



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:33 AM UTC

PDB ID : 8H5Y / pdb_00008h5y
Title : Crystal structure of RadD- ADP complex
Authors : Yan, X.X.; Tian, L.F.
Deposited on : 2022-10-14
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

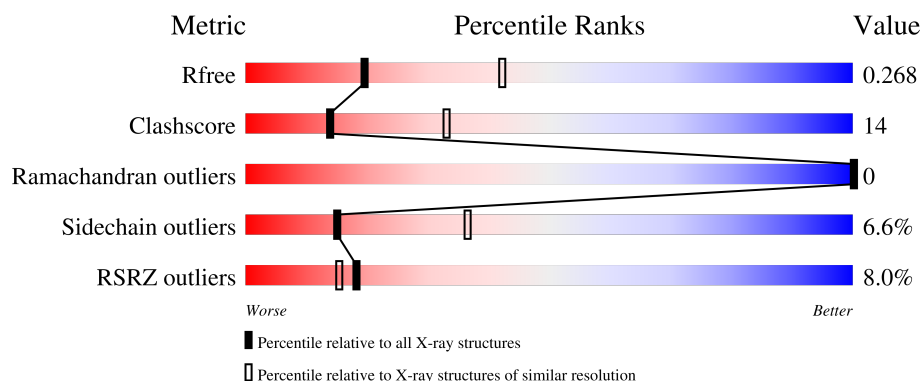
1 Overall quality at a glance

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	586	5% 66% 27% • •
1	B	586	11% 66% 28% • •

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8956 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.

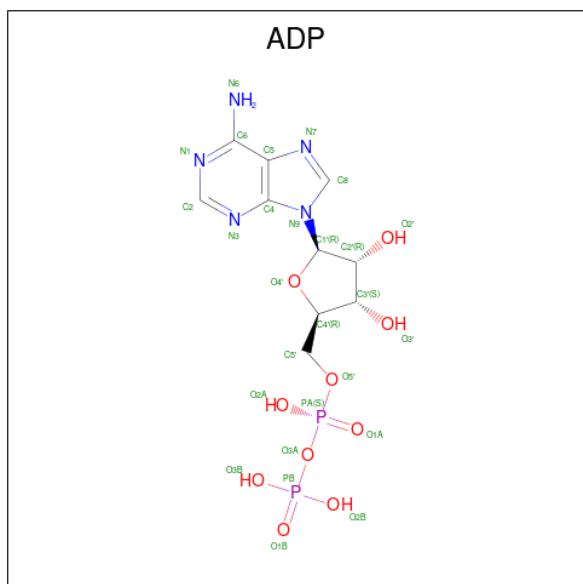
- Molecule 1 is a protein called Putative DNA repair helicase RadD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	568	Total	C	N	O	S	0	2	0
			4349	2779	778	775	17			
1	A	564	Total	C	N	O	S	0	2	0
			4336	2769	771	778	18			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

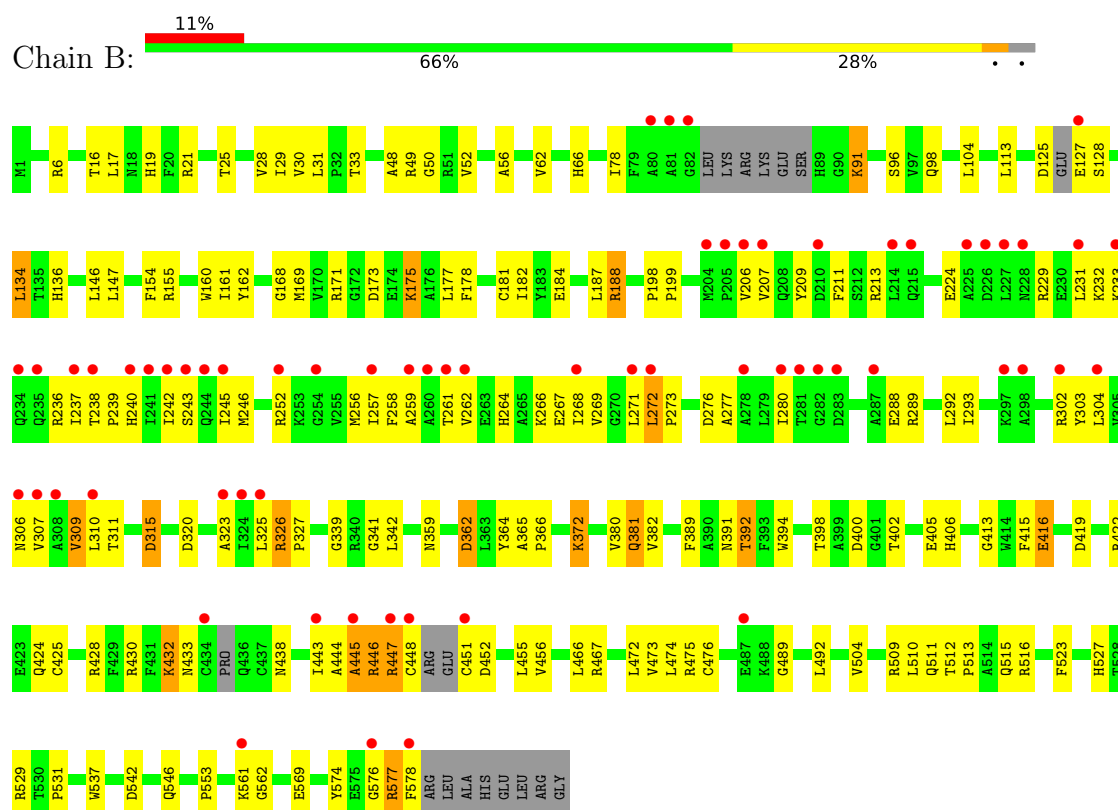
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	131	Total	O	0	0
			131	131		
5	A	82	Total	O	0	0
			82	82		

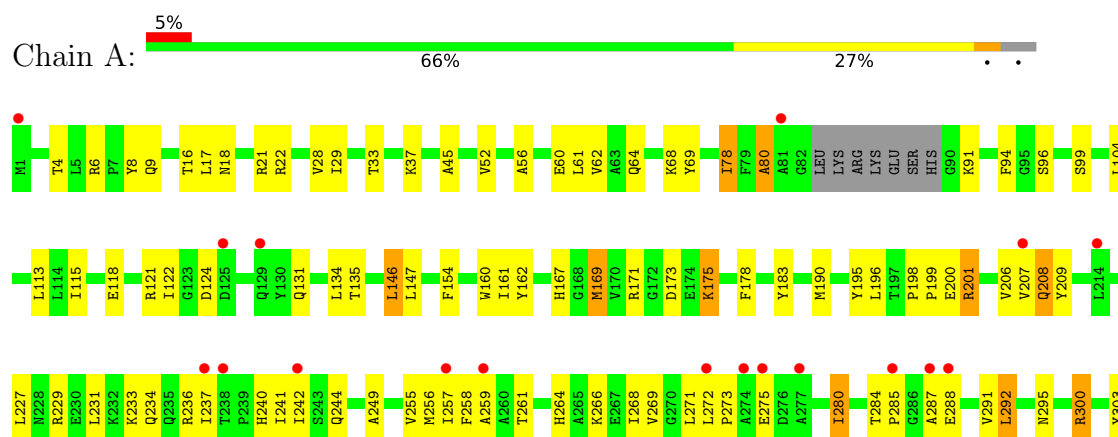
3 Residue-property plots

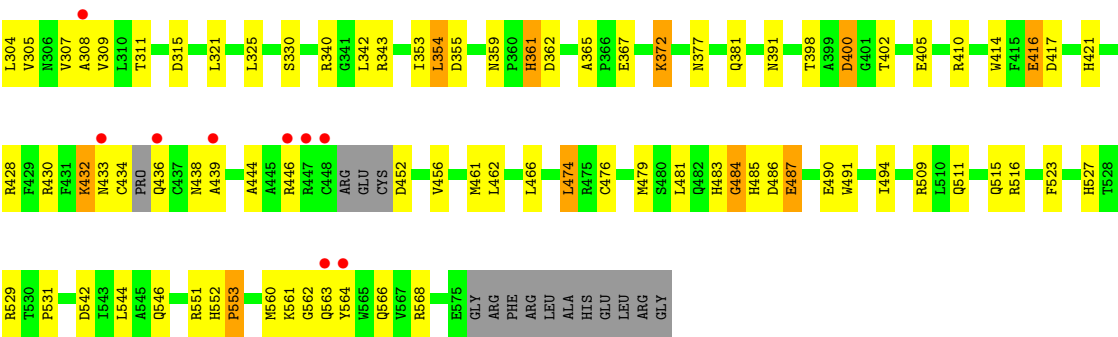
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Putative DNA repair helicase RadD



• Molecule 1: Putative DNA repair helicase RadD





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.09Å 78.77Å 110.24Å 90.00° 99.56° 90.00°	Depositor
Resolution (Å)	19.96 – 2.70 19.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.96-2.70) 99.0 (19.96-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 2.71Å)	Xtriage
Refinement program	PHENIX 1.12-2829_1692	Depositor
R, R_{free}	0.223 , 0.269 0.224 , 0.268	Depositor DCC
R_{free} test set	1852 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.1	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	0.93	EDS
Total number of atoms	8956	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.4613e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ADP, MG, ZN

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	0.62	3/4440 (0.1%)	0.84	7/6037 (0.1%)
1	B	0.60	2/4453 (0.0%)	0.84	9/6053 (0.1%)
All	All	0.61	5/8893 (0.1%)	0.84	16/12090 (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	4
1	B	0	2
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	553	PRO	C-O	-8.39	1.14	1.23
1	B	447	ARG	CA-C	-7.57	1.43	1.52
1	B	447	ARG	C-O	-7.17	1.16	1.23
1	A	198	PRO	CA-C	6.04	1.57	1.52
1	A	551	ARG	C-O	-5.16	1.17	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	VAL	CA-C-N	-8.27	109.33	121.24
1	A	309	VAL	C-N-CA	-8.27	109.33	121.24
1	B	49	ARG	CA-C-N	-7.50	106.70	121.41
1	B	49	ARG	C-N-CA	-7.50	106.70	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	446	ARG	N-CA-C	6.83	123.99	112.99
1	B	33	THR	CA-C-N	-6.83	108.02	121.41
1	B	33	THR	C-N-CA	-6.83	108.02	121.41
1	B	577	ARG	CA-C-N	6.45	133.32	121.70
1	B	577	ARG	C-N-CA	6.45	133.32	121.70
1	B	447	ARG	N-CA-C	6.29	117.86	107.73
1	B	445	ALA	CB-CA-C	5.77	121.90	110.42
1	A	564	TYR	CA-C-N	5.74	132.50	121.54
1	A	564	TYR	C-N-CA	5.74	132.50	121.54
1	A	354	LEU	CB-CG-CD2	-5.63	93.81	110.70
1	A	80	ALA	N-CA-CB	-5.32	101.51	110.49
1	A	309	VAL	CA-CB-CG1	5.11	119.09	110.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	ASP	Peptide
1	A	273	PRO	Peptide
1	A	308	ALA	Peptide
1	A	484	GLY	Peptide
1	B	229	ARG	Peptide
1	B	50	GLY	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	4336	0	4178	118	0
1	B	4349	0	4185	128	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	2	0
3	B	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	82	0	0	8	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	131	0	0	7	1
All	All	8956	0	8387	246	1

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 (246) 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:434:CYS:N	5:A:701:HOH:O	1.62	1.24
1:B:433:ASN:ND2	1:B:448:CYS:O	1.99	0.96
1:B:428:ARG:NH1	1:B:438:ASN:OD1	2.00	0.95
1:B:206:VAL:HG13	1:B:207:VAL:HG22	1.49	0.93
1:B:243:SER:HA	1:B:246:MET:HE2	1.57	0.86
1:B:315:ASP:N	1:B:315:ASP:OD1	2.07	0.86
1:B:272:LEU:HD11	1:B:277:ALA:HB2	1.60	0.83
1:A:433:ASN:C	5:A:701:HOH:O	2.02	0.80
1:B:405:GLU:HG2	1:B:529:ARG:HB3	1.63	0.79
1:A:405:GLU:HG3	1:A:529:ARG:HB3	1.66	0.78
1:A:291:VAL:O	1:A:295:ASN:ND2	2.17	0.77
1:A:321:LEU:HD21	1:A:354:LEU:HD12	1.66	0.76
1:B:362[A]:ASP:HB2	1:B:365:ALA:HB2	1.68	0.76
1:A:242:ILE:HD11	1:A:272:LEU:HD21	1.68	0.75
1:B:433:ASN:O	5:B:701:HOH:O	2.05	0.73
1:B:271:LEU:O	5:B:702:HOH:O	2.09	0.70
1:A:372:LYS:NZ	1:A:377:ASN:O	2.25	0.69
1:B:574:TYR:CZ	1:B:576:GLY:O	2.47	0.68
1:A:37:LYS:HG2	3:A:602:ADP:O2B	1.94	0.67
1:B:256:MET:HE1	1:B:311:THR:HG21	1.76	0.67
1:B:272:LEU:HB2	1:B:273:PRO:HD2	1.75	0.67
1:B:280:ILE:HG13	1:B:306:ASN:HB3	1.78	0.66
1:B:432:LYS:HE3	1:B:455:LEU:HD13	1.77	0.66
1:B:444:ALA:HB2	1:B:455:LEU:HD21	1.76	0.66
1:B:259:ALA:HB1	1:B:264:HIS:HB3	1.78	0.65
1:A:432:LYS:NZ	1:A:439:ALA:O	2.29	0.64
1:B:447:ARG:N	1:B:451:CYS:O	2.31	0.63
1:A:18:ASN:HB3	1:A:22:ARG:HH22	1.64	0.63
1:A:434:CYS:CA	5:A:701:HOH:O	2.24	0.63
1:B:267:GLU:O	1:B:271:LEU:HD23	1.99	0.63
1:A:285:PRO:HB2	1:A:288:GLU:H	1.63	0.62
1:B:257:ILE:HG12	1:B:323:ALA:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:ARG:HA	1:B:578:PHE:HB2	1.82	0.61
1:B:574:TYR:OH	1:B:576:GLY:O	2.15	0.61
1:B:513:PRO:HB3	1:B:516[A]:ARG:HH21	1.63	0.61
1:B:430:ARG:CZ	1:B:531:PRO:HG3	2.31	0.61
1:A:444:ALA:O	1:A:452:ASP:HA	2.01	0.61
1:A:428:ARG:HD3	1:A:438:ASN:OD1	2.00	0.60
1:A:280:ILE:HG12	1:A:304:LEU:HD11	1.82	0.60
1:B:398:THR:HG23	1:B:400:ASP:H	1.66	0.60
1:B:444:ALA:O	1:B:445:ALA:C	2.44	0.60
1:A:241:ILE:HG21	1:A:325:LEU:HD11	1.82	0.60
1:A:436:GLN:HA	5:A:701:HOH:O	2.02	0.60
1:B:432:LYS:HE2	1:B:438:ASN:O	2.02	0.60
1:A:295:ASN:HA	1:A:300:ARG:HH11	1.66	0.60
1:B:169:MET:HG3	1:B:389:PHE:HZ	1.67	0.60
1:B:211:PHE:CD1	1:B:231:LEU:HD12	2.36	0.59
1:A:315:ASP:O	1:A:343:ARG:NH2	2.36	0.59
1:B:264:HIS:O	1:B:268:ILE:HG13	2.01	0.59
1:A:242:ILE:HG21	1:A:271:LEU:HB3	1.84	0.59
1:A:434:CYS:HA	1:A:436:GLN:HA	1.86	0.58
1:A:486:ASP:HB2	1:A:487:GLU:OE2	2.04	0.57
1:A:259:ALA:HB3	1:A:307:VAL:HG22	1.85	0.57
1:B:272:LEU:HD11	1:B:277:ALA:CB	2.34	0.56
1:B:239:PRO:HA	1:B:242:ILE:HG22	1.86	0.56
1:B:280:ILE:CG1	1:B:306:ASN:HB3	2.34	0.56
1:A:64:GLN:O	1:A:68:LYS:HG3	2.05	0.56
1:B:381:GLN:HA	1:B:391:ASN:O	2.06	0.56
1:A:160:TRP:CE2	1:A:171:ARG:HD2	2.41	0.56
1:A:68:LYS:NZ	3:A:602:ADP:O1B	2.40	0.55
1:B:444:ALA:C	1:B:446:ARG:N	2.64	0.55
1:A:321:LEU:HD21	1:A:354:LEU:CD1	2.36	0.55
1:B:509:ARG:O	1:B:515:GLN:HB3	2.06	0.55
1:B:245:ILE:HG21	1:B:257:ILE:HD11	1.88	0.55
1:A:476:CYS:HB3	1:A:553:PRO:O	2.06	0.55
1:A:566:GLN:HE21	1:A:568:ARG:HE	1.55	0.55
1:B:372:LYS:HB2	1:B:372:LYS:NZ	2.22	0.55
1:A:264:HIS:O	1:A:268:ILE:HG13	2.07	0.55
1:A:355:ASP:OD1	1:A:359:ASN:HB2	2.07	0.55
1:A:146:LEU:HD22	1:A:178:PHE:HE1	1.72	0.54
1:B:66:HIS:CD2	1:B:78:ILE:HB	2.42	0.54
1:A:80:ALA:O	1:A:99:SER:OG	2.25	0.54
1:B:246:MET:SD	5:B:702:HOH:O	2.58	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362[B]:ASP:HB3	1:B:365:ALA:HB2	1.88	0.54
1:A:29:ILE:HG23	1:A:183:TYR:HB3	1.89	0.54
1:A:52:VAL:HG22	1:A:113:LEU:HB3	1.89	0.54
1:A:237:ILE:HA	1:A:240:HIS:HD2	1.73	0.54
1:B:29:ILE:HG13	1:B:147:LEU:HD11	1.90	0.53
1:A:398:THR:HG23	1:A:400:ASP:H	1.74	0.53
1:B:257:ILE:HG23	1:B:325:LEU:HD23	1.91	0.53
1:B:56:ALA:O	1:B:96:SER:HA	2.08	0.53
1:A:446:ARG:O	1:A:452:ASP:N	2.42	0.53
1:A:511:GLN:O	1:A:516:ARG:NH1	2.40	0.53
1:A:484:GLY:HA3	1:A:491:TRP:CZ2	2.43	0.53
1:A:242:ILE:HD11	1:A:272:LEU:CD2	2.37	0.53
1:B:52:VAL:HG22	1:B:113:LEU:HB3	1.90	0.53
1:B:447:ARG:HA	1:B:451:CYS:N	2.23	0.53
1:B:476:CYS:HB3	1:B:553:PRO:O	2.08	0.53
1:B:258:PHE:CD1	1:B:306:ASN:ND2	2.75	0.52
1:A:6:ARG:HD3	1:A:195:TYR:CE1	2.45	0.52
1:A:33:THR:HG21	1:A:340:ARG:HH12	1.75	0.52
1:B:28:VAL:HG13	1:B:178:PHE:CG	2.44	0.52
1:B:289:ARG:O	1:B:293:ILE:HG23	2.08	0.52
1:B:309:VAL:O	1:B:311:THR:HG23	2.08	0.52
1:B:266:LYS:HA	1:B:269:VAL:HG12	1.90	0.52
1:A:131[A]:GLN:OE1	1:A:135:THR:HG23	2.10	0.51
1:B:160:TRP:CE2	1:B:171:ARG:HD2	2.45	0.51
1:A:162:TYR:HA	1:A:178:PHE:O	2.11	0.51
1:A:154:PHE:HB2	1:A:160:TRP:CE3	2.45	0.51
1:A:257:ILE:HG13	1:A:325:LEU:HD23	1.92	0.51
1:B:512:THR:O	1:B:516[A]:ARG:HG3	2.11	0.51
1:A:485:HIS:O	5:A:703:HOH:O	2.20	0.51
1:A:481:LEU:HD22	1:A:494:ILE:HG13	1.93	0.51
1:A:17:LEU:O	1:A:21:ARG:HG3	2.11	0.51
1:A:261:THR:OG1	1:A:264:HIS:HB2	2.09	0.51
1:B:169:MET:HG3	1:B:389:PHE:CZ	2.47	0.50
1:B:475:ARG:NH1	5:B:705:HOH:O	2.37	0.50
1:A:430:ARG:CZ	1:A:531:PRO:HG3	2.42	0.50
1:B:162:TYR:HA	1:B:178:PHE:O	2.12	0.50
1:A:167:HIS:HB3	1:A:169[B]:MET:HE1	1.93	0.50
1:B:467:ARG:NH2	5:B:708:HOH:O	2.44	0.50
1:B:444:ALA:O	1:B:452:ASP:HA	2.11	0.50
1:A:255:VAL:HG22	1:A:321:LEU:HB3	1.94	0.49
1:A:16:THR:OG1	1:A:29:ILE:HD11	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:PRO:HB3	1:B:516[A]:ARG:NH2	2.28	0.49
1:B:326:ARG:HG2	1:B:327:PRO:N	2.28	0.49
1:B:372:LYS:HB2	1:B:372:LYS:HZ3	1.77	0.49
1:A:487:GLU:CD	1:A:487:GLU:H	2.21	0.49
1:B:173:ASP:C	1:B:175:LYS:H	2.21	0.48
1:B:238:THR:HB	1:B:239:PRO:HD3	1.96	0.48
1:A:287:ALA:O	1:A:291:VAL:HG23	2.13	0.48
1:B:382:VAL:HG21	1:B:406:HIS:CD2	2.47	0.48
1:B:256:MET:CE	1:B:311:THR:HG21	2.42	0.48
1:B:288:GLU:O	1:B:292:LEU:HG	2.14	0.48
1:A:355:ASP:CG	1:A:359:ASN:HB2	2.37	0.48
1:B:326:ARG:O	1:B:359:ASN:ND2	2.39	0.48
1:B:447:ARG:O	1:B:448:CYS:C	2.55	0.48
1:A:29:ILE:HG13	1:A:147:LEU:HD11	1.96	0.48
1:A:115:ILE:HA	1:A:147:LEU:O	2.14	0.48
1:A:21:ARG:NH2	5:A:709:HOH:O	2.46	0.47
1:A:284:THR:HG22	1:A:285:PRO:O	2.13	0.47
1:B:398:THR:HG22	1:B:402:THR:HB	1.96	0.47
1:B:160:TRP:CZ2	1:B:171:ARG:HD2	2.49	0.47
1:A:414:TRP:HZ3	1:A:416:GLU:HG3	1.79	0.47
1:A:208:GLN:HG2	1:A:209:TYR:O	2.14	0.47
1:A:257:ILE:HG23	1:A:305:VAL:HA	1.97	0.47
1:A:62:VAL:HG21	1:A:96:SER:HB3	1.97	0.46
1:B:372:LYS:HA	1:B:394:TRP:CE2	2.50	0.46
1:A:173:ASP:OD2	1:A:175:LYS:HG3	2.14	0.46
1:B:17:LEU:O	1:B:21:ARG:HG3	2.15	0.46
1:A:201:ARG:HD2	1:A:361:HIS:NE2	2.31	0.46
1:A:206:VAL:HG13	1:A:207:VAL:HG22	1.96	0.46
1:A:410:ARG:HD2	1:A:438:ASN:HD21	1.80	0.46
1:B:48:ALA:O	1:B:91:LYS:NZ	2.48	0.46
1:B:207:VAL:HB	1:B:237:ILE:HD11	1.98	0.46
1:A:461:MET:HE3	1:A:461:MET:HB3	1.85	0.46
1:B:29:ILE:HG22	1:B:31:LEU:HG	1.99	0.45
1:B:419:ASP:HB3	5:B:726:HOH:O	2.15	0.45
1:A:160:TRP:CZ2	1:A:171:ARG:HD2	2.52	0.45
1:A:8:TYR:CE1	1:A:9:GLN:HG3	2.51	0.45
1:A:362:ASP:HB2	1:A:365:ALA:CB	2.45	0.45
1:A:523:PHE:O	1:A:527:HIS:HB2	2.16	0.45
1:A:295:ASN:HA	1:A:300:ARG:NH1	2.31	0.45
1:A:542:ASP:O	1:A:546:GLN:HG3	2.16	0.45
1:A:288:GLU:O	1:A:292:LEU:HD22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ASP:OD2	1:B:302:ARG:HD3	2.17	0.45
1:A:462:LEU:O	1:A:466:LEU:HG	2.17	0.45
1:B:154:PHE:HB2	1:B:160:TRP:CE3	2.52	0.45
1:B:472:LEU:HD12	1:B:473:VAL:H	1.82	0.45
1:A:362:ASP:OD1	1:A:362:ASP:N	2.45	0.45
1:B:19:HIS:HE1	1:B:25:THR:O	2.00	0.44
1:B:523:PHE:O	1:B:527:HIS:HB2	2.17	0.44
1:A:433:ASN:O	1:A:434:CYS:HB3	2.17	0.44
1:B:146:LEU:HD22	1:B:178:PHE:HE1	1.82	0.44
1:A:362:ASP:HB2	1:A:365:ALA:HB2	2.00	0.44
1:A:483:HIS:HD2	1:A:544:LEU:HD22	1.82	0.44
1:A:560:MET:CE	1:A:563:GLN:O	2.65	0.44
1:A:474:LEU:H	1:A:474:LEU:HD12	1.83	0.44
1:A:190:MET:HB3	1:A:196:LEU:HG	1.99	0.44
1:A:206:VAL:HG12	1:A:244:GLN:OE1	2.18	0.44
1:A:330:SER:HB2	1:A:367:GLU:OE1	2.17	0.44
1:B:231:LEU:HD23	1:B:231:LEU:HA	1.79	0.44
1:B:516[B]:ARG:HG2	1:B:537:TRP:CH2	2.52	0.44
1:A:78:ILE:HA	1:A:94:PHE:O	2.18	0.44
1:A:561:LYS:HA	1:A:562:GLY:HA2	1.53	0.44
1:A:484:GLY:O	1:A:490:GLU:HA	2.18	0.44
1:B:512:THR:HB	1:B:513:PRO:HD2	2.00	0.43
1:A:199:PRO:HB3	1:A:342:LEU:HD21	2.00	0.43
1:B:271:LEU:HD13	1:B:271:LEU:HA	1.76	0.43
1:B:489:GLY:HA3	1:B:511:GLN:HB2	2.01	0.43
1:A:61:LEU:HD22	1:A:118:GLU:OE2	2.18	0.43
1:A:432:LYS:HE2	1:A:438:ASN:O	2.17	0.43
1:A:28:VAL:HG23	1:A:178:PHE:CG	2.54	0.43
1:B:207:VAL:CG2	1:B:237:ILE:HD11	2.48	0.43
1:B:398:THR:HG23	1:B:400:ASP:N	2.32	0.43
1:B:134:LEU:HD21	1:B:146:LEU:HD12	2.01	0.43
1:B:188:ARG:HD3	1:B:364:TYR:CD2	2.54	0.43
1:A:121:ARG:O	1:A:122:ILE:C	2.61	0.43
1:A:201:ARG:HG2	1:A:353:ILE:O	2.19	0.43
1:B:30:VAL:HB	1:B:184:GLU:HG3	2.01	0.43
1:B:161:ILE:HD11	1:B:177:LEU:HD12	2.01	0.43
1:B:424:GLN:HG2	1:B:425:CYS:O	2.19	0.43
1:B:561:LYS:HA	1:B:562:GLY:HA2	1.41	0.43
1:A:400:ASP:OD1	1:A:400:ASP:N	2.51	0.43
1:B:261:THR:O	1:B:307:VAL:HG21	2.19	0.42
1:B:492:LEU:HB2	1:B:510:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:LEU:HA	1:B:466:LEU:HD23	1.77	0.42
1:B:416:GLU:HG2	1:B:422:ARG:HB2	2.00	0.42
1:A:266:LYS:O	1:A:269:VAL:HG12	2.19	0.42
1:B:125:ASP:HA	1:B:127:GLU:HA	2.01	0.42
1:B:168:GLY:O	1:B:413:GLY:HA2	2.19	0.42
1:B:233:LYS:H	1:B:233:LYS:HG2	1.67	0.42
1:A:362:ASP:HA	5:A:734:HOH:O	2.19	0.42
1:A:479:MET:HG2	1:A:552:HIS:HB3	2.02	0.42
1:B:239:PRO:HG3	1:B:271:LEU:HG	2.00	0.42
1:B:380:VAL:O	1:B:392:THR:HA	2.19	0.42
1:B:398:THR:CG2	1:B:402:THR:HB	2.50	0.42
1:B:252:ARG:HD3	1:B:320:ASP:OD2	2.20	0.42
1:B:474:LEU:HD21	1:B:504:VAL:HG12	2.01	0.41
1:A:256:MET:CE	1:A:311:THR:HG21	2.50	0.41
1:B:311:THR:O	1:B:315:ASP:OD1	2.37	0.41
1:A:45:ALA:O	1:A:91:LYS:HE2	2.20	0.41
1:A:256:MET:HE2	1:A:258:PHE:CZ	2.56	0.41
1:B:28:VAL:HG23	1:B:181:CYS:HA	2.03	0.41
1:B:62:VAL:HG21	1:B:96:SER:HB3	2.02	0.41
1:B:542:ASP:O	1:B:546:GLN:HG3	2.20	0.41
1:B:173:ASP:C	1:B:175:LYS:N	2.79	0.41
1:B:259:ALA:HB3	1:B:307:VAL:CG2	2.50	0.41
1:A:154:PHE:HB2	1:A:160:TRP:CZ3	2.55	0.41
1:B:187:LEU:O	1:B:188:ARG:C	2.64	0.41
1:B:198:PRO:HA	1:B:199:PRO:HD3	1.97	0.41
1:A:56:ALA:HB1	1:A:61:LEU:HD23	2.01	0.41
1:A:161:ILE:HD12	1:A:161:ILE:HA	1.90	0.41
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.91	0.41
1:B:104:LEU:HD23	1:B:104:LEU:HA	1.84	0.41
1:B:280:ILE:HG13	1:B:306:ASN:CB	2.49	0.41
1:B:240:HIS:O	1:B:243:SER:OG	2.39	0.41
1:B:341:GLY:C	1:B:342:LEU:HD23	2.46	0.41
1:A:69:TYR:OH	5:A:702:HOH:O	2.15	0.41
1:A:381:GLN:HA	1:A:391:ASN:O	2.20	0.41
1:B:444:ALA:O	1:B:446:ARG:N	2.53	0.41
1:A:249:ALA:HB2	1:A:255:VAL:HG21	2.02	0.41
1:A:417:ASP:OD1	1:A:421:HIS:N	2.54	0.41
1:B:16:THR:HA	1:B:182:ILE:CD1	2.51	0.41
1:B:134:LEU:HA	1:B:134:LEU:HD23	1.75	0.40
1:B:242:ILE:HD12	1:B:245:ILE:HB	2.03	0.40
1:B:104:LEU:HD13	1:B:136:HIS:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:HD23	1:A:104:LEU:HA	1.85	0.40
1:A:271:LEU:HA	1:A:271:LEU:HD23	1.91	0.40
1:B:366:PRO:HB3	5:B:824:HOH:O	2.20	0.40
1:A:249:ALA:HB3	1:A:303:TYR:OH	2.21	0.40
1:B:272:LEU:HD13	1:B:303:TYR:CD2	2.56	0.40
1:B:339:GLY:HA2	1:B:342:LEU:HG	2.03	0.40
1:A:234:GLN:C	1:A:236:ARG:H	2.29	0.40
1:A:509:ARG:O	1:A:515:GLN:HB3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:816:HOH:O	5:A:714:HOH:O[2_748]	1.79	0.41

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	558/586 (95%)	501 (90%)	57 (10%)	0	100	100
1	B	560/586 (96%)	500 (89%)	60 (11%)	0	100	100
All	All	1118/1172 (95%)	1001 (90%)	117 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	430/491 (88%)	403 (94%)	27 (6%)	16	39
1	B	428/491 (87%)	397 (93%)	31 (7%)	13	32
All	All	858/982 (87%)	800 (93%)	58 (7%)	15	35

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	6	ARG
1	B	91	LYS
1	B	98	GLN
1	B	128	SER
1	B	134	LEU
1	B	155	ARG
1	B	175	LYS
1	B	188	ARG
1	B	209	TYR
1	B	213	ARG
1	B	224	GLU
1	B	232	LYS
1	B	236	ARG
1	B	262	VAL
1	B	272	LEU
1	B	304	LEU
1	B	309	VAL
1	B	310	LEU
1	B	315	ASP
1	B	326	ARG
1	B	362[A]	ASP
1	B	362[B]	ASP
1	B	372	LYS
1	B	381	GLN
1	B	392	THR
1	B	415	PHE
1	B	416	GLU
1	B	432	LYS
1	B	443	ILE
1	B	456	VAL
1	B	569	GLU
1	A	4	THR
1	A	60	GLU

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Mol	Chain	Res	Type
1	A	78	ILE
1	A	134	LEU
1	A	146	LEU
1	A	169[A]	MET
1	A	169[B]	MET
1	A	175	LYS
1	A	200	GLU
1	A	201	ARG
1	A	208	GLN
1	A	229	ARG
1	A	231	LEU
1	A	233	LYS
1	A	275	GLU
1	A	280	ILE
1	A	292	LEU
1	A	300	ARG
1	A	361	HIS
1	A	372	LYS
1	A	400	ASP
1	A	402	THR
1	A	416	GLU
1	A	432	LYS
1	A	456	VAL
1	A	474	LEU
1	A	487	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	18	ASN
1	B	19	HIS
1	B	23	HIS
1	B	66	HIS
1	B	70	GLN
1	B	193	HIS
1	B	412	GLN
1	B	421	HIS
1	A	240	HIS
1	A	483	HIS
1	A	546	GLN
1	A	566	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are 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
3	ADP	A	602	4	28,29,29	1.87	5 (17%)	43,45,45	1.80	11 (25%)
3	ADP	B	602	4	28,29,29	1.73	6 (21%)	43,45,45	1.95	8 (18%)

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	602	4	-	0/16/32/32	0/3/3/3
3	ADP	B	602	4	-	0/16/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	ADP	C5-C4	5.38	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	ADP	PA-O3A	5.32	1.65	1.59
3	B	602	ADP	C5-C4	4.96	1.47	1.39
3	B	602	ADP	PA-O3A	4.35	1.64	1.59
3	A	602	ADP	C5-C6	3.19	1.49	1.41
3	B	602	ADP	C5-N7	-3.01	1.33	1.39
3	B	602	ADP	C8-N7	2.97	1.37	1.31
3	A	602	ADP	C8-N7	2.70	1.36	1.31
3	A	602	ADP	C5-N7	-2.59	1.34	1.39
3	B	602	ADP	C5-C6	2.30	1.47	1.41
3	B	602	ADP	C8-N9	-2.11	1.34	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	ADP	C5-C4-N3	-6.62	117.60	126.72
3	B	602	ADP	N3-C4-N9	5.33	136.24	127.17
3	A	602	ADP	C5-C4-N3	-4.98	119.86	126.72
3	B	602	ADP	C2-N3-C4	3.96	121.51	111.83
3	A	602	ADP	N3-C4-N9	3.79	133.60	127.17
3	A	602	ADP	C4-C5-N7	-3.56	106.51	110.58
3	A	602	ADP	C2-N3-C4	3.34	119.98	111.83
3	B	602	ADP	N3-C2-N1	-3.27	123.63	128.58
3	A	602	ADP	N3-C2-N1	-3.24	123.68	128.58
3	B	602	ADP	C4-C5-N7	-3.14	107.00	110.58
3	A	602	ADP	C5'-C4'-C3'	-2.90	104.78	115.21
3	A	602	ADP	C5-N7-C8	2.65	107.61	103.45
3	A	602	ADP	C2-N1-C6	2.60	123.00	118.73
3	B	602	ADP	C4-N9-C8	2.40	108.26	105.74
3	B	602	ADP	C5-N7-C8	2.28	107.03	103.45
3	A	602	ADP	C6-C5-N7	2.25	136.44	132.09
3	A	602	ADP	C4-N9-C8	2.18	108.03	105.74
3	B	602	ADP	O3B-PB-O2B	2.12	115.74	107.80
3	A	602	ADP	O2A-PA-O1A	2.09	122.17	112.44

There are no chirality outliers.

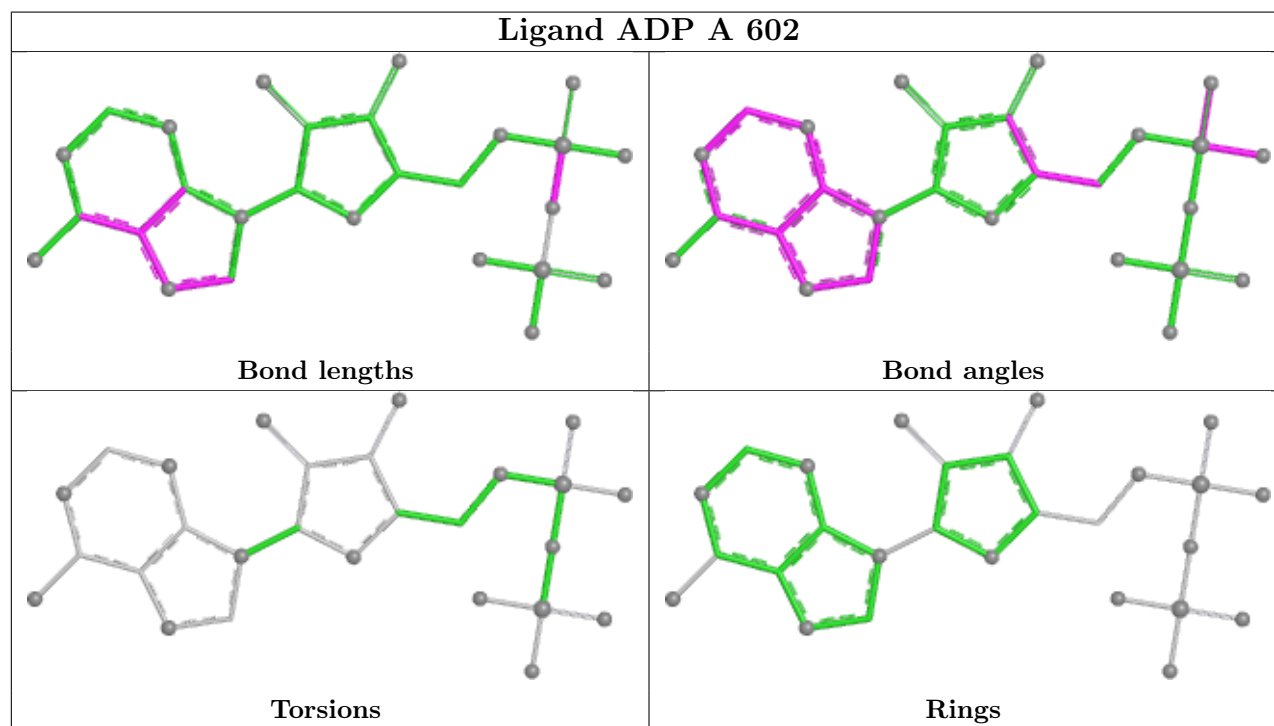
There are no torsion outliers.

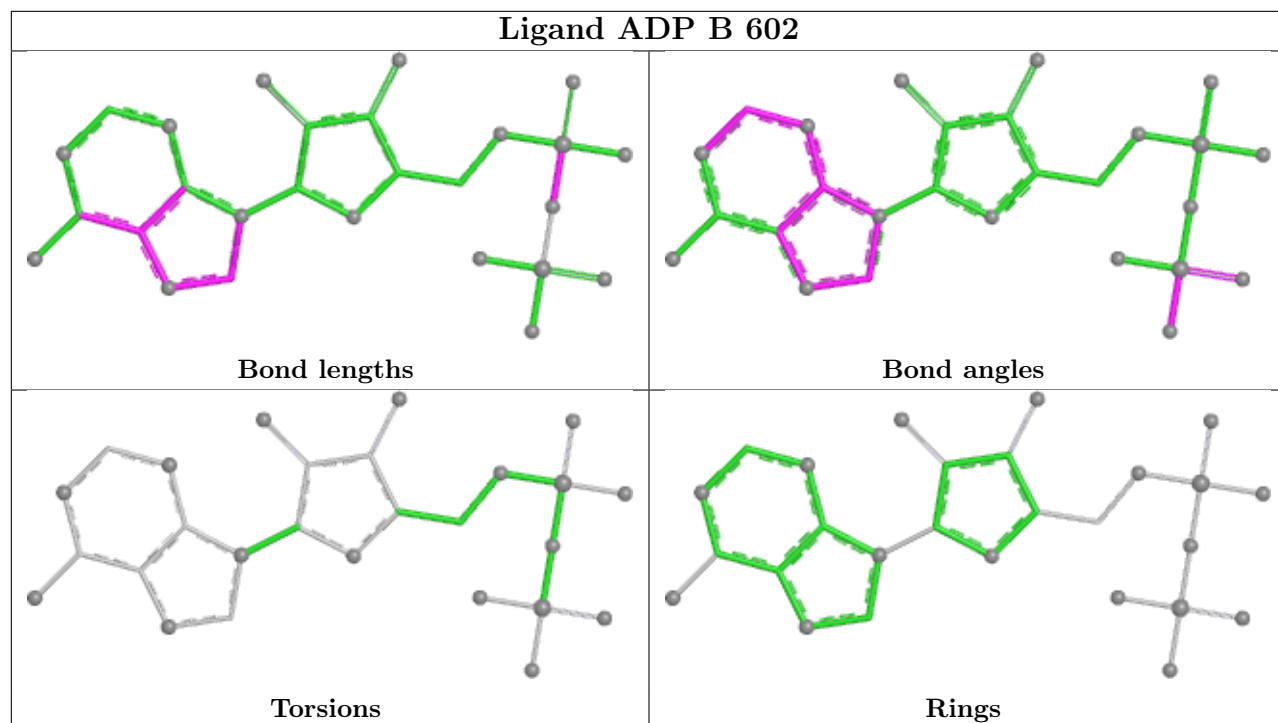
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	ADP	2	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	564/586 (96%)	0.25	27 (4%) 35 32	12, 41, 78, 92	2 (0%)
1	B	568/586 (96%)	0.40	64 (11%) 10 8	14, 41, 88, 113	2 (0%)
All	All	1132/1172 (96%)	0.33	91 (8%) 18 15	12, 41, 85, 113	4 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	233	LYS	5.0
1	B	272	LEU	4.7
1	B	238	THR	4.5
1	B	281	THR	4.2
1	B	231	LEU	4.1
1	A	448	CYS	3.9
1	B	278	ALA	3.8
1	A	274	ALA	3.8
1	A	308	ALA	3.7
1	B	228	ASN	3.7
1	B	257	ILE	3.7
1	A	1	MET	3.7
1	B	259	ALA	3.7
1	A	207	VAL	3.7
1	B	451	CYS	3.5
1	A	447	ARG	3.4
1	B	260	ALA	3.2
1	B	287	ALA	3.2
1	B	214	LEU	3.1
1	A	287	ALA	3.1
1	A	242	ILE	3.1
1	B	298	ALA	3.0
1	B	307	VAL	3.0
1	B	304	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	214	LEU	3.0
1	B	434	CYS	3.0
1	B	235	GLN	3.0
1	B	262	VAL	2.9
1	B	127	GLU	2.9
1	B	207	VAL	2.9
1	B	297	LYS	2.9
1	B	561	LYS	2.9
1	B	234	GLN	2.9
1	A	129	GLN	2.9
1	B	447	ARG	2.9
1	B	226	ASP	2.9
1	B	448	CYS	2.9
1	B	283	ASP	2.8
1	A	564	TYR	2.8
1	B	308	ALA	2.8
1	B	578	PHE	2.8
1	B	237	ILE	2.8
1	B	261	THR	2.8
1	B	205	PRO	2.7
1	B	310	LEU	2.6
1	B	306	ASN	2.6
1	B	282	GLY	2.6
1	B	206	VAL	2.5
1	B	244	GLN	2.5
1	A	433	ASN	2.5
1	A	257	ILE	2.5
1	B	227	LEU	2.5
1	A	272	LEU	2.5
1	A	288	GLU	2.5
1	B	204	MET	2.5
1	B	245	ILE	2.4
1	A	436	GLN	2.4
1	B	81	ALA	2.4
1	A	563	GLN	2.4
1	B	487	GLU	2.4
1	A	125	ASP	2.4
1	B	323	ALA	2.4
1	B	268	ILE	2.4
1	B	271	LEU	2.4
1	A	277	ALA	2.4
1	B	242	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	240	HIS	2.3
1	B	576	GLY	2.3
1	B	225	ALA	2.3
1	B	241	ILE	2.3
1	B	252	ARG	2.3
1	B	215	GLN	2.3
1	B	445	ALA	2.3
1	B	324	ILE	2.2
1	A	259	ALA	2.2
1	A	439	ALA	2.2
1	B	325	LEU	2.2
1	B	443	ILE	2.2
1	A	81	ALA	2.1
1	B	280	ILE	2.1
1	A	237	ILE	2.1
1	B	302	ARG	2.1
1	A	275	GLU	2.1
1	A	446	ARG	2.1
1	A	285	PRO	2.1
1	B	210	ASP	2.1
1	B	80	ALA	2.0
1	B	243	SER	2.0
1	B	254	GLY	2.0
1	A	238	THR	2.0
1	B	82	GLY	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 ⓘ

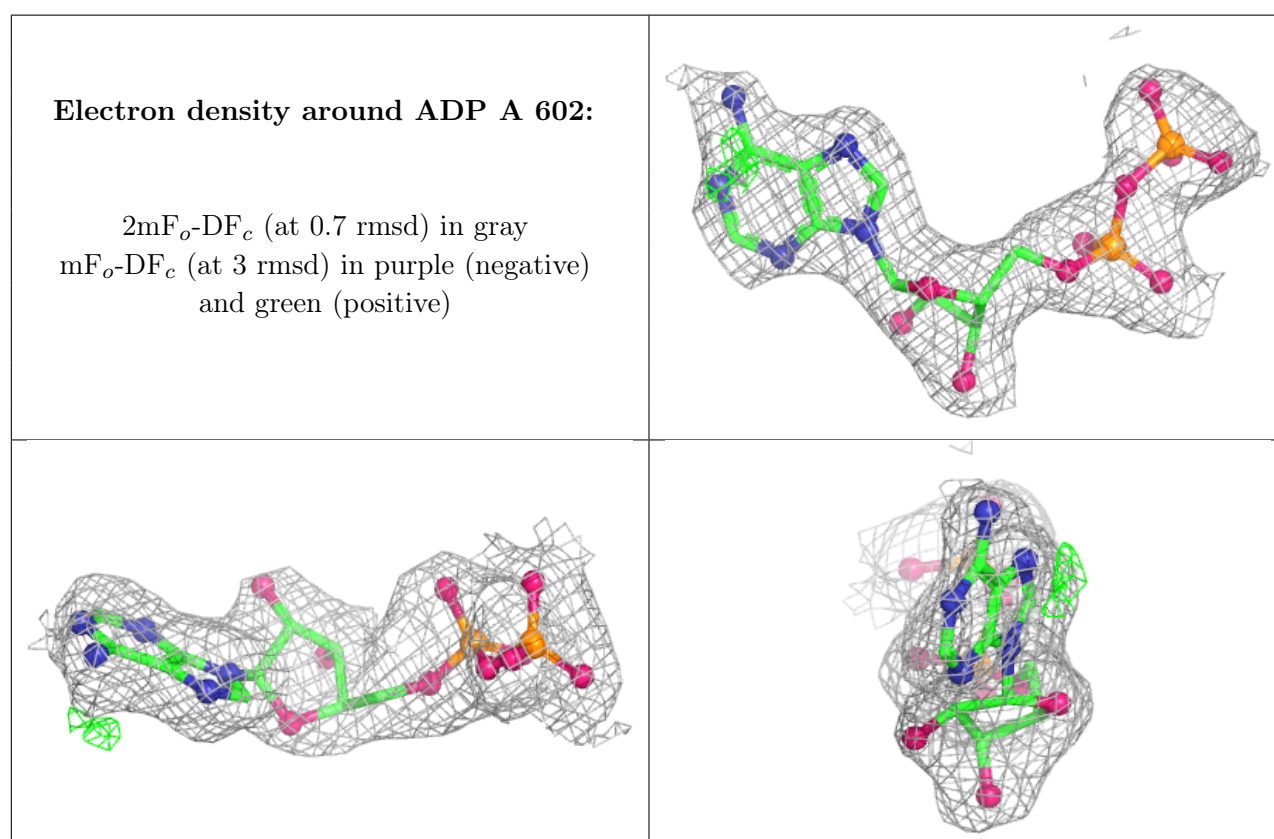
There are no oligosaccharides in this entry.

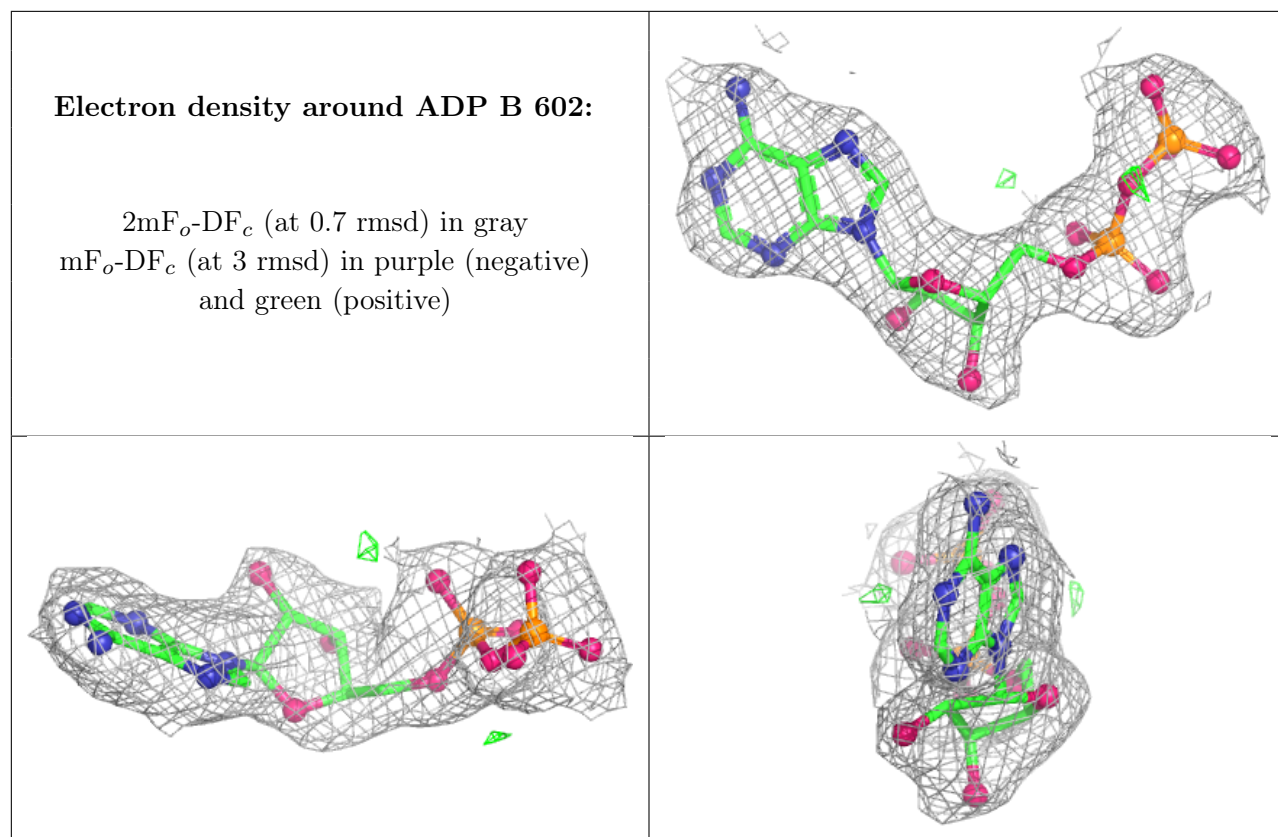
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	B	603	1/1	0.97	0.24	29,29,29,29	0
3	ADP	A	602	27/27	0.98	0.07	19,28,35,37	0
3	ADP	B	602	27/27	0.98	0.06	23,34,39,40	0
4	MG	A	603	1/1	0.98	0.05	17,17,17,17	0
2	ZN	B	601	1/1	0.99	0.04	30,30,30,30	0
2	ZN	A	601	1/1	1.00	0.05	33,33,33,33	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.