Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 06:46 am BST

PDB ID	:	3AUY
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 (i) symbol.

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

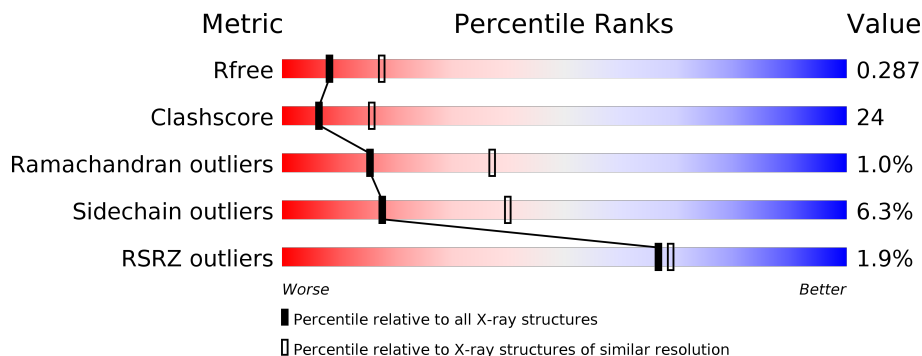|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.287
Clashscore		24
Ramachandran outliers		1.0%
Sidechain outliers		6.3%
RSRZ outliers		1.9%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	62% · 33% · ·
1	B	371	3% · 49% · 42% · 5% ·

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 2938	C 1883	N 502	O 544	S 9	0	0	0
1	B	357	Total 2869	C 1842	N 487	O 532	S 8	0	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
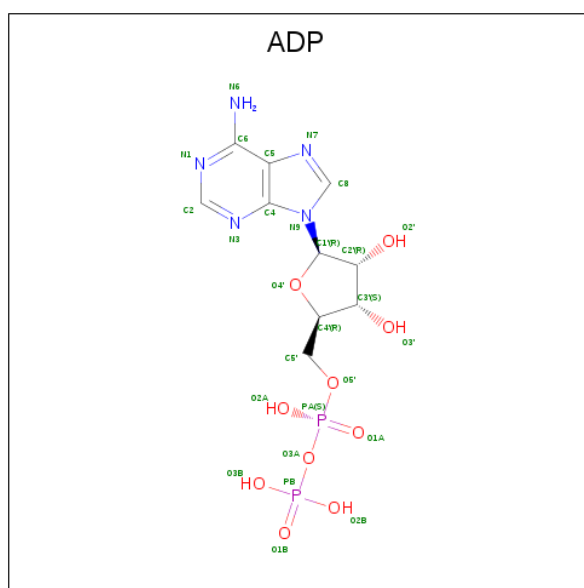
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA double-strand break repair rad50 ATPase
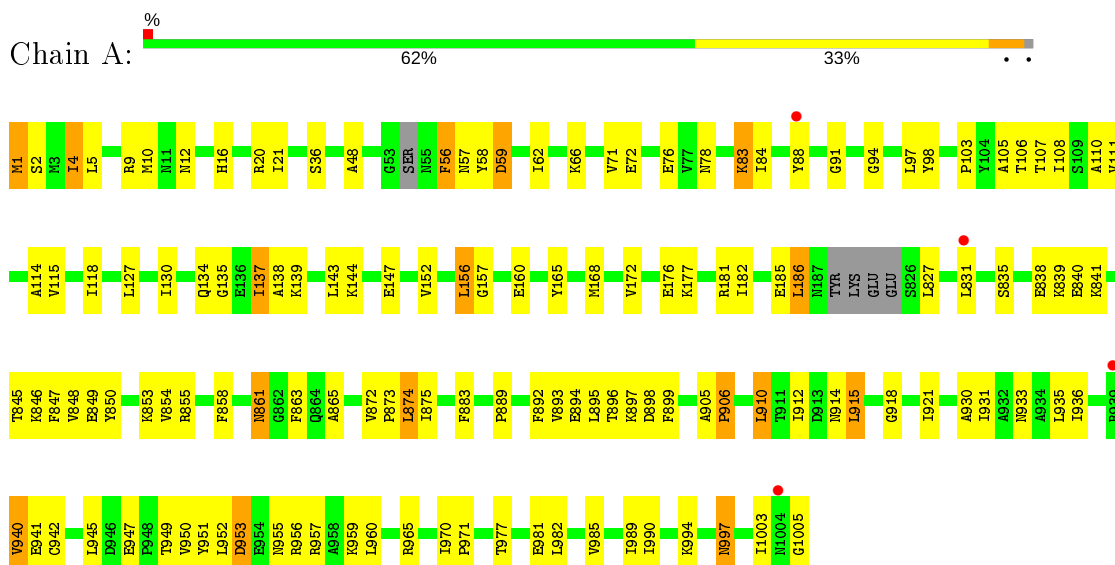
- Molecule 1: DNA double-strand break repair rad50 ATPase
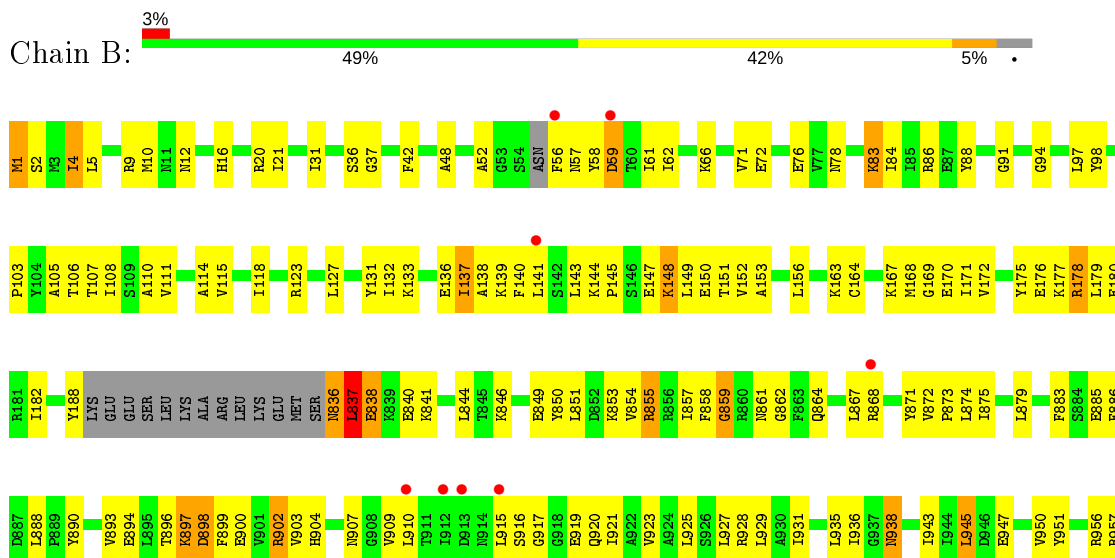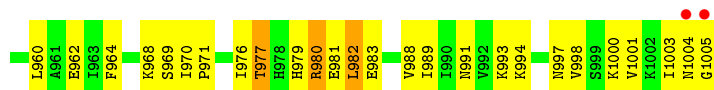
4 Data and refinement statistics (i)

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 72.30 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.40-2.70) 98.7 (72.30-2.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.80 (at 2.62Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.296 0.220 , 0.287	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)	0.34 , 58.0	EDS
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.45	0/2980	0.65	0/3991
1	B	0.42	0/2912	0.64	1/3903 (0.0%)
All	All	0.43	0/5892	0.65	1/7894 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	838	GLU	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2938	0	3031	114	0
1	B	2869	0	2948	176	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5932	0	6003	282	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 24.

All (282) 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:1:MET:HA	1:A:1:MET:HE2	1.49	0.95
1:A:949:THR:HG22	1:A:960:LEU:HD23	1.49	0.92
1:B:977:THR:HG23	1:B:979:HIS:H	1.39	0.87
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: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:B:1003:ILE:C	1:B:1004:ASN:HD22	1.85	0.78
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
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: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:938:ASN:C	1:B:938:ASN:HD22	1.96	0.68
1:B:144:LYS:HB3	1:B:145:PRO:HD2	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:1:MET:HA	1:B:1:MET:CE	2.27	0.64
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:169:GLY:O	1:B:172:VAL:HG22	1.98	0.63
1:B:4:ILE:HG23	1:B:76:GLU:HB3	1.80	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: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:A:1:MET:HA	1:A:1:MET:CE	2.25	0.61
1:B:896:THR:C	1:B:898:ASP:H	2.03	0.61
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
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:1:MET:HA	1:B:1:MET:HE3	1.85	0.58
1:B:851:LEU:O	1:B:855:ARG:HB2	2.03	0.58
1:B:149:LEU:HD23	1:B:898:ASP:HB3	1.84	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:A:56:PHE:C	1:A:56:PHE:CD2	2.76	0.58
1:B:883:PHE:CZ	1:B:923:VAL:HG22	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ILE:HD11	1:A:921:ILE:HG23	1.86	0.58
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:HG22	1:A:106:THR:O	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: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: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
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:HD13	1:B:837:LEU:O	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:141:LEU:HD11	1:B:921:ILE:HG12	1.91	0.53
1:B:139:LYS:O	1:B:143:LEU:HD23	2.08	0.53
1:B:4:ILE:HD13	1:B:4:ILE:C	2.29	0.53
1:A:854:VAL:CG1	1:B:854:VAL:HG21	2.37	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: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:896:THR:OG1	1:A:898:ASP:OD2	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:925:LEU:O	1:B:929:LEU:HG	2.09	0.52
1:B:857:ILE:HG22	1:B:857:ILE:O	2.09	0.52
1:A:845:THR:O	1:A:848:VAL:HG12	2.10	0.52
1:A:94:GLY:N	1:A:108:ILE:HD11	2.25	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:A:10:MET:HE2	1:A:16:HIS:HB2	1.91	0.51
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:896:THR:C	1:B:898:ASP:N	2.62	0.51
1:B:991:ASN:HB3	1:B:993:LYS:HE2	1.92	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
1:B:57:ASN:OD1	1:B:59:ASP:HB2	2.10	0.50
1:A:4:ILE:C	1:A:4:ILE:HD13	2.31	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:CE	1:A:144:LYS:HA	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: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:B:10:MET:HE2	1:B:16:HIS:HB2	1.95	0.48
1:A:48:ALA:HB2	1:A:71:VAL:CG1	2.43	0.48
1:B:12:ASN:CG	1:B:66:LYS:HG2	2.34	0.48
1:A:846:LYS:HE2	1:A:850:TYR:CE1	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LEU:HB3	1:B:867:LEU:HD22	1.95	0.47
1:A:949:THR:HB	1:A:957:ARG:HG3	1.95	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:12:ASN:CG	1:A:66:LYS:HG2	2.36	0.46
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: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
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:HH21	1:B:20:ARG:HG2	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:B:178:ARG:C	1:B:180:GLU:N	2.69	0.45
1:A:997:ASN:HD22	1:A:997:ASN:HA	1.62	0.45
1:B:84:ILE:HB	1:B:97:LEU:HD13	1.98	0.45
1:B:136:GLU:OE2	1:B:928:ARG:NE	2.40	0.45
1:B:4:ILE:CG2	1:B:76:GLU:HB3	2.45	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:B:147:GLU:O	1:B:150:GLU:HB3	2.16	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:903:VAL:O	1:B:910:LEU:N	2.39	0.45
1:B:1004:ASN:HB3	1:B:1005:GLY:H	1.30	0.45
1:B:20:ARG:NH2	1:B:20:ARG:HG2	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:848:VAL:CG1	1:A:849:GLU:N	2.81	0.44
1:B:164:CYS:O	1:B:168:MET:HG3	2.16	0.44
1:B:1:MET:SD	1:B:78:ASN:OD1	2.76	0.44
1:B:894:GLU:HB2	1:B:904:HIS:CE1	2.53	0.44
1:B:957:ARG:HG3	1:B:957:ARG:HH21	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:A:48:ALA:HB2	1:A:71:VAL:HG12	1.99	0.44
1:B:883:PHE:CE2	1:B:893:VAL:HG21	2.53	0.44
1:B:938:ASN:C	1:B:938:ASN:ND2	2.69	0.44
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.77	0.43
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:148:LYS:O	1:B:152:VAL:HG23	2.18	0.43
1:A:845:THR:C	1:A:848:VAL:HG12	2.39	0.43
1:B:175:TYR:CD1	1:B:844:LEU:HD22	2.54	0.43
1:A:152:VAL:O	1:A:156:LEU:HD22	2.19	0.43
1:A:88:TYR:OH	1:A:91:GLY:HA2	2.18	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:B:48:ALA:HB2	1:B:71:VAL:HG12	2.00	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:134:GLN:HG3	1:A:950:VAL:HG21	2.01	0.43
1:B:858:PHE:C	1:B:862:GLY:HA3	2.39	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: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:114:ALA:O	1:B:118:ILE:HG13	2.20	0.42
1:B:98:TYR:CD1	1:B:103:PRO:HA	2.54	0.42
1:A:977:THR:HG21	1:A:982:LEU:HD12	2.02	0.42
1:A:98:TYR:CD1	1:A:103:PRO:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:861:ASN:HA	1:A:865:ALA:HB2	2.02	0.42
1:B:873:PRO:HG2	1:B:874:LEU:H	1.84	0.42
1:B:943:ILE:CG2	1:B:943:ILE:O	2.67	0.42
1:B:175:TYR:HA	1:B:175:TYR:HD1	1.77	0.42
1:B:921:ILE:HD11	1:B:956:ARG:CD	2.49	0.41
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:B:42:PHE:CE2	1:B:976:ILE:HD11	2.55	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:994:LYS:CE	1:A:997:ASN:HD22	2.31	0.41
1:B:1:MET:HE2	1:B:2:SER:H	1.84	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: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:NH2	1:A:20:ARG:HG2	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:114:ALA:O	1:A:118:ILE:HG13	2.21	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:9:ARG:HB3	1:B:9:ARG:CZ	2.50	0.41
1:A:9:ARG:CZ	1:A:9:ARG:HB3	2.51	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:O	1:B:998:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	25	50
1	B	351/371 (95%)	309 (88%)	37 (10%)	5 (1%)	11	28
All	All	711/742 (96%)	637 (90%)	67 (9%)	7 (1%)	15	37

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%)	300 (94%)	19 (6%)	19	42
1	B	311/324 (96%)	290 (93%)	21 (7%)	16	36
All	All	630/648 (97%)	590 (94%)	40 (6%)	18	40

All (40) 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	56	PHE
1	A	59	ASP
1	A	83	LYS
1	A	137	ILE
1	A	156	LEU
1	A	186	LEU
1	A	861	ASN
1	A	874	LEU
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	997	ASN
1	B	1	MET
1	B	4	ILE
1	B	5	LEU
1	B	59	ASP
1	B	83	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	855	ARG
1	B	898	ASP
1	B	902	ARG
1	B	907	ASN

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Mol	Chain	Res	Type
1	B	938	ASN
1	B	945	LEU
1	B	977	THR
1	B	980	ARG
1	B	981	GLU
1	B	982	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) 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	A	1004	ASN
1	B	11	ASN
1	B	78	ASN
1	B	904	HIS
1	B	914	ASN
1	B	955	ASN
1	B	1004	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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	B	1006	3	24,29,29	1.96	7 (29%)	29,45,45	1.99	3 (10%)
2	ADP	A	1006	3	24,29,29	1.85	4 (16%)	29,45,45	1.85	3 (10%)

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	B	1006	3	-	2/12/32/32	0/3/3/3
2	ADP	A	1006	3	-	1/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1006	ADP	C4-N3	5.58	1.43	1.35
2	B	1006	ADP	C4-N3	4.69	1.42	1.35
2	B	1006	ADP	C2-N3	4.40	1.39	1.32
2	A	1006	ADP	C2-N3	4.17	1.38	1.32
2	B	1006	ADP	C3'-C4'	-3.00	1.45	1.53
2	B	1006	ADP	O5'-C5'	-2.61	1.34	1.44
2	A	1006	ADP	O4'-C1'	2.35	1.44	1.41
2	B	1006	ADP	O4'-C1'	2.35	1.44	1.41
2	B	1006	ADP	PB-O3B	2.27	1.63	1.54
2	A	1006	ADP	PB-O3B	2.19	1.63	1.54
2	B	1006	ADP	C8-N7	-2.08	1.31	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1006	ADP	O3'-C3'-C4'	-7.63	88.99	111.05
2	A	1006	ADP	O3'-C3'-C4'	-6.31	92.81	111.05
2	A	1006	ADP	C3'-C2'-C1'	5.50	109.25	100.98
2	B	1006	ADP	C3'-C2'-C1'	4.73	108.10	100.98
2	B	1006	ADP	O4'-C4'-C3'	2.75	110.56	105.11
2	A	1006	ADP	C4-C5-N7	2.11	111.60	109.40

There are no chirality outliers.
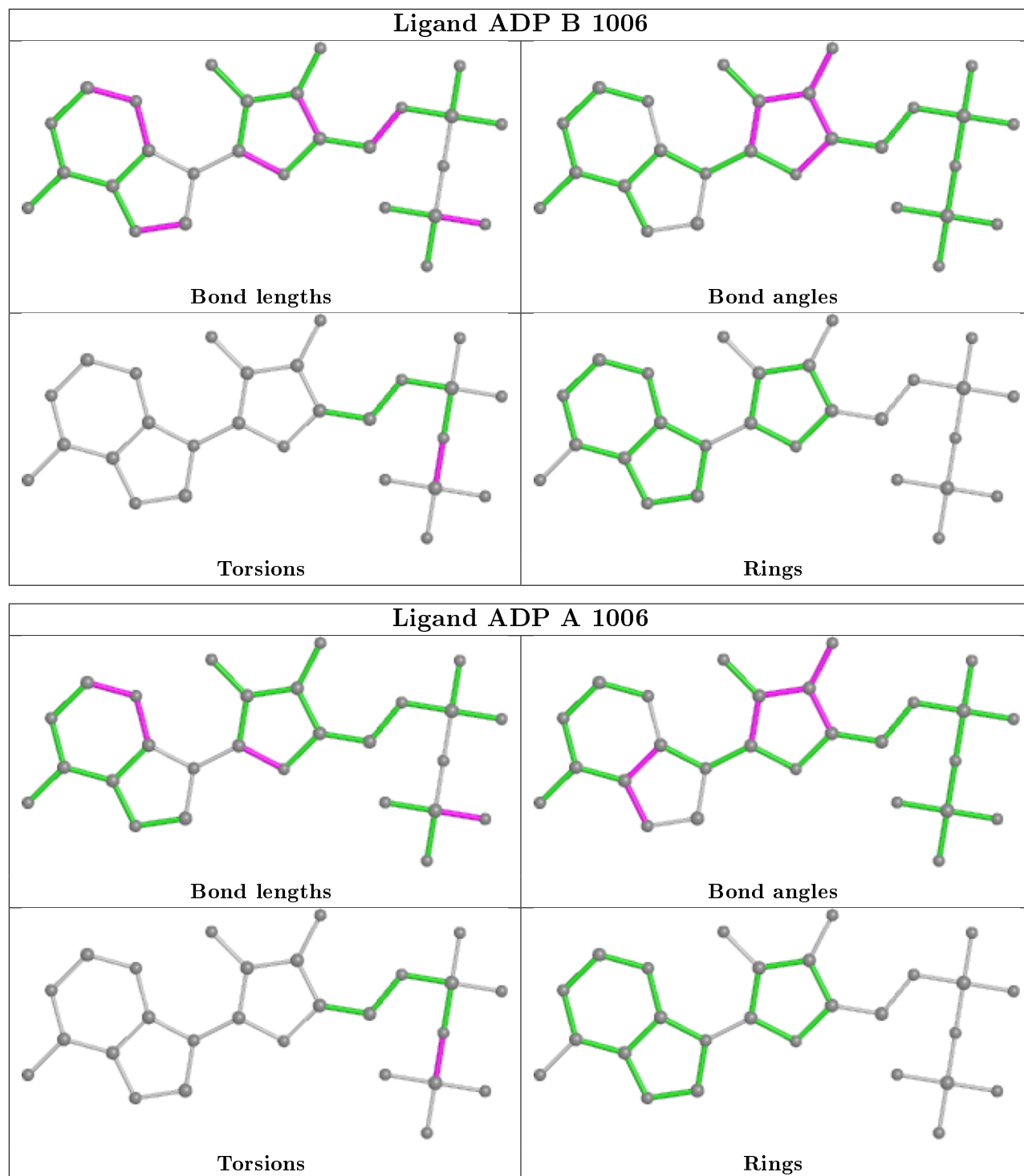
All (3) torsion outliers are listed below:

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 then 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.

Ligand ADP B 1006

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 1006

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

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 (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(Å²)	Q<0.9
1	A	366/371 (98%)	-0.01	4 (1%)	80	82	26, 47, 73, 95	0
1	B	357/371 (96%)	0.24	10 (2%)	53	54	33, 59, 89, 99	0
All	All	723/742 (97%)	0.11	14 (1%)	66	69	26, 54, 85, 99	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1005	GLY	7.5
1	A	939	ARG	4.5
1	B	915	LEU	3.7
1	B	912	ILE	3.1
1	A	1004	ASN	2.7
1	B	141	LEU	2.7
1	B	868	ARG	2.6
1	B	910	LEU	2.6
1	B	913	ASP	2.5
1	B	56	PHE	2.4
1	B	1004	ASN	2.4
1	A	88	TYR	2.3
1	B	59	ASP	2.2
1	A	831	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.
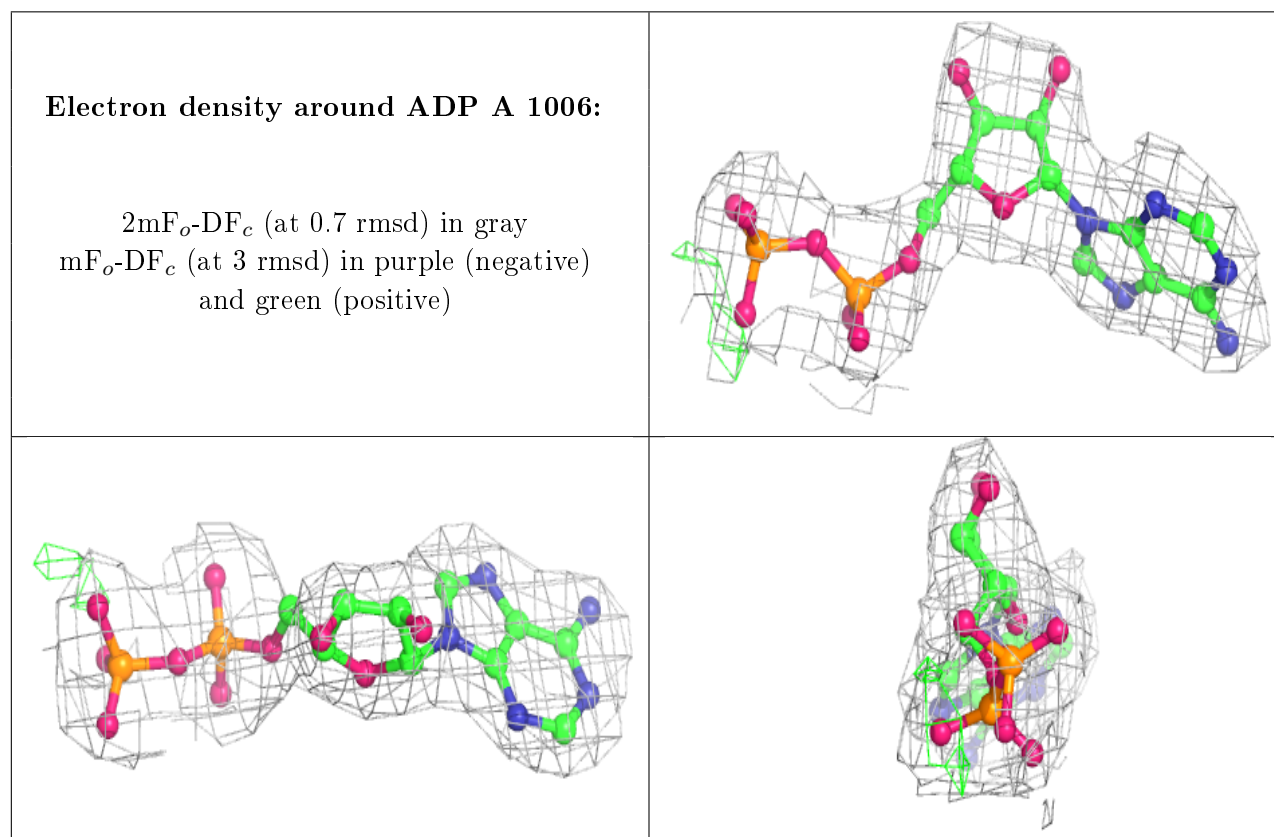
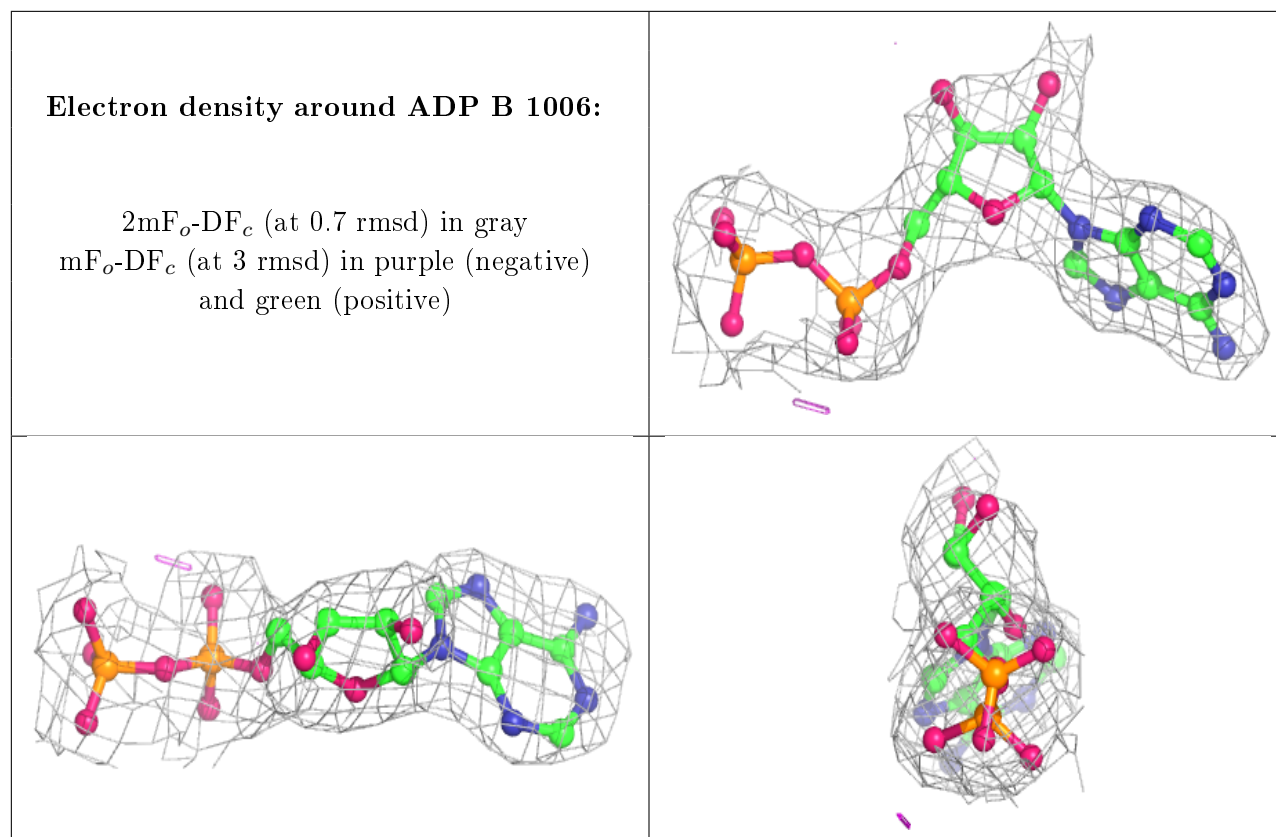## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	1007	1/1	0.89	0.19	35,35,35,35	0
2	ADP	A	1006	27/27	0.95	0.16	45,49,55,57	0
3	MG	B	1007	1/1	0.96	0.15	25,25,25,25	0
2	ADP	B	1006	27/27	0.97	0.15	51,55,60,62	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:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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.