	105.91	111.71
1	D	478	GLU	CA-C-N	-5.02	115.39	120.31
1	D	478	GLU	C-N-CA	-5.02	115.39	120.31

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	4009	0	3901	34	0
1	B	3933	0	3810	39	0
1	C	3925	0	3793	37	0
1	D	3909	0	3776	30	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	1	0
3	B	10	0	5	1	0
3	C	10	0	5	1	0
3	D	10	0	5	0	0
4	A	7	0	4	0	0
4	B	7	0	4	0	0
4	C	7	0	4	1	0
4	D	7	0	4	0	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
5	C	27	0	12	0	0
5	D	27	0	12	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
6	C	4	0	0	0	0
6	D	4	0	0	0	0
7	A	174	0	0	1	0
7	B	66	0	0	0	0
7	C	27	0	0	0	0
7	D	79	0	0	0	0
All	All	16327	0	15364	141	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 (141) 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:C:104:MET:HE2	1:C:204:ILE:HG22	1.43	1.00
1:D:255:ASP:HB3	1:D:258:GLU:HB2	1.56	0.88
1:C:104:MET:HE2	1:C:204:ILE:CG2	2.07	0.83
1:A:139:TYR:HB3	1:A:242:THR:HB	1.66	0.77
1:A:143:MET:HG3	1:A:242:THR:HG23	1.69	0.74
1:D:104:MET:HE2	1:D:204:ILE:HG13	1.71	0.72
1:D:250:GLY:HA2	1:D:367:SER:OG	1.93	0.69
1:C:54:HIS:HD2	1:C:56:TRP:H	1.40	0.69
1:D:173:LYS:O	1:D:173:LYS:HG2	1.93	0.67
1:B:365:MET:HE1	1:B:373:THR:CG2	2.27	0.65
1:C:104:MET:CE	1:C:204:ILE:HG22	2.23	0.64
1:B:28:ARG:HD3	1:B:28:ARG:C	2.23	0.64
1:A:29:GLU:OE2	3:A:519:GLU:HG3	1.98	0.64
1:C:354:MET:HA	1:C:354:MET:HE2	1.78	0.63
1:D:427:GLU:CB	1:D:427:GLU:OE2	2.46	0.63
1:B:509:PRO:HG2	1:B:512:VAL:HG13	1.82	0.61
1:D:327:ILE:CD1	1:D:354:MET:HE2	2.30	0.61
1:D:327:ILE:HD11	1:D:354:MET:HE2	1.81	0.61
1:A:245:SER:HB3	1:A:248:ASN:HB2	1.81	0.61
1:B:152:ASN:OD1	1:B:328:GLU:HG3	2.01	0.60
1:B:14:LYS:C	1:B:16:PRO:HD3	2.27	0.59
1:D:187:TYR:HE2	1:D:302:PRO:HB2	1.67	0.59
1:B:5:VAL:HG12	1:B:5:VAL:O	2.03	0.59
1:B:104:MET:HE3	1:B:204:ILE:HG13	1.84	0.58
1:C:286:LEU:O	1:C:287:GLN:HB3	2.03	0.58
1:B:267:ILE:HD11	1:B:296:GLU:HG2	1.87	0.56
1:C:5:VAL:HG12	1:C:5:VAL:O	2.04	0.56
1:C:491:GLU:HA	1:C:491:GLU:OE1	2.06	0.56
1:B:365:MET:HE1	1:B:373:THR:HG21	1.87	0.55
1:D:327:ILE:C	1:D:327:ILE:HD12	2.32	0.54
1:C:58:THR:OG1	1:C:59:THR:N	2.40	0.53
1:D:131:TYR:HB2	1:D:288:ILE:HD11	1.90	0.53
1:A:100:TRP:CH2	1:A:464:GLY:HA3	2.44	0.53
1:C:107:TYR:O	1:C:108:ILE:HG12	2.09	0.52
1:C:107:TYR:C	1:C:108:ILE:HG12	2.34	0.52
1:B:267:ILE:HD13	1:B:295:ILE:HA	1.91	0.52
1:A:476:ARG:HD2	7:A:548:HOH:O	2.10	0.52
1:A:104:MET:HE2	1:A:204:ILE:HG13	1.92	0.51
1:A:408:ASP:OD1	1:A:411:ARG:NH2	2.43	0.51
1:D:247:SER:C	1:D:249:LEU:H	2.19	0.51
1:C:228:LEU:HB2	1:C:231:ALA:HB2	1.91	0.51
1:D:431:LYS:O	1:D:435:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:ILE:CD1	1:B:296:GLU:HG2	2.41	0.51
1:B:187:TYR:OH	1:B:331:SER:OG	2.22	0.50
1:B:174:GLU:O	1:B:174:GLU:HG2	2.11	0.50
1:B:297:ASN:OD1	1:B:297:ASN:N	2.42	0.50
1:A:48:LEU:HD13	1:A:57:ILE:HG21	1.94	0.49
1:A:301:ALA:O	1:A:330:ARG:HD3	2.12	0.49
1:D:28:ARG:C	1:D:28:ARG:HD3	2.38	0.48
1:A:139:TYR:HB3	1:A:242:THR:CB	2.38	0.48
1:C:134:GLY:O	1:C:138:ARG:HG3	2.12	0.48
1:D:376:ASN:OD1	1:D:379:ARG:NH1	2.47	0.48
1:D:402:LEU:HB3	1:D:403:PRO:HD3	1.96	0.48
1:B:151:TYR:OH	1:B:351:ASP:OD1	2.32	0.48
1:C:151:TYR:OH	1:C:351:ASP:OD1	2.30	0.48
1:C:68:PHE:CD2	1:C:87:HIS:CE1	3.03	0.47
1:D:414:LYS:HE3	1:D:430:GLN:HB3	1.96	0.47
1:B:122:SER:HB3	1:B:503:GLU:HG3	1.94	0.47
1:D:402:LEU:C	1:D:402:LEU:HD23	2.38	0.47
1:C:94:MET:HE2	1:C:97:GLU:C	2.39	0.47
1:B:193:VAL:HG23	1:B:440:PHE:HZ	1.80	0.47
1:C:297:ASN:OD1	1:C:297:ASN:N	2.48	0.47
1:D:43:GLY:O	1:D:44:HIS:C	2.58	0.47
1:A:235:ARG:HD3	1:A:333:ASP:OD1	2.15	0.46
1:B:260:VAL:HG11	1:B:320:LEU:HG	1.97	0.46
1:C:92:ARG:HD2	1:C:476:ARG:O	2.15	0.46
1:D:206:SER:HB3	1:D:226:TYR:HE1	1.79	0.46
1:B:172:ALA:O	1:B:175:LYS:N	2.50	0.45
1:C:28:ARG:HD3	1:C:28:ARG:C	2.41	0.45
1:B:334:ILE:O	1:B:336:PRO:HD3	2.16	0.45
1:D:327:ILE:HD12	1:D:327:ILE:O	2.15	0.45
1:D:61:PHE:CG	1:D:144:GLN:HB3	2.52	0.45
1:A:243:ASN:OD1	1:A:243:ASN:N	2.43	0.45
1:B:24:ARG:HA	1:B:152:ASN:O	2.17	0.45
1:A:122:SER:HB3	1:A:503:GLU:HG3	1.99	0.45
1:B:172:ALA:O	1:B:173:LYS:C	2.58	0.45
1:C:167:ILE:O	1:C:167:ILE:HG13	2.16	0.45
1:A:267:ILE:HD13	1:A:293:LEU:HB2	1.98	0.44
1:B:100:TRP:CH2	1:B:464:GLY:HA3	2.52	0.44
1:A:3:PRO:HD3	1:A:190:PHE:CZ	2.52	0.44
1:C:249:LEU:HD23	1:C:249:LEU:HA	1.76	0.44
1:C:431:LYS:HE2	1:C:435:GLU:OE2	2.17	0.44
1:A:104:MET:CE	1:A:204:ILE:HG13	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:GLN:O	1:B:114:ILE:HD12	2.17	0.44
1:A:185:ARG:HB3	1:A:365:MET:HE2	1.99	0.44
1:D:320:LEU:HD12	1:D:320:LEU:HA	1.87	0.44
1:C:121:THR:O	1:C:126:ARG:NH2	2.51	0.44
1:D:15:HIS:N	1:D:16:PRO:HD3	2.33	0.44
1:D:508:GLU:H	1:D:508:GLU:CD	2.15	0.44
1:B:267:ILE:O	1:B:267:ILE:CG2	2.67	0.43
1:C:307:ARG:CZ	1:C:325:GLU:HB2	2.48	0.43
1:D:100:TRP:CH2	1:D:464:GLY:HA3	2.54	0.43
1:C:442:ASN:HA	1:C:443:PRO:HD2	1.90	0.43
1:B:1:MET:HE1	1:B:376:ASN:ND2	2.33	0.43
1:A:484:ARG:HA	1:A:484:ARG:HD3	1.85	0.43
1:A:130:LEU:HD11	1:A:285:ARG:HG3	2.00	0.43
1:A:43:GLY:O	1:A:44:HIS:C	2.61	0.43
1:A:142:LEU:HD12	1:A:142:LEU:HA	1.83	0.43
1:D:153:PHE:CD1	1:D:153:PHE:C	2.97	0.43
1:B:191:GLY:C	1:B:193:VAL:N	2.77	0.42
1:B:296:GLU:OE2	1:B:316:SER:OG	2.37	0.42
1:C:107:TYR:C	1:C:108:ILE:CG1	2.92	0.42
1:A:327:ILE:HD13	1:A:327:ILE:HA	1.73	0.42
1:B:267:ILE:O	1:B:267:ILE:HG22	2.18	0.42
1:C:272:GLU:O	1:C:273:GLU:C	2.62	0.42
1:B:225:MET:HE2	1:B:225:MET:HB3	1.93	0.42
1:A:291:ASN:O	1:A:292:VAL:C	2.62	0.42
3:C:2519:GLU:OE1	4:C:2520:CYS:HA	2.20	0.42
1:B:243:ASN:CG	1:B:300:TYR:CD2	2.97	0.42
1:C:226:TYR:CD1	1:C:226:TYR:N	2.87	0.42
1:D:228:LEU:HB2	1:D:231:ALA:HB2	2.01	0.42
1:D:255:ASP:HB3	1:D:258:GLU:CB	2.38	0.42
1:C:143:MET:O	1:C:143:MET:HG2	2.18	0.42
1:A:102:LEU:HD23	1:A:336:PRO:HB3	2.02	0.42
1:A:214:THR:HG21	1:A:239:LEU:HD21	2.02	0.42
1:B:43:GLY:O	1:B:44:HIS:C	2.63	0.42
1:C:123:ASN:OD1	1:C:510:PHE:HA	2.20	0.42
1:A:281:LYS:O	1:A:282:ASP:HB2	2.20	0.41
1:A:260:VAL:HG13	1:A:316:SER:HB2	2.02	0.41
1:B:122:SER:O	1:B:126:ARG:HG3	2.20	0.41
1:C:343:ASP:C	1:C:343:ASP:OD1	2.63	0.41
1:C:216:LEU:HA	1:C:217:PRO:HD3	1.81	0.41
1:C:512:VAL:O	1:C:515:GLU:HB3	2.21	0.41
1:C:171:ASP:O	1:C:172:ALA:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:THR:HA	1:D:71:PRO:HD3	1.83	0.41
1:A:354:MET:HE2	1:A:354:MET:HA	2.03	0.41
1:B:191:GLY:C	1:B:193:VAL:H	2.29	0.41
1:B:512:VAL:O	1:B:515:GLU:HG2	2.21	0.41
1:C:354:MET:HE2	1:C:354:MET:CA	2.48	0.41
1:A:267:ILE:O	1:A:267:ILE:HG22	2.19	0.40
1:A:514:LEU:C	1:A:516:LYS:H	2.29	0.40
1:C:61:PHE:CG	1:C:144:GLN:HB3	2.55	0.40
1:A:102:LEU:HD13	1:A:455:MET:CE	2.51	0.40
1:B:54:HIS:HB3	1:B:57:ILE:O	2.21	0.40
1:B:102:LEU:HD23	1:B:336:PRO:HB3	2.03	0.40
1:B:296:GLU:H	1:B:296:GLU:HG3	1.68	0.40
1:A:9:LEU:HD23	1:A:9:LEU:HA	1.92	0.40
1:A:514:LEU:C	1:A:516:LYS:N	2.79	0.40
1:C:54:HIS:CD2	1:C:57:ILE:H	2.40	0.40
1:B:29:GLU:OE2	3:B:1519:GLU:HB2	2.21	0.40
1:D:3:PRO:HD3	1:D:190:PHE:CZ	2.57	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	504/518 (97%)	488 (97%)	14 (3%)	2 (0%)	30	51
1	B	495/518 (96%)	481 (97%)	14 (3%)	0	100	100
1	C	494/518 (95%)	466 (94%)	25 (5%)	3 (1%)	21	42
1	D	491/518 (95%)	471 (96%)	19 (4%)	1 (0%)	43	66
All	All	1984/2072 (96%)	1906 (96%)	72 (4%)	6 (0%)	36	58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	248	ASN
1	A	515	GLU
1	C	122	SER
1	C	172	ALA
1	A	282	ASP
1	D	161	GLN

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	416/434 (96%)	405 (97%)	11 (3%)	40	68
1	B	401/434 (92%)	388 (97%)	13 (3%)	34	62
1	C	396/434 (91%)	380 (96%)	16 (4%)	28	55
1	D	400/434 (92%)	387 (97%)	13 (3%)	33	61
All	All	1613/1736 (93%)	1560 (97%)	53 (3%)	33	61

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	39	LEU
1	A	136	LYS
1	A	182	ARG
1	A	242	THR
1	A	243	ASN
1	A	279	ILE
1	A	311	SER
1	A	330	ARG
1	A	408	ASP
1	A	423	ILE
1	B	55	LYS
1	B	174	GLU
1	B	205	SER
1	B	247	SER
1	B	267	ILE

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Mol	Chain	Res	Type
1	B	297	ASN
1	B	306	LYS
1	B	386	LYS
1	B	456	ILE
1	B	458	THR
1	B	474	LEU
1	B	500	GLN
1	B	512	VAL
1	C	28	ARG
1	C	70	THR
1	C	92	ARG
1	C	108	ILE
1	C	143	MET
1	C	168	SER
1	C	204	ILE
1	C	206	SER
1	C	215	SER
1	C	255	ASP
1	C	268	LYS
1	C	297	ASN
1	C	393	ILE
1	C	423	ILE
1	C	431	LYS
1	C	515	GLU
1	D	157	MET
1	D	185	ARG
1	D	205	SER
1	D	223	SER
1	D	251	ILE
1	D	258	GLU
1	D	277	ILE
1	D	287	GLN
1	D	297	ASN
1	D	320	LEU
1	D	408	ASP
1	D	512	VAL
1	D	517	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	418	GLN

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Mol	Chain	Res	Type
1	B	44	HIS
1	B	404	GLN
1	B	418	GLN
1	C	17	GLN
1	C	54	HIS
1	C	378	ASN
1	D	144	GLN
1	D	404	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 29 ligands modelled in this entry, 13 are monoatomic - leaving 16 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	$\# Z > 2$
4	CYS	A	520	6	5,6,6	1.36	0	3,7,7	1.81	1 (33%)
6	AF3	C	2522	3,2,5,1	0,3,3	-	-	-		
6	AF3	D	3522	2,7,4,3,1,5	0,3,3	-	-	-		
5	ADP	D	3521	6,2	28,29,29	1.45	3 (10%)	43,45,45	1.98	11 (25%)
3	GLU	B	1519	6,2	8,9,9	1.11	0	8,11,11	0.93	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CYS	D	3520	6	5,6,6	1.27	0	3,7,7	1.75	1 (33%)
4	CYS	B	1520	-	5,6,6	0.97	0	3,7,7	1.41	1 (33%)
3	GLU	D	3519	6,2	8,9,9	1.05	0	8,11,11	1.13	1 (12%)
5	ADP	B	1521	6,2	28,29,29	1.37	4 (14%)	43,45,45	1.83	9 (20%)
3	GLU	C	2519	6,2	8,9,9	1.05	0	8,11,11	1.12	1 (12%)
5	ADP	C	2521	6,2	28,29,29	1.32	4 (14%)	43,45,45	1.98	10 (23%)
6	AF3	B	1522	3,2,5,1	0,3,3	-	-	-	-	-
3	GLU	A	519	6,2	8,9,9	1.25	0	8,11,11	1.32	1 (12%)
5	ADP	A	521	6,2	28,29,29	1.22	3 (10%)	43,45,45	2.27	14 (32%)
4	CYS	C	2520	-	5,6,6	1.08	0	3,7,7	1.22	0
6	AF3	A	522	2,7,4,3,5	0,3,3	-	-	-	-	-

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
4	CYS	A	520	6	-	0/6/6/6	-
5	ADP	D	3521	6,2	-	4/16/32/32	0/3/3/3
3	GLU	B	1519	6,2	-	4/9/9/9	-
4	CYS	D	3520	6	-	0/6/6/6	-
4	CYS	B	1520	-	-	0/6/6/6	-
3	GLU	D	3519	6,2	-	4/9/9/9	-
5	ADP	B	1521	6,2	-	4/16/32/32	0/3/3/3
3	GLU	C	2519	6,2	-	6/9/9/9	-
5	ADP	C	2521	6,2	-	4/16/32/32	0/3/3/3
3	GLU	A	519	6,2	-	7/9/9/9	-
5	ADP	A	521	6,2	-	2/16/32/32	0/3/3/3
4	CYS	C	2520	-	-	0/6/6/6	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	3521	ADP	C5-C4	4.71	1.47	1.39
5	B	1521	ADP	C5-C4	4.22	1.46	1.39
5	C	2521	ADP	C5-C4	4.00	1.46	1.39
5	A	521	ADP	C5-C4	3.60	1.45	1.39
5	D	3521	ADP	C8-N7	2.98	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	521	ADP	C8-N7	2.89	1.37	1.31
5	B	1521	ADP	C5-N7	-2.58	1.34	1.39
5	D	3521	ADP	C5-C6	2.58	1.48	1.41
5	C	2521	ADP	C5-N7	-2.58	1.34	1.39
5	A	521	ADP	C5-C6	2.54	1.48	1.41
5	C	2521	ADP	C8-N7	2.32	1.36	1.31
5	B	1521	ADP	C5-C6	2.21	1.47	1.41
5	C	2521	ADP	C5-C6	2.17	1.47	1.41
5	B	1521	ADP	PA-O3A	2.11	1.61	1.59

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1521	ADP	C5-C4-N3	-5.56	119.06	126.72
5	C	2521	ADP	C5-C4-N3	-5.47	119.18	126.72
5	A	521	ADP	N3-C2-N1	-4.98	121.04	128.58
5	D	3521	ADP	C5-C4-N3	-4.89	119.99	126.72
5	A	521	ADP	C4-N9-C8	4.73	110.70	105.74
5	A	521	ADP	C5-C4-N3	-4.70	120.25	126.72
5	C	2521	ADP	N3-C4-N9	4.43	134.69	127.17
5	B	1521	ADP	N3-C4-N9	4.42	134.68	127.17
5	A	521	ADP	N9-C8-N7	-4.33	107.80	113.94
5	D	3521	ADP	N3-C4-N9	4.16	134.24	127.17
5	B	1521	ADP	N3-C2-N1	-4.12	122.35	128.58
5	D	3521	ADP	C4-N9-C8	4.06	110.01	105.74
5	A	521	ADP	C2-N3-C4	4.06	121.75	111.83
5	A	521	ADP	C4-C5-N7	-4.04	105.96	110.58
5	B	1521	ADP	C2-N3-C4	3.98	121.55	111.83
5	A	521	ADP	C5-N7-C8	3.83	109.48	103.45
5	A	521	ADP	N3-C4-N9	3.83	133.69	127.17
5	C	2521	ADP	C4-C5-N7	-3.74	106.31	110.58
5	C	2521	ADP	C2-N3-C4	3.69	120.85	111.83
5	C	2521	ADP	N3-C2-N1	-3.54	123.23	128.58
5	C	2521	ADP	C4-N9-C8	3.53	109.44	105.74
5	D	3521	ADP	C2-N3-C4	3.49	120.36	111.83
5	C	2521	ADP	C5-N7-C8	3.47	108.91	103.45
5	D	3521	ADP	N9-C8-N7	-3.34	109.20	113.94
5	C	2521	ADP	N9-C8-N7	-3.33	109.21	113.94
5	A	521	ADP	C6-C5-N7	3.30	138.44	132.09
5	D	3521	ADP	O2A-PA-O3A	3.27	116.10	107.27
5	D	3521	ADP	N3-C2-N1	-3.16	123.80	128.58
5	D	3521	ADP	C4-C5-N7	-3.11	107.02	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1521	ADP	C4-C5-N7	-2.98	107.18	110.58
3	A	519	GLU	OXT-C-O	-2.93	117.44	124.08
5	A	521	ADP	C4-N9-C1'	-2.91	119.82	126.63
5	D	3521	ADP	C5-N7-C8	2.90	108.00	103.45
5	A	521	ADP	O2A-PA-O3A	2.86	114.99	107.27
4	D	3520	CYS	OXT-C-O	-2.83	117.67	124.08
5	A	521	ADP	O3'-C3'-C4'	-2.77	103.12	111.08
4	A	520	CYS	OXT-C-O	-2.74	117.85	124.08
5	A	521	ADP	C2-N1-C6	2.63	123.06	118.73
5	C	2521	ADP	O3'-C3'-C4'	-2.45	104.03	111.08
5	D	3521	ADP	C6-C5-N7	2.43	136.78	132.09
5	C	2521	ADP	C6-C5-N7	2.40	136.72	132.09
3	D	3519	GLU	OXT-C-O	-2.34	118.77	124.08
5	B	1521	ADP	C6-C5-N7	2.30	136.53	132.09
4	B	1520	CYS	OXT-C-O	-2.21	119.07	124.08
3	B	1519	GLU	OXT-C-O	-2.19	119.12	124.08
5	A	521	ADP	O3B-PB-O2B	2.11	115.70	107.80
3	C	2519	GLU	OXT-C-O	-2.09	119.33	124.08
5	B	1521	ADP	C4-N9-C8	2.07	107.91	105.74
5	D	3521	ADP	O3B-PB-O1B	2.05	118.82	110.83
5	B	1521	ADP	C5-N7-C8	2.03	106.64	103.45
5	B	1521	ADP	O3'-C3'-C4'	-2.01	105.32	111.08

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	2521	ADP	C5'-O5'-PA-O1A
3	A	519	GLU	OXT-C-CA-CB
5	B	1521	ADP	O4'-C4'-C5'-O5'
5	B	1521	ADP	C3'-C4'-C5'-O5'
5	D	3521	ADP	O4'-C4'-C5'-O5'
3	A	519	GLU	OXT-C-CA-N
3	A	519	GLU	O-C-CA-CB
3	C	2519	GLU	OXT-C-CA-CB
5	D	3521	ADP	C3'-C4'-C5'-O5'
3	C	2519	GLU	O-C-CA-CB
3	A	519	GLU	O-C-CA-N
3	D	3519	GLU	O-C-CA-CB
3	B	1519	GLU	O-C-CA-CB
3	C	2519	GLU	OXT-C-CA-N
5	B	1521	ADP	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
5	C	2521	ADP	PB-O3A-PA-O2A
3	B	1519	GLU	OXT-C-CA-CB
3	A	519	GLU	N-CA-CB-CG
3	D	3519	GLU	OXT-C-CA-CB
5	C	2521	ADP	C5'-O5'-PA-O3A
5	B	1521	ADP	PB-O3A-PA-O1A
5	C	2521	ADP	PB-O3A-PA-O1A
5	D	3521	ADP	PB-O3A-PA-O2A
3	C	2519	GLU	OE2-CD-CG-CB
3	C	2519	GLU	O-C-CA-N
3	D	3519	GLU	OE2-CD-CG-CB
3	B	1519	GLU	OE2-CD-CG-CB
3	C	2519	GLU	OE1-CD-CG-CB
3	B	1519	GLU	OE1-CD-CG-CB
3	D	3519	GLU	OE1-CD-CG-CB
3	A	519	GLU	OE2-CD-CG-CB
3	A	519	GLU	OE1-CD-CG-CB
5	A	521	ADP	PB-O3A-PA-O2A
5	A	521	ADP	O4'-C4'-C5'-O5'
5	D	3521	ADP	PB-O3A-PA-O1A

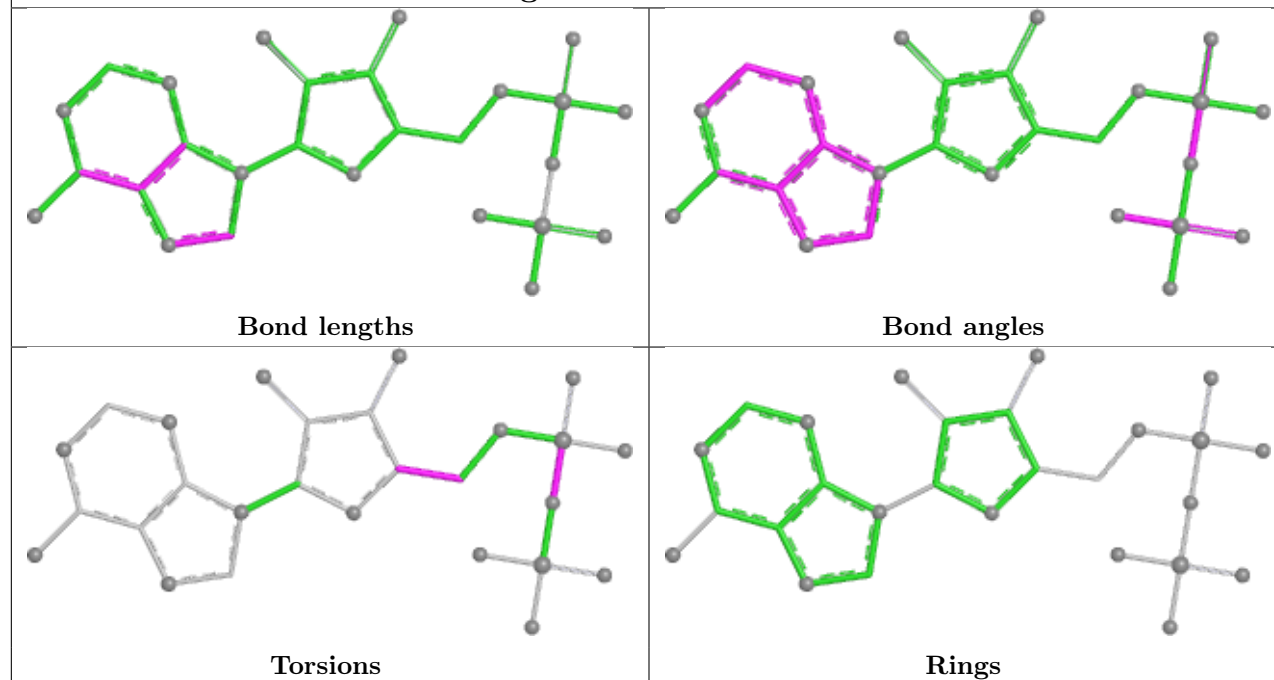
There are no ring outliers.

4 monomers are involved in 3 short contacts:

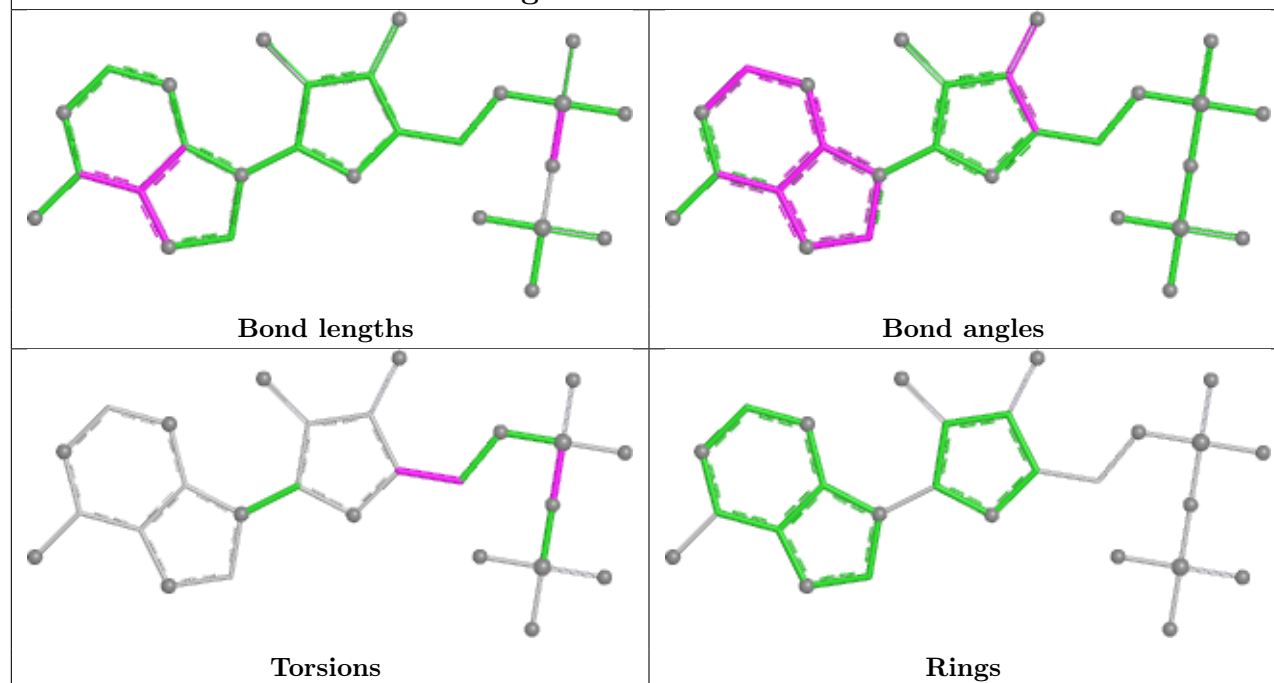
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1519	GLU	1	0
3	C	2519	GLU	1	0
3	A	519	GLU	1	0
4	C	2520	CYS	1	0

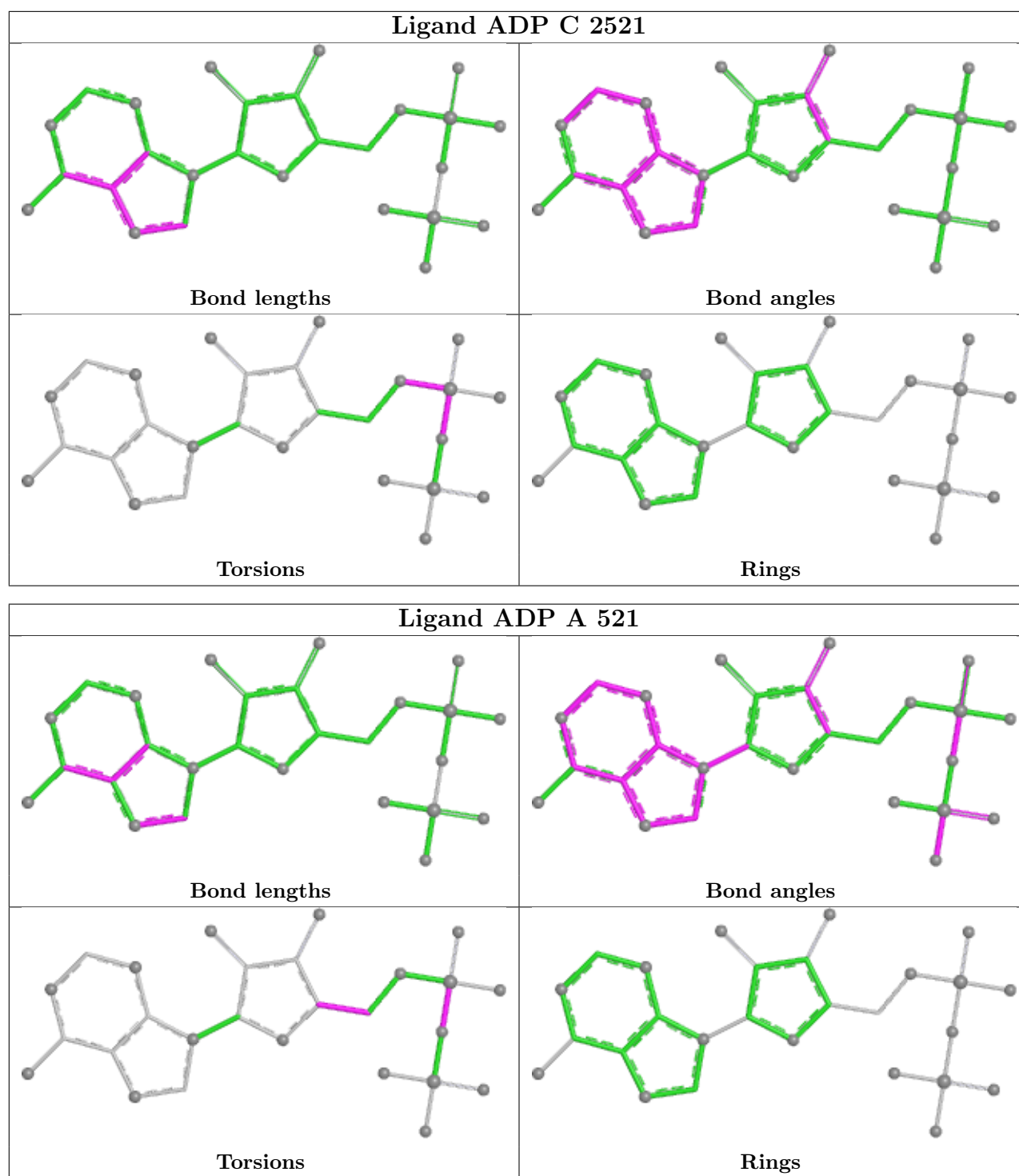
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand ADP D 3521



Ligand ADP B 1521





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.52	8 (1%) 70 66	18, 30, 53, 75	0
1	B	503/518 (97%)	-0.02	19 (3%) 44 38	26, 39, 61, 89	0
1	C	504/518 (97%)	0.24	26 (5%) 33 27	30, 45, 69, 84	0
1	D	499/518 (96%)	-0.07	21 (4%) 40 35	24, 40, 66, 91	0
All	All	2016/2072 (97%)	-0.09	74 (3%) 45 39	18, 39, 64, 91	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	247	SER	6.4
1	C	243	ASN	5.8
1	C	221	THR	5.3
1	B	243	ASN	4.9
1	B	518	ALA	4.5
1	B	248	ASN	4.4
1	C	248	ASN	4.2
1	D	242	THR	4.1
1	C	242	THR	4.1
1	B	247	SER	4.0
1	C	247	SER	4.0
1	B	215	SER	4.0
1	D	162	ALA	3.9
1	D	243	ASN	3.6
1	B	164	SER	3.5
1	B	172	ALA	3.4
1	A	272	GLU	3.4
1	C	109	ALA	3.4
1	D	283	GLY	3.4
1	C	163	LYS	3.4
1	C	110	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	512	VAL	3.4
1	C	518	ALA	3.3
1	D	110	GLU	3.3
1	D	248	ASN	3.3
1	C	167	ILE	3.3
1	B	516	LYS	3.3
1	C	284	LYS	3.2
1	C	311	SER	3.1
1	C	511	ALA	3.0
1	C	281	LYS	2.9
1	B	282	ASP	2.9
1	C	282	ASP	2.9
1	A	242	THR	2.8
1	C	209	LEU	2.8
1	D	222	GLU	2.8
1	B	281	LYS	2.8
1	B	508	GLU	2.8
1	C	283	GLY	2.8
1	C	497	ARG	2.7
1	C	516	LYS	2.7
1	D	111	GLY	2.7
1	C	486	GLU	2.7
1	A	517	HIS	2.7
1	B	174	GLU	2.6
1	B	500	GLN	2.6
1	D	223	SER	2.4
1	B	515	GLU	2.4
1	C	120	GLY	2.4
1	B	507	THR	2.4
1	C	500	GLN	2.4
1	D	279	ILE	2.3
1	A	214	THR	2.3
1	C	507	THR	2.3
1	A	243	ASN	2.2
1	D	249	LEU	2.2
1	C	474	LEU	2.2
1	B	173	LYS	2.2
1	D	174	GLU	2.2
1	D	395	CYS	2.2
1	D	312	GLY	2.2
1	D	157	MET	2.2
1	B	280	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	516	LYS	2.1
1	A	518	ALA	2.1
1	C	501	GLU	2.1
1	D	280	GLU	2.1
1	D	506	ASP	2.0
1	D	161	GLN	2.0
1	D	517	HIS	2.0
1	A	244	LYS	2.0
1	D	284	LYS	2.0
1	B	223	SER	2.0
1	C	143	MET	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
6	AF3	D	3522	4/4	0.78	0.16	57,58,58,62	0
6	AF3	B	1522	4/4	0.82	0.15	57,58,59,60	0
2	MG	A	526	1/1	0.82	0.09	44,44,44,44	0
3	GLU	A	519	10/10	0.83	0.21	68,69,71,71	0
6	AF3	A	522	4/4	0.84	0.15	49,51,52,55	0
6	AF3	C	2522	4/4	0.85	0.13	59,60,60,62	0
3	GLU	C	2519	10/10	0.90	0.12	67,68,69,70	0
3	GLU	D	3519	10/10	0.92	0.11	46,48,49,49	0
3	GLU	B	1519	10/10	0.93	0.11	50,52,54,54	0
4	CYS	C	2520	7/7	0.93	0.13	53,55,55,55	0
4	CYS	A	520	7/7	0.95	0.13	51,52,53,53	0
4	CYS	D	3520	7/7	0.95	0.13	50,52,54,54	0

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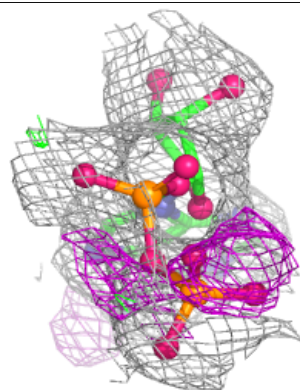
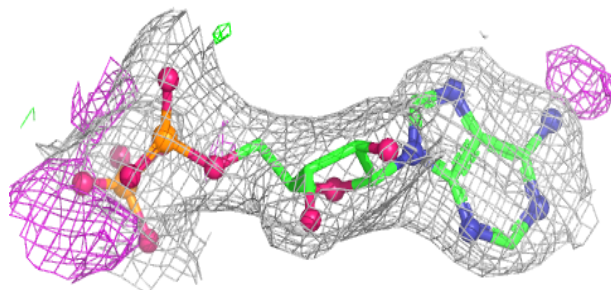
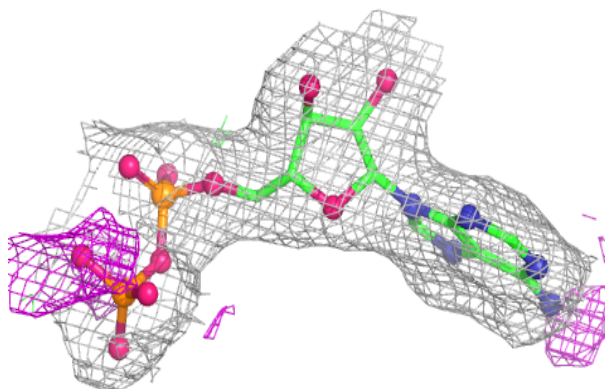
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	C	2525	1/1	0.96	0.05	45,45,45,45	0
4	CYS	B	1520	7/7	0.96	0.10	48,48,49,49	0
5	ADP	B	1521	27/27	0.97	0.07	33,36,37,38	0
5	ADP	C	2521	27/27	0.97	0.07	35,41,45,46	0
2	MG	B	1524	1/1	0.98	0.04	36,36,36,36	0
5	ADP	D	3521	27/27	0.98	0.05	31,34,37,37	0
2	MG	C	2524	1/1	0.98	0.04	47,47,47,47	0
2	MG	A	525	1/1	0.98	0.03	26,26,26,26	0
5	ADP	A	521	27/27	0.98	0.05	29,31,34,35	0
2	MG	A	524	1/1	0.98	0.03	34,34,34,34	0
2	MG	B	1523	1/1	0.99	0.04	45,45,45,45	0
2	MG	A	523	1/1	0.99	0.04	40,40,40,40	0
2	MG	D	3523	1/1	0.99	0.04	38,38,38,38	0
2	MG	D	3524	1/1	0.99	0.02	35,35,35,35	0
2	MG	B	1525	1/1	0.99	0.05	37,37,37,37	0
2	MG	C	2523	1/1	1.00	0.03	46,46,46,46	0
2	MG	D	3525	1/1	1.00	0.02	37,37,37,37	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.

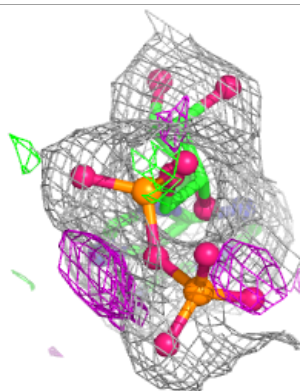
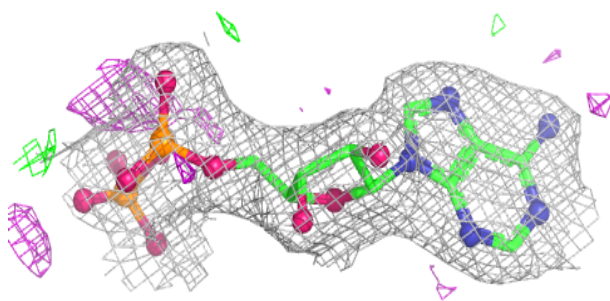
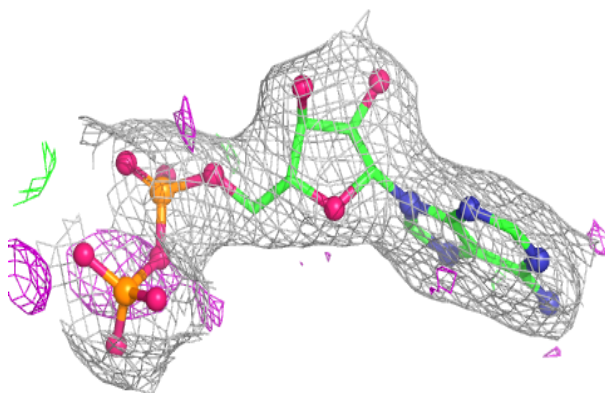
Electron density around ADP B 1521:

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

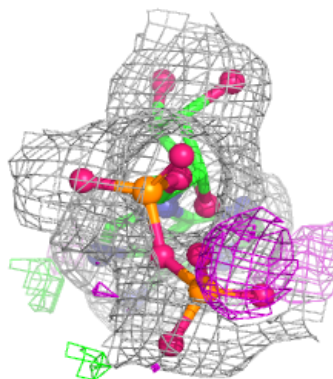
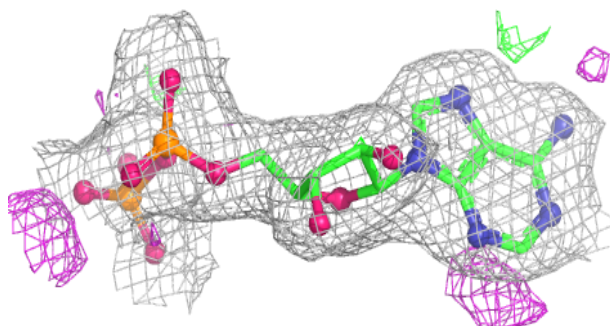
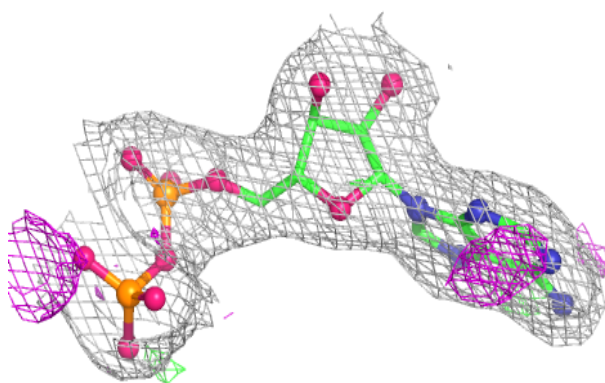


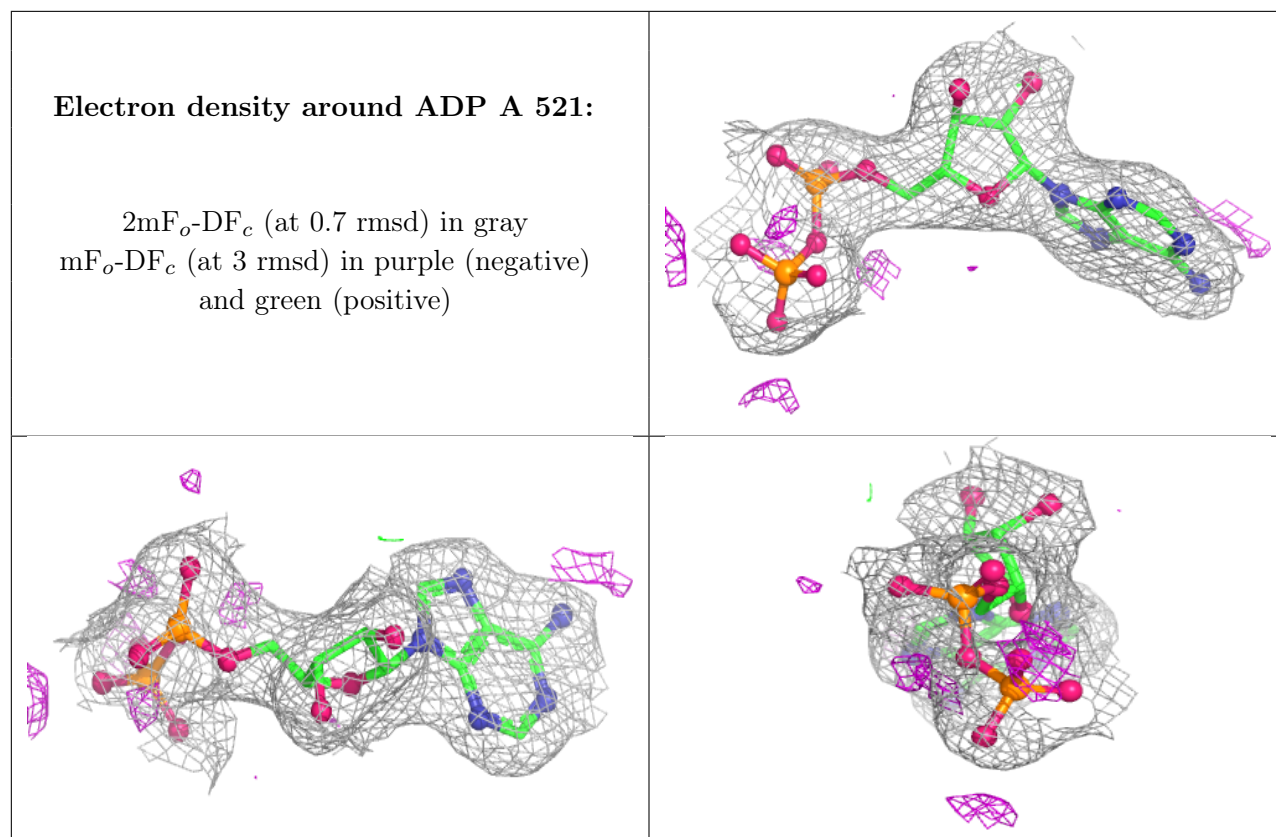
Electron density around ADP C 2521:

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

**Electron density around ADP D 3521:**

$2mF_o-DF_c$ (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.