



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:17 AM UTC

PDB ID : 3AUY / pdb_00003auy
Title : Crystal structure of Rad50 bound to ADP
Authors : Lim, H.S.; Cho, Y.
Deposited on : 2011-02-18
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

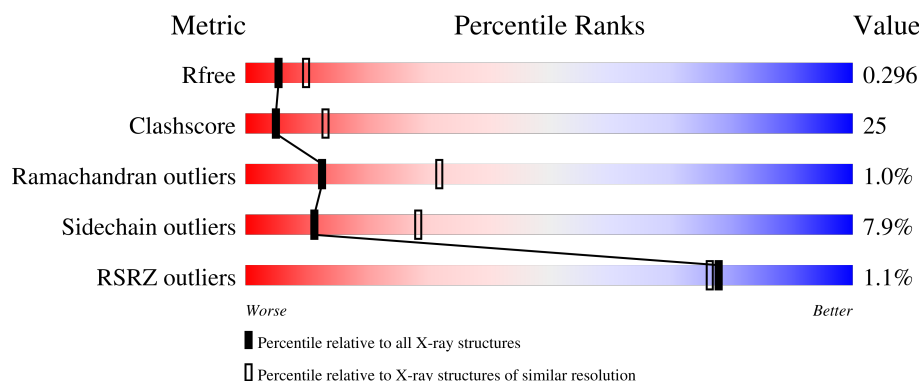
1 Overall quality at a glance

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	371	58% 35% 6%
1	B	371	45% 43% 8%

2 Entry composition [i](#)

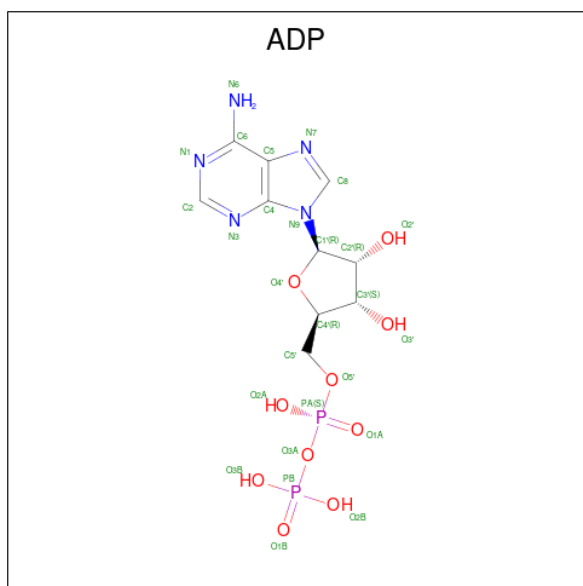
There are 4 unique types of molecules in this entry. The entry contains 5932 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA double-strand break repair rad50 ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2938	1883	502	544	9			
1	B	357	Total	C	N	O	S	0	0	0
			2869	1842	487	532	8			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total 39	O 39	0	0
4	B	30	Total 30	O 30	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.16Å 95.30Å 110.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.40 – 2.70 19.40 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.40-2.70) 98.6 (19.40-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.62Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.296 0.228 , 0.296	Depositor DCC
R_{free} test set	2287 reflections (9.12%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5932	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: 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	0.55	0/2980	0.98	12/3991 (0.3%)
1	B	0.49	0/2912	0.98	10/3903 (0.3%)
All	All	0.52	0/5892	0.98	22/7894 (0.3%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	838	GLU	N-CA-C	-12.96	97.44	113.38
1	A	950	VAL	N-CA-C	7.00	123.91	109.34
1	A	910	LEU	N-CA-C	6.95	118.96	110.41
1	B	118	ILE	N-CA-C	6.47	116.61	110.53
1	A	133	LYS	N-CA-C	6.45	119.04	110.53
1	A	118	ILE	N-CA-C	6.21	116.36	110.53
1	B	840	GLU	N-CA-C	-6.15	104.58	111.28
1	B	987	ASP	N-CA-C	-6.14	103.91	111.40
1	B	947	GLU	CA-C-N	6.00	126.78	120.12
1	B	947	GLU	C-N-CA	6.00	126.78	120.12
1	A	987	ASP	N-CA-C	-5.80	104.38	112.45
1	B	1001	VAL	N-CA-C	5.78	116.18	107.75
1	B	43	GLU	N-CA-C	-5.71	105.06	111.28
1	A	43	GLU	N-CA-C	-5.66	105.11	111.28
1	A	152	VAL	N-CA-C	-5.53	105.33	110.53
1	A	986	ALA	N-CA-C	5.50	119.02	110.17
1	A	838	GLU	N-CA-C	-5.25	105.64	111.36
1	A	165	TYR	N-CA-C	-5.20	105.61	111.28
1	A	162	GLU	N-CA-C	-5.20	105.52	111.14
1	B	970	ILE	CA-C-N	5.13	125.42	119.47
1	B	970	ILE	C-N-CA	5.13	125.42	119.47
1	A	859	GLY	N-CA-C	5.05	120.24	112.51

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	2938	0	3031	121	0
1	B	2869	0	2948	184	0
2	A	27	0	12	0	0
2	B	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	39	0	0	1	0
4	B	30	0	0	2	0
All	All	5932	0	6003	297	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 25.

All (297) 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:949:THR:HG22	1:A:960:LEU:HD23	1.49	0.92
1:B:1:MET:HE2	1:B:1:MET:HA	1.55	0.89
1:B:977:THR:HG23	1:B:979:HIS:H	1.39	0.87
1:A:1:MET:HA	1:A:1:MET:HE2	1.55	0.85
1:B:72:GLU:OE1	1:B:83:LYS:HE3	1.78	0.84
1:A:989:ILE:HD12	1:A:1005:GLY:HA3	1.61	0.83
1:B:1003:ILE:C	1:B:1004:ASN:HD22	1.85	0.83
1:B:980:ARG:O	1:B:983:GLU:HG2	1.79	0.82
1:A:72:GLU:OE1	1:A:83:LYS:HE3	1.79	0.82
1:A:144:LYS:HE2	1:A:144:LYS:HA	1.62	0.82
1:B:147:GLU:O	1:B:151:THR:HG22	1.81	0.80
1:A:57:ASN:HD21	1:A:59:ASP:HB2	1.46	0.80
1:A:181:ARG:O	1:A:185:GLU:HG3	1.82	0.79
1:A:107:THR:HG23	1:A:110:ALA:H	1.50	0.77
1:B:107:THR:HG23	1:B:110:ALA:H	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:858:PHE:HA	1:B:862:GLY:HA3	1.67	0.75
1:B:903:VAL:HG21	1:B:915:LEU:HD11	1.68	0.75
1:B:894:GLU:HB3	1:B:902:ARG:HB2	1.69	0.74
1:A:854:VAL:HG11	1:B:854:VAL:HG21	1.68	0.73
1:B:938:ASN:C	1:B:938:ASN:HD22	1.96	0.72
1:A:57:ASN:ND2	1:A:59:ASP:HB2	2.04	0.72
1:B:917:GLY:HA2	1:B:920:GLN:HG3	1.73	0.71
1:B:123:ARG:HD2	4:B:1024:HOH:O	1.91	0.71
1:B:143:LEU:HB3	1:B:147:GLU:HB2	1.74	0.69
1:B:994:LYS:HE2	1:B:997:ASN:HA	1.73	0.69
1:B:143:LEU:HD12	1:B:147:GLU:HG3	1.72	0.69
1:B:983:GLU:HB2	1:B:989:ILE:HD13	1.73	0.69
1:B:144:LYS:HB3	1:B:145:PRO:HD2	1.75	0.67
1:A:1:MET:HA	1:A:1:MET:CE	2.25	0.67
1:A:4:ILE:HG23	1:A:76:GLU:HB3	1.77	0.67
1:B:902:ARG:NH1	1:B:909:VAL:HG11	2.10	0.67
1:B:902:ARG:HH11	1:B:909:VAL:HG11	1.58	0.67
1:A:921:ILE:HD11	1:A:956:ARG:HB3	1.77	0.66
1:A:872:VAL:HB	1:A:873:PRO:HD3	1.77	0.66
1:A:953:ASP:OD2	1:A:956:ARG:HG3	1.96	0.66
1:A:143:LEU:HB3	1:A:147:GLU:HB2	1.78	0.66
1:B:983:GLU:HB2	1:B:989:ILE:CD1	2.27	0.65
1:B:896:THR:C	1:B:898:ASP:H	2.03	0.65
1:A:918:GLY:HA2	1:A:959:LYS:HD3	1.78	0.65
1:A:157:GLY:O	1:A:160:GLU:HB2	1.97	0.65
1:A:947:GLU:HB3	1:A:950:VAL:CG2	2.27	0.64
1:A:850:TYR:CZ	1:B:853:LYS:HD3	2.32	0.64
1:A:905:ALA:HB1	1:A:906:PRO:HD2	1.79	0.64
1:B:4:ILE:HG23	1:B:76:GLU:HB3	1.80	0.63
1:B:169:GLY:O	1:B:172:VAL:HG22	1.98	0.63
1:A:56:PHE:C	1:A:56:PHE:CD2	2.76	0.63
1:A:57:ASN:HD21	1:A:59:ASP:CB	2.11	0.62
1:B:885:GLU:OE1	1:B:968:LYS:N	2.32	0.62
1:B:167:LYS:O	1:B:170:GLU:HG2	1.99	0.62
1:A:947:GLU:O	1:A:950:VAL:HG23	1.99	0.62
1:B:1:MET:HA	1:B:1:MET:CE	2.27	0.62
1:B:858:PHE:CA	1:B:862:GLY:HA3	2.29	0.62
1:B:921:ILE:HD11	1:B:956:ARG:HD3	1.80	0.62
1:A:994:LYS:HE3	1:A:997:ASN:HA	1.82	0.62
1:B:950:VAL:O	1:B:951:TYR:HB2	2.01	0.61
1:A:835:SER:O	1:A:839:LYS:HG2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:GLU:HB3	1:A:950:VAL:HG23	1.83	0.60
1:B:838:GLU:O	1:B:841:LYS:HB3	2.01	0.60
1:A:853:LYS:HD3	1:B:850:TYR:CE1	2.37	0.60
1:B:864:GLN:O	1:B:868:ARG:HG3	2.00	0.60
1:B:868:ARG:HD3	1:B:897:LYS:HG2	1.83	0.60
1:A:849:GLU:OE2	1:A:853:LYS:NZ	2.34	0.60
1:B:36:SER:HA	1:B:994:LYS:HB2	1.83	0.60
1:B:868:ARG:HD3	1:B:897:LYS:O	2.03	0.59
1:A:139:LYS:HE2	1:B:88:TYR:OH	2.03	0.59
1:B:143:LEU:HD12	1:B:147:GLU:CG	2.32	0.59
1:A:165:TYR:O	1:A:855:ARG:NH1	2.36	0.59
1:B:163:LYS:O	1:B:167:LYS:HG2	2.03	0.58
1:B:149:LEU:HD23	1:B:898:ASP:HB3	1.84	0.58
1:B:851:LEU:O	1:B:855:ARG:HB2	2.03	0.58
1:B:994:LYS:CE	1:B:997:ASN:HA	2.33	0.58
1:A:168:MET:O	1:A:172:VAL:HG23	2.03	0.58
1:B:177:LYS:O	1:B:180:GLU:HB2	2.03	0.58
1:B:883:PHE:CZ	1:B:923:VAL:HG22	2.38	0.58
1:B:4:ILE:HD13	1:B:4:ILE:C	2.29	0.58
1:A:137:ILE:HD11	1:A:921:ILE:HG23	1.86	0.58
1:A:1:MET:HE3	1:A:938:ASN:HD21	1.69	0.57
1:B:172:VAL:O	1:B:176:GLU:HG3	2.04	0.57
1:A:892:PHE:CZ	1:A:894:GLU:HG3	2.40	0.57
1:B:2:SER:HB2	1:B:936:ILE:HD12	1.86	0.57
1:A:36:SER:HA	1:A:994:LYS:HB2	1.85	0.57
1:A:106:THR:O	1:A:106:THR:HG22	2.04	0.57
1:B:998:VAL:HG12	1:B:1000:LYS:HE3	1.85	0.57
1:A:138:ALA:HB2	1:A:952:LEU:CD1	2.34	0.57
1:B:916:SER:HB3	1:B:919:GLU:OE1	2.05	0.56
1:B:931:ILE:O	1:B:935:LEU:HD23	2.05	0.56
1:B:896:THR:C	1:B:898:ASP:N	2.62	0.56
1:B:871:TYR:O	1:B:875:ILE:HG13	2.06	0.56
1:A:130:ILE:HG13	1:A:942:CYS:O	2.06	0.55
1:B:836:ASN:O	1:B:838:GLU:N	2.33	0.55
1:A:172:VAL:O	1:A:176:GLU:HG3	2.06	0.55
1:B:143:LEU:O	1:B:148:LYS:HE3	2.06	0.55
1:A:4:ILE:HD13	1:A:4:ILE:C	2.31	0.55
1:A:955:ASN:ND2	1:A:959:LYS:HE2	2.21	0.55
1:A:875:ILE:HG21	1:A:895:LEU:HD22	1.89	0.55
1:A:930:ALA:HA	1:A:933:ASN:HD22	1.72	0.55
1:B:106:THR:HG22	1:B:106:THR:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:ARG:HG3	1:A:985:VAL:HG22	1.90	0.54
1:B:56:PHE:HZ	1:B:61:ILE:HG23	1.73	0.54
1:B:837:LEU:O	1:B:837:LEU:HD13	2.08	0.54
1:B:57:ASN:HD21	1:B:59:ASP:CB	2.20	0.54
1:A:848:VAL:HG13	1:A:849:GLU:N	2.23	0.54
1:B:875:ILE:O	1:B:879:LEU:HB2	2.08	0.53
1:B:894:GLU:HB2	1:B:904:HIS:HE1	1.73	0.53
1:B:57:ASN:HD21	1:B:59:ASP:HB3	1.74	0.53
1:B:182:ILE:HG21	1:B:841:LYS:HB2	1.91	0.53
1:B:943:ILE:HG23	1:B:943:ILE:O	2.09	0.53
1:B:139:LYS:O	1:B:143:LEU:HD23	2.08	0.53
1:B:141:LEU:HD11	1:B:921:ILE:HG12	1.91	0.53
1:A:854:VAL:CG1	1:B:854:VAL:HG21	2.37	0.53
1:B:12:ASN:CG	1:B:66:LYS:HG2	2.34	0.53
1:B:868:ARG:HG2	1:B:868:ARG:HH11	1.75	0.52
1:B:960:LEU:HG	1:B:964:PHE:CE2	2.44	0.52
1:A:10:MET:HE2	1:A:16:HIS:HB2	1.90	0.52
1:B:31:ILE:CD1	1:B:983:GLU:HB3	2.39	0.52
1:A:21:ILE:N	1:A:21:ILE:HD12	2.25	0.52
1:A:898:ASP:O	1:A:899:PHE:HB2	2.09	0.52
1:B:886:PHE:HB2	1:B:888:LEU:HD23	1.91	0.52
1:B:896:THR:OG1	1:B:900:GLU:HB3	2.09	0.52
1:B:925:LEU:O	1:B:929:LEU:HG	2.09	0.52
1:B:857:ILE:O	1:B:857:ILE:HG22	2.09	0.52
1:A:94:GLY:N	1:A:108:ILE:HD11	2.25	0.52
1:A:845:THR:O	1:A:848:VAL:HG12	2.10	0.52
1:B:902:ARG:HH11	1:B:902:ARG:HB3	1.75	0.52
1:B:957:ARG:HD3	1:B:979:HIS:ND1	2.25	0.52
1:B:176:GLU:O	1:B:180:GLU:HG2	2.11	0.51
1:A:2:SER:HB2	1:A:936:ILE:CD1	2.41	0.51
1:B:991:ASN:HB3	1:B:993:LYS:HE2	1.92	0.51
1:A:12:ASN:CG	1:A:66:LYS:HG2	2.36	0.51
1:A:941:GLU:O	1:A:971:PRO:HG2	2.10	0.51
1:A:883:PHE:CD1	1:A:893:VAL:HG21	2.45	0.51
1:B:21:ILE:N	1:B:21:ILE:HD12	2.25	0.51
1:A:4:ILE:CG2	1:A:76:GLU:HB3	2.40	0.51
1:B:896:THR:O	1:B:898:ASP:N	2.44	0.51
1:A:875:ILE:CG2	1:A:895:LEU:HD22	2.41	0.50
1:A:912:ILE:HA	1:A:915:LEU:HD22	1.93	0.50
1:B:167:LYS:HA	1:B:170:GLU:HG2	1.91	0.50
1:B:846:LYS:O	1:B:849:GLU:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ASN:OD1	1:B:59:ASP:HB2	2.10	0.50
1:B:133:LYS:O	1:B:136:GLU:HG3	2.11	0.50
1:B:148:LYS:HA	1:B:151:THR:CG2	2.42	0.49
1:B:145:PRO:O	1:B:149:LEU:HD13	2.12	0.49
1:B:837:LEU:HD22	1:B:840:GLU:H	1.77	0.49
1:B:921:ILE:HD11	1:B:956:ARG:HB3	1.93	0.49
1:A:847:PHE:CE1	1:B:857:ILE:HD13	2.47	0.49
1:A:144:LYS:HA	1:A:144:LYS:CE	2.38	0.49
1:B:168:MET:O	1:B:172:VAL:HG13	2.13	0.49
1:A:994:LYS:HE3	1:A:997:ASN:HD22	1.78	0.49
1:B:857:ILE:O	1:B:857:ILE:CG2	2.61	0.48
1:B:938:ASN:C	1:B:938:ASN:ND2	2.69	0.48
1:A:135:GLY:O	1:A:139:LYS:HG3	2.13	0.48
1:B:86:ARG:HD2	4:B:1013:HOH:O	2.13	0.48
1:A:918:GLY:CA	1:A:959:LYS:HD3	2.42	0.48
1:A:48:ALA:HB2	1:A:71:VAL:CG1	2.43	0.48
1:A:846:LYS:HE2	1:A:850:TYR:CE1	2.48	0.48
1:A:845:THR:C	1:A:848:VAL:HG12	2.39	0.48
1:A:905:ALA:HB1	1:A:906:PRO:CD	2.44	0.48
1:A:97:LEU:HB3	1:A:105:ALA:HB3	1.96	0.47
1:B:156:LEU:HB3	1:B:867:LEU:HD22	1.95	0.47
1:B:858:PHE:C	1:B:862:GLY:HA3	2.39	0.47
1:A:949:THR:HB	1:A:957:ARG:HG3	1.95	0.47
1:B:10:MET:HE2	1:B:16:HIS:HB2	1.96	0.47
1:B:890:TYR:OH	1:B:915:LEU:HD22	2.14	0.47
1:B:48:ALA:HB2	1:B:71:VAL:CG1	2.45	0.47
1:A:898:ASP:OD2	1:A:898:ASP:N	2.45	0.47
1:B:988:VAL:HG12	1:B:989:ILE:N	2.29	0.47
4:A:1049:HOH:O	1:B:108:ILE:HB	2.15	0.47
1:B:883:PHE:CD2	1:B:893:VAL:HG21	2.50	0.47
1:B:921:ILE:CG2	1:B:960:LEU:HD13	2.44	0.47
1:A:2:SER:HB2	1:A:936:ILE:HD12	1.96	0.47
1:A:874:LEU:N	1:A:874:LEU:HD23	2.30	0.47
1:B:868:ARG:NH1	1:B:899:PHE:CE1	2.83	0.47
1:A:182:ILE:HD11	1:A:840:GLU:OE1	2.15	0.46
1:B:37:GLY:HA2	2:B:1006:ADP:O1A	2.15	0.46
1:B:179:LEU:HD21	1:B:844:LEU:HB2	1.98	0.46
1:B:178:ARG:C	1:B:180:GLU:N	2.69	0.46
1:B:868:ARG:O	1:B:872:VAL:HB	2.15	0.46
1:B:879:LEU:HD13	1:B:927:LEU:HA	1.98	0.46
1:B:1003:ILE:O	1:B:1004:ASN:ND2	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ILE:HB	1:A:97:LEU:HD13	1.97	0.46
1:A:950:VAL:HG12	1:A:951:TYR:CD1	2.51	0.46
1:B:20:ARG:HG2	1:B:20:ARG:HH21	1.80	0.46
1:B:137:ILE:HG23	1:B:138:ALA:H	1.81	0.46
1:A:1003:ILE:HD12	1:A:1003:ILE:O	2.16	0.46
1:A:910:LEU:H	1:A:910:LEU:HG	1.55	0.45
1:B:97:LEU:HB3	1:B:105:ALA:HB3	1.96	0.45
1:A:997:ASN:HA	1:A:997:ASN:HD22	1.62	0.45
1:B:84:ILE:HB	1:B:97:LEU:HD13	1.98	0.45
1:B:4:ILE:CG2	1:B:76:GLU:HB3	2.45	0.45
1:B:136:GLU:OE2	1:B:928:ARG:NE	2.40	0.45
1:A:933:ASN:OD1	1:A:940:VAL:HG12	2.17	0.45
1:A:152:VAL:HG22	1:A:931:ILE:HD11	1.98	0.45
1:A:863:PHE:CD1	1:B:171:ILE:HG23	2.52	0.45
1:B:58:TYR:O	1:B:62:ILE:HG13	2.17	0.45
1:B:147:GLU:O	1:B:150:GLU:HB3	2.16	0.45
1:B:903:VAL:O	1:B:910:LEU:N	2.39	0.45
1:B:20:ARG:HG2	1:B:20:ARG:NH2	2.32	0.45
1:B:1004:ASN:HB3	1:B:1005:GLY:H	1.30	0.45
1:A:57:ASN:ND2	1:A:59:ASP:CB	2.75	0.45
1:B:21:ILE:HG13	1:B:1001:VAL:HG11	1.99	0.45
1:B:133:LYS:HB2	1:B:133:LYS:NZ	2.32	0.45
1:B:858:PHE:HA	1:B:862:GLY:CA	2.44	0.45
1:A:872:VAL:HG21	1:A:897:LYS:HA	1.98	0.44
1:A:871:TYR:O	1:A:872:VAL:C	2.58	0.44
1:B:876:GLN:O	1:B:877:LYS:C	2.61	0.44
1:A:20:ARG:HH21	1:A:20:ARG:HG2	1.83	0.44
1:A:58:TYR:O	1:A:62:ILE:HG13	2.17	0.44
1:B:962:GLU:OE2	1:B:962:GLU:HA	2.16	0.44
1:A:1:MET:SD	1:A:78:ASN:OD1	2.75	0.44
1:B:1:MET:SD	1:B:78:ASN:OD1	2.76	0.44
1:B:164:CYS:O	1:B:168:MET:HG3	2.16	0.44
1:B:894:GLU:HB2	1:B:904:HIS:CE1	2.53	0.44
1:B:957:ARG:HH21	1:B:957:ARG:HG3	1.82	0.44
1:B:153:ALA:HA	1:B:156:LEU:HD23	1.98	0.44
1:B:858:PHE:O	1:B:859:GLY:O	2.35	0.44
1:B:905:ALA:O	1:B:906:PRO:C	2.61	0.44
1:A:48:ALA:HB2	1:A:71:VAL:HG12	1.99	0.44
1:B:70:TYR:CD1	1:B:70:TYR:C	2.95	0.44
1:B:883:PHE:CE2	1:B:893:VAL:HG21	2.53	0.44
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:VAL:HG11	1:B:899:PHE:HB3	1.99	0.43
1:B:977:THR:HG21	1:B:982:LEU:HD22	2.00	0.43
1:B:188:TYR:CD1	1:B:188:TYR:C	2.96	0.43
1:A:848:VAL:CG1	1:A:849:GLU:N	2.81	0.43
1:B:148:LYS:O	1:B:152:VAL:HG23	2.18	0.43
1:B:175:TYR:CD1	1:B:844:LEU:HD22	2.54	0.43
1:A:88:TYR:OH	1:A:91:GLY:HA2	2.18	0.43
1:A:152:VAL:O	1:A:156:LEU:HD22	2.19	0.43
1:A:896:THR:OG1	1:A:898:ASP:OD2	2.26	0.43
1:B:48:ALA:HB2	1:B:71:VAL:HG12	2.00	0.43
1:B:94:GLY:N	1:B:108:ILE:HD11	2.34	0.43
1:B:127:LEU:HD12	1:B:127:LEU:HA	1.91	0.43
1:B:180:GLU:OE2	1:B:180:GLU:HA	2.18	0.43
1:A:134:GLN:HG3	1:A:950:VAL:HG21	2.01	0.43
1:A:841:LYS:O	1:A:845:THR:HG23	2.18	0.43
1:A:910:LEU:HB3	1:A:914:ASN:HB2	1.99	0.43
1:A:955:ASN:HD21	1:A:959:LYS:HE2	1.83	0.43
1:B:861:ASN:HA	1:B:864:GLN:HG3	2.00	0.43
1:B:953:ASP:O	1:B:954:GLU:C	2.62	0.43
1:A:970:ILE:HA	1:A:971:PRO:HD2	1.81	0.43
1:B:143:LEU:CD1	1:B:147:GLU:HG3	2.46	0.42
1:B:147:GLU:C	1:B:151:THR:HG22	2.44	0.42
1:B:98:TYR:CD1	1:B:103:PRO:HA	2.54	0.42
1:B:114:ALA:O	1:B:118:ILE:HG13	2.20	0.42
1:A:98:TYR:CD1	1:A:103:PRO:HA	2.55	0.42
1:A:977:THR:HG21	1:A:982:LEU:HD12	2.02	0.42
1:B:921:ILE:HD11	1:B:956:ARG:CG	2.49	0.42
1:B:943:ILE:HG22	1:B:970:ILE:HG21	2.01	0.42
1:A:107:THR:O	1:A:108:ILE:C	2.62	0.42
1:B:131:TYR:CE2	1:B:133:LYS:HG2	2.55	0.42
1:B:139:LYS:HA	1:B:143:LEU:HD23	2.00	0.42
1:B:902:ARG:HD2	1:B:909:VAL:HG11	2.01	0.42
1:A:850:TYR:O	1:A:851:LEU:C	2.63	0.42
1:B:980:ARG:O	1:B:981:GLU:C	2.61	0.42
1:A:861:ASN:HA	1:A:865:ALA:HB2	2.02	0.42
1:B:166:GLN:O	1:B:167:LYS:C	2.61	0.42
1:B:873:PRO:HG2	1:B:874:LEU:H	1.84	0.42
1:B:943:ILE:O	1:B:943:ILE:CG2	2.67	0.42
1:B:175:TYR:HD1	1:B:175:TYR:HA	1.77	0.42
1:B:42:PHE:CE2	1:B:976:ILE:HD11	2.55	0.41
1:B:921:ILE:HD11	1:B:956:ARG:CD	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:945:LEU:N	1:B:945:LEU:CD2	2.82	0.41
1:B:947:GLU:HG2	1:B:977:THR:HA	2.02	0.41
1:A:827:LEU:O	1:A:831:LEU:HG	2.20	0.41
1:A:835:SER:O	1:A:838:GLU:HB2	2.21	0.41
1:A:858:PHE:HZ	1:B:168:MET:HG3	1.86	0.41
1:A:916:SER:O	1:A:917:GLY:C	2.64	0.41
1:A:994:LYS:CE	1:A:997:ASN:HD22	2.31	0.41
1:A:953:ASP:OD2	1:A:956:ARG:CG	2.66	0.41
1:B:1:MET:HG3	1:B:78:ASN:HD21	1.85	0.41
1:B:178:ARG:O	1:B:179:LEU:C	2.61	0.41
1:A:70:TYR:CD1	1:A:70:TYR:C	2.99	0.41
1:B:156:LEU:HD12	1:B:871:TYR:CD2	2.56	0.41
1:A:186:LEU:HG	1:A:838:GLU:OE2	2.20	0.41
1:B:141:LEU:HD22	1:B:920:GLN:HB3	2.02	0.41
1:A:20:ARG:HG2	1:A:20:ARG:NH2	2.35	0.41
1:B:957:ARG:HD3	1:B:979:HIS:CE1	2.55	0.41
1:B:836:ASN:OD1	1:B:837:LEU:N	2.53	0.41
1:B:969:SER:O	1:B:971:PRO:HD3	2.20	0.41
1:A:21:ILE:CG2	1:A:990:ILE:HD13	2.51	0.41
1:A:9:ARG:CZ	1:A:9:ARG:HB3	2.51	0.41
1:A:114:ALA:O	1:A:118:ILE:HG13	2.21	0.41
1:A:946:ASP:O	1:A:947:GLU:C	2.64	0.41
1:B:9:ARG:HB3	1:B:9:ARG:CZ	2.50	0.41
1:B:98:TYR:HD1	1:B:103:PRO:HA	1.86	0.41
1:B:111:VAL:O	1:B:115:VAL:HG23	2.20	0.41
1:B:88:TYR:OH	1:B:91:GLY:HA2	2.20	0.41
1:A:127:LEU:HD12	1:A:127:LEU:HA	1.93	0.40
1:A:883:PHE:CE1	1:A:893:VAL:HG21	2.56	0.40
1:B:977:THR:HG21	1:B:982:LEU:CD2	2.51	0.40
1:A:111:VAL:O	1:A:115:VAL:HG23	2.21	0.40
1:B:132:ILE:HD12	1:B:945:LEU:CD1	2.51	0.40
1:B:861:ASN:HA	1:B:864:GLN:CG	2.50	0.40
1:B:998:VAL:HG12	1:B:998:VAL:O	2.21	0.40
1:A:177:LYS:O	1:A:181:ARG:HG2	2.21	0.40
1:B:175:TYR:CE1	1:B:844:LEU:HD22	2.56	0.40
1:B:107:THR:HG23	1:B:110:ALA:N	2.28	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	360/371 (97%)	328 (91%)	30 (8%)	2 (1%)	21	44
1	B	351/371 (95%)	309 (88%)	37 (10%)	5 (1%)	9	23
All	All	711/742 (96%)	637 (90%)	67 (9%)	7 (1%)	12	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	837	LEU
1	B	859	GLY
1	B	897	LYS
1	A	953	ASP
1	B	148	LYS
1	B	52	ALA
1	A	889	PRO

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	319/324 (98%)	296 (93%)	23 (7%)	13	32
1	B	311/324 (96%)	284 (91%)	27 (9%)	9	24
All	All	630/648 (97%)	580 (92%)	50 (8%)	11	28

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	ILE
1	A	5	LEU
1	A	11	ASN
1	A	56	PHE
1	A	59	ASP
1	A	137	ILE
1	A	156	LEU
1	A	167	LYS
1	A	186	LEU
1	A	861	ASN
1	A	874	LEU
1	A	893	VAL
1	A	898	ASP
1	A	906	PRO
1	A	910	LEU
1	A	915	LEU
1	A	935	LEU
1	A	940	VAL
1	A	945	LEU
1	A	981	GLU
1	A	985	VAL
1	A	997	ASN
1	B	1	MET
1	B	4	ILE
1	B	5	LEU
1	B	11	ASN
1	B	59	ASP
1	B	83	LYS
1	B	133	LYS
1	B	137	ILE
1	B	140	PHE
1	B	178	ARG
1	B	188	TYR
1	B	836	ASN
1	B	837	LEU
1	B	843	LYS
1	B	898	ASP
1	B	902	ARG
1	B	906	PRO
1	B	907	ASN
1	B	935	LEU
1	B	938	ASN

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Mol	Chain	Res	Type
1	B	945	LEU
1	B	957	ARG
1	B	977	THR
1	B	980	ARG
1	B	981	GLU
1	B	982	LEU
1	B	985	VAL

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	57	ASN
1	A	78	ASN
1	A	134	GLN
1	A	187	ASN
1	A	861	ASN
1	A	938	ASN
1	A	955	ASN
1	A	978	HIS
1	A	979	HIS
1	A	997	ASN
1	B	57	ASN
1	B	78	ASN
1	B	116	ASN
1	B	904	HIS
1	B	914	ASN
1	B	955	ASN
1	B	997	ASN
1	B	1004	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 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	$\# Z > 2$
2	ADP	A	1006	3	28,29,29	1.76	4 (14%)	43,45,45	1.55	4 (9%)
2	ADP	B	1006	3	28,29,29	1.77	6 (21%)	43,45,45	1.68	4 (9%)

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
2	ADP	A	1006	3	-	1/16/32/32	0/3/3/3
2	ADP	B	1006	3	-	2/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1006	ADP	C4-N3	4.78	1.43	1.34
2	A	1006	ADP	PA-O3A	4.18	1.64	1.59
2	B	1006	ADP	C4-N3	4.12	1.42	1.34
2	B	1006	ADP	PA-O3A	3.22	1.63	1.59
2	B	1006	ADP	C3'-C4'	-3.02	1.45	1.53
2	B	1006	ADP	C2-N3	2.96	1.39	1.33
2	A	1006	ADP	C2-N3	2.75	1.38	1.33
2	B	1006	ADP	O5'-C5'	-2.60	1.34	1.44
2	B	1006	ADP	PB-O3B	2.36	1.63	1.54
2	A	1006	ADP	PB-O3B	2.29	1.63	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1006	ADP	O3'-C3'-C4'	-7.69	88.99	111.08
2	A	1006	ADP	O3'-C3'-C4'	-6.36	92.81	111.08
2	A	1006	ADP	C3'-C2'-C1'	4.12	109.25	101.46
2	B	1006	ADP	C3'-C2'-C1'	3.51	108.10	101.46
2	B	1006	ADP	O4'-C4'-C3'	2.73	110.56	105.15
2	A	1006	ADP	O3A-PA-O1A	-2.34	103.66	110.70
2	B	1006	ADP	C5'-C4'-C3'	-2.08	107.71	115.21
2	A	1006	ADP	O2A-PA-O3A	2.01	112.69	107.27

There are no chirality outliers.

All (3) torsion outliers are listed below:

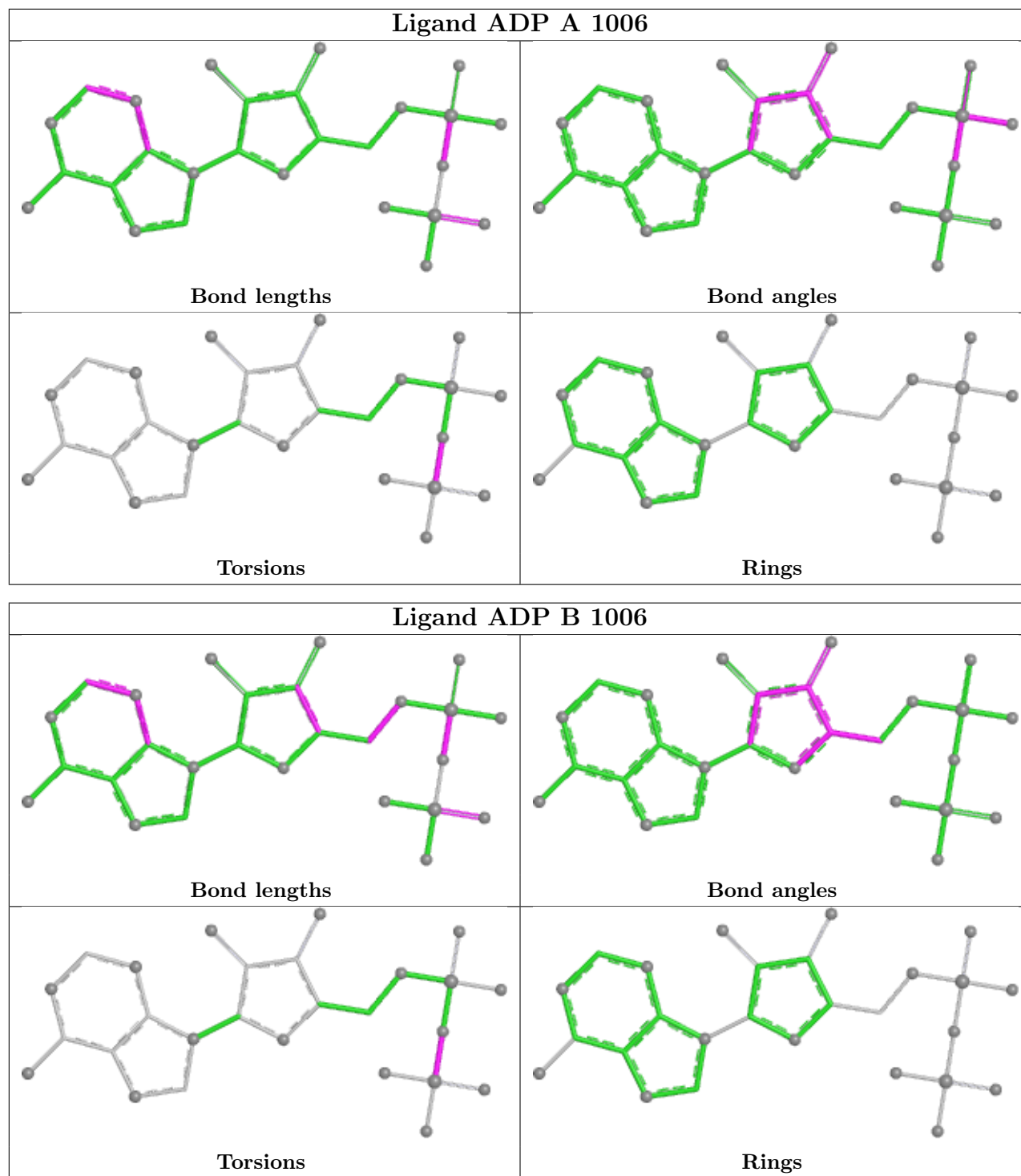
Mol	Chain	Res	Type	Atoms
2	A	1006	ADP	PA-O3A-PB-O2B
2	B	1006	ADP	PA-O3A-PB-O1B
2	B	1006	ADP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1006	ADP	1	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	366/371 (98%)	-0.20	4 (1%) 78 76	26, 47, 73, 95	0
1	B	357/371 (96%)	0.10	4 (1%) 78 76	33, 59, 89, 99	0
All	All	723/742 (97%)	-0.05	8 (1%) 78 76	26, 54, 85, 99	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1005	GLY	2.7
1	A	78	ASN	2.4
1	A	1005	GLY	2.4
1	B	140	PHE	2.4
1	A	939	ARG	2.3
1	A	93	GLY	2.2
1	B	81	ASN	2.2
1	B	912	ILE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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,

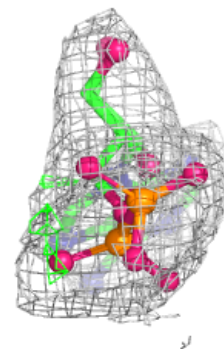
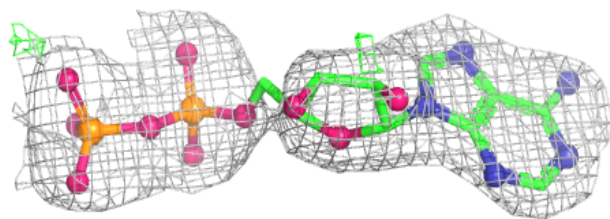
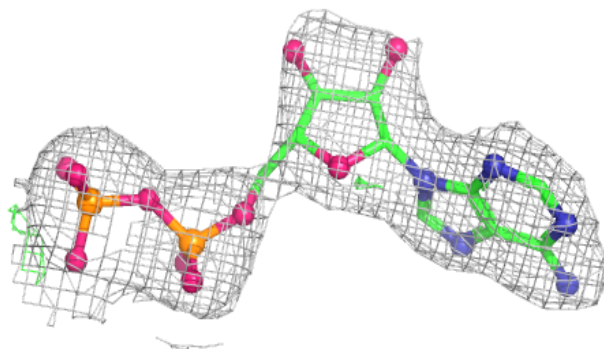
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	A	1006	27/27	0.94	0.08	45,49,55,57	0
2	ADP	B	1006	27/27	0.95	0.07	51,55,60,62	0
3	MG	A	1007	1/1	0.95	0.13	35,35,35,35	0
3	MG	B	1007	1/1	0.97	0.08	25,25,25,25	0

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

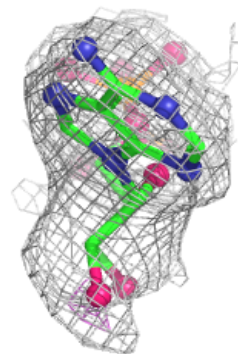
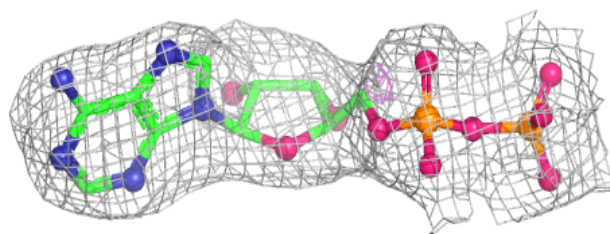
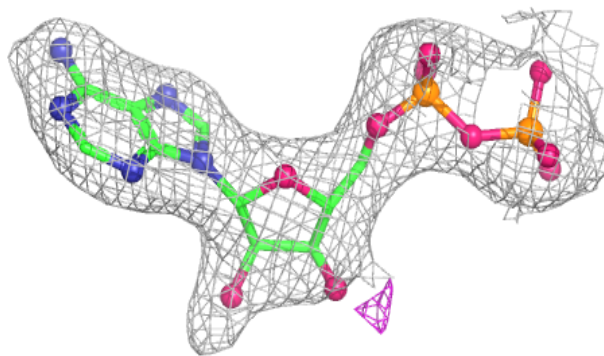
Electron density around ADP A 1006:

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



Electron density around ADP B 1006:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.