



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2021 – 06:19 PM EDT

PDB ID : 2D33  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

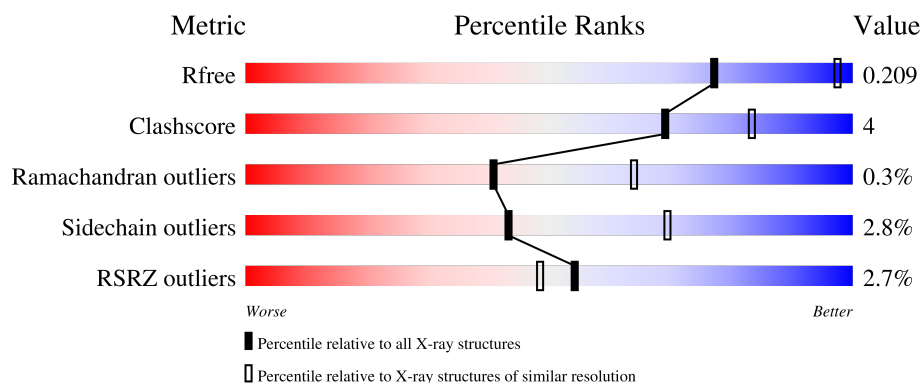
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




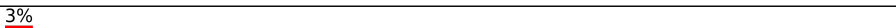
The reported resolution of this entry is 2.60 Å.

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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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  $\geq 3$ , 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	
1	B	518	
1	C	518	
1	D	518	

## 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			

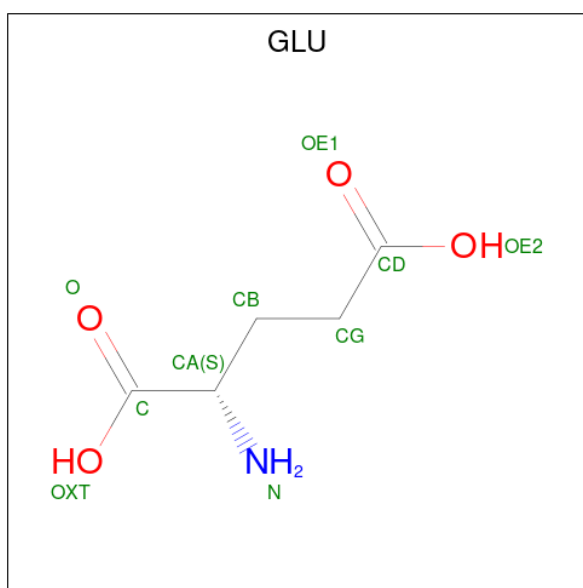
There are 16 discrepancies between the modelled and reference sequences:

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 (three-letter code: MG) (formula: Mg).

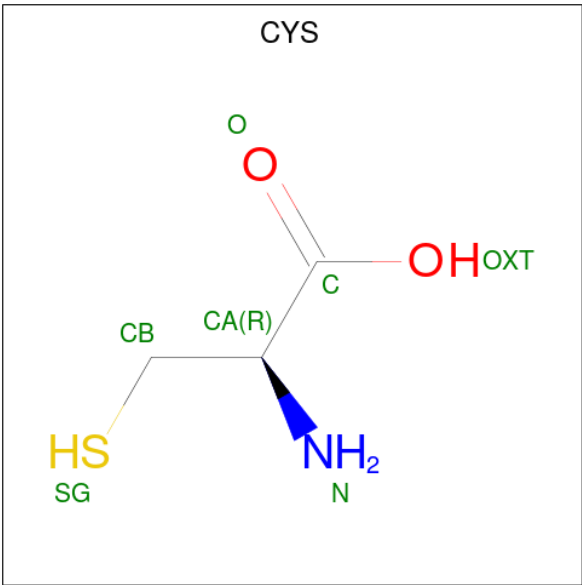
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Mg 4 4	0	0
2	B	3	Total Mg 3 3	0	0
2	C	3	Total Mg 3 3	0	0
2	D	3	Total Mg 3 3	0	0

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



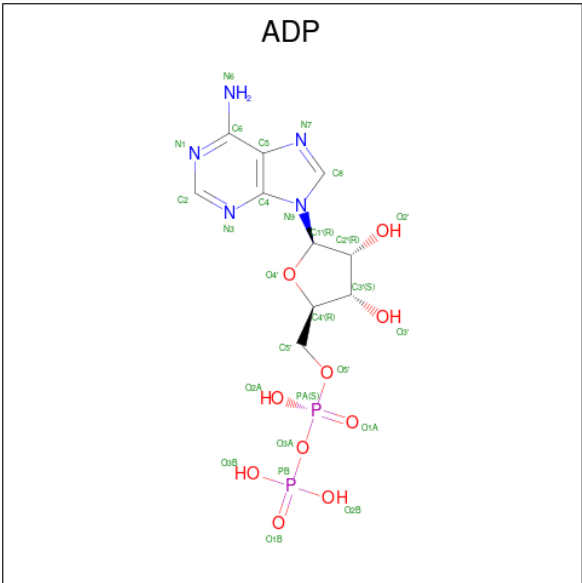
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 10 5 1 4	0	0
3	B	1	Total C N O 10 5 1 4	0	0
3	C	1	Total C N O 10 5 1 4	0	0
3	D	1	Total C N O 10 5 1 4	0	0

- Molecule 4 is CYSTEINE (three-letter code: CYS) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>S).



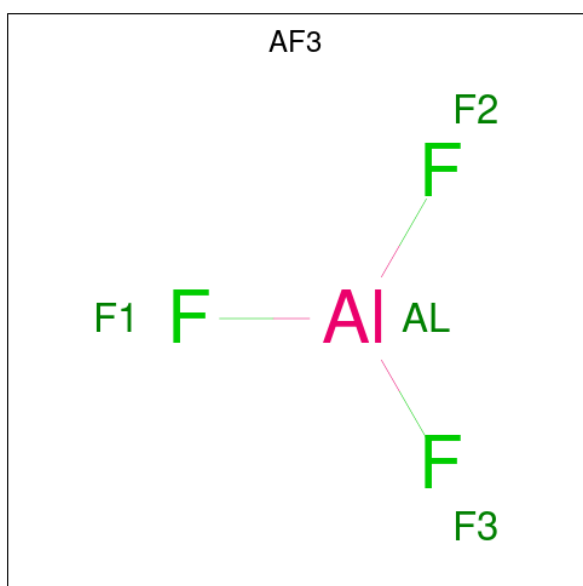
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
4	B	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
4	C	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
4	D	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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 (three-letter code: AF3) (formula:  $\text{AlF}_3$ ).



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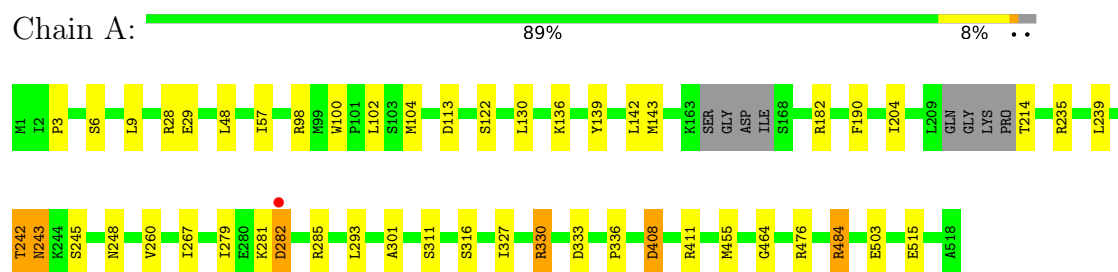
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	27	Total	O	0	0
			27	27		
7	D	79	Total	O	0	0
			79	79		

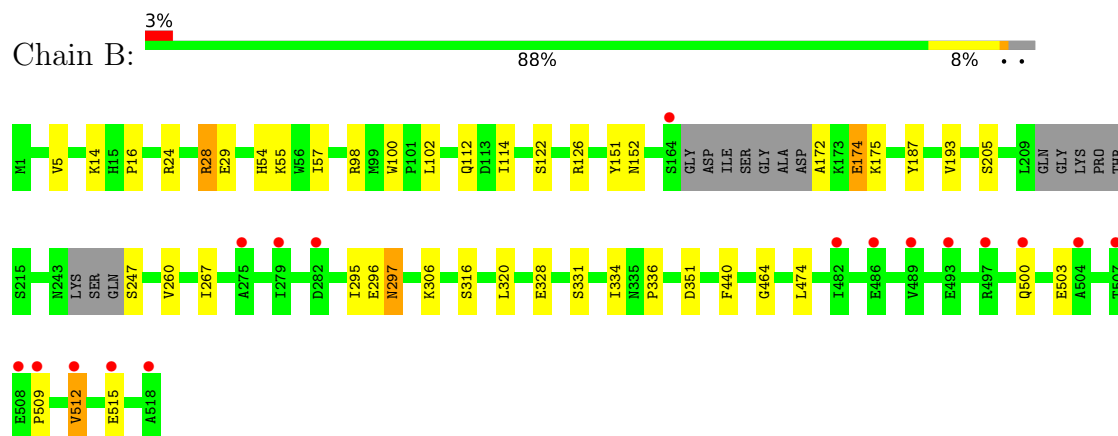
### 3 Residue-property plots

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.

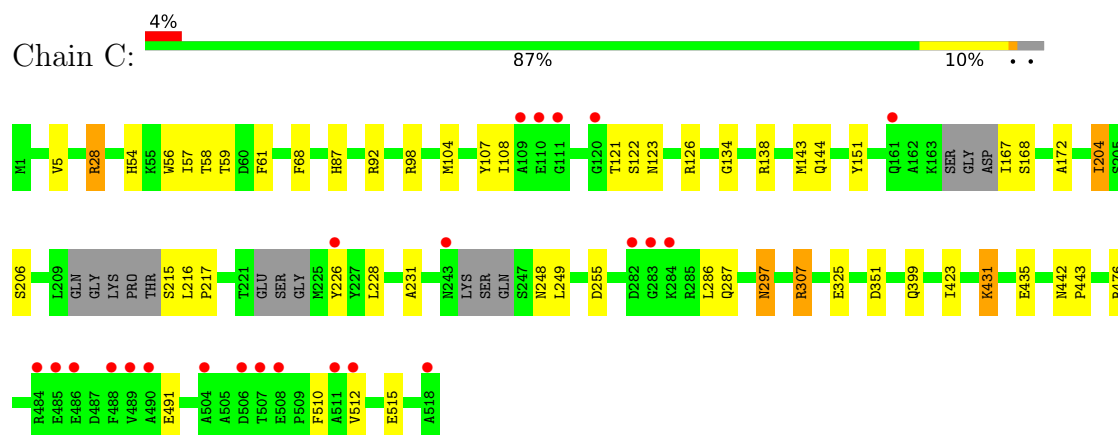
#### • Molecule 1: Glutamate–cysteine ligase



#### • Molecule 1: Glutamate–cysteine ligase

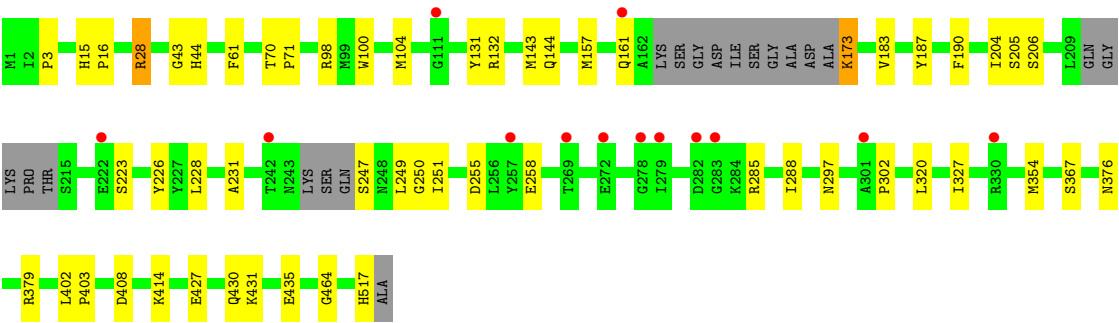
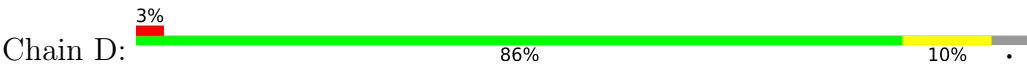


#### • Molecule 1: Glutamate–cysteine ligase





● Molecule 1: Glutamate–cysteine ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	325.23Å 325.23Å 105.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.60 39.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.60) 100.0 (39.76-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 40.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.83	0/4096	0.81	1/5547 (0.0%)
1	B	0.67	0/4019	0.73	0/5447
1	C	0.63	0/4010	0.68	0/5431
1	D	0.70	0/3993	0.74	2/5414 (0.0%)
All	All	0.71	0/16118	0.74	3/21839 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	A	113	ASP	CB-CG-OD1	-5.67	113.19	118.30
1	D	285	ARG	NE-CZ-NH1	-5.32	117.64	120.30

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	28	0
1	B	3933	0	3810	29	0
1	C	3925	0	3793	31	0
1	D	3909	0	3776	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	116	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 (116) 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:D:255:ASP:HB3	1:D:258:GLU:HB2	1.56	0.88
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:C:104:MET:HE2	1:C:204:ILE:HG22	1.71	0.71
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:C:104:MET:CE	1:C:204:ILE:HG22	2.23	0.69
1:D:173:LYS:O	1:D:173:LYS:HG2	1.93	0.67
1:A:29:GLU:OE2	3:A:519:GLU:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:28:ARG:HD3	1:B:28:ARG:C	2.23	0.59
1:C:286:LEU:O	1:C:287:GLN:HB3	2.03	0.58
1:B:187:TYR:OH	1:B:331:SER:OG	2.22	0.58
1:C:5:VAL:HG12	1:C:5:VAL:O	2.04	0.57
1:B:267:ILE:HD11	1:B:296:GLU:HG2	1.87	0.56
1:C:491:GLU:HA	1:C:491:GLU:OE1	2.06	0.56
1:B:14:LYS:C	1:B:16:PRO:HD3	2.27	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: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:408:ASP:OD1	1:A:411:ARG:NH2	2.43	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
1:B:267:ILE:CD1	1:B:296:GLU:HG2	2.41	0.51
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:D:327:ILE:C	1:D:327:ILE:HD12	2.32	0.49
1:A:301:ALA:O	1:A:330:ARG:HD3	2.12	0.49
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:A:104:MET:HE2	1:A:204:ILE:HG13	1.95	0.47
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:C:107:TYR:C	1:C:108:ILE:HG12	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:SER:C	1:D:249:LEU:H	2.19	0.47
1:D:104:MET:CE	1:D:204:ILE:HG13	2.45	0.46
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: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: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
1:B:112:GLN:O	1:B:114:ILE:HD12	2.17	0.44
1:D:28:ARG:C	1:D:28:ARG:HD3	2.38	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: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:104:MET:HE1	1:C:204:ILE:HG22	2.01	0.43
1:C:442:ASN:HA	1:C:443:PRO:HD2	1.90	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:142:LEU:HD12	1:A:142:LEU:HA	1.83	0.43
1:D:402:LEU:C	1:D:402:LEU:HD23	2.38	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:104:MET:HE1	1:C:204:ILE:CG2	2.49	0.42
3:C:2519:GLU:OE1	4:C:2520:CYS:HA	2.20	0.42
1:D:43:GLY:O	1:D:44:HIS:C	2.58	0.42
1:C:226:TYR:CD1	1:C:226:TYR:N	2.87	0.42
1:D:183:VAL:CG1	1:D:354:MET:HE3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:70:THR:HA	1:D:71:PRO:HD3	1.83	0.41
1:C:28:ARG:C	1:C:28:ARG:HD3	2.41	0.41
1:B:512:VAL:O	1:B:515:GLU:HG2	2.21	0.41
1:A:267:ILE:O	1:A:267:ILE:HG22	2.19	0.40
1:B:296:GLU:OE2	1:B:316:SER:OG	2.37	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: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 [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%)	488 (97%)	14 (3%)	2 (0%)	34 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	495/518 (96%)	481 (97%)	14 (3%)	0	100	100
1	C	494/518 (95%)	466 (94%)	25 (5%)	3 (1%)	25	47
1	D	491/518 (95%)	471 (96%)	19 (4%)	1 (0%)	47	71
All	All	1984/2072 (96%)	1906 (96%)	72 (4%)	6 (0%)	41	64

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%)	404 (97%)	12 (3%)	42	68
1	B	401/434 (92%)	390 (97%)	11 (3%)	44	71
1	C	396/434 (91%)	384 (97%)	12 (3%)	41	67
1	D	400/434 (92%)	389 (97%)	11 (3%)	43	69
All	All	1613/1736 (93%)	1567 (97%)	46 (3%)	43	68

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	28	ARG
1	A	98	ARG
1	A	136	LYS
1	A	182	ARG

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Mol	Chain	Res	Type
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	484	ARG
1	B	28	ARG
1	B	55	LYS
1	B	98	ARG
1	B	174	GLU
1	B	205	SER
1	B	247	SER
1	B	297	ASN
1	B	306	LYS
1	B	474	LEU
1	B	500	GLN
1	B	512	VAL
1	C	28	ARG
1	C	98	ARG
1	C	168	SER
1	C	204	ILE
1	C	206	SER
1	C	215	SER
1	C	255	ASP
1	C	297	ASN
1	C	307	ARG
1	C	399	GLN
1	C	423	ILE
1	C	431	LYS
1	D	28	ARG
1	D	98	ARG
1	D	143	MET
1	D	157	MET
1	D	173	LYS
1	D	205	SER
1	D	223	SER
1	D	251	ILE
1	D	297	ASN
1	D	408	ASP
1	D	517	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	418	GLN
1	B	418	GLN
1	C	54	HIS
1	C	418	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 monosaccharides 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	C	2520	-	3,6,6	1.33	1 (33%)	1,7,7	0.54	0
3	GLU	B	1519	2,6	2,9,9	1.14	0	2,11,11	0.86	0
4	CYS	D	3520	6	3,6,6	1.57	0	1,7,7	0.89	0
3	GLU	A	519	2,6	2,9,9	1.28	0	2,11,11	0.67	0
5	ADP	C	2521	2,6	24,29,29	1.04	3 (12%)	29,45,45	1.47	3 (10%)
6	AF3	A	522	7,5,3,2,4	0,3,3	-	-	-	-	-
4	CYS	B	1520	-	3,6,6	0.83	0	1,7,7	0.81	0
3	GLU	D	3519	2,6	2,9,9	0.34	0	2,11,11	1.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	AF3	B	1522	1,3,5,2	0,3,3	-	-	-		
5	ADP	B	1521	2,6	24,29,29	0.95	1 (4%)	29,45,45	1.42	3 (10%)
6	AF3	D	3522	7,1,5,3,2,4	0,3,3	-	-	-		
6	AF3	C	2522	1,3,5,2	0,3,3	-	-	-		
4	CYS	A	520	6	3,6,6	1.52	0	1,7,7	0.73	0
3	GLU	C	2519	2,6	2,9,9	0.87	0	2,11,11	0.80	0
5	ADP	A	521	2,6	24,29,29	0.87	1 (4%)	29,45,45	1.82	7 (24%)
5	ADP	D	3521	2,6	24,29,29	1.14	3 (12%)	29,45,45	1.42	4 (13%)

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	C	2520	-	-	0/2/6/6	-
3	GLU	B	1519	2,6	-	0/3/9/9	-
4	CYS	D	3520	6	-	0/2/6/6	-
3	GLU	A	519	2,6	-	1/3/9/9	-
5	ADP	C	2521	2,6	-	5/12/32/32	0/3/3/3
4	CYS	B	1520	-	-	0/2/6/6	-
3	GLU	D	3519	2,6	-	0/3/9/9	-
5	ADP	B	1521	2,6	-	4/12/32/32	0/3/3/3
4	CYS	A	520	6	-	0/2/6/6	-
3	GLU	C	2519	2,6	-	0/3/9/9	-
5	ADP	A	521	2,6	-	2/12/32/32	0/3/3/3
5	ADP	D	3521	2,6	-	3/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	3521	ADP	C5-C4	2.48	1.47	1.40
5	D	3521	ADP	C2'-C1'	-2.34	1.50	1.53
4	C	2520	CYS	CA-N	2.18	1.51	1.47
5	C	2521	ADP	C2'-C1'	-2.16	1.50	1.53
5	B	1521	ADP	C5-C4	2.15	1.46	1.40
5	C	2521	ADP	O4'-C1'	2.09	1.44	1.41
5	D	3521	ADP	C2-N3	2.07	1.35	1.32
5	C	2521	ADP	C5-C4	2.00	1.46	1.40
5	A	521	ADP	C2'-C1'	-2.00	1.50	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	521	ADP	N3-C2-N1	-4.89	121.04	128.68
5	B	1521	ADP	N3-C2-N1	-4.05	122.35	128.68
5	A	521	ADP	C1'-N9-C4	-3.88	119.82	126.64
5	C	2521	ADP	N3-C2-N1	-3.49	123.23	128.68
5	A	521	ADP	C4-C5-N7	-3.30	105.96	109.40
5	D	3521	ADP	N3-C2-N1	-3.12	123.80	128.68
5	C	2521	ADP	C4-C5-N7	-2.96	106.31	109.40
5	A	521	ADP	O3'-C3'-C4'	-2.74	103.12	111.05
5	B	1521	ADP	PA-O3A-PB	-2.62	123.83	132.83
5	D	3521	ADP	C1'-N9-C4	-2.56	122.14	126.64
5	A	521	ADP	PA-O3A-PB	-2.55	124.07	132.83
5	A	521	ADP	C2-N1-C6	2.51	123.06	118.75
5	C	2521	ADP	O3'-C3'-C4'	-2.43	104.03	111.05
5	D	3521	ADP	C4-C5-N7	-2.28	107.02	109.40
5	B	1521	ADP	C4-C5-N7	-2.13	107.18	109.40
5	A	521	ADP	O3B-PB-O2B	2.11	115.70	107.64
5	D	3521	ADP	O3B-PB-O1B	2.08	118.82	110.68

There are no chirality outliers.

All (15) torsion outliers are listed below:

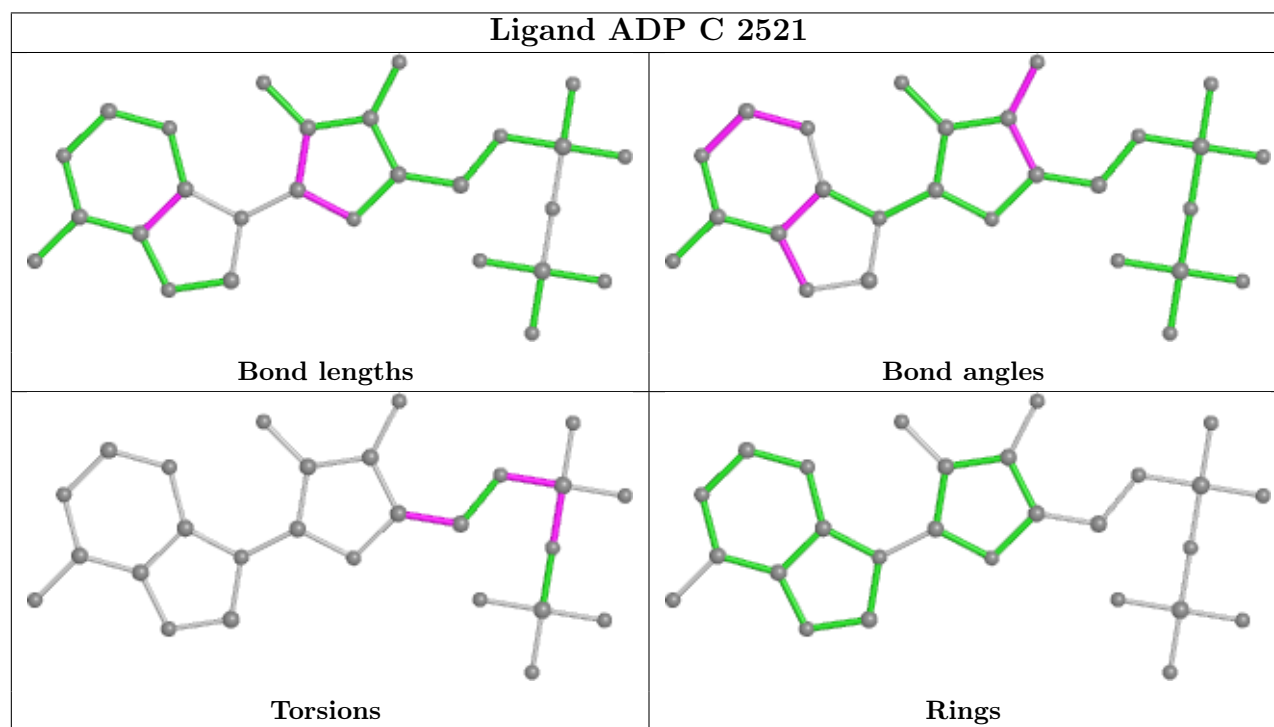
Mol	Chain	Res	Type	Atoms
5	C	2521	ADP	C5'-O5'-PA-O1A
5	D	3521	ADP	O4'-C4'-C5'-O5'
5	B	1521	ADP	O4'-C4'-C5'-O5'
5	B	1521	ADP	C3'-C4'-C5'-O5'
5	D	3521	ADP	C3'-C4'-C5'-O5'
5	C	2521	ADP	C5'-O5'-PA-O3A
5	B	1521	ADP	PB-O3A-PA-O2A
5	C	2521	ADP	PB-O3A-PA-O2A
3	A	519	GLU	N-CA-CB-CG
5	B	1521	ADP	PB-O3A-PA-O1A
5	C	2521	ADP	PB-O3A-PA-O1A
5	D	3521	ADP	PB-O3A-PA-O2A
5	A	521	ADP	O4'-C4'-C5'-O5'
5	C	2521	ADP	O4'-C4'-C5'-O5'
5	A	521	ADP	PB-O3A-PA-O2A

There are no ring outliers.

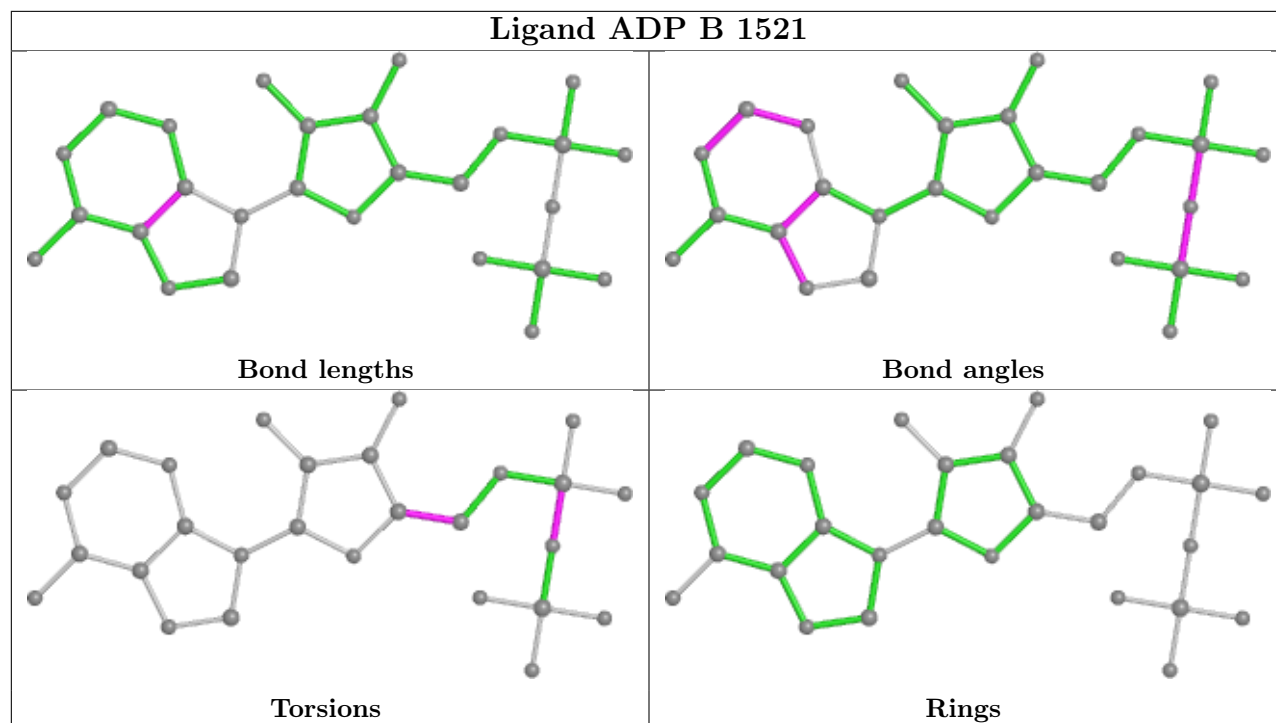
4 monomers are involved in 3 short contacts:

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

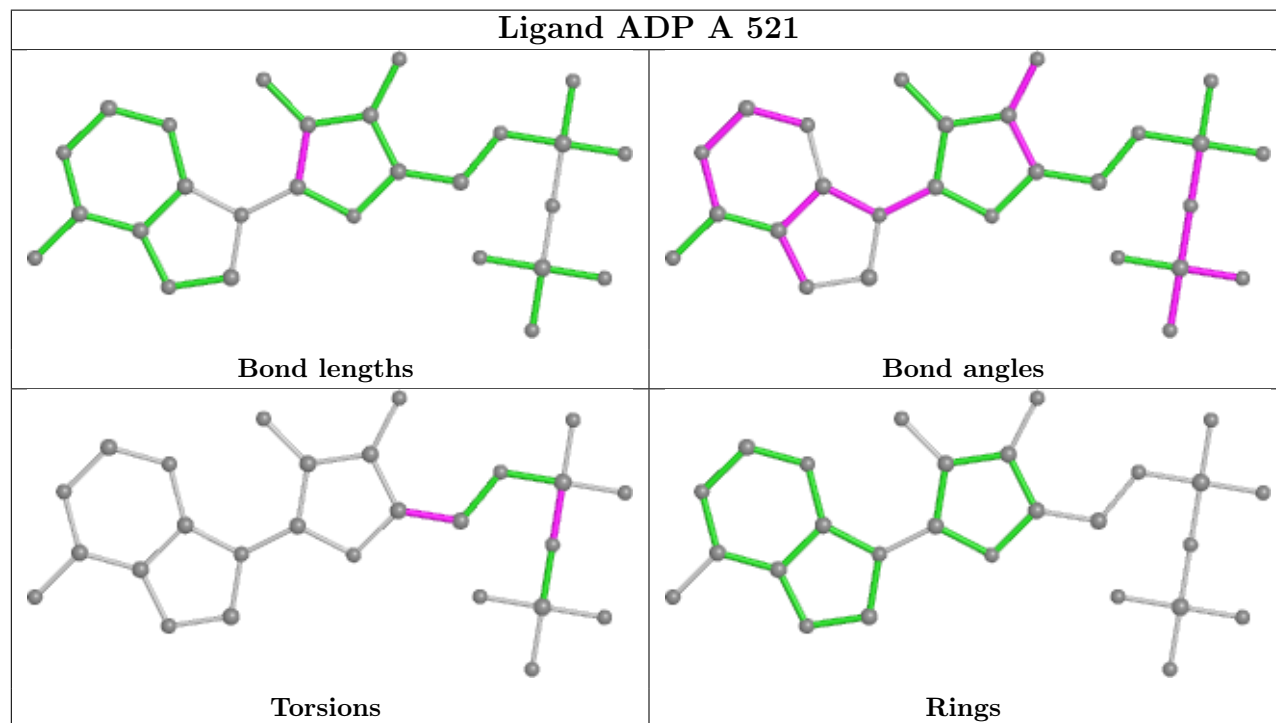
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

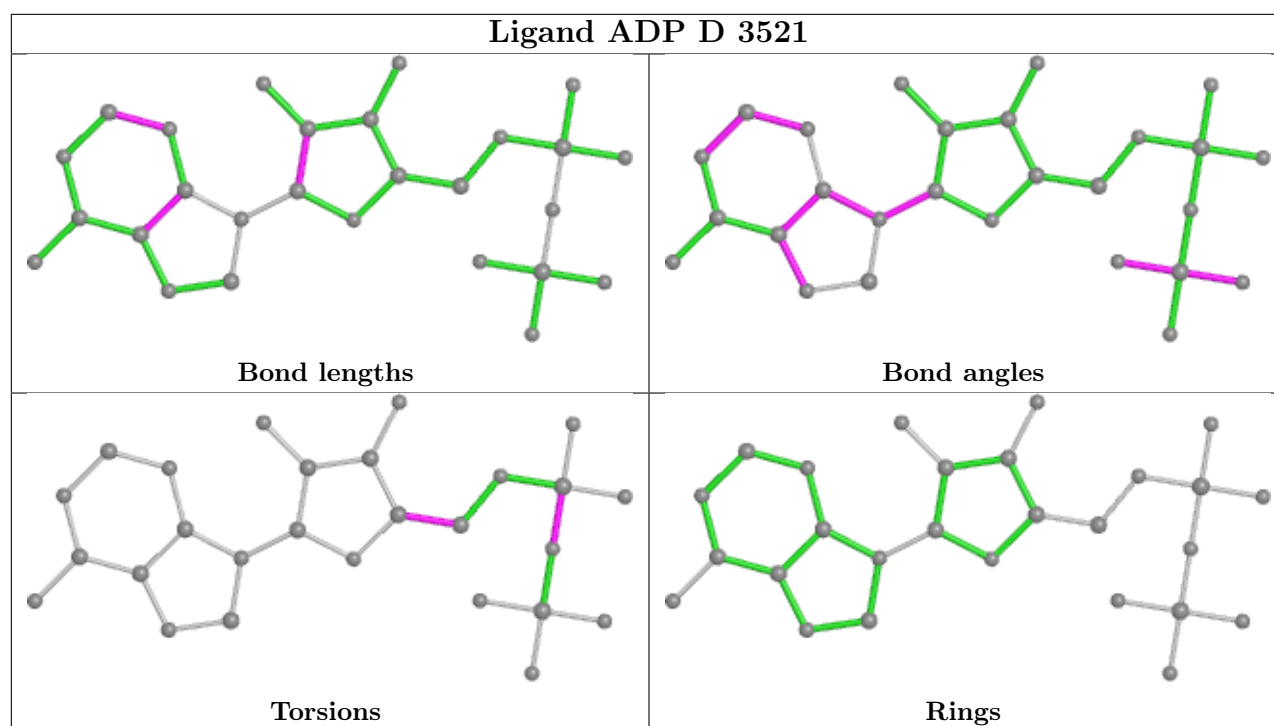


## Ligand ADP B 1521



## Ligand ADP A 521





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	510/518 (98%)	-0.40	1 (0%) 95 95	18, 30, 53, 75	0
1	B	503/518 (97%)	-0.20	17 (3%) 45 38	26, 39, 61, 89	0
1	C	504/518 (97%)	-0.06	23 (4%) 32 26	30, 45, 69, 84	0
1	D	499/518 (96%)	-0.13	13 (2%) 56 50	24, 40, 66, 91	0
All	All	2016/2072 (97%)	-0.20	54 (2%) 54 48	18, 39, 64, 91	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	518	ALA	6.6
1	C	109	ALA	5.1
1	C	507	THR	4.4
1	C	111	GLY	3.9
1	B	164	SER	3.8
1	B	500	GLN	3.4
1	C	486	GLU	3.4
1	C	518	ALA	3.1
1	D	279	ILE	3.1
1	D	257	TYR	3.0
1	B	507	THR	3.0
1	D	283	GLY	3.0
1	D	161	GLN	2.9
1	D	272	GLU	2.9
1	B	512	VAL	2.9
1	C	110	GLU	2.8
1	C	504	ALA	2.8
1	C	489	VAL	2.8
1	C	120	GLY	2.8
1	D	282	ASP	2.7
1	C	512	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	283	GLY	2.6
1	D	242	THR	2.6
1	C	508	GLU	2.5
1	C	226	TYR	2.5
1	D	301	ALA	2.5
1	B	508	GLU	2.5
1	B	489	VAL	2.5
1	B	493	GLU	2.5
1	C	506	ASP	2.4
1	C	511	ALA	2.4
1	B	275	ALA	2.4
1	B	486	GLU	2.4
1	D	269	THR	2.3
1	C	485	GLU	2.3
1	B	515	GLU	2.3
1	B	497	ARG	2.3
1	B	282	ASP	2.2
1	D	278	GLY	2.2
1	C	243	ASN	2.2
1	C	490	ALA	2.2
1	A	282	ASP	2.2
1	D	222	GLU	2.2
1	C	484	ARG	2.2
1	D	330	ARG	2.2
1	C	282	ASP	2.2
1	B	504	ALA	2.2
1	B	279	ILE	2.1
1	B	509	PRO	2.1
1	D	111	GLY	2.1
1	C	284	LYS	2.1
1	B	482	ILE	2.1
1	C	488	PHE	2.1
1	C	161	GLN	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

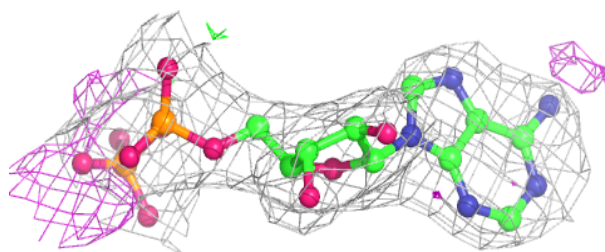
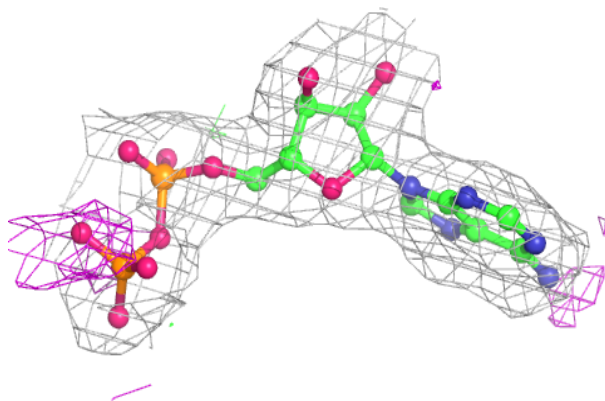
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	AF3	D	3522	4/4	0.87	0.23	57,58,58,62	0
3	GLU	A	519	10/10	0.88	0.26	68,69,71,71	0
6	AF3	A	522	4/4	0.89	0.17	49,51,52,55	0
2	MG	A	526	1/1	0.89	0.12	44,44,44,44	0
6	AF3	B	1522	4/4	0.90	0.19	57,58,59,60	0
4	CYS	C	2520	7/7	0.91	0.17	53,55,55,55	0
6	AF3	C	2522	4/4	0.93	0.17	59,60,60,62	0
2	MG	C	2525	1/1	0.94	0.19	45,45,45,45	0
3	GLU	D	3519	10/10	0.94	0.37	46,48,49,49	0
4	CYS	A	520	7/7	0.94	0.15	51,52,53,53	0
2	MG	D	3523	1/1	0.94	0.23	38,38,38,38	0
3	GLU	C	2519	10/10	0.95	0.25	67,68,69,70	0
4	CYS	D	3520	7/7	0.95	0.19	50,52,54,54	0
3	GLU	B	1519	10/10	0.96	0.20	50,52,54,54	0
4	CYS	B	1520	7/7	0.96	0.15	48,48,49,49	0
2	MG	C	2523	1/1	0.96	0.15	46,46,46,46	0
2	MG	A	525	1/1	0.96	0.13	26,26,26,26	0
2	MG	A	524	1/1	0.97	0.18	34,34,34,34	0
2	MG	C	2524	1/1	0.97	0.20	47,47,47,47	0
2	MG	B	1524	1/1	0.97	0.19	36,36,36,36	0
5	ADP	B	1521	27/27	0.97	0.14	33,36,37,38	0
2	MG	D	3524	1/1	0.98	0.20	35,35,35,35	0
5	ADP	C	2521	27/27	0.98	0.14	35,41,45,46	0
5	ADP	D	3521	27/27	0.98	0.15	31,34,37,37	0
2	MG	D	3525	1/1	0.98	0.17	37,37,37,37	0
2	MG	A	523	1/1	0.98	0.11	40,40,40,40	0
2	MG	B	1525	1/1	0.98	0.10	37,37,37,37	0
2	MG	B	1523	1/1	0.98	0.14	45,45,45,45	0
5	ADP	A	521	27/27	0.99	0.13	29,31,34,35	0

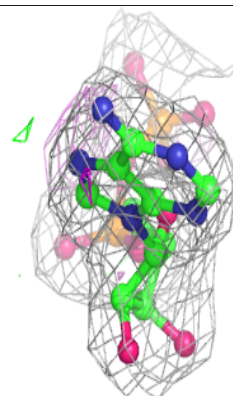
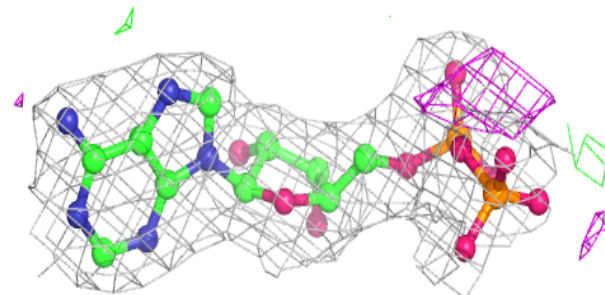
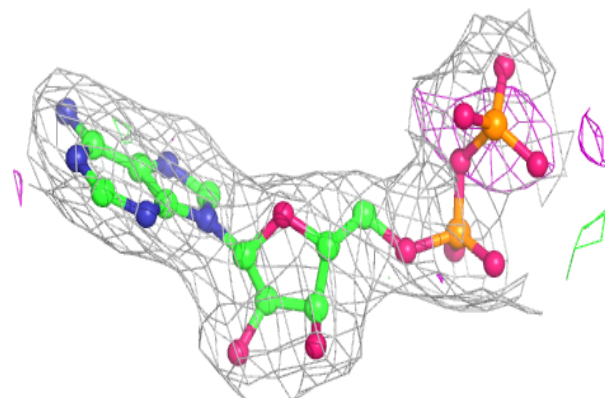
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

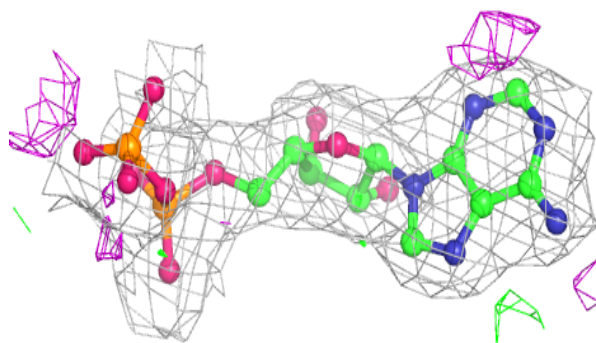
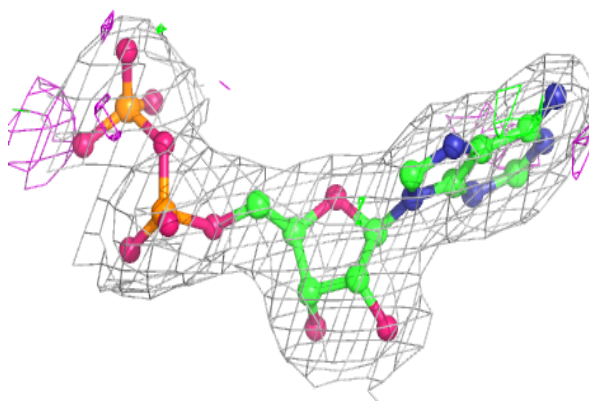
**Electron density around ADP C 2521:**

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

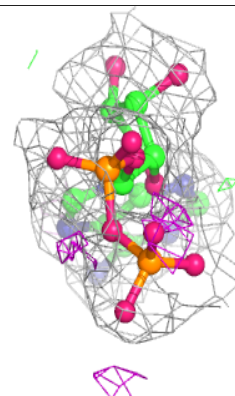
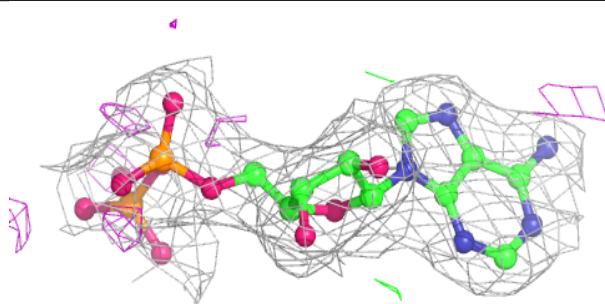
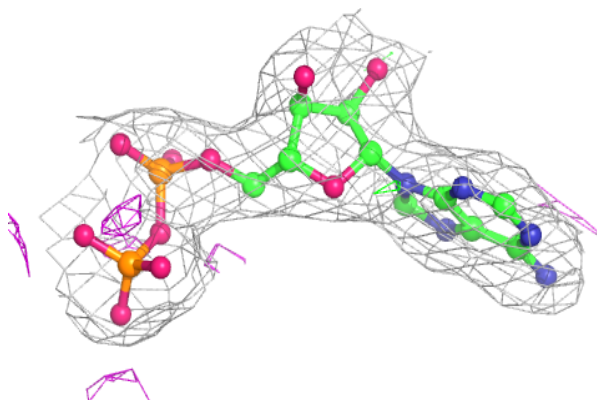


**Electron density around ADP D 3521:**

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

**Electron density around ADP A 521:**

$2mF_o-DF_c$  (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.