



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:04 pm BST

PDB ID : 4IC7
Title : Crystal structure of the ERK5 kinase domain in complex with an MKK5 binding fragment
Authors : Gogl, G.; Remenyi, A.
Deposited on : 2012-12-10
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 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

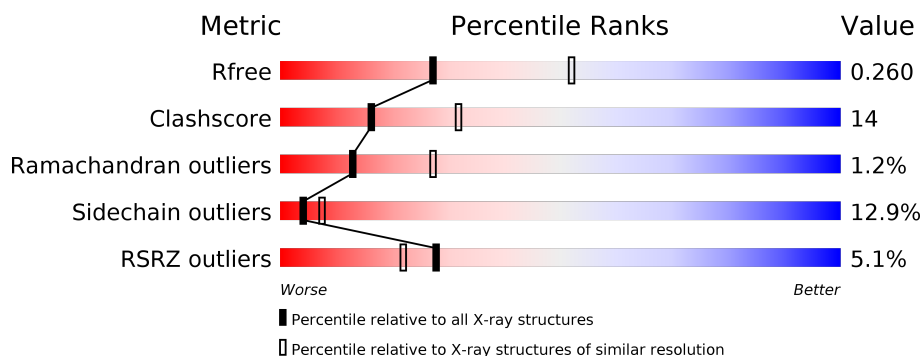
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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 on 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	442	<div> <div>3%</div> <div> <div></div> <div>55%</div> <div>21%</div> <div>•</div> <div>20%</div> </div> </div>
1	D	442	<div> <div>7%</div> <div> <div></div> <div>54%</div> <div>21%</div> <div>•</div> <div>20%</div> </div> </div>
2	B	126	<div> <div></div> <div> <div>50%</div> <div>34%</div> <div>11%</div> <div>• •</div> </div> </div>
2	E	126	<div> <div>4%</div> <div> <div></div> <div>58%</div> <div>26%</div> <div>• •</div> <div>12%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7394 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 Mitogen-activated protein kinase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2775	1776	488	498	13			
1	D	353	Total	C	N	O	S	0	0	0
			2675	1713	471	478	13			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q13164
A	0	SER	-	EXPRESSION TAG	UNP Q13164
A	432	SER	-	EXPRESSION TAG	UNP Q13164
A	433	GLY	-	EXPRESSION TAG	UNP Q13164
A	434	ARG	-	EXPRESSION TAG	UNP Q13164
A	435	HIS	-	EXPRESSION TAG	UNP Q13164
A	436	HIS	-	EXPRESSION TAG	UNP Q13164
A	437	HIS	-	EXPRESSION TAG	UNP Q13164
A	438	HIS	-	EXPRESSION TAG	UNP Q13164
A	439	HIS	-	EXPRESSION TAG	UNP Q13164
A	440	HIS	-	EXPRESSION TAG	UNP Q13164
D	-1	GLY	-	EXPRESSION TAG	UNP Q13164
D	0	SER	-	EXPRESSION TAG	UNP Q13164
D	432	SER	-	EXPRESSION TAG	UNP Q13164
D	433	GLY	-	EXPRESSION TAG	UNP Q13164
D	434	ARG	-	EXPRESSION TAG	UNP Q13164
D	435	HIS	-	EXPRESSION TAG	UNP Q13164
D	436	HIS	-	EXPRESSION TAG	UNP Q13164
D	437	HIS	-	EXPRESSION TAG	UNP Q13164
D	438	HIS	-	EXPRESSION TAG	UNP Q13164
D	439	HIS	-	EXPRESSION TAG	UNP Q13164
D	440	HIS	-	EXPRESSION TAG	UNP Q13164

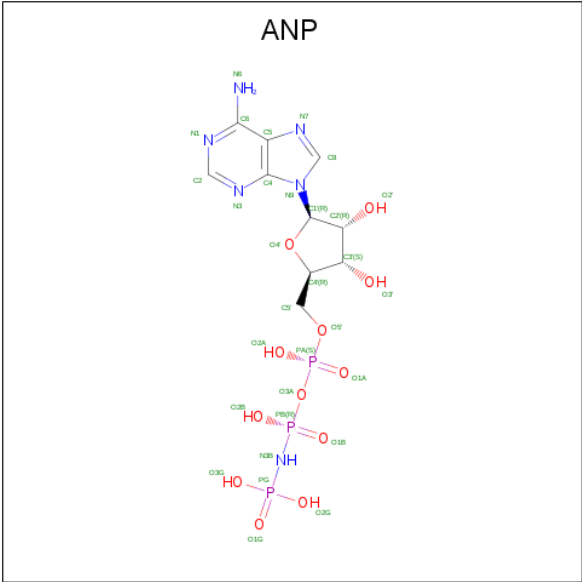
- Molecule 2 is a protein called Dual specificity mitogen-activated protein kinase kinase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	111	Total	C	N	O	S	0	0	0
			859	544	145	166	4			
2	B	123	Total	C	N	O	S	0	0	0
			940	592	166	178	4			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	14	GLY	-	EXPRESSION TAG	UNP Q13163
E	15	SER	-	EXPRESSION TAG	UNP Q13163
E	131	SER	-	EXPRESSION TAG	UNP Q13163
E	132	GLY	-	EXPRESSION TAG	UNP Q13163
E	133	ARG	-	EXPRESSION TAG	UNP Q13163
E	134	HIS	-	EXPRESSION TAG	UNP Q13163
E	135	HIS	-	EXPRESSION TAG	UNP Q13163
E	136	HIS	-	EXPRESSION TAG	UNP Q13163
E	137	HIS	-	EXPRESSION TAG	UNP Q13163
E	138	HIS	-	EXPRESSION TAG	UNP Q13163
E	139	HIS	-	EXPRESSION TAG	UNP Q13163
B	14	GLY	-	EXPRESSION TAG	UNP Q13163
B	15	SER	-	EXPRESSION TAG	UNP Q13163
B	131	SER	-	EXPRESSION TAG	UNP Q13163
B	132	GLY	-	EXPRESSION TAG	UNP Q13163
B	133	ARG	-	EXPRESSION TAG	UNP Q13163
B	134	HIS	-	EXPRESSION TAG	UNP Q13163
B	135	HIS	-	EXPRESSION TAG	UNP Q13163
B	136	HIS	-	EXPRESSION TAG	UNP Q13163
B	137	HIS	-	EXPRESSION TAG	UNP Q13163
B	138	HIS	-	EXPRESSION TAG	UNP Q13163
B	139	HIS	-	EXPRESSION TAG	UNP Q13163

- 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	0	0
			31	10	6	12	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

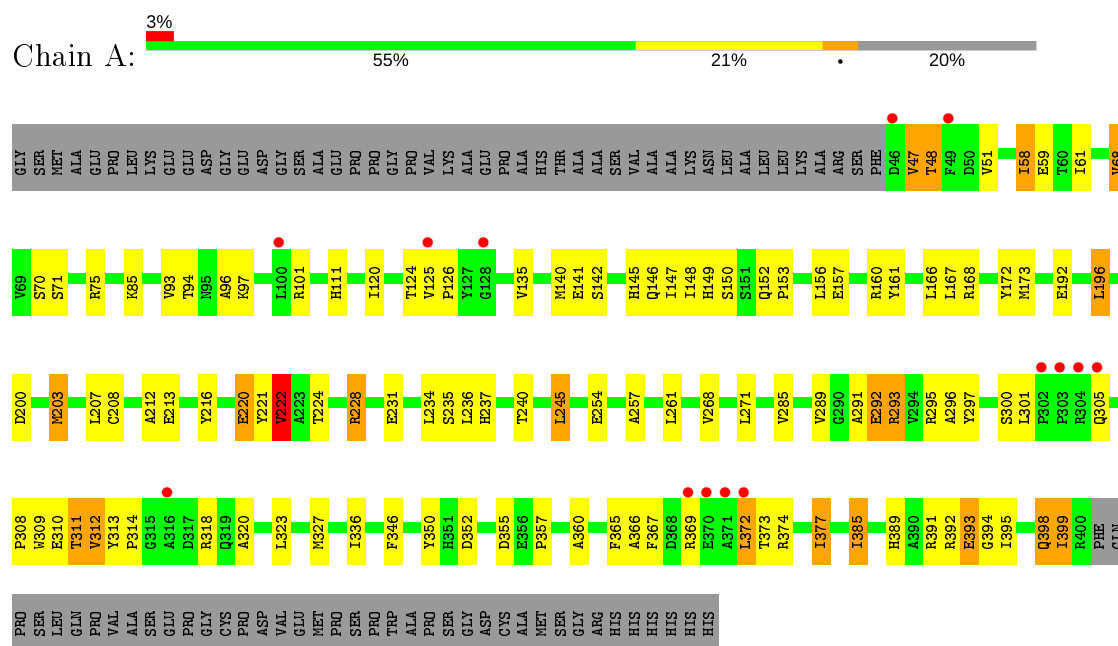
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total	O	0	0
			36	36		
4	D	32	Total	O	0	0
			32	32		
4	E	10	Total	O	0	0
			10	10		
4	B	5	Total	O	0	0
			5	5		

3 Residue-property plots [i](#)

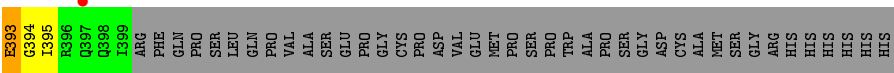
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Mitogen-activated protein kinase 7

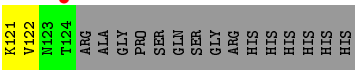


• Molecule 1: Mitogen-activated protein kinase 7

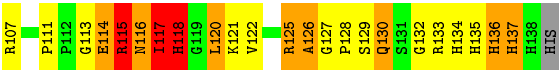
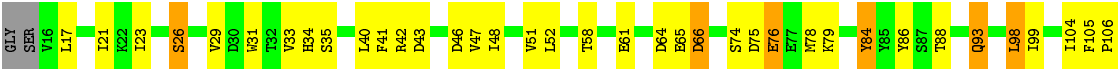




• Molecule 2: Dual specificity mitogen-activated protein kinase kinase 5



• Molecule 2: Dual specificity mitogen-activated protein kinase kinase 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	69.37Å 69.37Å 271.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.27 – 2.60 48.27 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.27-2.60) 94.5 (48.27-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.211 , 0.258 0.213 , 0.260	Depositor DCC
R_{free} test set	1958 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	56.8	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 76.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.104 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7394	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.42	0/2843	0.72	6/3865 (0.2%)
1	D	0.40	0/2740	0.71	2/3735 (0.1%)
2	B	0.44	0/961	0.76	1/1311 (0.1%)
2	E	0.40	0/876	0.69	2/1194 (0.2%)
All	All	0.41	0/7420	0.72	11/10105 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	D	0	3
2	B	0	5
2	E	0	1
All	All	0	12

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	196	LEU	CA-CB-CG	7.55	132.67	115.30
1	A	196	LEU	CA-CB-CG	6.37	129.95	115.30
1	A	394	GLY	N-CA-C	-5.93	98.27	113.10
1	A	292	GLU	N-CA-C	5.92	126.97	111.00
1	A	207	LEU	CB-CA-C	5.73	121.09	110.20
2	E	120	LEU	CA-CB-CG	5.45	127.83	115.30
2	E	118	HIS	N-CA-C	5.40	125.57	111.00
1	A	360	ALA	C-N-CD	5.31	139.56	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	118	HIS	N-CA-C	5.24	125.14	111.00
1	D	392	ARG	C-N-CA	5.09	134.41	121.70
1	A	222	VAL	N-CA-C	-5.06	97.35	111.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	292	GLU	Peptide
1	A	366	ALA	Peptide
1	A	51	VAL	Peptide
2	B	115	ARG	Sidechain
2	B	117	ILE	Peptide
2	B	126	ALA	Peptide
2	B	130	GLN	Peptide
2	B	136	HIS	Peptide
1	D	292	GLU	Peptide
1	D	367	PHE	Peptide
1	D	392	ARG	Peptide
2	E	117	ILE	Peptide

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	2775	0	2698	74	0
1	D	2675	0	2551	70	0
2	B	940	0	891	52	0
2	E	859	0	828	28	0
3	A	31	0	11	3	0
3	D	31	0	13	8	0
4	A	36	0	0	4	0
4	B	5	0	0	1	0
4	D	32	0	0	2	0
4	E	10	0	0	0	0
All	All	7394	0	6992	206	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 14.

All (206) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:THR:O	1:A:85:LYS:NZ	1.99	0.95
2:E:112:PRO:HA	2:E:114:GLU:H	1.39	0.88
2:E:116:ASN:H	2:E:116:ASN:ND2	1.71	0.87
2:B:116:ASN:N	2:B:116:ASN:HD22	1.72	0.87
3:D:501:ANP:H8	3:D:501:ANP:H3'	1.57	0.87
1:D:393:GLU:OE2	1:D:394:GLY:N	2.07	0.86
2:E:116:ASN:N	2:E:116:ASN:HD22	1.75	0.84
2:E:116:ASN:ND2	2:E:116:ASN:N	2.23	0.83
1:D:232:LEU:HD11	1:D:243:ILE:HD12	1.62	0.79
1:D:361:PRO:HD2	2:E:42:ARG:NH1	1.98	0.78
1:A:391:ARG:NH2	2:B:46:ASP:OD2	2.16	0.78
1:D:392:ARG:HA	1:D:393:GLU:HB3	1.66	0.77
2:B:93:GLN:HG3	2:B:99:ILE:HD11	1.65	0.77
2:B:111:PRO:O	2:B:113:GLY:HA3	1.84	0.77
1:D:65:ALA:O	3:D:501:ANP:O2B	2.02	0.77
1:D:245:LEU:HD13	4:D:626:HOH:O	1.84	0.76
2:E:115:ARG:HD2	2:E:118:HIS:O	1.88	0.74
1:D:59:GLU:HB3	1:D:71:SER:HB3	1.69	0.73
1:A:297:TYR:HA	1:A:300:SER:HB3	1.71	0.73
1:A:97:LYS:NZ	1:A:101:ARG:HH22	1.86	0.72
1:A:309:TRP:HA	1:A:312:VAL:HG13	1.71	0.72
2:B:127:GLY:HA2	2:B:133:ARG:CB	2.20	0.71
1:A:145:HIS:CD2	2:B:128:PRO:HA	2.26	0.70
2:B:116:ASN:ND2	2:B:116:ASN:N	2.38	0.70
1:D:147:ILE:HD12	2:E:120:LEU:HD21	1.73	0.70
3:D:501:ANP:O1A	3:D:501:ANP:N3B	2.25	0.69
1:D:277:VAL:HG22	1:D:278:LEU:HD12	1.74	0.69
2:E:43:ASP:N	2:E:43:ASP:OD1	2.26	0.69
1:A:220:GLU:HG2	1:A:221:TYR:H	1.59	0.68
2:B:33:VAL:HG12	2:B:34:HIS:H	1.59	0.68
3:D:501:ANP:H3'	3:D:501:ANP:C8	2.24	0.68
1:A:96:ALA:HB1	1:A:377:ILE:HG21	1.77	0.67
1:A:355:ASP:OD2	4:A:612:HOH:O	2.12	0.66
2:B:116:ASN:H	2:B:116:ASN:ND2	1.92	0.66
2:B:29:VAL:HG11	2:B:51:VAL:HG11	1.77	0.66
1:D:233:MET:HE1	1:D:270:GLN:HG2	1.78	0.65
1:A:308:PRO:HG2	1:A:311:THR:HG23	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:MET:O	3:D:501:ANP:H2	1.96	0.64
2:B:113:GLY:N	4:B:204:HOH:O	2.31	0.64
1:A:120:ILE:HG21	1:A:385:ILE:HG12	1.80	0.63
1:D:181:ARG:HG2	1:D:243:ILE:HD11	1.80	0.63
1:A:393:GLU:HG2	1:A:395:ILE:HB	1.81	0.63
2:E:40:LEU:HB2	2:E:43:ASP:OD1	1.98	0.63
2:B:76:GLU:O	2:B:79:LYS:N	2.28	0.62
1:D:391:ARG:O	1:D:393:GLU:HB3	1.99	0.62
1:D:309:TRP:HA	1:D:312:VAL:HG13	1.82	0.62
1:A:203:MET:SD	1:A:221:TYR:HA	2.40	0.61
1:D:387:ASP:O	1:D:391:ARG:HB3	2.01	0.60
1:D:142:SER:OG	1:D:143:ASP:N	2.34	0.60
1:A:147:ILE:HG23	2:B:120:LEU:HD11	1.84	0.59
1:A:234:LEU:HD21	1:A:271:LEU:HD11	1.83	0.59
2:B:127:GLY:O	2:B:129:SER:N	2.36	0.59
2:B:23:ILE:HG13	2:B:26:SER:HB2	1.85	0.59
2:E:23:ILE:HD12	2:E:24:PRO:HD2	1.85	0.59
1:D:206:GLY:HA2	1:D:217:PHE:HE1	1.67	0.58
1:D:220:GLU:OE2	1:D:221:TYR:N	2.36	0.58
1:D:120:ILE:HG21	1:D:385:ILE:HG12	1.85	0.57
1:A:245:LEU:HD22	1:A:336:ILE:O	2.05	0.57
2:B:34:HIS:HB2	2:B:35:SER:C	2.25	0.56
1:A:350:TYR:OH	4:A:605:HOH:O	2.18	0.56
1:A:398:GLN:HG3	1:D:237:HIS:CG	2.40	0.56
1:A:140:MET:O	3:A:501:ANP:H2	2.04	0.56
1:A:146:GLN:O	1:A:150:SER:OG	2.23	0.56
1:A:296:ALA:O	1:A:297:TYR:HB3	2.07	0.55
1:A:59:GLU:O	1:A:70:SER:OG	2.22	0.55
1:A:369:ARG:HA	1:A:372:LEU:HD12	1.88	0.55
1:D:349:LYS:NZ	2:E:117:ILE:HD11	2.22	0.54
2:E:112:PRO:HA	2:E:114:GLU:N	2.16	0.54
1:A:393:GLU:OE2	1:A:393:GLU:O	2.26	0.54
1:A:291:ALA:C	1:A:293:ARG:HA	2.28	0.54
1:D:126:PRO:HG2	1:D:130:PHE:H	1.72	0.54
1:D:281:PRO:HD2	1:D:298:ILE:HD13	1.90	0.54
1:A:161:TYR:CE2	2:B:115:ARG:HG3	2.43	0.54
2:B:122:VAL:HG13	2:B:125:ARG:HD2	1.91	0.53
1:D:185:PRO:HD3	1:D:251:ILE:HG12	1.91	0.53
2:E:37:PRO:HB2	2:E:38:GLN:HG2	1.90	0.53
1:D:265:LYS:HB2	1:D:269:HIS:ND1	2.24	0.53
1:D:360:ALA:HB3	2:E:42:ARG:NH1	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:GLU:OE1	1:A:160:ARG:NH1	2.38	0.52
1:A:94:THR:HA	1:A:97:LYS:HE3	1.92	0.52
1:D:83:ILE:HD13	1:D:136:VAL:HG22	1.90	0.52
1:A:291:ALA:O	1:A:293:ARG:HA	2.08	0.52
2:B:40:LEU:HB2	2:B:43:ASP:OD2	2.09	0.52
1:D:386:GLU:HA	1:D:389:HIS:HB2	1.91	0.52
1:D:161:TYR:CZ	2:E:115:ARG:HB2	2.45	0.52
1:D:231:GLU:OE1	1:D:335:ARG:NH2	2.38	0.52
2:B:64:ASP:HA	2:B:84:TYR:CZ	2.45	0.52
1:A:300:SER:OG	1:A:301:LEU:N	2.43	0.52
2:B:66:ASP:OD1	2:B:66:ASP:N	2.40	0.52
1:D:225:ARG:HB3	1:D:233:MET:HE1	1.92	0.51
1:A:200:ASP:OD2	3:A:501:ANP:O1B	2.28	0.51
1:A:148:ILE:HD13	1:A:254:GLU:HG2	1.92	0.51
1:D:291:ALA:O	1:D:293:ARG:HA	2.10	0.51
1:A:261:LEU:HD13	1:A:313:TYR:OH	2.10	0.51
1:D:240:THR:O	1:D:243:ILE:HG23	2.10	0.51
1:D:214:HIS:C	1:D:216:TYR:H	2.14	0.50
1:A:221:TYR:CG	1:A:222:VAL:N	2.79	0.50
1:D:166:LEU:HD11	1:D:248:VAL:HG22	1.93	0.50
2:E:34:HIS:HB2	2:E:35:SER:HA	1.92	0.50
1:A:240:THR:N	4:A:604:HOH:O	2.26	0.50
1:A:257:ALA:HB2	1:A:313:TYR:HE1	1.77	0.50
2:B:33:VAL:HG12	2:B:34:HIS:N	2.26	0.50
1:D:393:GLU:O	1:D:395:ILE:N	2.45	0.50
2:B:116:ASN:C	2:B:117:ILE:HG12	2.27	0.50
1:D:395:ILE:HG23	2:E:31:TRP:CD1	2.47	0.49
1:A:357:PRO:HG3	2:B:58:THR:HG21	1.93	0.49
1:D:211:PRO:HB2	2:B:26:SER:HB3	1.94	0.49
1:D:293:ARG:CB	1:D:296:ALA:H	2.26	0.49
1:D:379:GLU:HA	1:D:382:VAL:HB	1.94	0.49
1:A:221:TYR:OH	1:A:228:ARG:HD2	2.12	0.49
2:B:115:ARG:HD2	2:B:118:HIS:N	2.27	0.49
1:D:392:ARG:HA	1:D:393:GLU:CB	2.40	0.48
3:D:501:ANP:O2A	3:D:501:ANP:O1B	2.32	0.48
1:D:97:LYS:O	1:D:99:THR:N	2.47	0.48
2:B:61:GLU:HG3	2:B:105:PHE:HB2	1.96	0.48
1:A:93:VAL:O	1:A:97:LYS:HG3	2.14	0.47
1:A:149:HIS:HB3	2:B:129:SER:CB	2.44	0.47
1:A:75:ARG:HH11	1:D:339:ALA:HB2	1.80	0.47
2:B:48:ILE:HD13	2:B:106:PRO:HG3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLN:HG2	4:A:609:HOH:O	2.13	0.47
2:E:47:VAL:O	2:E:51:VAL:HG13	2.13	0.47
1:A:97:LYS:HZ2	1:A:101:ARG:HH22	1.59	0.47
1:A:111:HIS:CE1	1:A:168:ARG:NH1	2.83	0.47
1:D:218:MET:HE1	1:D:232:LEU:HB3	1.97	0.47
2:B:126:ALA:HB1	2:B:135:HIS:HB2	1.96	0.46
1:A:152:GLN:HG2	1:A:153:PRO:HD2	1.97	0.46
1:A:212:ALA:HA	1:A:213:GLU:HA	1.53	0.46
1:A:220:GLU:HG2	1:A:221:TYR:N	2.28	0.46
2:B:125:ARG:HG2	2:B:125:ARG:HH11	1.81	0.46
1:D:393:GLU:C	1:D:393:GLU:OE2	2.54	0.46
1:A:152:GLN:OE1	2:B:120:LEU:HD13	2.15	0.46
1:D:379:GLU:O	1:D:383:ALA:N	2.48	0.46
2:E:61:GLU:OE2	2:E:107:ARG:NH1	2.48	0.46
2:E:120:LEU:HD22	2:E:121:LYS:N	2.30	0.46
1:A:47:VAL:HB	1:A:68:VAL:HG11	1.97	0.46
1:A:146:GLN:OE1	2:B:125:ARG:HB3	2.16	0.46
1:A:120:ILE:O	1:A:389:HIS:HE1	1.99	0.46
1:A:161:TYR:CZ	2:B:115:ARG:HB2	2.51	0.46
2:B:43:ASP:O	2:B:47:VAL:HG23	2.15	0.46
1:A:392:ARG:HA	1:A:393:GLU:HB3	1.98	0.46
1:A:142:SER:HA	2:B:125:ARG:NH1	2.31	0.46
2:B:134:HIS:O	2:B:135:HIS:CG	2.69	0.46
1:A:141:GLU:OE1	1:A:192:GLU:N	2.40	0.45
1:A:58:ILE:O	1:A:59:GLU:HG2	2.17	0.45
1:A:237:HIS:CG	1:A:237:HIS:O	2.69	0.45
1:D:352:ASP:HB3	1:D:355:ASP:HB3	1.98	0.45
2:B:132:GLY:HA3	2:B:133:ARG:HA	1.44	0.45
2:B:41:PHE:HB2	2:B:78:MET:HG3	1.99	0.45
1:A:97:LYS:HZ3	1:A:101:ARG:HH22	1.62	0.45
1:D:296:ALA:HA	1:D:299:GLN:HB2	1.98	0.45
1:D:77:THR:HG22	1:D:79:GLN:H	1.82	0.45
2:E:110:LYS:HD2	2:E:114:GLU:HB3	1.99	0.45
1:A:352:ASP:HB3	1:A:355:ASP:HB3	1.98	0.45
1:D:176:ALA:HB2	1:D:359:CYS:HB3	1.98	0.45
1:D:392:ARG:H	1:D:392:ARG:HG3	1.48	0.45
1:D:95:ASN:OD1	1:D:95:ASN:N	2.50	0.45
1:A:145:HIS:HD2	2:B:128:PRO:HA	1.80	0.45
2:E:103:GLN:HG2	2:E:105:PHE:CZ	2.52	0.44
1:D:234:LEU:HD21	1:D:271:LEU:HD11	2.00	0.44
1:A:111:HIS:HD2	1:A:172:TYR:CD2	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:ASN:H	2:B:116:ASN:HD22	1.44	0.44
2:B:42:ARG:HD3	2:B:42:ARG:HA	1.65	0.44
1:D:82:ALA:HB2	1:D:139:LEU:HD23	1.99	0.44
2:B:136:HIS:O	2:B:137:HIS:HB2	2.16	0.44
1:D:184:LYS:NZ	4:D:614:HOH:O	2.39	0.44
1:A:395:ILE:HG23	2:B:31:TRP:CD1	2.53	0.44
2:B:21:ILE:HG12	2:B:104:ILE:HD11	2.00	0.43
3:D:501:ANP:C3'	3:D:501:ANP:C8	2.86	0.43
1:D:209:THR:O	1:D:214:HIS:HE1	2.01	0.43
1:D:143:ASP:O	1:D:147:ILE:HG12	2.18	0.43
1:D:254:GLU:O	1:D:258:ARG:N	2.52	0.43
1:A:58:ILE:HG13	2:E:76:GLU:HG3	2.00	0.42
1:D:144:LEU:HB3	1:D:185:PRO:HB3	2.00	0.42
1:A:167:LEU:HA	1:A:167:LEU:HD23	1.80	0.42
1:D:72:ALA:HB3	1:D:81:VAL:HG12	2.01	0.42
1:D:69:VAL:HG12	1:D:70:SER:H	1.85	0.42
1:A:146:GLN:OE1	2:B:126:ALA:N	2.51	0.42
2:B:114:GLU:HG2	2:B:114:GLU:H	1.49	0.42
2:E:48:ILE:O	2:E:52:LEU:N	2.47	0.42
1:A:142:SER:HB2	2:B:122:VAL:HG13	2.01	0.42
1:D:122:ARG:HA	1:D:123:PRO:HD2	1.84	0.42
1:D:98:ARG:NH2	3:D:501:ANP:O1G	2.53	0.42
1:D:86:ILE:CG2	1:D:89:ALA:HB2	2.50	0.42
1:A:125:VAL:HA	1:A:126:PRO:HA	1.92	0.42
2:B:74:SER:C	2:B:75:ASP:O	2.58	0.42
1:A:231:GLU:HA	1:A:236:LEU:HD12	2.02	0.41
1:A:310:GLU:O	1:A:314:PRO:HA	2.19	0.41
1:D:121:LEU:HA	1:D:121:LEU:HD12	1.71	0.41
1:A:289:VAL:O	1:A:295:ARG:NH1	2.52	0.41
2:E:120:LEU:HD22	2:E:121:LYS:H	1.84	0.41
1:A:323:LEU:O	1:A:327:MET:HG3	2.20	0.41
2:E:17:LEU:HD12	2:E:18:VAL:H	1.85	0.41
2:B:122:VAL:CG1	2:B:125:ARG:HD2	2.51	0.41
1:D:98:ARG:HB3	1:D:99:THR:H	1.74	0.41
2:E:23:ILE:HD13	2:E:52:LEU:HD21	2.03	0.41
1:D:368:ASP:HB3	1:D:369:ARG:H	1.72	0.41
1:A:293:ARG:HG2	1:A:295:ARG:HE	1.86	0.41
2:B:86:TYR:HD1	2:B:86:TYR:HA	1.74	0.41
2:E:64:ASP:CB	2:E:68:ASP:HB2	2.51	0.40
2:B:98:LEU:H	2:B:98:LEU:HD23	1.87	0.40
1:D:55:TYR:HD2	1:D:121:LEU:HD21	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:GLU:O	1:D:314:PRO:HA	2.22	0.40
1:A:320:ALA:HB2	1:A:346:PHE:CE1	2.57	0.40
3:A:501:ANP:H8	3:A:501:ANP:O5'	2.21	0.40
1:D:86:ILE:HG22	1:D:89:ALA:HB2	2.03	0.40
1:A:399:ILE:HG13	1:A:399:ILE:O	2.22	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	353/442 (80%)	324 (92%)	25 (7%)	4 (1%)	14	30
1	D	351/442 (79%)	303 (86%)	44 (12%)	4 (1%)	14	30
2	B	121/126 (96%)	103 (85%)	17 (14%)	1 (1%)	19	39
2	E	109/126 (86%)	101 (93%)	6 (6%)	2 (2%)	8	16
All	All	934/1136 (82%)	831 (89%)	92 (10%)	11 (1%)	13	27

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	VAL
1	A	385	ILE
1	D	367	PHE
2	E	16	VAL
1	D	385	ILE
1	A	216	TYR
1	A	372	LEU
1	D	368	ASP
1	D	371	ALA
2	B	117	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	122	VAL

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	283/373 (76%)	249 (88%)	34 (12%)	5	9
1	D	262/373 (70%)	231 (88%)	31 (12%)	5	9
2	B	98/110 (89%)	77 (79%)	21 (21%)	1	1
2	E	92/110 (84%)	83 (90%)	9 (10%)	8	15
All	All	735/966 (76%)	640 (87%)	95 (13%)	4	7

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	VAL
1	A	48	THR
1	A	58	ILE
1	A	61	ILE
1	A	68	VAL
1	A	71	SER
1	A	124	THR
1	A	135	VAL
1	A	156	LEU
1	A	166	LEU
1	A	173	MET
1	A	196	LEU
1	A	203	MET
1	A	208	CYS
1	A	220	GLU
1	A	224	THR
1	A	228	ARG
1	A	235	SER
1	A	245	LEU
1	A	268	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	285	VAL
1	A	293	ARG
1	A	305	GLN
1	A	311	THR
1	A	312	VAL
1	A	318	ARG
1	A	365	PHE
1	A	367	PHE
1	A	373	THR
1	A	374	ARG
1	A	377	ILE
1	A	393	GLU
1	A	398	GLN
1	A	399	ILE
1	D	59	GLU
1	D	63	ASN
1	D	81	VAL
1	D	83	ILE
1	D	90	PHE
1	D	95	ASN
1	D	121	LEU
1	D	141	GLU
1	D	156	LEU
1	D	166	LEU
1	D	170	LEU
1	D	196	LEU
1	D	219	THR
1	D	220	GLU
1	D	224	THR
1	D	243	ILE
1	D	245	LEU
1	D	265	LYS
1	D	277	VAL
1	D	285	VAL
1	D	294	VAL
1	D	298	ILE
1	D	311	THR
1	D	312	VAL
1	D	326	ARG
1	D	365	PHE
1	D	368	ASP
1	D	389	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	391	ARG
1	D	392	ARG
1	D	393	GLU
2	E	43	ASP
2	E	57	THR
2	E	65	GLU
2	E	84	TYR
2	E	98	LEU
2	E	116	ASN
2	E	117	ILE
2	E	118	HIS
2	E	120	LEU
2	B	17	LEU
2	B	26	SER
2	B	52	LEU
2	B	65	GLU
2	B	66	ASP
2	B	76	GLU
2	B	84	TYR
2	B	88	THR
2	B	93	GLN
2	B	98	LEU
2	B	107	ARG
2	B	114	GLU
2	B	115	ARG
2	B	116	ASN
2	B	117	ILE
2	B	118	HIS
2	B	120	LEU
2	B	121	LYS
2	B	125	ARG
2	B	130	GLN
2	B	137	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
2	E	116	ASN
2	B	116	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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	A	501	-	29,33,33	2.68	10 (34%)	31,52,52	2.39	9 (29%)
3	ANP	D	501	-	29,33,33	2.65	11 (37%)	31,52,52	2.66	8 (25%)

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	A	501	-	-	3/14/38/38	0/3/3/3
3	ANP	D	501	-	-	3/14/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	ANP	PB-O1B	8.25	1.59	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	ANP	PB-O1B	7.89	1.58	1.46
3	A	501	ANP	C2'-C1'	-5.49	1.45	1.53
3	D	501	ANP	C2'-C1'	-5.26	1.45	1.53
3	A	501	ANP	C2'-C3'	-4.95	1.39	1.53
3	A	501	ANP	PB-N3B	4.58	1.75	1.63
3	D	501	ANP	C2'-C3'	-4.57	1.40	1.53
3	D	501	ANP	PB-N3B	4.53	1.75	1.63
3	A	501	ANP	O4'-C4'	-3.75	1.36	1.45
3	D	501	ANP	O4'-C4'	-3.36	1.37	1.45
3	A	501	ANP	O2'-C2'	-2.71	1.36	1.43
3	A	501	ANP	O3'-C3'	-2.71	1.36	1.43
3	D	501	ANP	C3'-C4'	-2.62	1.46	1.53
3	A	501	ANP	C6-N6	2.57	1.43	1.34
3	A	501	ANP	C3'-C4'	-2.56	1.46	1.53
3	D	501	ANP	O3'-C3'	-2.52	1.37	1.43
3	D	501	ANP	C6-N6	2.51	1.43	1.34
3	A	501	ANP	PG-O1G	2.44	1.50	1.46
3	D	501	ANP	O2'-C2'	-2.35	1.37	1.43
3	D	501	ANP	PG-O1G	2.27	1.49	1.46
3	D	501	ANP	PB-O3A	-2.04	1.56	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	ANP	O1B-PB-N3B	-10.26	96.66	111.77
3	A	501	ANP	O1B-PB-N3B	-9.58	97.66	111.77
3	D	501	ANP	O2B-PB-O3A	5.01	121.35	104.64
3	A	501	ANP	O2B-PB-O3A	4.91	121.03	104.64
3	D	501	ANP	O2B-PB-O1B	4.65	119.68	109.92
3	D	501	ANP	PA-O3A-PB	-4.63	116.32	132.62
3	D	501	ANP	N3-C2-N1	-3.22	123.65	128.68
3	A	501	ANP	O2B-PB-O1B	3.10	116.42	109.92
3	A	501	ANP	N3-C2-N1	-2.81	124.28	128.68
3	A	501	ANP	C3'-C2'-C1'	2.70	105.04	100.98
3	D	501	ANP	O3A-PB-N3B	-2.68	99.16	106.59
3	A	501	ANP	C4-C5-N7	-2.60	106.69	109.40
3	A	501	ANP	O5'-C5'-C4'	2.59	117.91	108.99
3	D	501	ANP	O5'-C5'-C4'	2.37	117.16	108.99
3	D	501	ANP	C4-C5-N7	-2.36	106.94	109.40
3	A	501	ANP	O3G-PG-O2G	-2.13	101.95	107.64
3	A	501	ANP	PA-O3A-PB	-2.13	125.12	132.62

There are no chirality outliers.

All (6) torsion outliers are listed below:

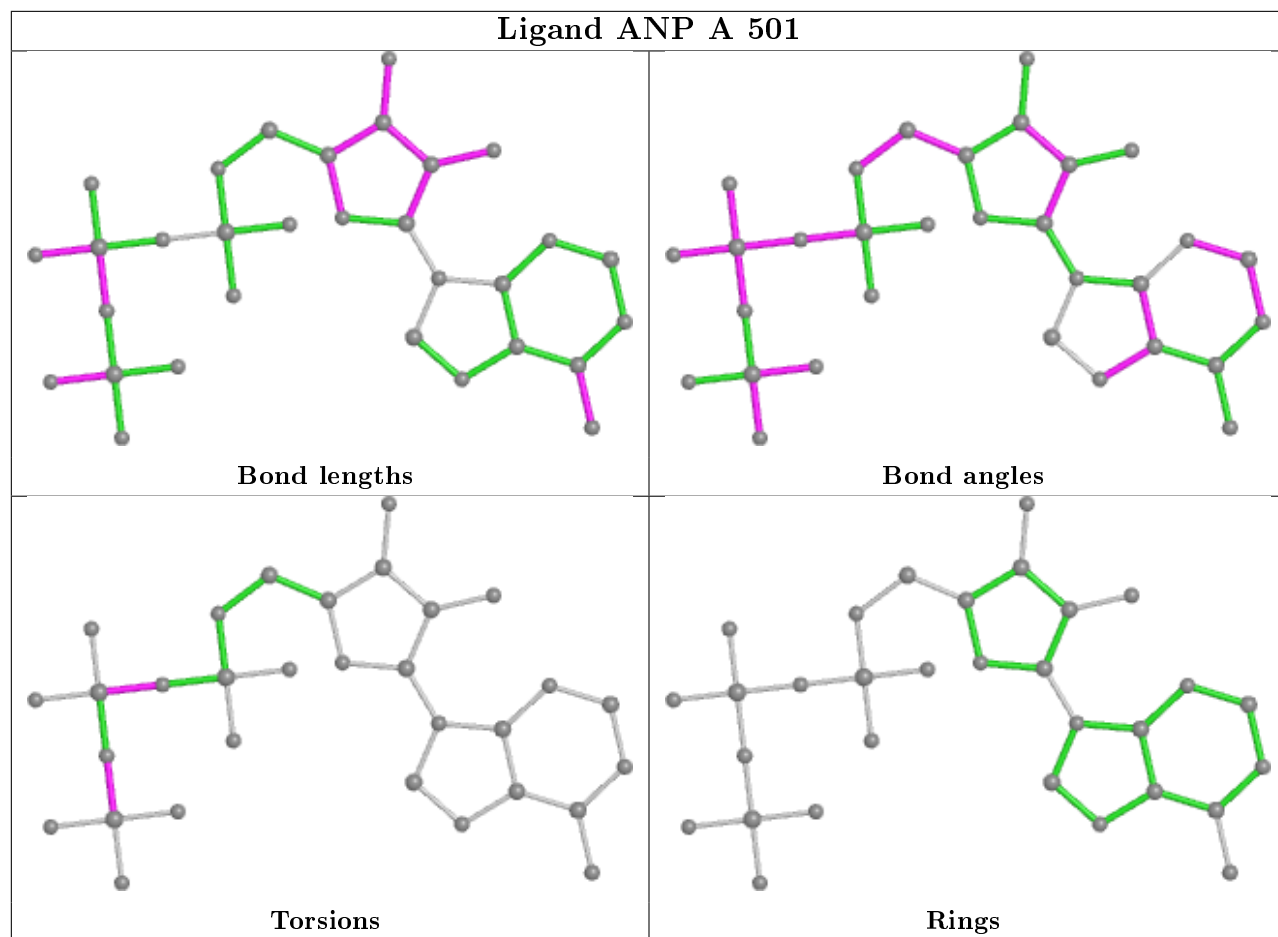
Mol	Chain	Res	Type	Atoms
3	A	501	ANP	PB-N3B-PG-O1G
3	A	501	ANP	PA-O3A-PB-O1B
3	A	501	ANP	PA-O3A-PB-O2B
3	D	501	ANP	PB-N3B-PG-O1G
3	D	501	ANP	PG-N3B-PB-O1B
3	D	501	ANP	C4'-C5'-O5'-PA

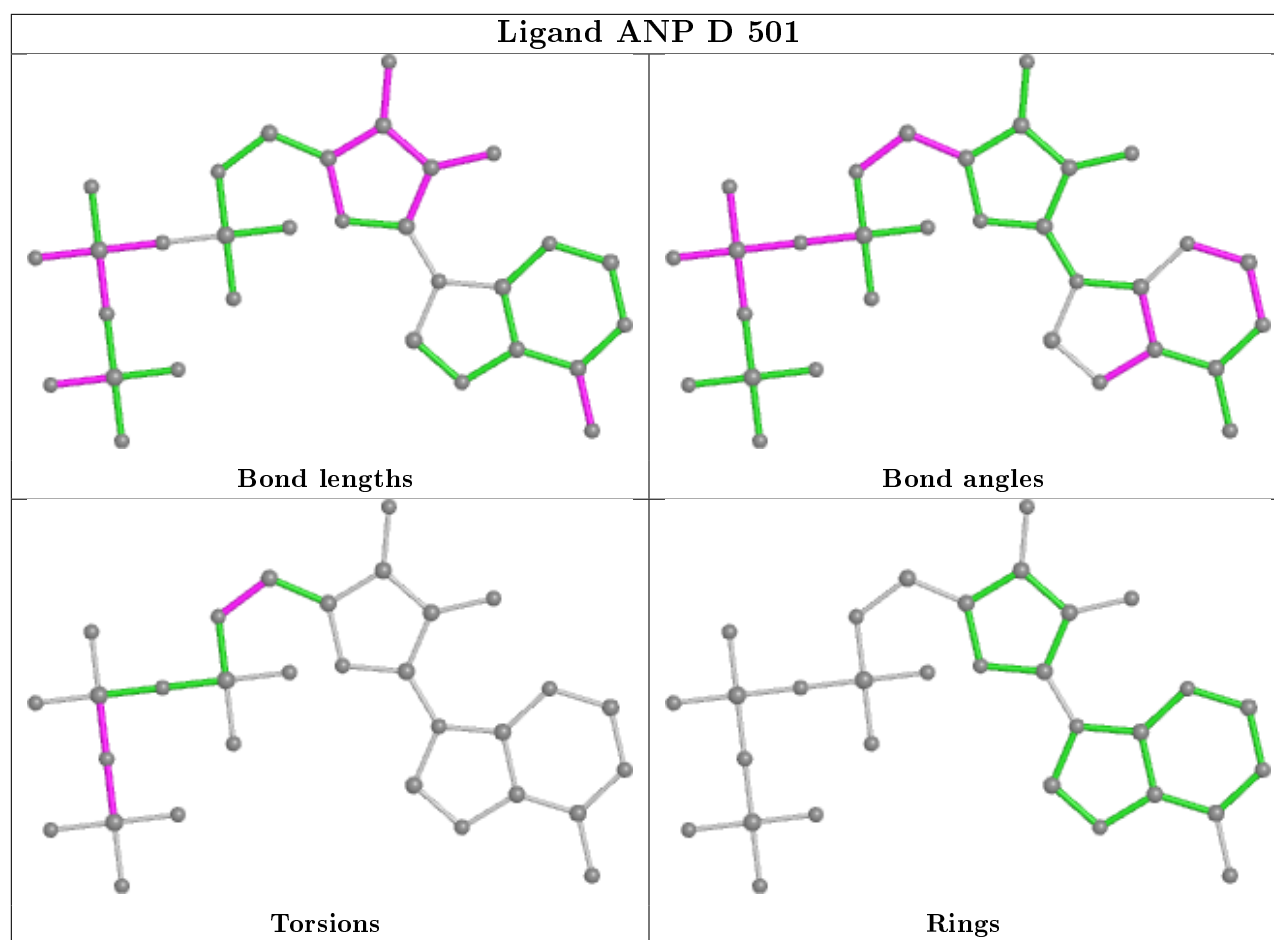
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	ANP	3	0
3	D	501	ANP	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	355/442 (80%)	0.15	14 (3%) 39 32	49, 82, 141, 206	0
1	D	353/442 (79%)	0.47	29 (8%) 11 8	49, 84, 162, 184	0
2	B	123/126 (97%)	-0.01	0 100 100	60, 92, 131, 152	0
2	E	111/126 (88%)	0.21	5 (4%) 33 26	62, 89, 150, 182	0
All	All	942/1136 (82%)	0.26	48 (5%) 28 22	49, 85, 153, 206	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	371	ALA	13.4
1	A	369	ARG	10.5
1	D	47	VAL	6.4
1	D	124	THR	5.8
1	D	134	TYR	5.5
1	D	55	TYR	5.2
1	A	370	GLU	4.6
2	E	35	SER	4.2
1	D	120	ILE	4.1
1	A	372	LEU	3.9
1	D	121	LEU	3.9
2	E	15	SER	3.8
1	D	123	PRO	3.7
1	D	96	ALA	3.6
1	D	390	ALA	3.5
2	E	124	THR	3.3
1	D	57	ILE	3.1
1	D	54	GLU	3.1
1	D	53	ASP	3.1
1	D	122	ARG	2.8
1	D	51	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	68	VAL	2.7
1	D	90	PHE	2.7
1	A	302	PRO	2.6
1	A	125	VAL	2.6
1	A	316	ALA	2.6
1	D	48	THR	2.6
2	E	36	GLY	2.6
1	D	292	GLU	2.5
1	D	58	ILE	2.5
1	A	305	GLN	2.4
1	A	303	PRO	2.4
2	E	23	ILE	2.4
1	D	69	VAL	2.4
1	D	80	GLN	2.3
1	D	73	ARG	2.3
1	D	153	PRO	2.3
1	D	135	VAL	2.3
1	D	59	GLU	2.2
1	D	136	VAL	2.2
1	A	128	GLY	2.2
1	D	56	GLU	2.1
1	A	49	PHE	2.1
1	A	46	ASP	2.1
1	D	397	GLN	2.0
1	A	100	LEU	2.0
1	A	304	ARG	2.0
1	D	50	ASP	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 carbohydrates in this entry.

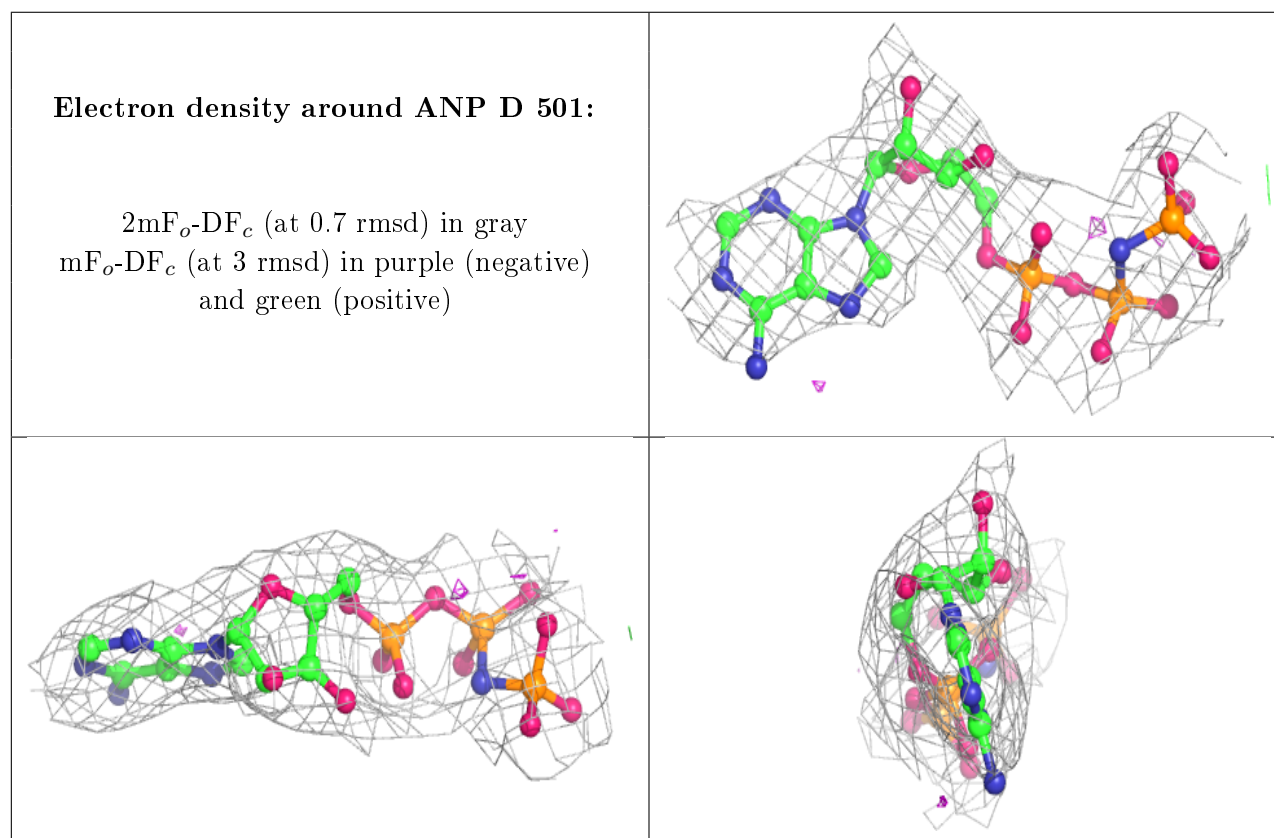
6.4 Ligands [i](#)

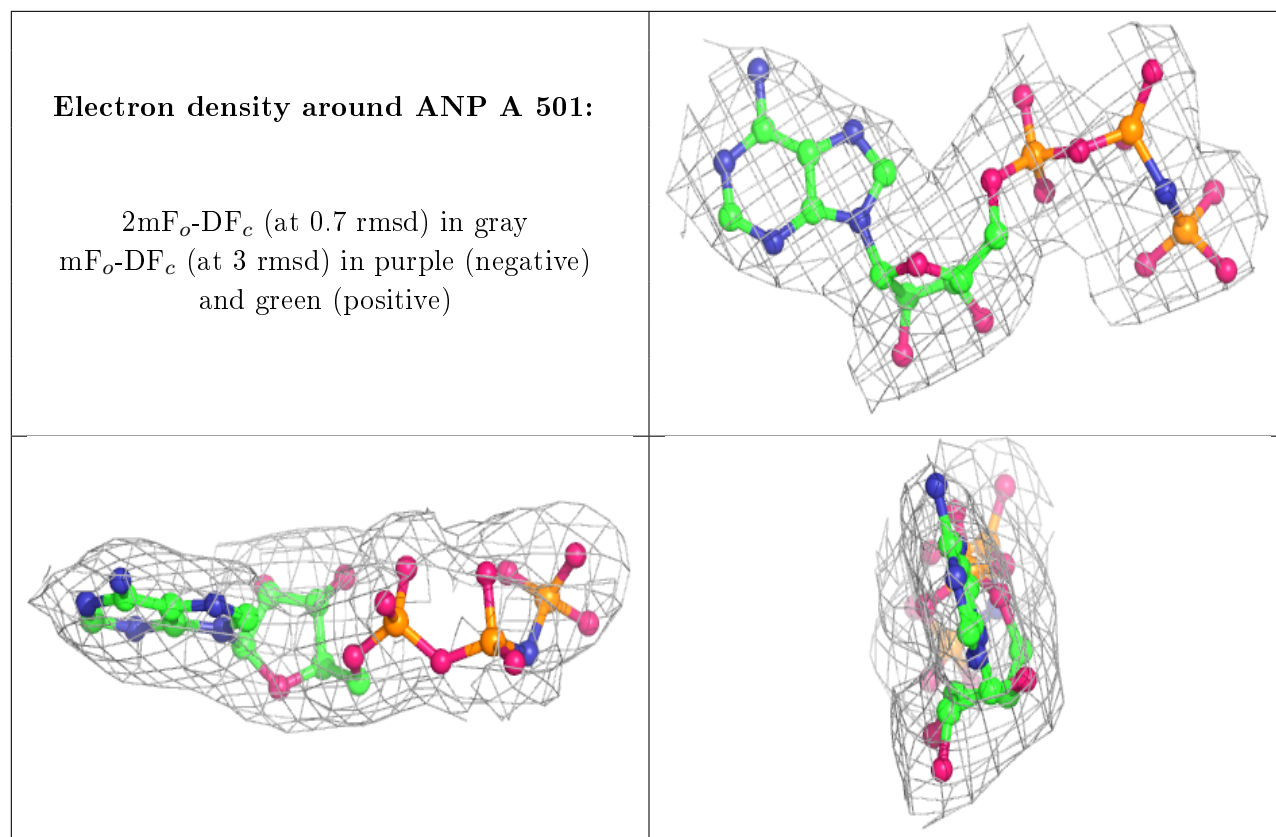
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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(Å ²)	Q<0.9
3	ANP	D	501	31/31	0.83	0.17	90,121,213,278	0
3	ANP	A	501	31/31	0.96	0.11	66,80,236,380	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.