



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 04:47 PM EDT

PDB ID : 1XTJ / pdb_00001xtj
Title : structure of human UAP56 in complex with ADP
Authors : Shi, H.; Cordin, O.; Minder, C.M.; Linder, P.; Xu, R.-M.
Deposited on : 2004-10-22
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

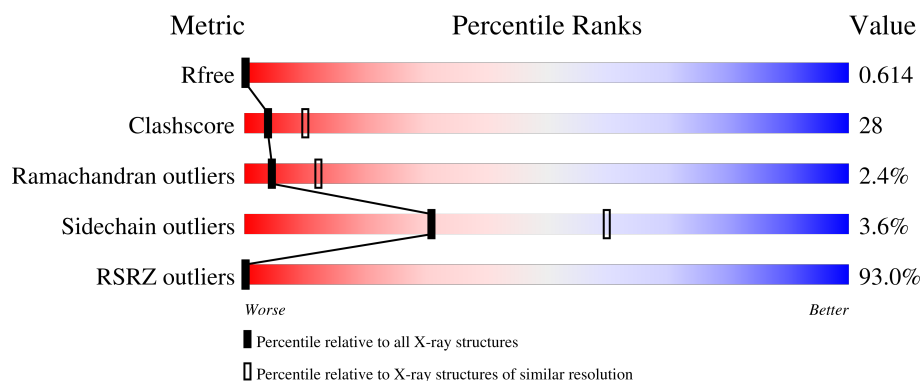
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	386	<p>90% 51% 40% 6% . .</p>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3139 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 Probable ATP-dependent RNA helicase p47.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			3022	1923	525	553	21			

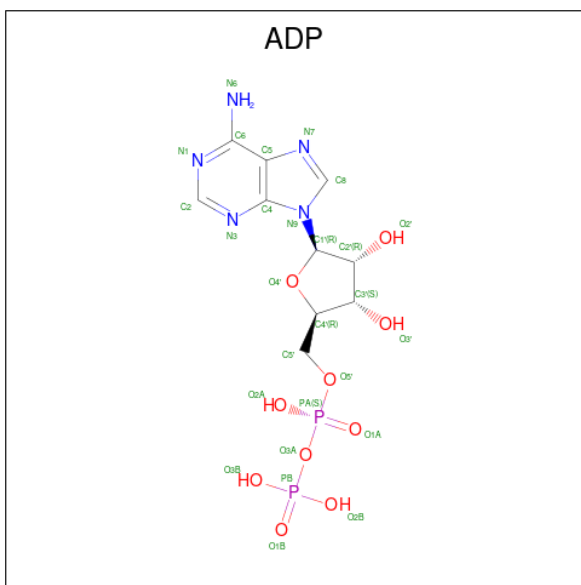
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLY	-	cloning artifact	UNP Q13838
A	39	SER	-	cloning artifact	UNP Q13838
A	40	PRO	-	cloning artifact	UNP Q13838
A	41	GLY	-	cloning artifact	UNP Q13838
A	42	HIS	-	cloning artifact	UNP Q13838
A	43	MET	-	cloning artifact	UNP Q13838

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

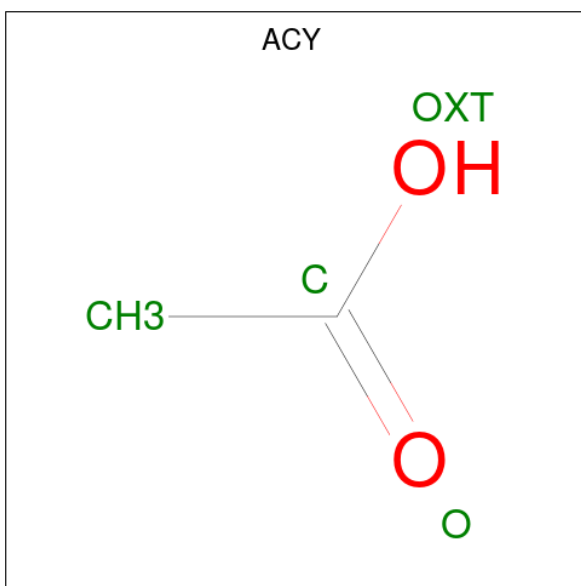
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

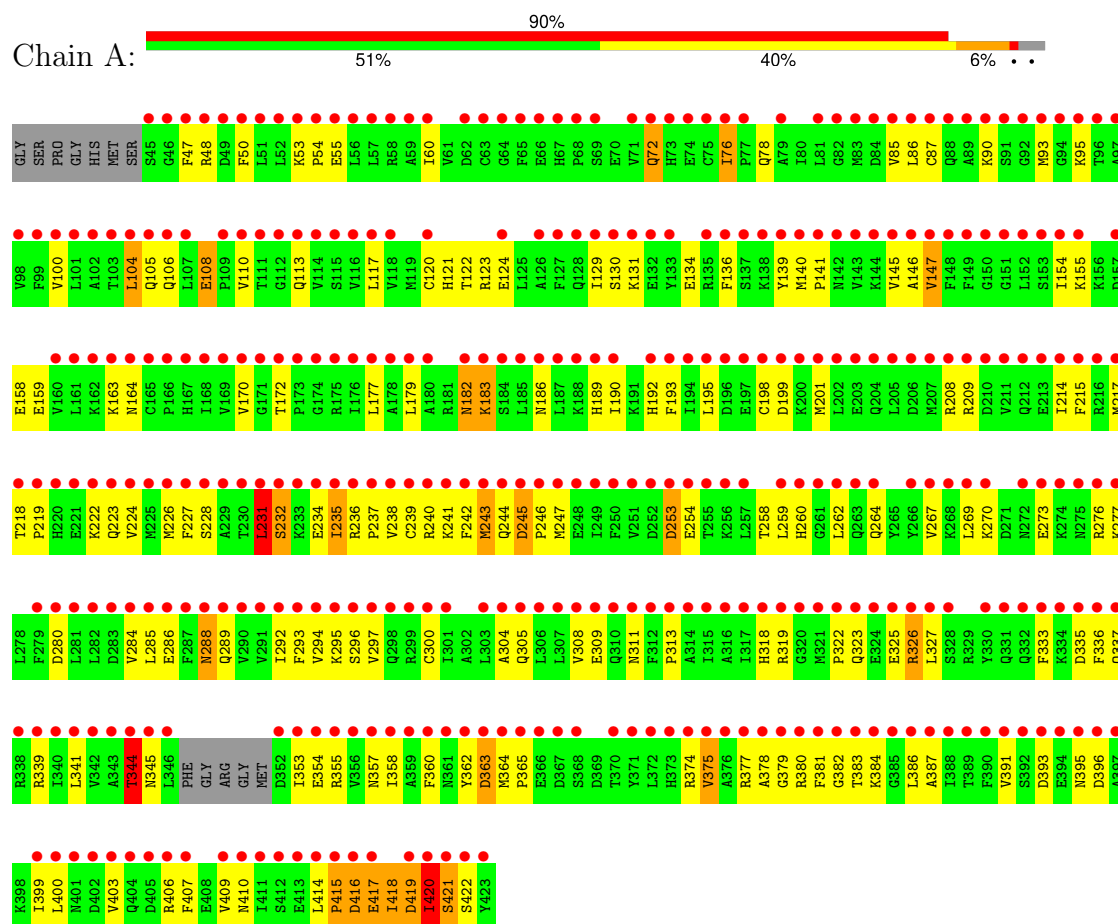
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	85	Total	O	0	0
			85	85		

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: Probable ATP-dependent RNA helicase p47



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.99Å 78.20Å 63.19Å 90.00° 103.42° 90.00°	Depositor
Resolution (Å)	32.70 – 2.70 32.70 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (32.70-2.70) 77.8 (32.70-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.25Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.300 0.591 , 0.614	Depositor DCC
R_{free} test set	797 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	1.723	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.53 , 483.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.36	EDS
Total number of atoms	3139	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, 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	0.46	0/3075	1.05	21/4137 (0.5%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	LEU	N-CA-C	-9.52	101.35	113.16
1	A	344	THR	N-CA-C	-9.00	102.43	113.41
1	A	375	VAL	N-CA-C	8.99	119.54	110.82
1	A	288	ASN	N-CA-C	-8.31	102.96	113.43
1	A	418	ILE	N-CA-C	-7.07	105.72	113.43
1	A	296	SER	N-CA-C	6.48	119.08	110.53
1	A	243	MET	N-CA-C	6.37	119.33	109.07
1	A	182	ASN	N-CA-C	-6.11	104.62	111.28
1	A	95	LYS	N-CA-C	5.89	118.59	111.40
1	A	270	LYS	N-CA-C	-5.83	101.84	110.46
1	A	419	ASP	CA-C-O	5.77	121.28	117.94
1	A	245	ASP	CA-C-N	5.62	126.09	120.52
1	A	245	ASP	C-N-CA	5.62	126.09	120.52
1	A	76	ILE	CB-CA-C	-5.49	108.53	114.35
1	A	419	ASP	CB-CA-C	-5.44	109.24	117.07
1	A	355	ARG	N-CA-C	-5.43	106.50	113.02
1	A	108	GLU	CA-C-N	5.40	125.41	119.90
1	A	108	GLU	C-N-CA	5.40	125.41	119.90
1	A	311	ASN	N-CA-C	5.33	119.09	112.58
1	A	172	THR	CA-C-N	5.27	125.33	119.32
1	A	172	THR	C-N-CA	5.27	125.33	119.32

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	3022	0	3054	173	0
2	A	1	0	0	0	0
3	A	27	0	12	0	0
4	A	4	0	3	0	0
5	A	85	0	0	8	0
All	All	3139	0	3069	173	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 28.

All (173) 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:364:MET:HE1	1:A:400:LEU:HD13	1.51	0.92
1:A:262:LEU:HD21	1:A:375:VAL:HG12	1.52	0.90
1:A:106:GLN:HE22	1:A:223:GLN:HE22	1.23	0.83
1:A:417:GLU:HG2	1:A:418:ILE:HG13	1.61	0.82
1:A:53:LYS:HG3	1:A:105:GLN:HE22	1.45	0.81
1:A:93:MET:HE1	1:A:254:GLU:H	1.46	0.80
1:A:120:CYS:SG	1:A:129:ILE:HD12	2.25	0.77
1:A:192:HIS:HD2	1:A:223:GLN:HE21	1.32	0.76
1:A:391:VAL:HG13	1:A:396:ASP:HB2	1.69	0.73
1:A:319:ARG:H	1:A:344:THR:HG21	1.51	0.73
1:A:313:PRO:HG2	1:A:339:ARG:HB2	1.72	0.71
1:A:179:LEU:HA	1:A:182:ASN:HD22	1.55	0.71
1:A:267:VAL:HG13	5:A:584:HOH:O	1.90	0.70
1:A:93:MET:HE1	1:A:254:GLU:N	2.08	0.69
1:A:269:LEU:HD22	1:A:273:GLU:HB3	1.76	0.68
1:A:130:SER:HB2	1:A:147:VAL:HG13	1.75	0.68
1:A:198:CYS:SG	1:A:226:MET:HB3	2.34	0.67
1:A:53:LYS:HG3	1:A:105:GLN:NE2	2.10	0.66
1:A:262:LEU:HD21	1:A:375:VAL:CG1	2.24	0.66
1:A:284:VAL:HG21	5:A:611:HOH:O	1.96	0.65
1:A:319:ARG:HG3	1:A:345:ASN:HD21	1.61	0.64
1:A:226:MET:HE3	1:A:243:MET:HE2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:HB3	1:A:201:MET:HE1	1.79	0.63
1:A:406:ARG:HH11	1:A:406:ARG:HB3	1.62	0.63
1:A:190:ILE:HB	1:A:218:THR:HG23	1.80	0.63
1:A:214:ILE:HA	1:A:217:MET:CE	2.29	0.63
1:A:145:VAL:HG12	1:A:146:ALA:N	2.14	0.63
1:A:269:LEU:HD11	1:A:277:LYS:HG3	1.80	0.63
1:A:319:ARG:N	1:A:344:THR:HG21	2.13	0.63
1:A:106:GLN:NE2	1:A:223:GLN:HE22	1.97	0.62
1:A:236:ARG:N	1:A:237:PRO:HD2	2.14	0.62
1:A:258:THR:HG22	1:A:260:HIS:H	1.63	0.62
1:A:110:VAL:HG11	1:A:113:GLN:NE2	2.15	0.62
1:A:232:SER:HB3	1:A:235:ILE:HB	1.81	0.61
1:A:259:LEU:HD21	1:A:264:GLN:HE22	1.64	0.61
1:A:47:PHE:O	1:A:50:PHE:HB2	2.01	0.61
1:A:420:ILE:HD13	1:A:420:ILE:N	2.16	0.60
1:A:90:LYS:O	1:A:93:MET:HB2	2.00	0.60
1:A:420:ILE:HG12	1:A:421:SER:H	1.67	0.60
1:A:155:LYS:O	1:A:159:GLU:HG3	2.02	0.60
1:A:297:VAL:HG22	1:A:318:HIS:HB2	1.84	0.59
1:A:159:GLU:HB3	1:A:163:LYS:NZ	2.16	0.59
1:A:294:VAL:HG21	1:A:300:CYS:HA	1.83	0.59
1:A:54:PRO:HG2	1:A:55:GLU:OE2	2.02	0.59
1:A:319:ARG:NE	1:A:345:ASN:OD1	2.36	0.59
1:A:333:PHE:CE1	1:A:341:LEU:HB2	2.37	0.58
1:A:195:LEU:HB3	1:A:201:MET:CE	2.34	0.57
1:A:192:HIS:HD2	1:A:223:GLN:NE2	2.02	0.57
1:A:384:LYS:HB3	5:A:632:HOH:O	2.04	0.56
1:A:182:ASN:O	1:A:183:LYS:HB2	2.06	0.56
1:A:288:ASN:H	1:A:357:ASN:HD22	1.54	0.56
1:A:377:ARG:HD3	1:A:384:LYS:O	2.06	0.55
1:A:294:VAL:HG12	1:A:362:TYR:CD2	2.41	0.55
1:A:380:ARG:NE	1:A:380:ARG:HA	2.22	0.55
1:A:218:THR:HG23	1:A:219:PRO:HD2	1.89	0.54
1:A:288:ASN:HB2	1:A:357:ASN:HD21	1.72	0.54
1:A:86:LEU:HD12	1:A:226:MET:HB2	1.90	0.54
1:A:285:LEU:HD13	1:A:358:ILE:HD13	1.90	0.54
1:A:243:MET:HB3	1:A:246:PRO:HB3	1.90	0.54
1:A:391:VAL:HG13	1:A:396:ASP:CB	2.38	0.54
1:A:305:GLN:HA	5:A:624:HOH:O	2.08	0.54
1:A:294:VAL:HA	1:A:363:ASP:OD1	2.07	0.54
1:A:55:GLU:H	1:A:55:GLU:CD	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:HD22	1:A:201:MET:HE1	1.90	0.53
1:A:415:PRO:O	1:A:416:ASP:HB3	2.09	0.53
1:A:179:LEU:HA	1:A:182:ASN:ND2	2.23	0.53
1:A:409:VAL:HG12	1:A:410:ASN:H	1.73	0.53
1:A:419:ASP:C	1:A:420:ILE:HD13	2.34	0.53
1:A:335:ASP:OD2	1:A:337:GLN:HB2	2.07	0.52
1:A:53:LYS:H	1:A:105:GLN:HE22	1.57	0.52
1:A:289:GLN:HG3	1:A:336:PHE:HE1	1.74	0.52
1:A:409:VAL:HG12	1:A:410:ASN:N	2.25	0.52
1:A:123:ARG:HG2	1:A:124:GLU:OE2	2.10	0.52
1:A:48:ARG:C	1:A:50:PHE:H	2.15	0.52
1:A:154:ILE:HD11	1:A:182:ASN:HD21	1.75	0.51
1:A:131:LYS:HD2	1:A:134:GLU:OE2	2.11	0.51
1:A:294:VAL:HG21	1:A:300:CYS:CA	2.40	0.51
1:A:208:ARG:HH21	1:A:238:VAL:HG22	1.75	0.51
1:A:240:ARG:HH11	1:A:240:ARG:HB2	1.76	0.51
1:A:406:ARG:HB3	1:A:406:ARG:NH1	2.25	0.51
1:A:193:PHE:O	1:A:224:VAL:HA	2.12	0.50
1:A:195:LEU:HD22	1:A:201:MET:CE	2.41	0.50
1:A:258:THR:HG22	1:A:260:HIS:N	2.26	0.50
1:A:214:ILE:HA	1:A:217:MET:HE3	1.92	0.50
1:A:214:ILE:HA	1:A:217:MET:HE2	1.93	0.50
1:A:238:VAL:HG12	1:A:242:PHE:HE1	1.77	0.50
1:A:243:MET:HE3	1:A:246:PRO:HG3	1.94	0.49
1:A:399:ILE:O	1:A:403:VAL:HG23	2.12	0.49
1:A:239:CYS:SG	1:A:243:MET:HE2	2.52	0.49
1:A:417:GLU:HG2	1:A:418:ILE:N	2.26	0.49
1:A:234:GLU:OE2	1:A:234:GLU:HA	2.13	0.49
1:A:323:GLN:O	1:A:327:LEU:HG	2.12	0.49
1:A:139:TYR:C	1:A:141:PRO:HD3	2.37	0.49
1:A:333:PHE:CD1	1:A:341:LEU:HB2	2.48	0.49
1:A:218:THR:HG22	1:A:222:LYS:HD3	1.94	0.49
1:A:293:PHE:O	1:A:362:TYR:HB3	2.12	0.49
1:A:326:ARG:HB2	1:A:326:ARG:HH11	1.77	0.49
1:A:195:LEU:HB2	1:A:198:CYS:SG	2.52	0.49
1:A:72:GLN:O	1:A:76:ILE:HB	2.12	0.48
1:A:105:GLN:HE21	1:A:105:GLN:HA	1.78	0.48
1:A:130:SER:HB2	1:A:147:VAL:CG1	2.43	0.48
1:A:232:SER:CB	1:A:235:ILE:HB	2.44	0.48
1:A:238:VAL:HG12	1:A:242:PHE:CE1	2.49	0.47
1:A:100:VAL:HG11	1:A:136:PHE:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:HD22	1:A:273:GLU:CB	2.43	0.47
1:A:313:PRO:CG	1:A:339:ARG:HB2	2.42	0.47
1:A:420:ILE:CG1	1:A:421:SER:H	2.25	0.47
1:A:164:ASN:HB2	5:A:596:HOH:O	2.14	0.47
1:A:358:ILE:HG12	1:A:386:LEU:HD23	1.97	0.47
1:A:145:VAL:HG12	1:A:146:ALA:H	1.79	0.47
1:A:218:THR:CG2	1:A:219:PRO:HD2	2.43	0.47
1:A:186:ASN:HD21	1:A:189:HIS:CE1	2.32	0.47
1:A:239:CYS:C	1:A:241:LYS:H	2.23	0.47
1:A:393:ASP:OD1	1:A:395:ASN:HB2	2.14	0.47
1:A:364:MET:SD	1:A:365:PRO:HD2	2.55	0.47
1:A:353:ILE:O	1:A:354:GLU:HB2	2.15	0.47
1:A:186:ASN:HD21	1:A:189:HIS:HE1	1.62	0.46
1:A:326:ARG:HH11	1:A:326:ARG:CB	2.27	0.46
1:A:365:PRO:HB3	1:A:374:ARG:NH1	2.31	0.46
1:A:215:PHE:CD1	1:A:242:PHE:HD2	2.33	0.46
1:A:147:VAL:HA	1:A:170:VAL:O	2.16	0.46
1:A:240:ARG:HB2	1:A:240:ARG:NH1	2.31	0.46
1:A:154:ILE:O	1:A:158:GLU:HG3	2.16	0.45
1:A:420:ILE:HG12	1:A:421:SER:N	2.29	0.45
1:A:182:ASN:O	1:A:183:LYS:CB	2.64	0.45
1:A:209:ARG:HH11	1:A:209:ARG:HG2	1.81	0.45
1:A:305:GLN:O	1:A:309:GLU:HG3	2.17	0.45
1:A:236:ARG:N	1:A:237:PRO:CD	2.79	0.45
1:A:420:ILE:O	1:A:421:SER:HB3	2.16	0.45
1:A:322:PRO:HD2	1:A:325:GLU:OE2	2.17	0.45
1:A:117:LEU:HB2	1:A:190:ILE:HD12	1.99	0.45
1:A:286:GLU:OE2	1:A:422:SER:OG	2.31	0.44
1:A:292:ILE:HA	1:A:360:PHE:HB2	1.98	0.44
1:A:159:GLU:HB3	1:A:163:LYS:HZ2	1.80	0.44
1:A:232:SER:OG	1:A:235:ILE:HD13	2.17	0.44
1:A:60:ILE:HD13	1:A:136:PHE:CE1	2.52	0.44
1:A:100:VAL:O	1:A:104:LEU:HB2	2.17	0.44
1:A:226:MET:HE1	1:A:239:CYS:HA	1.99	0.44
1:A:289:GLN:HA	1:A:339:ARG:O	2.17	0.44
1:A:113:GLN:HA	5:A:561:HOH:O	2.16	0.44
1:A:407:PHE:O	1:A:409:VAL:N	2.50	0.44
1:A:297:VAL:HG13	1:A:318:HIS:CD2	2.53	0.44
1:A:53:LYS:NZ	5:A:587:HOH:O	2.50	0.44
1:A:319:ARG:HB2	1:A:344:THR:HG21	1.99	0.44
1:A:140:MET:N	1:A:141:PRO:HD3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLN:O	1:A:245:ASP:C	2.61	0.43
1:A:358:ILE:CD1	1:A:386:LEU:HD23	2.48	0.43
1:A:415:PRO:O	1:A:416:ASP:CB	2.66	0.43
1:A:48:ARG:C	1:A:50:PHE:N	2.76	0.43
1:A:304:ALA:O	1:A:308:VAL:HG23	2.18	0.43
1:A:192:HIS:CD2	1:A:223:GLN:HE21	2.23	0.43
1:A:78:GLN:HG2	1:A:247:MET:SD	2.59	0.43
1:A:121:HIS:CD2	1:A:122:THR:HG23	2.54	0.43
1:A:106:GLN:HE22	1:A:223:GLN:NE2	2.04	0.42
1:A:93:MET:HE1	1:A:253:ASP:HA	2.01	0.42
1:A:145:VAL:CG1	1:A:146:ALA:N	2.80	0.42
1:A:318:HIS:HA	1:A:344:THR:HB	2.02	0.42
1:A:78:GLN:N	1:A:78:GLN:CD	2.78	0.42
1:A:85:VAL:HG12	1:A:86:LEU:N	2.35	0.42
1:A:414:LEU:HD12	1:A:415:PRO:HD2	2.01	0.42
1:A:87:CYS:O	1:A:227:PHE:HA	2.20	0.42
1:A:208:ARG:NH2	1:A:238:VAL:CG2	2.83	0.42
1:A:189:HIS:HB2	5:A:634:HOH:O	2.20	0.41
1:A:379:GLY:O	1:A:380:ARG:NE	2.50	0.41
1:A:231:LEU:HD23	1:A:231:LEU:N	2.36	0.41
1:A:177:LEU:HD13	1:A:214:ILE:HG13	2.01	0.41
1:A:382:GLY:O	1:A:383:THR:HG23	2.21	0.41
1:A:375:VAL:CG1	1:A:387:ALA:HB2	2.51	0.41
1:A:353:ILE:HG12	1:A:381:PHE:HE1	1.86	0.41
1:A:358:ILE:HG12	1:A:386:LEU:HB3	2.03	0.41
1:A:276:ARG:HG2	1:A:280:ASP:OD2	2.21	0.40
1:A:86:LEU:HB2	1:A:243:MET:HE1	2.02	0.40
1:A:106:GLN:O	1:A:108:GLU:HG3	2.21	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	370/386 (96%)	333 (90%)	28 (8%)	9 (2%)	4	12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	PRO
1	A	416	ASP
1	A	420	ILE
1	A	421	SER
1	A	183	LYS
1	A	295	LYS
1	A	417	GLU
1	A	378	ALA
1	A	232	SER

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	337/347 (97%)	325 (96%)	12 (4%)	31	60

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	104	LEU
1	A	147	VAL
1	A	199	ASP
1	A	228	SER
1	A	231	LEU
1	A	235	ILE
1	A	253	ASP
1	A	326	ARG
1	A	344	THR
1	A	363	ASP
1	A	420	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	88	GLN
1	A	105	GLN
1	A	113	GLN
1	A	182	ASN
1	A	189	HIS
1	A	192	HIS
1	A	212	GLN
1	A	223	GLN
1	A	264	GLN
1	A	305	GLN
1	A	323	GLN
1	A	331	GLN
1	A	332	GLN
1	A	337	GLN
1	A	357	ASN
1	A	404	GLN
1	A	410	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	ACY	A	500	-	3,3,3	1.63	0	3,3,3	1.32	0
3	ADP	A	550	2	28,29,29	1.23	4 (14%)	43,45,45	1.15	2 (4%)

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	ADP	A	550	2	-	5/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	550	ADP	C2-N1	2.90	1.39	1.33
3	A	550	ADP	C6-N6	-2.38	1.28	1.34
3	A	550	ADP	C1'-N9	2.37	1.52	1.46
3	A	550	ADP	PA-O3A	-2.02	1.57	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	550	ADP	N3-C2-N1	-3.70	122.98	128.58
3	A	550	ADP	C2-N1-C6	3.05	123.73	118.73

There are no chirality outliers.

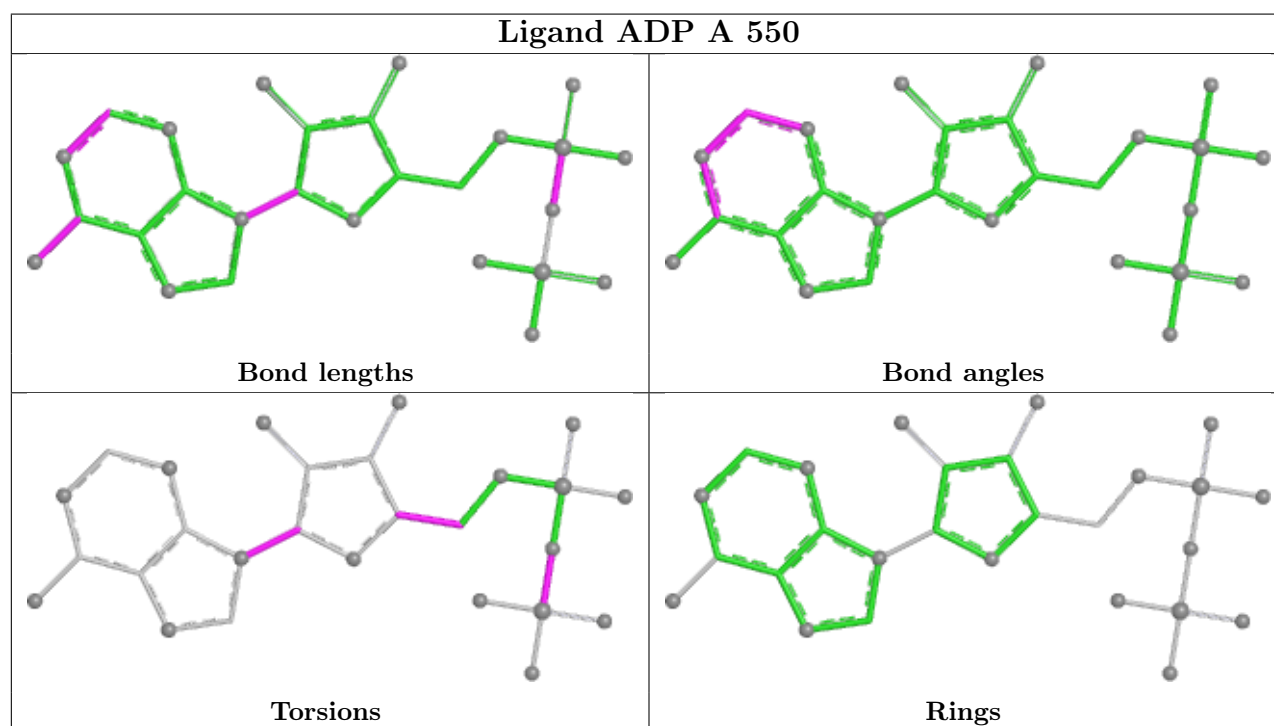
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	550	ADP	PA-O3A-PB-O3B
3	A	550	ADP	O4'-C4'-C5'-O5'
3	A	550	ADP	PA-O3A-PB-O2B
3	A	550	ADP	C2'-C1'-N9-C8
3	A	550	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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	374/386 (96%)	3.94	348 (93%) 0 0	14, 42, 79, 101	0

All (348) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	ALA	11.2
1	A	65	PHE	10.7
1	A	150	GLY	10.1
1	A	69	SER	9.4
1	A	126	ALA	8.9
1	A	316	ALA	8.9
1	A	243	MET	8.2
1	A	138	LYS	7.9
1	A	64	GLY	7.6
1	A	171	GLY	7.6
1	A	237	PRO	7.4
1	A	149	PHE	7.2
1	A	250	PHE	7.1
1	A	330	TYR	7.0
1	A	359	ALA	6.9
1	A	199	ASP	6.9
1	A	387	ALA	6.9
1	A	116	VAL	6.8
1	A	343	ALA	6.7
1	A	399	ILE	6.7
1	A	196	ASP	6.6
1	A	306	LEU	6.5
1	A	94	GLY	6.4
1	A	63	CYS	6.3
1	A	157	ASP	6.3
1	A	87	CYS	6.2
1	A	361	ASN	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	386	LEU	6.1
1	A	279	PHE	6.1
1	A	59	ALA	6.1
1	A	71	VAL	6.1
1	A	354	GLU	6.0
1	A	340	ILE	6.0
1	A	189	HIS	6.0
1	A	275	ASN	5.9
1	A	266	TYR	5.9
1	A	421	SER	5.8
1	A	362	TYR	5.8
1	A	416	ASP	5.8
1	A	54	PRO	5.8
1	A	251	VAL	5.7
1	A	267	VAL	5.7
1	A	146	ALA	5.7
1	A	371	TYR	5.7
1	A	292	ILE	5.6
1	A	320	GLY	5.6
1	A	289	GLN	5.6
1	A	227	PHE	5.6
1	A	165	CYS	5.6
1	A	269	LEU	5.6
1	A	105	GLN	5.6
1	A	253	ASP	5.5
1	A	113	GLN	5.5
1	A	333	PHE	5.5
1	A	190	ILE	5.5
1	A	91	SER	5.5
1	A	294	VAL	5.5
1	A	206	ASP	5.4
1	A	75	CYS	5.4
1	A	56	LEU	5.4
1	A	205	LEU	5.4
1	A	383	THR	5.4
1	A	173	PRO	5.4
1	A	342	VAL	5.3
1	A	378	ALA	5.3
1	A	388	ILE	5.3
1	A	263	GLN	5.2
1	A	127	PHE	5.2
1	A	352	ASP	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	396	ASP	5.2
1	A	404	GLN	5.2
1	A	60	ILE	5.2
1	A	230	THR	5.1
1	A	417	GLU	5.1
1	A	169	VAL	5.1
1	A	376	ALA	5.1
1	A	203	GLU	5.1
1	A	84	ASP	5.1
1	A	322	PRO	5.1
1	A	357	ASN	5.1
1	A	152	LEU	5.1
1	A	401	ASN	5.0
1	A	99	PHE	5.0
1	A	162	LYS	5.0
1	A	163	LYS	5.0
1	A	112	GLY	4.9
1	A	242	PHE	4.9
1	A	214	ILE	4.9
1	A	85	VAL	4.9
1	A	414	LEU	4.9
1	A	232	SER	4.9
1	A	114	VAL	4.9
1	A	284	VAL	4.9
1	A	168	ILE	4.8
1	A	314	ALA	4.8
1	A	130	SER	4.8
1	A	272	ASN	4.8
1	A	55	GLU	4.7
1	A	218	THR	4.7
1	A	73	HIS	4.7
1	A	303	LEU	4.7
1	A	177	LEU	4.7
1	A	262	LEU	4.7
1	A	282	LEU	4.7
1	A	154	ILE	4.7
1	A	259	LEU	4.7
1	A	317	ILE	4.6
1	A	129	ILE	4.6
1	A	397	ALA	4.5
1	A	400	LEU	4.5
1	A	353	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	79	ALA	4.5
1	A	201	MET	4.4
1	A	76	ILE	4.4
1	A	264	GLN	4.4
1	A	235	ILE	4.4
1	A	249	ILE	4.4
1	A	373	HIS	4.4
1	A	324	GLU	4.4
1	A	184	SER	4.4
1	A	141	PRO	4.4
1	A	355	ARG	4.4
1	A	245	ASP	4.3
1	A	229	ALA	4.3
1	A	377	ARG	4.3
1	A	233	LYS	4.3
1	A	178	ALA	4.3
1	A	375	VAL	4.3
1	A	97	ALA	4.3
1	A	224	VAL	4.3
1	A	270	LYS	4.2
1	A	194	ILE	4.2
1	A	247	MET	4.2
1	A	318	HIS	4.2
1	A	310	GLN	4.2
1	A	212	GLN	4.2
1	A	321	MET	4.2
1	A	363	ASP	4.1
1	A	412	SER	4.1
1	A	180	ALA	4.1
1	A	120	CYS	4.1
1	A	291	VAL	4.1
1	A	308	VAL	4.1
1	A	53	LYS	4.1
1	A	46	GLY	4.1
1	A	118	VAL	4.1
1	A	72	GLN	4.0
1	A	382	GLY	4.0
1	A	327	LEU	4.0
1	A	193	PHE	4.0
1	A	381	PHE	4.0
1	A	153	SER	4.0
1	A	132	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	406	ARG	4.0
1	A	215	PHE	4.0
1	A	96	THR	4.0
1	A	185	LEU	4.0
1	A	164	ASN	4.0
1	A	195	LEU	4.0
1	A	283	ASP	4.0
1	A	339	ARG	3.9
1	A	280	ASP	3.9
1	A	117	LEU	3.9
1	A	202	LEU	3.9
1	A	372	LEU	3.9
1	A	217	MET	3.9
1	A	182	ASN	3.9
1	A	161	LEU	3.9
1	A	260	HIS	3.9
1	A	281	LEU	3.9
1	A	151	GLY	3.9
1	A	47	PHE	3.9
1	A	98	VAL	3.9
1	A	313	PRO	3.8
1	A	239	CYS	3.8
1	A	246	PRO	3.8
1	A	49	ASP	3.8
1	A	268	LYS	3.8
1	A	139	TYR	3.8
1	A	137	SER	3.8
1	A	380	ARG	3.8
1	A	223	GLN	3.8
1	A	228	SER	3.7
1	A	57	LEU	3.7
1	A	89	ALA	3.7
1	A	174	GLY	3.7
1	A	319	ARG	3.7
1	A	148	PHE	3.7
1	A	293	PHE	3.7
1	A	407	PHE	3.7
1	A	166	PRO	3.7
1	A	423	TYR	3.7
1	A	50	PHE	3.7
1	A	226	MET	3.7
1	A	88	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	231	LEU	3.6
1	A	238	VAL	3.6
1	A	356	VAL	3.6
1	A	186	ASN	3.6
1	A	300	CYS	3.6
1	A	364	MET	3.6
1	A	360	PHE	3.6
1	A	297	VAL	3.6
1	A	309	GLU	3.6
1	A	133	TYR	3.6
1	A	100	VAL	3.6
1	A	86	LEU	3.6
1	A	104	LEU	3.6
1	A	101	LEU	3.6
1	A	274	LYS	3.6
1	A	110	VAL	3.5
1	A	170	VAL	3.5
1	A	296	SER	3.5
1	A	392	SER	3.5
1	A	143	VAL	3.5
1	A	379	GLY	3.5
1	A	338	ARG	3.5
1	A	252	ASP	3.5
1	A	179	LEU	3.5
1	A	111	THR	3.4
1	A	301	ILE	3.4
1	A	358	ILE	3.4
1	A	391	VAL	3.4
1	A	176	ILE	3.4
1	A	95	LYS	3.4
1	A	336	PHE	3.4
1	A	93	MET	3.4
1	A	131	LYS	3.4
1	A	222	LYS	3.4
1	A	389	THR	3.4
1	A	257	LEU	3.4
1	A	315	ILE	3.3
1	A	103	THR	3.3
1	A	92	GLY	3.3
1	A	216	ARG	3.3
1	A	374	ARG	3.3
1	A	62	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	405	ASP	3.3
1	A	241	LYS	3.3
1	A	385	GLY	3.3
1	A	107	LEU	3.3
1	A	197	GLU	3.3
1	A	145	VAL	3.3
1	A	240	ARG	3.3
1	A	276	ARG	3.3
1	A	307	LEU	3.3
1	A	188	LYS	3.3
1	A	325	GLU	3.2
1	A	328	SER	3.2
1	A	411	ILE	3.2
1	A	144	LYS	3.2
1	A	409	VAL	3.2
1	A	74	GLU	3.2
1	A	344	THR	3.2
1	A	420	ILE	3.2
1	A	335	ASP	3.2
1	A	366	GLU	3.2
1	A	287	PHE	3.1
1	A	311	ASN	3.1
1	A	419	ASP	3.1
1	A	219	PRO	3.1
1	A	337	GLN	3.1
1	A	207	MET	3.1
1	A	200	LYS	3.0
1	A	422	SER	3.0
1	A	285	LEU	3.0
1	A	254	GLU	3.0
1	A	48	ARG	3.0
1	A	115	SER	3.0
1	A	393	ASP	3.0
1	A	82	GLY	2.9
1	A	403	VAL	2.9
1	A	323	GLN	2.9
1	A	209	ARG	2.9
1	A	345	ASN	2.9
1	A	136	PHE	2.9
1	A	415	PRO	2.9
1	A	128	GLN	2.9
1	A	52	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	211	VAL	2.9
1	A	183	LYS	2.9
1	A	346	LEU	2.9
1	A	413	GLU	2.8
1	A	402	ASP	2.8
1	A	331	GLN	2.8
1	A	155	LYS	2.8
1	A	370	THR	2.8
1	A	225	MET	2.8
1	A	208	ARG	2.8
1	A	204	GLN	2.8
1	A	410	ASN	2.8
1	A	298	GLN	2.7
1	A	192	HIS	2.7
1	A	124	GLU	2.7
1	A	395	ASN	2.7
1	A	135	ARG	2.7
1	A	51	LEU	2.7
1	A	368	SER	2.7
1	A	77	PRO	2.7
1	A	332	GLN	2.7
1	A	175	ARG	2.7
1	A	326	ARG	2.7
1	A	286	GLU	2.6
1	A	68	PRO	2.6
1	A	277	LYS	2.6
1	A	295	LYS	2.6
1	A	160	VAL	2.6
1	A	256	LYS	2.6
1	A	367	ASP	2.5
1	A	236	ARG	2.5
1	A	220	HIS	2.5
1	A	198	CYS	2.5
1	A	288	ASN	2.5
1	A	261	GLY	2.5
1	A	244	GLN	2.5
1	A	167	HIS	2.5
1	A	58	ARG	2.4
1	A	255	THR	2.4
1	A	341	LEU	2.4
1	A	273	GLU	2.4
1	A	312	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	83	MET	2.4
1	A	299	ARG	2.4
1	A	90	LYS	2.4
1	A	290	VAL	2.3
1	A	142	ASN	2.3
1	A	140	MET	2.3
1	A	248	GLU	2.3
1	A	394	GLU	2.3
1	A	45	SER	2.3
1	A	109	PRO	2.3
1	A	213	GLU	2.3
1	A	106	GLN	2.3
1	A	67	HIS	2.2
1	A	210	ASP	2.2
1	A	305	GLN	2.2
1	A	365	PRO	2.2
1	A	66	GLU	2.2
1	A	172	THR	2.2
1	A	221	GLU	2.2
1	A	334	LYS	2.1
1	A	390	PHE	2.1
1	A	304	ALA	2.1
1	A	384	LYS	2.1
1	A	81	LEU	2.1
1	A	147	VAL	2.1
1	A	234	GLU	2.0
1	A	187	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

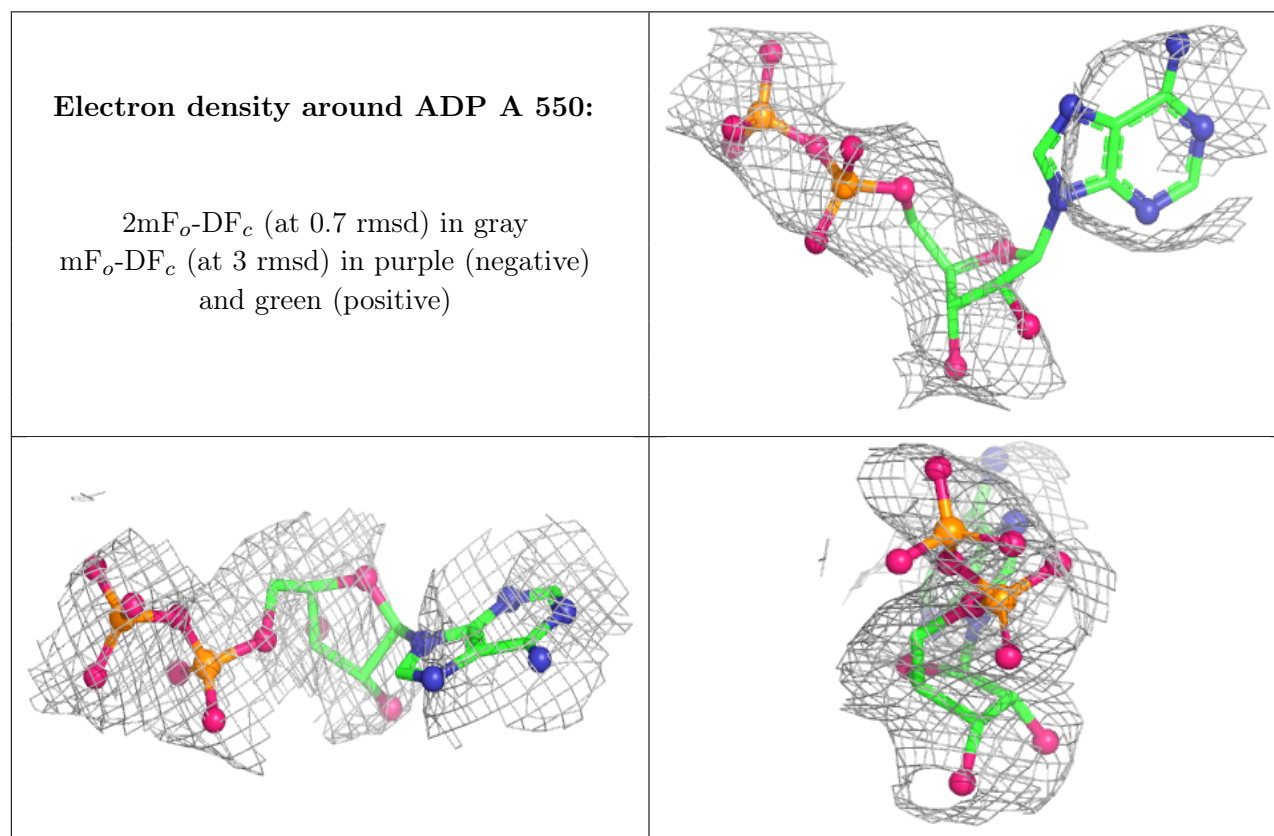
6.4 Ligands [i](#)

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

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ACY	A	500	4/4	0.57	0.28	66,66,66,66	0
3	ADP	A	550	27/27	0.59	0.25	32,41,44,47	0
2	MG	A	501	1/1	0.68	0.19	35,35,35,35	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.