



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:04 am BST

PDB ID : 3RUV  
Title : Crystal structure of Cpn-rls in complex with ATP analogue from *Methanococcus maripaludis*  
Authors : Pereira, J.H.; Ralston, C.Y.; Douglas, N.R.; Kumar, R.; McAndrew, R.P.; Knee, K.M.; King, J.A.; Frydman, J.; Adams, P.D.  
Deposited on : 2011-05-05  
Resolution : 2.24 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 : 2.11  
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) : 2.11

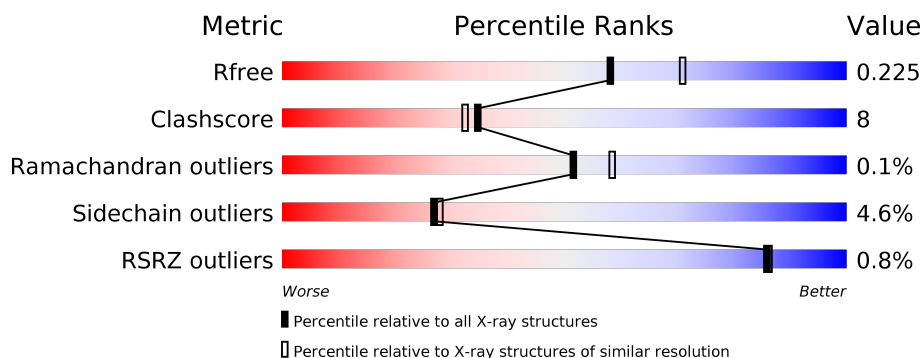
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.24 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 on 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	543	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• 5%</div> </div> </div>
1	B	543	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>• 5%</div> </div> </div>
1	C	543	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• 5%</div> </div> </div>
1	D	543	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• 5%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	D	548	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16211 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 Chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			3859	2397	666	771	25			
1	B	516	Total	C	N	O	S	0	0	0
			3859	2397	666	771	25			
1	C	516	Total	C	N	O	S	0	0	0
			3859	2397	666	771	25			
1	D	516	Total	C	N	O	S	0	0	0
			3859	2397	666	771	25			

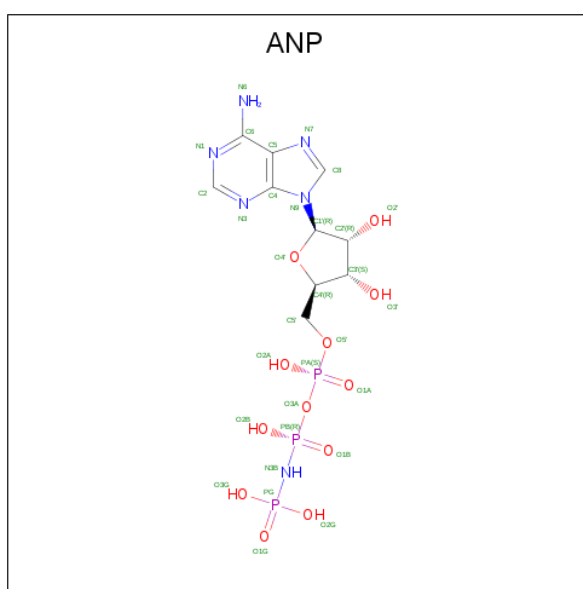
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
A	328	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
A	330	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
A	331	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
B	327	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
B	328	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
B	330	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
B	331	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
C	327	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
C	328	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
C	330	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
C	331	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
D	327	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
D	328	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
D	330	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
D	331	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

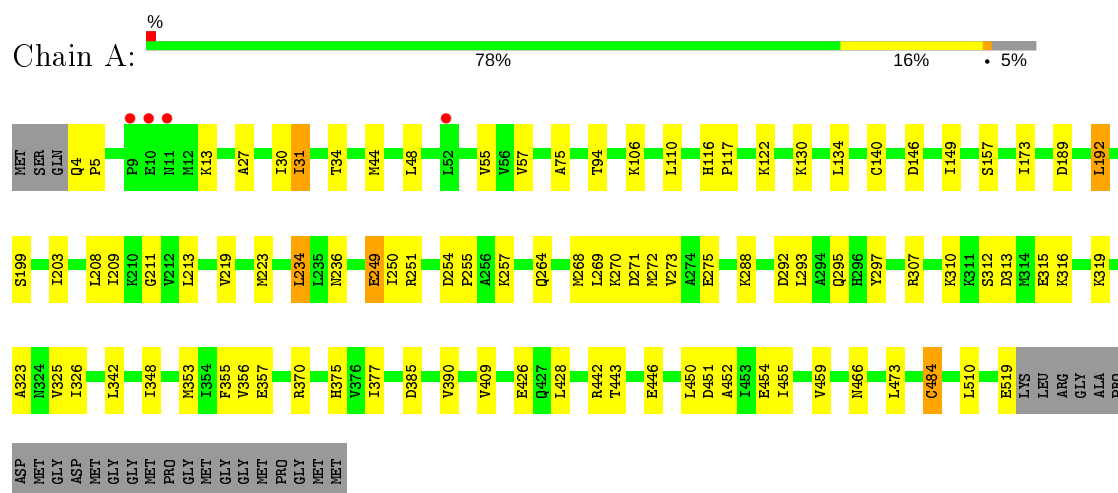
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	184	Total 184	O 184	0	0
5	B	133	Total 133	O 133	0	0
5	C	141	Total 141	O 141	0	0
5	D	125	Total 125	O 125	0	0

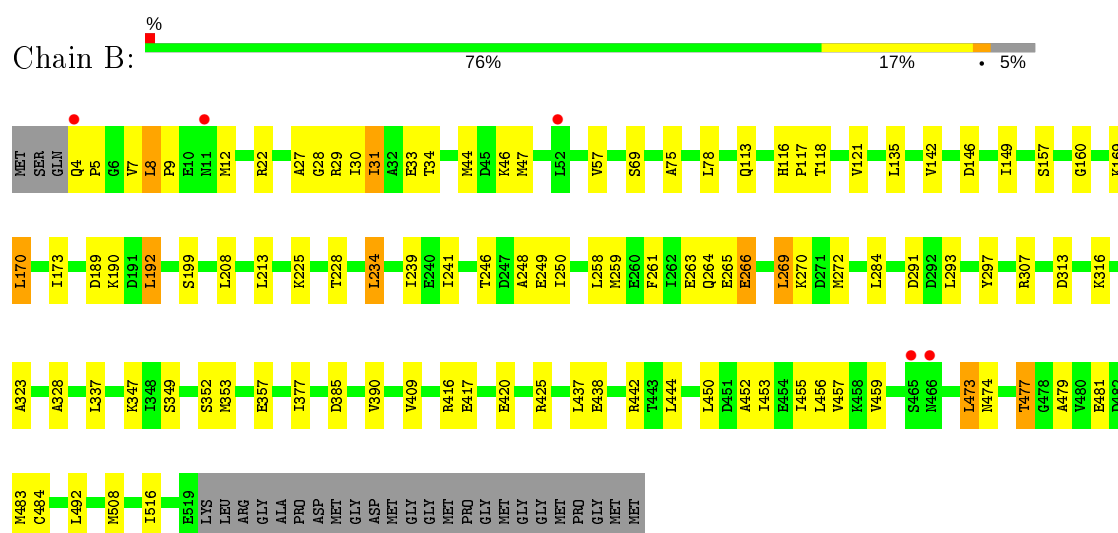
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Chaperonin



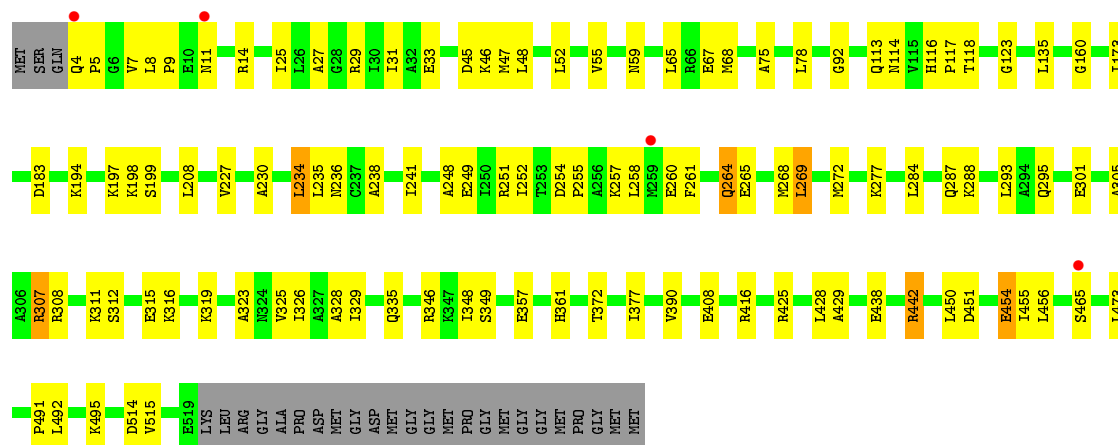
#### • Molecule 1: Chaperonin



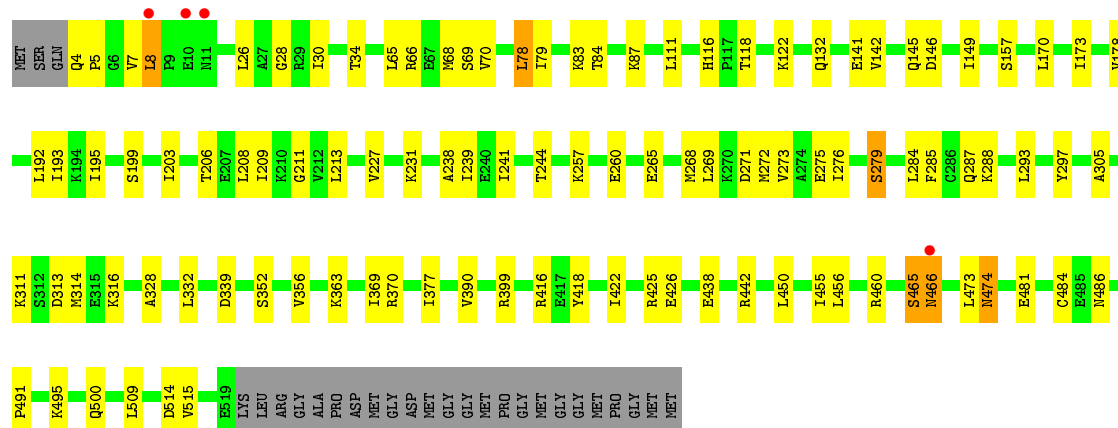
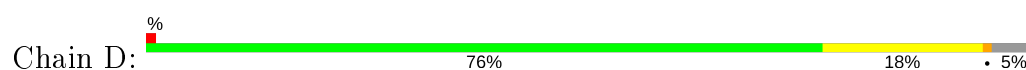
#### • Molecule 1: Chaperonin







### • Molecule 1: Chaperonin



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.02Å 184.48Å 184.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.81 – 2.24 48.81 – 2.24	Depositor EDS
% Data completeness (in resolution range)	90.4 (48.81-2.24) 99.7 (48.81-2.24)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.171 , 0.220 0.177 , 0.225	Depositor DCC
$R_{free}$ test set	6592 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16211	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, SO4

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	0.40	0/3883	0.54	0/5228
1	B	0.37	0/3883	0.53	0/5228
1	C	0.40	0/3883	0.55	0/5228
1	D	0.36	0/3883	0.52	0/5228
All	All	0.38	0/15532	0.54	0/20912

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3859	0	4001	66	0
1	B	3859	0	4001	72	0
1	C	3859	0	4001	76	0
1	D	3859	0	4001	84	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	31	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	12	0	0
3	C	31	0	12	1	0
3	D	31	0	12	2	0
4	A	15	0	0	0	0
4	B	15	0	0	1	0
4	C	15	0	0	0	0
4	D	15	0	0	2	0
5	A	184	0	0	2	0
5	B	133	0	0	1	0
5	C	141	0	0	1	0
5	D	125	0	0	0	0
All	All	16211	0	16051	262	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 8.

All (262) 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:241:ILE:H	1:D:241:ILE:HD12	1.41	0.84
1:A:234:LEU:HD22	1:A:323:ALA:HB3	1.61	0.82
1:D:287:GLN:HE22	1:D:311:LYS:HE3	1.47	0.79
1:D:455:ILE:HD13	1:D:473:LEU:HD22	1.64	0.78
1:C:234:LEU:HD22	1:C:323:ALA:HB3	1.66	0.76
1:B:9:PRO:HG2	1:B:12:MET:HE3	1.69	0.75
1:B:269:LEU:HD12	1:B:272:MET:HE1	1.69	0.74
1:C:264:GLN:HE21	1:C:264:GLN:HA	1.53	0.74
1:B:455:ILE:HD12	1:B:473:LEU:HD13	1.71	0.73
1:B:234:LEU:HD22	1:B:323:ALA:HB3	1.70	0.73
1:B:442:ARG:HG3	1:B:452:ALA:HB1	1.69	0.72
1:D:65:LEU:HB3	1:D:79:ILE:HD12	1.71	0.72
1:D:30:ILE:O	1:D:34:THR:HG23	1.90	0.71
1:B:189:ASP:HB3	1:B:192:LEU:HD22	1.72	0.70
1:B:293:LEU:HD13	1:C:328:ALA:HB2	1.73	0.70
1:D:285:PHE:HB3	1:D:314:MET:HE1	1.73	0.70
1:A:293:LEU:HD13	1:B:328:ALA:HB2	1.74	0.69
1:A:140:CYS:SG	5:A:596:HOH:O	2.49	0.69
1:B:263:GLU:HA	1:B:266:GLU:HG3	1.74	0.69
1:A:313:ASP:OD1	1:A:316:LYS:HE2	1.92	0.69
1:D:66:ARG:HD3	4:D:548:SO4:O3	1.92	0.68
1:C:236:ASN:HD22	1:C:325:VAL:HG12	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ARG:O	1:C:33:GLU:HG3	1.94	0.67
1:D:116:HIS:HD2	1:D:118:THR:OG1	1.77	0.67
1:A:450:LEU:HD12	1:A:473:LEU:HD21	1.77	0.66
1:A:484:CYS:SG	5:A:596:HOH:O	2.52	0.66
1:B:4:GLN:HG3	1:B:5:PRO:HD2	1.78	0.66
1:C:249:GLU:HG2	1:C:251:ARG:HH12	1.60	0.66
1:B:474:ASN:HB3	1:B:477:THR:OG1	1.97	0.65
1:C:27:ALA:HA	1:D:7:VAL:CG2	2.27	0.65
1:C:235:LEU:HD13	1:C:329:ILE:HD13	1.79	0.64
1:D:28:GLY:HA2	1:D:78:LEU:HD22	1.78	0.64
1:B:31:ILE:HG13	1:B:75:ALA:HB1	1.80	0.63
1:B:30:ILE:O	1:B:34:THR:HG23	1.99	0.63
1:A:375:HIS:HB3	1:B:508:MET:HE1	1.80	0.63
1:B:239:ILE:HD11	1:B:284:LEU:HD21	1.81	0.62
1:C:315:GLU:O	1:C:319:LYS:HG2	1.99	0.62
1:D:241:ILE:HG13	1:D:269:LEU:HD21	1.80	0.62
1:A:442:ARG:HG3	1:A:452:ALA:HB1	1.81	0.61
1:C:451:ASP:OD2	1:C:454:GLU:HG2	2.00	0.61
1:C:293:LEU:HD13	1:D:328:ALA:HB2	1.83	0.61
1:B:47:MET:HE3	1:C:515:VAL:HG13	1.82	0.61
1:B:225:LYS:HD2	4:B:547:SO4:O3	2.00	0.60
1:A:173:ILE:HG23	1:A:208:LEU:HB2	1.84	0.60
1:A:189:ASP:HB3	1:A:192:LEU:HD22	1.83	0.60
1:A:30:ILE:O	1:A:34:THR:HG23	2.01	0.60
1:B:173:ILE:HG23	1:B:208:LEU:HB2	1.84	0.59
1:B:269:LEU:HD12	1:B:272:MET:CE	2.30	0.59
1:D:313:ASP:OD1	1:D:316:LYS:HE2	2.01	0.59
1:C:249:GLU:HG2	1:C:251:ARG:NH1	2.17	0.59
1:A:268:MET:O	1:A:272:MET:HG3	2.03	0.59
1:B:477:THR:HB	1:B:479:ALA:H	1.67	0.59
1:A:249:GLU:HG2	1:A:251:ARG:HH12	1.66	0.59
1:A:122:LYS:HD3	1:A:426:GLU:CD	2.23	0.59
1:D:285:PHE:CB	1:D:314:MET:HE1	2.32	0.59
1:A:271:ASP:O	1:A:275:GLU:HG3	2.02	0.59
1:A:251:ARG:NH1	1:B:249:GLU:HB2	2.19	0.58
1:D:238:ALA:HB2	1:D:288:LYS:HB2	1.85	0.58
1:C:349:SER:HB3	1:D:87:LYS:NZ	2.17	0.58
1:A:450:LEU:CD1	1:A:473:LEU:HD21	2.34	0.58
1:B:113:GLN:HG3	1:B:113:GLN:O	2.03	0.58
1:A:4:GLN:HB2	1:A:5:PRO:HD2	1.86	0.58
1:B:46:LYS:HD2	1:C:514:ASP:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:MET:HG3	1:D:68:MET:O	2.05	0.56
1:C:268:MET:O	1:C:272:MET:HG3	2.05	0.56
1:D:146:ASP:O	1:D:149:ILE:HG22	2.06	0.56
1:D:241:ILE:HD12	1:D:241:ILE:N	2.17	0.56
1:D:293:LEU:HG	1:D:297:TYR:CE2	2.41	0.56
1:C:173:ILE:HG23	1:C:208:LEU:HB2	1.87	0.56
1:A:236:ASN:HB2	1:A:325:VAL:HG12	1.88	0.56
1:A:249:GLU:HG2	1:A:251:ARG:NH1	2.21	0.55
1:D:132:GLN:HE21	1:D:500:GLN:HE21	1.54	0.55
1:C:116:HIS:CD2	1:C:117:PRO:HD2	2.41	0.55
1:A:213:LEU:HD23	1:A:353:MET:CE	2.36	0.55
1:B:293:LEU:HG	1:B:297:TYR:CE2	2.42	0.55
1:D:195:ILE:HG23	1:D:369:ILE:HD12	1.89	0.54
1:D:287:GLN:NE2	1:D:311:LYS:HE3	2.18	0.54
1:D:442:ARG:HH11	1:D:442:ARG:HG2	1.73	0.54
1:A:48:LEU:HD23	1:B:516:ILE:HB	1.90	0.54
1:C:265:GLU:O	1:C:268:MET:HG2	2.08	0.53
1:A:236:ASN:O	1:A:288:LYS:HE2	2.08	0.53
1:C:227:VAL:HG22	1:C:230:ALA:HB2	1.90	0.53
1:A:116:HIS:CD2	1:A:117:PRO:HD2	2.43	0.53
1:B:44:MET:HE1	1:C:118:THR:HG23	1.89	0.53
1:A:31:ILE:HG13	1:A:75:ALA:HB1	1.91	0.53
1:B:116:HIS:CD2	1:B:117:PRO:HD2	2.43	0.53
1:B:347:LYS:HD3	1:B:352:SER:HB3	1.91	0.53
1:D:416:ARG:HH22	1:D:438:GLU:CD	2.12	0.53
1:B:146:ASP:O	1:B:149:ILE:HG22	2.09	0.53
1:C:160:GLY:O	5:C:596:HOH:O	2.18	0.52
1:D:83:LYS:HE2	4:D:548:SO4:O3	2.09	0.52
1:B:27:ALA:HA	1:C:7:VAL:HG21	1.91	0.52
1:A:57:VAL:HG22	1:B:508:MET:CE	2.39	0.52
1:D:211:GLY:HA3	1:D:356:VAL:O	2.10	0.52
1:A:313:ASP:HA	1:A:316:LYS:HE2	1.92	0.52
1:B:160:GLY:O	5:B:594:HOH:O	2.19	0.52
1:C:45:ASP:OD1	1:C:59:ASN:HB2	2.09	0.52
1:A:409:VAL:HG11	1:A:459:VAL:HG12	1.92	0.52
1:D:116:HIS:CD2	1:D:118:THR:OG1	2.62	0.52
1:C:277:LYS:HE3	1:C:301:GLU:OE1	2.09	0.52
1:D:239:ILE:HD11	1:D:284:LEU:HD21	1.90	0.52
1:D:314:MET:HA	1:D:314:MET:CE	2.40	0.52
1:D:425:ARG:HG2	1:D:425:ARG:HH11	1.74	0.51
1:B:241:ILE:HD11	1:B:265:GLU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:GLU:O	1:B:420:GLU:HB2	2.10	0.51
1:C:27:ALA:HA	1:D:7:VAL:HG22	1.92	0.51
1:A:443:THR:HA	1:A:446:GLU:HG2	1.93	0.51
1:B:313:ASP:OD1	1:B:316:LYS:HE2	2.10	0.51
1:D:142:VAL:HG13	1:D:149:ILE:HG21	1.92	0.51
1:D:241:ILE:CD1	1:D:241:ILE:H	2.17	0.51
1:B:259:MET:HE1	1:C:268:MET:CE	2.40	0.51
1:A:146:ASP:OD2	1:A:149:ILE:HD12	2.11	0.50
1:C:455:ILE:HD12	1:C:473:LEU:HD13	1.92	0.50
1:A:315:GLU:O	1:A:319:LYS:HG2	2.12	0.50
1:C:27:ALA:HA	1:D:7:VAL:HG21	1.94	0.50
1:D:450:LEU:HD12	1:D:473:LEU:HD21	1.94	0.49
1:A:292:ASP:O	1:A:295:GLN:HB2	2.12	0.49
1:A:44:MET:HE2	1:A:44:MET:HA	1.94	0.49
1:D:239:ILE:O	1:D:239:ILE:HG22	2.11	0.49
1:A:213:LEU:HD23	1:A:353:MET:HE1	1.94	0.49
1:A:264:GLN:O	1:A:268:MET:HG3	2.13	0.49
1:B:28:GLY:HA2	1:B:78:LEU:HD22	1.94	0.49
1:C:198:LYS:HG2	1:C:348:ILE:HG12	1.95	0.49
1:D:178:VAL:HA	1:D:193:ILE:HD11	1.95	0.49
1:A:273:VAL:HG21	1:A:297:TYR:HB2	1.95	0.48
1:B:442:ARG:HG3	1:B:452:ALA:CB	2.39	0.48
1:D:279:SER:OG	1:D:332:LEU:HG	2.13	0.48
1:C:25:ILE:O	1:C:29:ARG:HG3	2.13	0.48
1:D:199:SER:HA	1:D:377:ILE:HD11	1.94	0.48
1:A:451:ASP:HB3	1:A:454:GLU:HG2	1.95	0.48
1:C:252:ILE:HD13	1:C:258:LEU:HD23	1.96	0.48
1:C:46:LYS:HD3	1:D:514:ASP:HB3	1.94	0.48
1:C:47:MET:HE2	1:D:515:VAL:HG22	1.94	0.48
1:A:255:PRO:HD3	1:B:261:PHE:CZ	2.49	0.48
1:A:219:VAL:HG12	1:A:223:MET:HE1	1.95	0.47
1:D:293:LEU:HG	1:D:297:TYR:HE2	1.76	0.47
1:D:231:LYS:N	1:D:231:LYS:HD2	2.29	0.47
1:A:519:GLU:O	1:A:519:GLU:HG2	2.14	0.47
1:B:453:ILE:O	1:B:457:VAL:HG23	2.14	0.47
1:C:238:ALA:HB2	1:C:288:LYS:HB3	1.96	0.47
1:B:264:GLN:HE21	1:B:264:GLN:HA	1.79	0.47
1:A:310:LYS:HE2	1:A:313:ASP:OD2	2.15	0.47
1:B:118:THR:HA	1:B:121:VAL:HG22	1.96	0.47
1:B:27:ALA:HA	1:C:7:VAL:CG2	2.45	0.47
1:A:250:ILE:HB	1:B:248:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:MET:CE	1:B:483:MET:HA	2.45	0.47
1:C:241:ILE:HD11	1:C:269:LEU:HD22	1.97	0.47
1:C:199:SER:HA	1:C:377:ILE:HD11	1.96	0.47
1:C:346:ARG:NH2	1:C:357:GLU:OE2	2.42	0.47
1:A:130:LYS:HE3	1:A:134:LEU:HD21	1.96	0.47
1:A:409:VAL:HG21	1:A:459:VAL:HG11	1.97	0.46
1:C:197:LYS:O	1:C:198:LYS:HD2	2.15	0.46
1:B:69:SER:O	1:C:9:PRO:HG3	2.15	0.46
1:B:313:ASP:HA	1:B:316:LYS:HE2	1.98	0.46
1:A:375:HIS:HB3	1:B:508:MET:CE	2.43	0.46
1:B:9:PRO:HG2	1:B:12:MET:CE	2.44	0.46
1:C:65:LEU:HD23	1:C:68:MET:HE1	1.98	0.46
1:D:206:THR:HG23	1:D:369:ILE:HA	1.96	0.46
1:D:314:MET:HA	1:D:314:MET:HE2	1.98	0.46
1:D:28:GLY:CA	1:D:78:LEU:HD22	2.43	0.46
1:A:213:LEU:HD11	1:A:355:PHE:CD1	2.51	0.46
1:B:199:SER:HA	1:B:377:ILE:HD11	1.97	0.46
1:A:57:VAL:HG22	1:B:508:MET:HE2	1.97	0.46
1:C:293:LEU:CD1	1:D:328:ALA:HB2	2.46	0.46
1:C:123:GLY:HA3	1:C:429:ALA:HB3	1.97	0.46
1:C:287:GLN:NE2	1:C:311:LYS:HG2	2.31	0.46
1:D:287:GLN:HE22	1:D:311:LYS:CE	2.21	0.46
1:D:450:LEU:CD1	1:D:473:LEU:HD21	2.46	0.45
1:A:375:HIS:O	1:B:508:MET:HE1	2.15	0.45
1:C:372:THR:O	1:D:84:THR:HG21	2.16	0.45
1:B:409:VAL:HG11	1:B:459:VAL:HG12	1.98	0.45
1:D:203:ILE:HA	1:D:370:ARG:O	2.17	0.45
1:B:313:ASP:HA	1:B:316:LYS:HG2	1.99	0.45
1:D:474:ASN:HD21	3:D:545:ANP:HN62	1.63	0.45
1:D:157:SER:HB2	1:D:390:VAL:HG21	1.98	0.45
1:A:209:ILE:HG23	1:A:357:GLU:HB3	1.99	0.45
1:A:116:HIS:CG	1:A:117:PRO:HD2	2.51	0.45
1:C:307:ARG:NH1	1:C:308:ARG:NH2	2.64	0.45
1:A:211:GLY:HA3	1:A:356:VAL:O	2.17	0.44
1:B:416:ARG:HH22	1:B:438:GLU:CD	2.20	0.44
1:C:252:ILE:CD1	1:C:258:LEU:HD23	2.48	0.44
1:C:284:LEU:O	1:C:305:ALA:HA	2.16	0.44
1:C:408:GLU:OE2	1:C:495:LYS:NZ	2.44	0.44
1:D:390:VAL:HG12	1:D:491:PRO:HG2	2.00	0.44
1:C:47:MET:HE2	1:D:515:VAL:CG2	2.48	0.44
1:D:265:GLU:O	1:D:269:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:ASP:HA	1:D:316:LYS:HE2	2.00	0.44
1:D:209:ILE:HD13	1:D:213:LEU:HD11	1.99	0.44
1:A:106:LYS:HA	1:A:106:LYS:HD3	1.89	0.43
1:A:254:ASP:HA	1:A:255:PRO:HD2	1.69	0.43
1:A:199:SER:HA	1:A:377:ILE:HD11	1.99	0.43
1:D:122:LYS:HD3	1:D:426:GLU:CD	2.38	0.43
1:D:273:VAL:HG21	1:D:297:TYR:HB2	2.01	0.43
1:A:157:SER:HB2	1:A:390:VAL:HG21	2.00	0.43
1:C:194:LYS:HB2	1:C:316:LYS:CE	2.47	0.43
1:C:416:ARG:NH2	1:C:438:GLU:OE2	2.51	0.43
1:D:363:LYS:HD3	1:D:363:LYS:HA	1.60	0.43
1:A:442:ARG:HG2	1:A:442:ARG:HH11	1.83	0.43
1:D:284:LEU:O	1:D:305:ALA:HA	2.18	0.43
1:D:418:TYR:CE2	1:D:422:ILE:HD11	2.54	0.43
1:A:455:ILE:HD12	1:A:473:LEU:HD13	1.99	0.43
1:B:456:LEU:HA	1:B:456:LEU:HD23	1.84	0.43
1:B:31:ILE:CG1	1:B:75:ALA:HB1	2.46	0.43
1:D:141:GLU:HG2	1:D:399:ARG:NH1	2.34	0.43
1:D:465:SER:O	1:D:466:ASN:C	2.57	0.42
1:B:157:SER:HB2	1:B:390:VAL:HG21	2.01	0.42
1:C:257:LYS:HA	1:C:260:GLU:HB2	2.01	0.42
1:A:451:ASP:OD2	1:A:454:GLU:HG2	2.19	0.42
1:C:4:GLN:HA	1:C:5:PRO:HA	1.78	0.42
1:A:270:LYS:HG3	1:A:297:TYR:CE2	2.54	0.42
1:A:250:ILE:HB	1:B:248:ALA:CB	2.49	0.42
1:C:135:LEU:HB3	1:C:492:LEU:HD11	2.00	0.42
1:C:349:SER:HB3	1:D:87:LYS:HZ1	1.82	0.42
1:A:27:ALA:HA	1:B:7:VAL:HG21	2.00	0.42
1:C:390:VAL:HB	1:C:491:PRO:CG	2.49	0.42
1:C:65:LEU:HA	1:C:68:MET:HE2	2.02	0.42
1:D:474:ASN:ND2	3:D:545:ANP:HN62	2.18	0.42
1:C:295:GLN:HE22	1:C:307:ARG:HH21	1.66	0.42
1:C:438:GLU:O	1:C:442:ARG:HB2	2.20	0.42
1:C:48:LEU:HD13	1:C:67:GLU:HB2	2.01	0.42
1:D:257:LYS:HE2	1:D:260:GLU:OE1	2.20	0.42
1:D:276:ILE:O	1:D:279:SER:HB2	2.18	0.42
1:C:442:ARG:HD3	1:C:456:LEU:HD22	2.02	0.42
1:B:169:LYS:O	1:B:173:ILE:HG13	2.19	0.42
1:C:349:SER:HB3	1:D:87:LYS:HZ3	1.84	0.42
1:D:481:GLU:OE1	1:D:486:ASN:ND2	2.51	0.42
1:B:269:LEU:HA	1:B:272:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:ILE:HD13	1:D:284:LEU:HD22	2.02	0.41
1:A:255:PRO:HA	1:B:261:PHE:CE1	2.55	0.41
1:C:183:ASP:C	1:C:183:ASP:OD1	2.59	0.41
1:C:442:ARG:HH11	1:C:442:ARG:HG2	1.86	0.41
1:A:203:ILE:HA	1:A:370:ARG:O	2.19	0.41
1:C:442:ARG:HD3	1:C:456:LEU:CD2	2.50	0.41
1:D:4:GLN:HB3	1:D:5:PRO:HD3	2.03	0.41
1:D:68:MET:O	1:D:70:VAL:HG23	2.20	0.41
1:A:257:LYS:HA	1:A:257:LYS:HD3	1.81	0.41
1:B:270:LYS:HG2	1:B:297:TYR:CZ	2.55	0.41
1:B:29:ARG:O	1:B:33:GLU:HG3	2.21	0.41
1:B:213:LEU:HG	1:B:353:MET:HE3	2.03	0.41
1:C:254:ASP:HA	1:C:255:PRO:HD2	1.85	0.41
1:D:271:ASP:O	1:D:275:GLU:HG3	2.21	0.41
1:B:135:LEU:HB3	1:B:492:LEU:HD11	2.02	0.41
1:A:375:HIS:C	1:B:508:MET:HE1	2.40	0.41
1:B:250:ILE:HB	1:C:248:ALA:HB2	2.02	0.41
1:B:258:LEU:HD23	1:B:258:LEU:HA	1.80	0.41
1:D:173:ILE:HG23	1:D:208:LEU:HB2	2.02	0.41
1:D:268:MET:O	1:D:272:MET:HG3	2.21	0.41
1:C:92:GLY:HA2	3:C:545:ANP:O2B	2.21	0.41
1:D:456:LEU:O	1:D:460:ARG:HG3	2.20	0.41
1:C:31:ILE:HG13	1:C:75:ALA:HB1	2.02	0.41
1:C:14:ARG:HA	1:C:515:VAL:O	2.21	0.41
1:D:509:LEU:HD23	1:D:509:LEU:HA	1.94	0.41
1:D:7:VAL:HG12	1:D:8:LEU:HD13	2.02	0.41
1:D:192:LEU:HA	1:D:192:LEU:HD23	1.95	0.40
1:B:170:LEU:HD23	1:B:170:LEU:HA	1.86	0.40
1:C:450:LEU:HD12	1:C:473:LEU:HD21	2.03	0.40
1:D:146:ASP:CG	1:D:149:ILE:HG22	2.41	0.40
1:C:261:PHE:HB3	1:D:244:THR:HG21	2.03	0.40
1:B:8:LEU:H	1:B:8:LEU:HD12	1.86	0.40
1:A:94:THR:H	3:A:545:ANP:HNB1	1.69	0.40
1:C:113:GLN:O	1:C:114:ASN:HB2	2.21	0.40
1:C:235:LEU:HD13	1:C:329:ILE:CD1	2.49	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	514/543 (95%)	503 (98%)	11 (2%)	0	100	100
1	B	514/543 (95%)	504 (98%)	10 (2%)	0	100	100
1	C	514/543 (95%)	503 (98%)	10 (2%)	1 (0%)	47	53
1	D	514/543 (95%)	503 (98%)	9 (2%)	2 (0%)	34	35
All	All	2056/2172 (95%)	2013 (98%)	40 (2%)	3 (0%)	51	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	465	SER
1	D	69	SER
1	D	466	ASN

### 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	412/430 (96%)	394 (96%)	18 (4%)	28	30
1	B	412/430 (96%)	385 (93%)	27 (7%)	16	14
1	C	412/430 (96%)	395 (96%)	17 (4%)	30	33
1	D	412/430 (96%)	398 (97%)	14 (3%)	37	42
All	All	1648/1720 (96%)	1572 (95%)	76 (5%)	27	28

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	31	ILE
1	A	55	VAL
1	A	110	LEU
1	A	192	LEU
1	A	234	LEU
1	A	249	GLU
1	A	269	LEU
1	A	307	ARG
1	A	312	SER
1	A	326	ILE
1	A	342	LEU
1	A	348	ILE
1	A	385	ASP
1	A	428	LEU
1	A	466	ASN
1	A	484	CYS
1	A	510	LEU
1	B	8	LEU
1	B	22	ARG
1	B	31	ILE
1	B	57	VAL
1	B	142	VAL
1	B	170	LEU
1	B	190	LYS
1	B	192	LEU
1	B	228	THR
1	B	234	LEU
1	B	246	THR
1	B	266	GLU
1	B	269	LEU
1	B	291	ASP
1	B	307	ARG
1	B	337	LEU
1	B	349	SER
1	B	357	GLU
1	B	385	ASP
1	B	425	ARG
1	B	437	LEU
1	B	444	LEU
1	B	450	LEU
1	B	473	LEU
1	B	477	THR

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Mol	Chain	Res	Type
1	B	481	GLU
1	B	484	CYS
1	C	8	LEU
1	C	11	ASN
1	C	52	LEU
1	C	55	VAL
1	C	78	LEU
1	C	234	LEU
1	C	264	GLN
1	C	269	LEU
1	C	307	ARG
1	C	312	SER
1	C	326	ILE
1	C	335	GLN
1	C	361	HIS
1	C	425	ARG
1	C	428	LEU
1	C	442	ARG
1	C	454	GLU
1	D	8	LEU
1	D	26	LEU
1	D	78	LEU
1	D	111	LEU
1	D	145	GLN
1	D	170	LEU
1	D	227	VAL
1	D	279	SER
1	D	339	ASP
1	D	352	SER
1	D	465	SER
1	D	474	ASN
1	D	484	CYS
1	D	495	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	264	GLN
1	A	500	GLN
1	B	264	GLN
1	B	287	GLN

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Mol	Chain	Res	Type
1	B	296	HIS
1	B	427	GLN
1	B	500	GLN
1	C	4	GLN
1	C	264	GLN
1	C	287	GLN
1	C	500	GLN
1	D	116	HIS
1	D	125	GLN
1	D	264	GLN
1	D	287	GLN
1	D	296	HIS
1	D	474	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 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
3	ANP	D	545	2	29,33,33	2.27	9 (31%)	31,52,52	1.43	4 (12%)
4	SO4	C	548	-	4,4,4	0.13	0	6,6,6	0.13	0
3	ANP	C	545	2	29,33,33	2.18	8 (27%)	31,52,52	1.47	6 (19%)
4	SO4	B	548	-	4,4,4	0.17	0	6,6,6	0.09	0
4	SO4	D	548	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	A	547	-	4,4,4	0.13	0	6,6,6	0.14	0
4	SO4	A	546	-	4,4,4	0.15	0	6,6,6	0.17	0
4	SO4	D	546	-	4,4,4	0.14	0	6,6,6	0.20	0
4	SO4	B	546	-	4,4,4	0.17	0	6,6,6	0.20	0
4	SO4	D	547	-	4,4,4	0.15	0	6,6,6	0.15	0
4	SO4	C	546	-	4,4,4	0.17	0	6,6,6	0.25	0
4	SO4	A	548	-	4,4,4	0.14	0	6,6,6	0.09	0
3	ANP	A	545	2	29,33,33	2.14	9 (31%)	31,52,52	1.43	3 (9%)
4	SO4	B	547	-	4,4,4	0.17	0	6,6,6	0.11	0
3	ANP	B	545	2	29,33,33	2.19	8 (27%)	31,52,52	1.45	5 (16%)
4	SO4	C	547	-	4,4,4	0.12	0	6,6,6	0.17	0

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
3	ANP	D	545	2	-	4/14/38/38	0/3/3/3
3	ANP	A	545	2	-	4/14/38/38	0/3/3/3
3	ANP	C	545	2	-	4/14/38/38	0/3/3/3
3	ANP	B	545	2	-	4/14/38/38	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	545	ANP	PB-O1B	6.76	1.56	1.46
3	B	545	ANP	PB-O1B	6.73	1.56	1.46
3	A	545	ANP	PB-O1B	6.20	1.56	1.46
3	D	545	ANP	PG-O1G	6.13	1.55	1.46
3	C	545	ANP	PG-O1G	6.03	1.55	1.46
3	C	545	ANP	PB-O1B	5.81	1.55	1.46
3	B	545	ANP	PG-O1G	5.44	1.54	1.46
3	A	545	ANP	PG-O1G	4.90	1.53	1.46
3	C	545	ANP	O2'-C2'	-3.17	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	545	ANP	PG-O3G	-3.07	1.48	1.56
3	A	545	ANP	PG-O3G	-3.05	1.48	1.56
3	C	545	ANP	C2'-C1'	-3.01	1.49	1.53
3	C	545	ANP	PG-O3G	-3.00	1.48	1.56
3	A	545	ANP	O2'-C2'	-2.87	1.36	1.43
3	B	545	ANP	C2'-C1'	-2.76	1.49	1.53
3	D	545	ANP	O2'-C2'	-2.72	1.36	1.43
3	B	545	ANP	O2'-C2'	-2.72	1.36	1.43
3	C	545	ANP	C2'-C3'	-2.72	1.45	1.53
3	A	545	ANP	O3'-C3'	-2.67	1.36	1.43
3	B	545	ANP	PG-O3G	-2.63	1.49	1.56
3	D	545	ANP	C2'-C1'	-2.58	1.49	1.53
3	D	545	ANP	C2'-C3'	-2.50	1.46	1.53
3	B	545	ANP	O3'-C3'	-2.50	1.37	1.43
3	B	545	ANP	C2'-C3'	-2.44	1.46	1.53
3	B	545	ANP	C6-N6	2.43	1.42	1.34
3	A	545	ANP	C2'-C1'	-2.32	1.50	1.53
3	A	545	ANP	C2'-C3'	-2.31	1.47	1.53
3	C	545	ANP	C6-N6	2.31	1.42	1.34
3	D	545	ANP	C6-N6	2.29	1.42	1.34
3	D	545	ANP	O3'-C3'	-2.29	1.37	1.43
3	A	545	ANP	C6-N6	2.26	1.42	1.34
3	C	545	ANP	O3'-C3'	-2.20	1.37	1.43
3	D	545	ANP	PG-N3B	2.16	1.69	1.63
3	A	545	ANP	PG-N3B	2.10	1.68	1.63

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	545	ANP	N3-C2-N1	-5.25	120.47	128.68
3	C	545	ANP	N3-C2-N1	-5.08	120.74	128.68
3	B	545	ANP	N3-C2-N1	-5.00	120.87	128.68
3	A	545	ANP	N3-C2-N1	-4.94	120.96	128.68
3	C	545	ANP	O1G-PG-N3B	-3.16	107.11	111.77
3	A	545	ANP	O3A-PB-N3B	2.50	113.54	106.59
3	B	545	ANP	PA-O3A-PB	-2.38	124.24	132.62
3	B	545	ANP	O3A-PB-N3B	2.32	113.02	106.59
3	B	545	ANP	C4-C5-N7	-2.21	107.10	109.40
3	D	545	ANP	O5'-C5'-C4'	2.19	116.52	108.99
3	C	545	ANP	N6-C6-N1	2.16	123.06	118.57
3	D	545	ANP	C4-C5-N7	-2.15	107.16	109.40
3	C	545	ANP	O3A-PB-N3B	2.12	112.47	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	545	ANP	C5-C6-N6	-2.11	117.15	120.35
3	A	545	ANP	C4-C5-N7	-2.07	107.24	109.40
3	D	545	ANP	O3A-PB-N3B	2.07	112.33	106.59
3	B	545	ANP	O5'-C5'-C4'	2.07	116.10	108.99
3	C	545	ANP	O5'-C5'-C4'	2.06	116.07	108.99

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	545	ANP	PB-N3B-PG-O1G
3	B	545	ANP	PB-N3B-PG-O1G
3	B	545	ANP	C5'-O5'-PA-O1A
3	A	545	ANP	PB-N3B-PG-O1G
3	C	545	ANP	PB-N3B-PG-O1G
3	A	545	ANP	PB-O3A-PA-O1A
3	D	545	ANP	PB-O3A-PA-O1A
3	B	545	ANP	PB-O3A-PA-O1A
3	D	545	ANP	PB-O3A-PA-O2A
3	B	545	ANP	PB-O3A-PA-O2A
3	A	545	ANP	PB-O3A-PA-O2A
3	C	545	ANP	PB-O3A-PA-O1A
3	C	545	ANP	PB-O3A-PA-O2A
3	D	545	ANP	C5'-O5'-PA-O1A
3	A	545	ANP	C5'-O5'-PA-O1A
3	C	545	ANP	C5'-O5'-PA-O1A

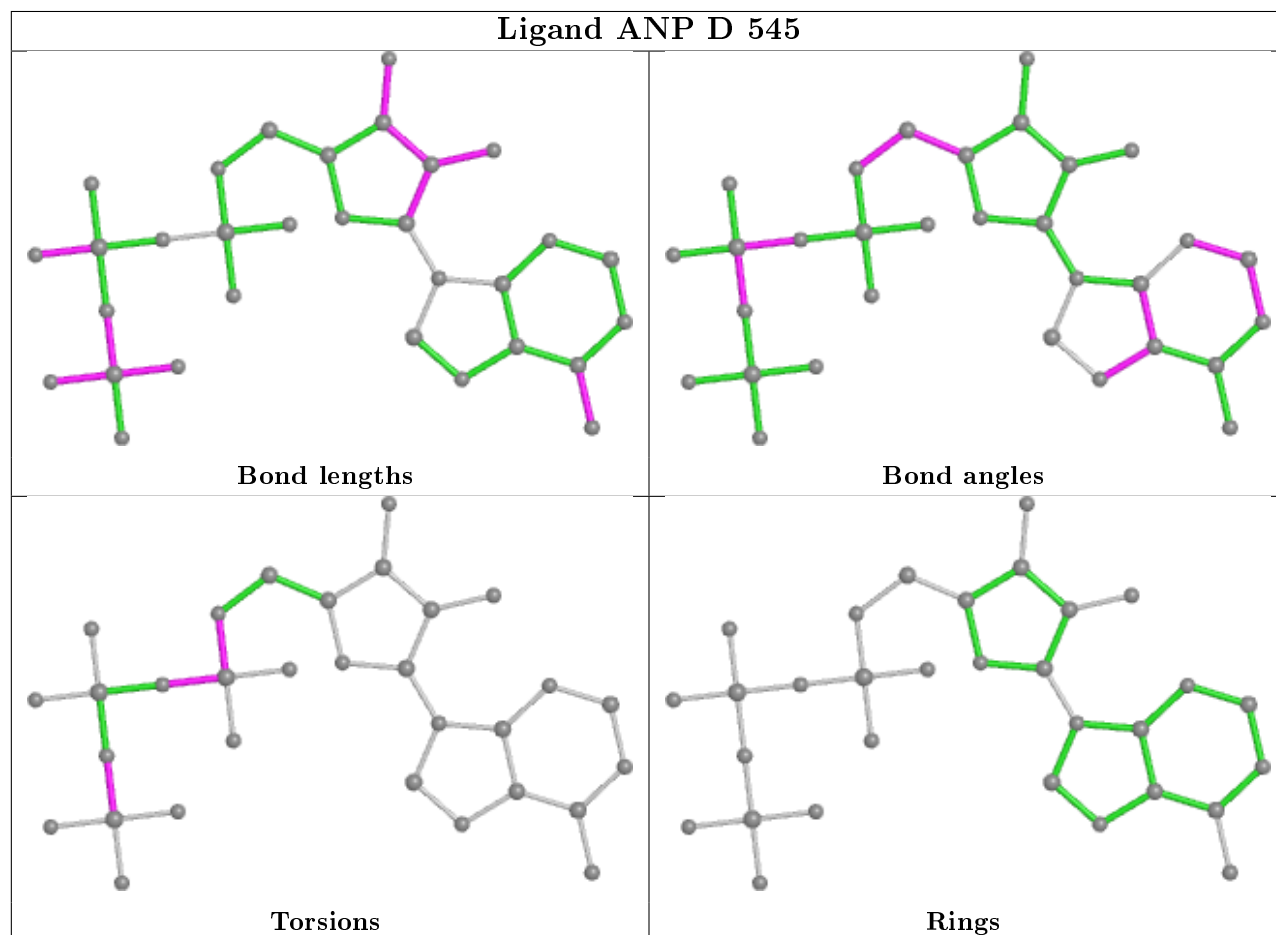
There are no ring outliers.

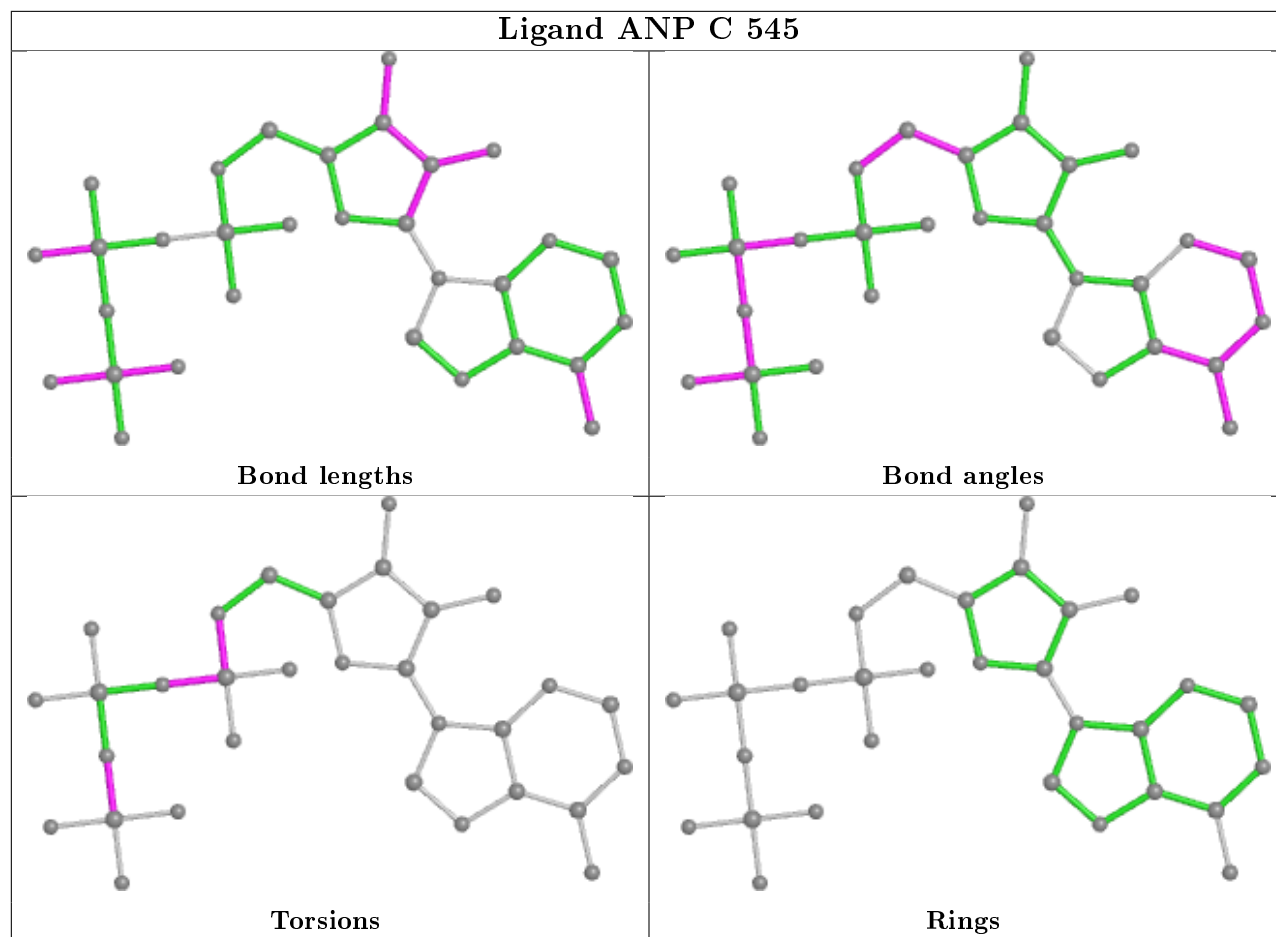
5 monomers are involved in 7 short contacts:

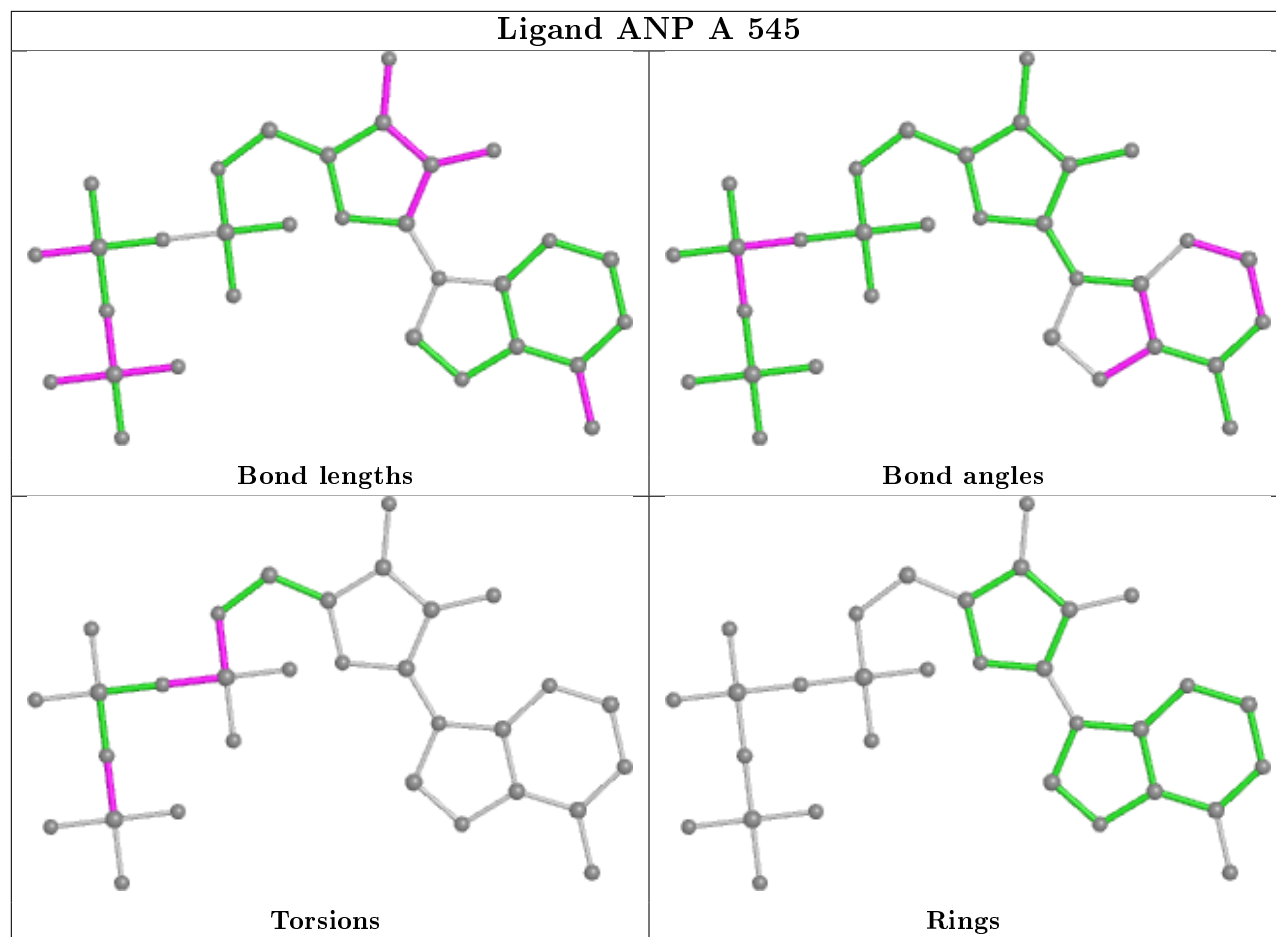
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	545	ANP	2	0
3	C	545	ANP	1	0
4	D	548	SO4	2	0
3	A	545	ANP	1	0
4	B	547	SO4	1	0

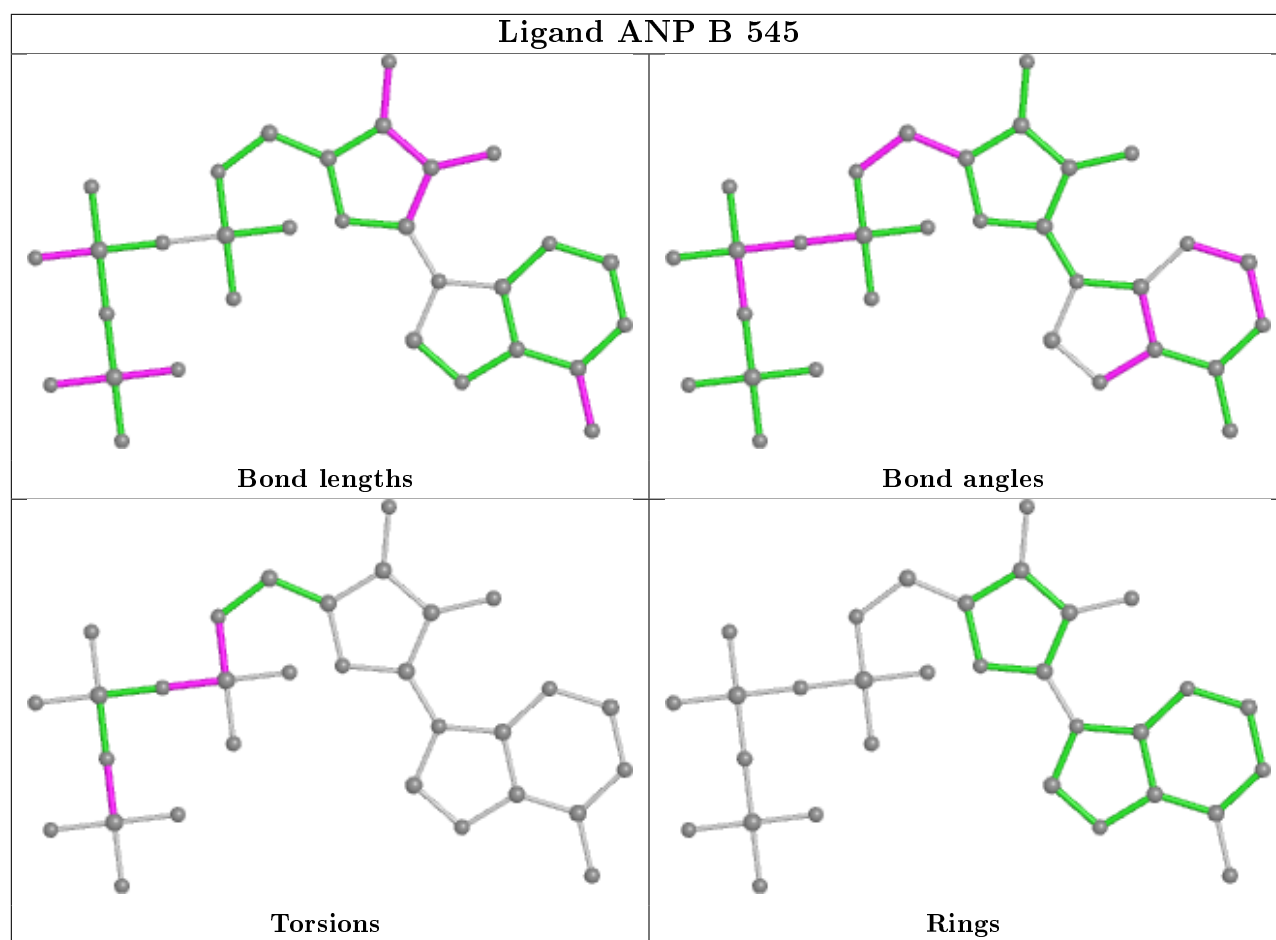
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 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	516/543 (95%)	-0.41	4 (0%) 86 86	21, 43, 79, 119	0
1	B	516/543 (95%)	-0.38	5 (0%) 82 83	26, 47, 83, 128	0
1	C	516/543 (95%)	-0.35	4 (0%) 86 86	21, 46, 82, 121	0
1	D	516/543 (95%)	-0.24	4 (0%) 86 86	28, 50, 85, 149	0
All	All	2064/2172 (95%)	-0.34	17 (0%) 86 86	21, 47, 83, 149	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	11	ASN	4.8
1	A	11	ASN	3.8
1	D	466	ASN	3.7
1	D	10	GLU	3.4
1	B	466	ASN	3.3
1	B	11	ASN	3.2
1	C	4	GLN	2.9
1	B	465	SER	2.7
1	A	10	GLU	2.6
1	B	52	LEU	2.4
1	A	9	PRO	2.4
1	C	11	ASN	2.2
1	C	259	MET	2.2
1	A	52	LEU	2.2
1	D	8	LEU	2.1
1	C	465	SER	2.1
1	B	4	GLN	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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

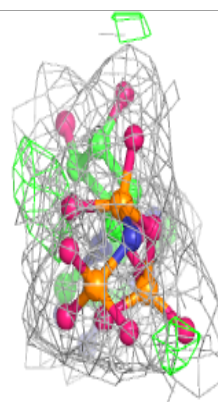
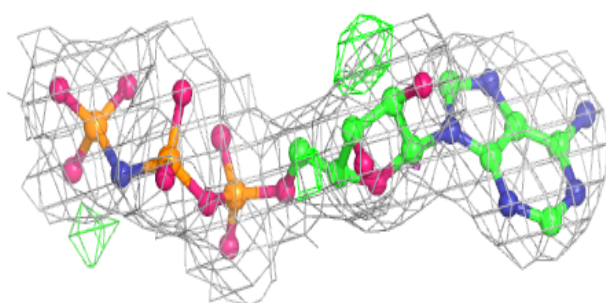
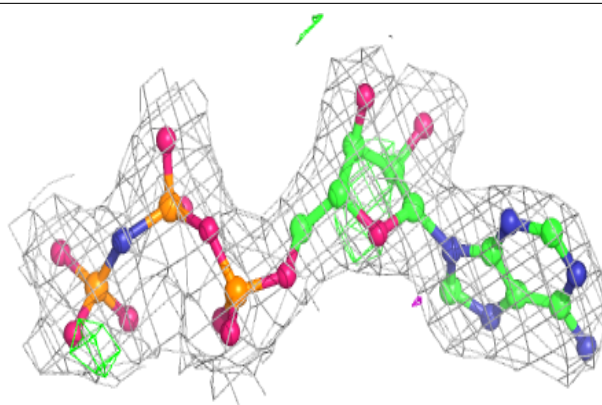
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	SO4	D	548	5/5	0.80	0.18	144,149,149,150	0
4	SO4	A	548	5/5	0.84	0.15	119,121,127,127	0
4	SO4	B	548	5/5	0.85	0.21	112,114,117,117	0
4	SO4	A	547	5/5	0.87	0.20	116,118,119,124	0
4	SO4	C	548	5/5	0.87	0.22	124,125,128,132	0
4	SO4	C	547	5/5	0.89	0.15	95,96,102,110	0
4	SO4	B	547	5/5	0.90	0.15	98,106,110,114	0
4	SO4	C	546	5/5	0.90	0.15	80,88,95,97	0
4	SO4	D	547	5/5	0.90	0.15	110,113,115,116	0
4	SO4	D	546	5/5	0.92	0.15	94,100,108,110	0
4	SO4	B	546	5/5	0.93	0.14	84,92,94,96	0
2	MG	B	549	1/1	0.94	0.08	37,37,37,37	0
4	SO4	A	546	5/5	0.94	0.07	74,87,95,96	0
2	MG	D	549	1/1	0.96	0.11	42,42,42,42	0
2	MG	C	549	1/1	0.96	0.10	38,38,38,38	0
2	MG	A	549	1/1	0.97	0.11	42,42,42,42	0
3	ANP	D	545	31/31	0.98	0.11	23,35,46,50	0
2	MG	A	544	1/1	0.98	0.13	27,27,27,27	0
2	MG	C	544	1/1	0.98	0.19	30,30,30,30	0
2	MG	B	544	1/1	0.99	0.16	33,33,33,33	0
3	ANP	C	545	31/31	0.99	0.12	21,30,39,43	0
3	ANP	B	545	31/31	0.99	0.11	19,33,46,50	0
2	MG	D	544	1/1	0.99	0.16	39,39,39,39	0
3	ANP	A	545	31/31	0.99	0.10	22,28,39,42	0

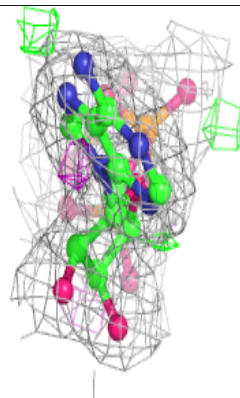
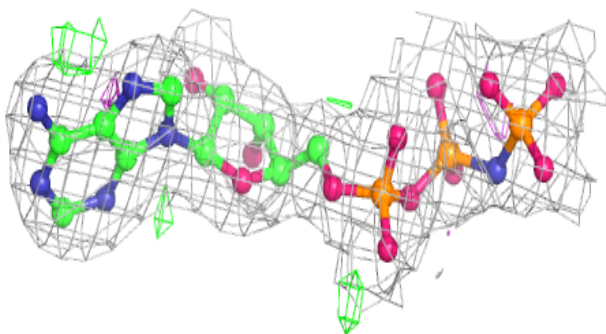
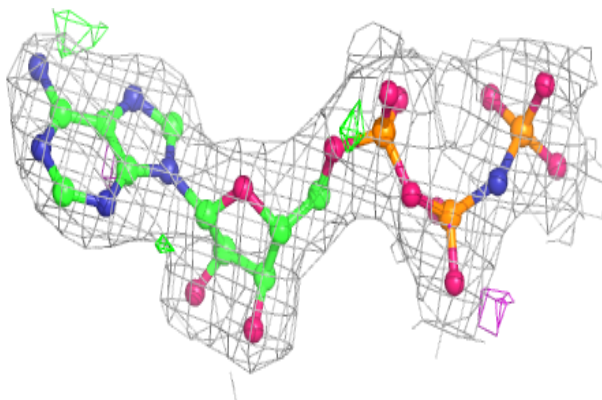
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ANP D 545:**

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

**Electron density around ANP C 545:**

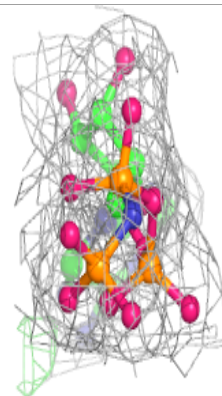
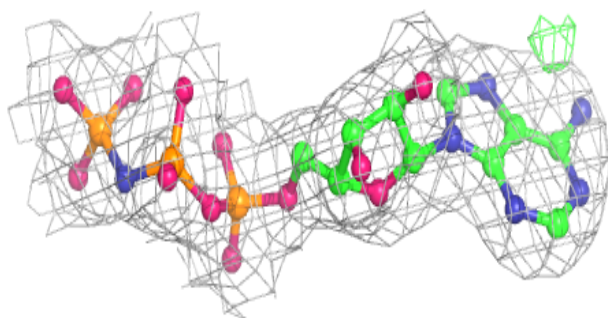
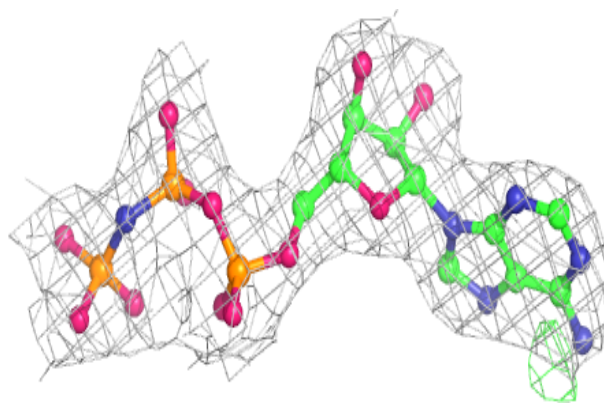
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



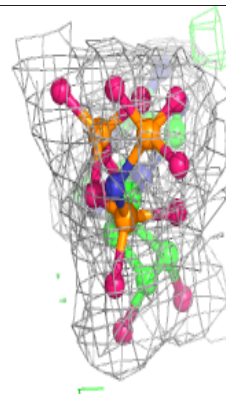
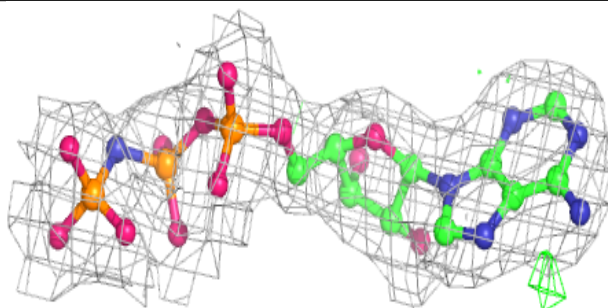
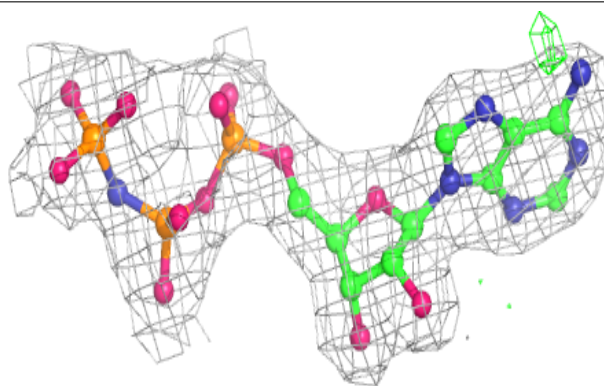


**Electron density around ANP B 545:**

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

**Electron density around ANP A 545:**

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



## 6.5 Other polymers

There are no such residues in this entry.