



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2026 – 11:36 pm BST

PDB ID : 4CEI / pdb_00004cei
Title : Crystal structure of ADPNP-bound AddAB with a forked DNA substrate
Authors : Krajewski, W.W.; Wilkinson, M.; Fu, X.; Cronin, N.B.; Wigley, D.
Deposited on : 2013-11-11
Resolution : 2.80 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 : 1.8.4, CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

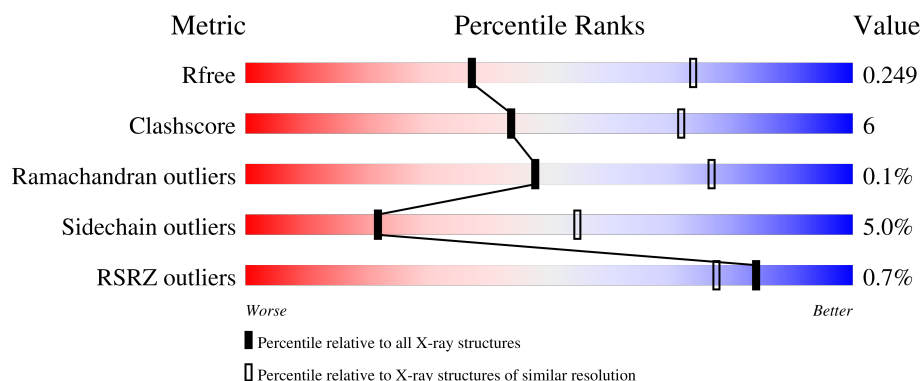
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

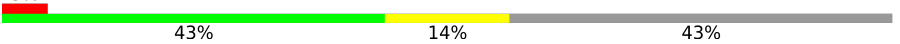
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	1232	 75% 18% • 5%
2	B	1166	 80% 18% ..
3	X	65	 5% 43% 14% 43%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19688 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 ATP-DEPENDENT HELICASE/NUCLEASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1170	Total	C	N	O	S	0	0	0
			9468	6040	1611	1790	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	780	GLY	ALA	variant	UNP P23478
A	1172	ALA	ASP	engineered mutation	UNP P23478

- Molecule 2 is a protein called ATP-DEPENDENT HELICASE/DEOXYRIBONUCLEASE SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1152	Total	C	N	O	S	0	1	0
			9383	5964	1605	1770	44			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	843	ASP	GLU	variant	UNP P23477
B	844	GLU	GLN	variant	UNP P23477
B	961	ALA	ASP	engineered mutation	UNP P23477

- Molecule 3 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	37	Total	C	N	O	P	0	0	0
			757	363	129	228	37			

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

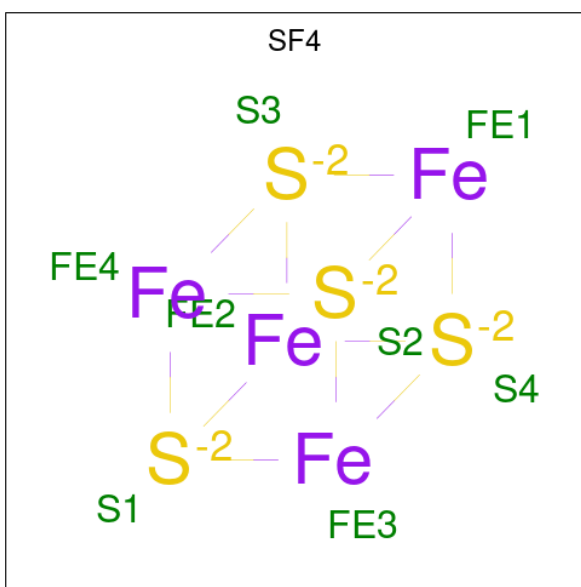


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	B	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			8	4	4		

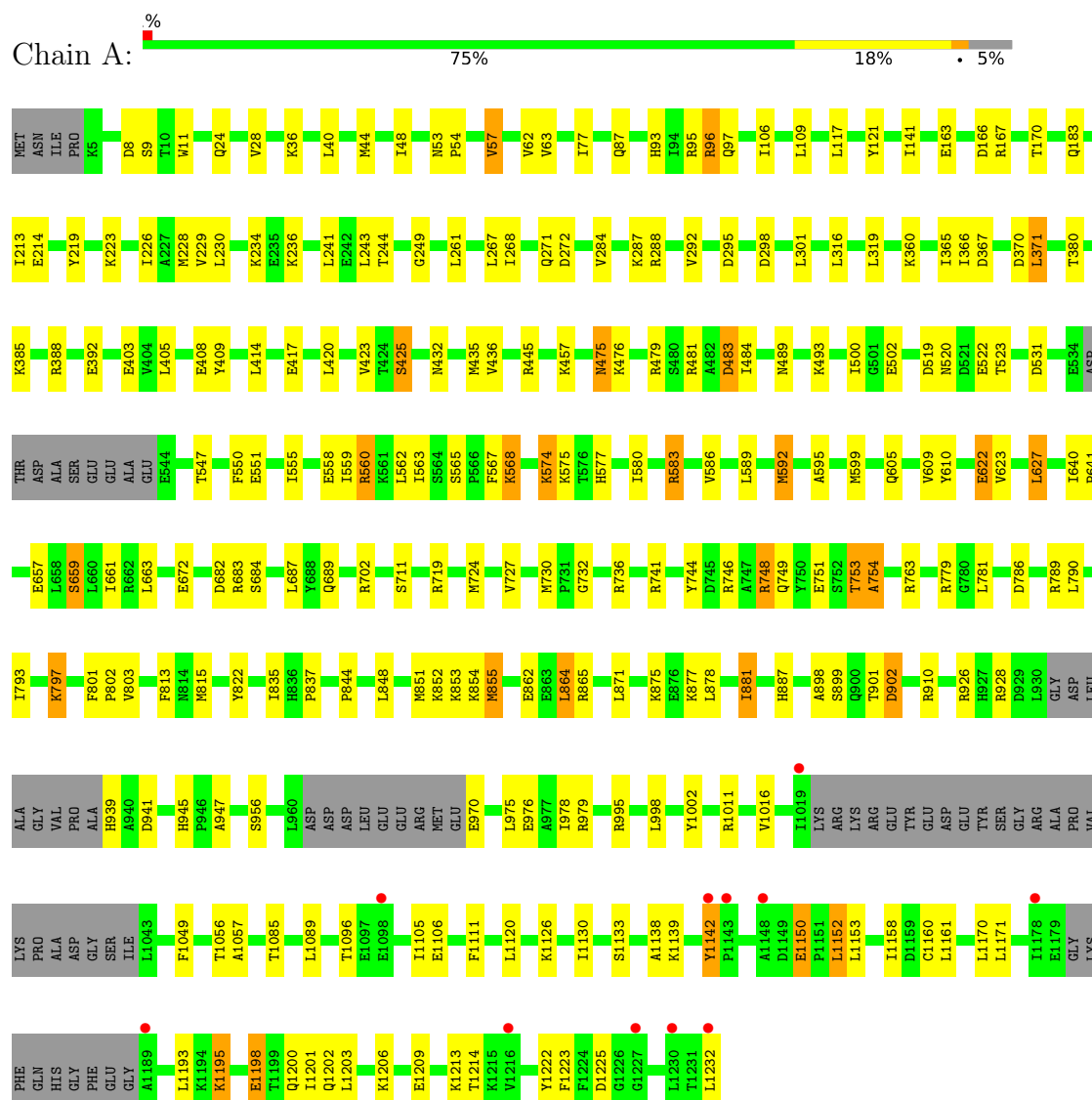
- Molecule 7 is water.

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

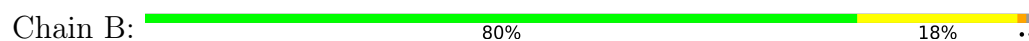
3 Residue-property plots

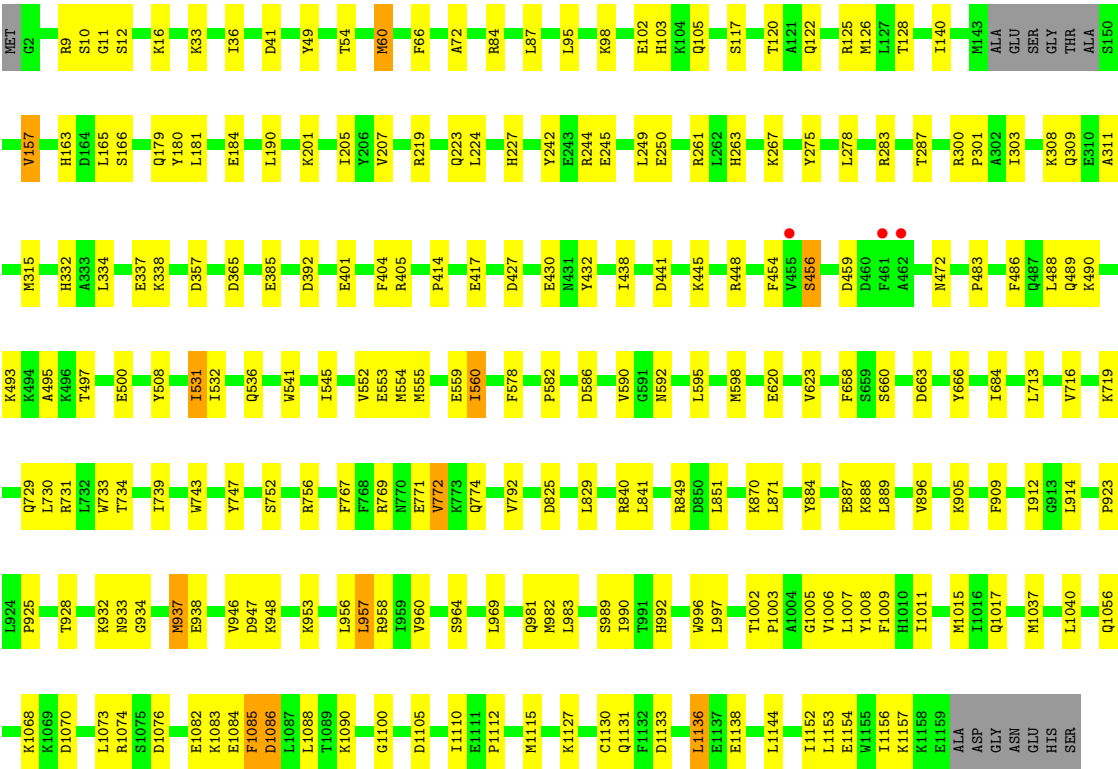
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ATP-DEPENDENT HELICASE/NUCLEASE SUBUNIT A

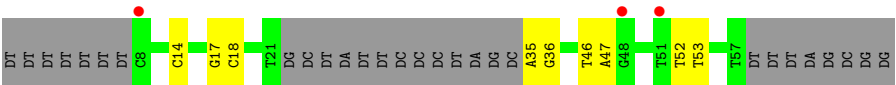


• Molecule 2: ATP-DEPENDENT HELICASE/DEOXYRIBONUCLEASE SUBUNIT B





● Molecule 3: DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.94Å 151.34Å 124.56Å 90.00° 95.95° 90.00°	Depositor
Resolution (Å)	29.95 – 2.80 29.95 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.95-2.80) 99.7 (29.95-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.195 , 0.240 0.205 , 0.249	Depositor DCC
R_{free} test set	3459 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19688	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 2.95% 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: MG, SF4, ANP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.30	0/9657	0.75	7/13034 (0.1%)
2	B	0.29	0/9577	0.74	8/12904 (0.1%)
3	X	0.25	0/845	0.56	0/1300
All	All	0.29	0/20079	0.74	15/27238 (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	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1142	TYR	CA-C-N	-6.42	113.37	119.85
1	A	1142	TYR	C-N-CA	-6.42	113.37	119.85
2	B	287	THR	CA-C-N	6.32	126.53	119.32
2	B	287	THR	C-N-CA	6.32	126.53	119.32
2	B	934	GLY	N-CA-C	-6.19	107.33	114.69
2	B	84	ARG	CA-C-N	6.17	126.18	119.89
2	B	84	ARG	C-N-CA	6.17	126.18	119.89
2	B	483	PRO	N-CA-C	6.09	118.13	110.70
1	A	899	SER	N-CA-C	-5.84	106.78	114.31
2	B	660	SER	CA-C-N	-5.58	114.82	120.85
2	B	660	SER	C-N-CA	-5.58	114.82	120.85
1	A	592	MET	CA-C-N	-5.46	114.47	119.82
1	A	592	MET	C-N-CA	-5.46	114.47	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1150	GLU	CA-C-N	-5.20	114.88	120.03
1	A	1150	GLU	C-N-CA	-5.20	114.88	120.03

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	574	LYS	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	9468	0	9441	137	1
2	B	9383	0	9329	117	1
3	X	757	0	423	6	0
4	A	31	0	13	0	0
4	B	31	0	13	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	8	0	0	1	0
7	A	4	0	0	0	0
7	B	4	0	0	0	0
All	All	19688	0	19219	239	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 6.

All (239) 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:380:THR:HG21	1:A:388:ARG:HH11	1.46	0.79
2:B:912:ILE:HD11	2:B:948:LYS:HB3	1.67	0.76
2:B:244:ARG:HE	2:B:245:GLU:H	1.34	0.74
1:A:28:VAL:HB	1:A:436:VAL:HG12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:896:VAL:HG21	2:B:1011:ILE:HG23	1.72	0.71
1:A:902:ASP:N	1:A:902:ASP:OD1	2.24	0.70
1:A:360:LYS:NZ	1:A:367:ASP:OD1	2.21	0.70
2:B:12:SER:HB3	2:B:278:LEU:HB3	1.73	0.68
1:A:719:ARG:NH1	2:B:365:ASP:OD1	2.25	0.68
2:B:947:ASP:HB2	2:B:958:ARG:HG2	1.76	0.67
2:B:392:ASP:OD2	2:B:405:ARG:NH2	2.29	0.66
1:A:1198:GLU:OE1	1:A:1202:GLN:NE2	2.29	0.65
2:B:283:ARG:HD3	4:B:2161:ANP:H4'	1.78	0.65
1:A:683:ARG:O	1:A:689:GLN:NE2	2.29	0.65
2:B:982:MET:HE3	2:B:1006:VAL:HB	1.80	0.63
2:B:592:ASN:ND2	2:B:595:LEU:H	1.97	0.63
1:A:1138:ALA:HA	1:A:1152:LEU:HD11	1.80	0.62
1:A:502:GLU:OE1	1:A:865:ARG:NH2	2.33	0.61
1:A:871:LEU:HD22	1:A:878:LEU:HD21	1.82	0.60
2:B:180:TYR:OH	2:B:553:GLU:OE1	2.19	0.60
2:B:459:ASP:O	2:B:870:LYS:NZ	2.35	0.60
2:B:263:HIS:NE2	2:B:275:TYR:OH	2.30	0.59
2:B:456:SER:HB2	2:B:459:ASP:HB2	1.83	0.59
1:A:555:ILE:HG12	1:A:881:ILE:HD12	1.85	0.59
2:B:909:PHE:HB3	2:B:947:ASP:HB3	1.83	0.58
2:B:1112:PRO:HG3	6:B:2160:SF4:S4	2.43	0.58
2:B:334:LEU:HD23	2:B:338:LYS:HG3	1.85	0.58
1:A:166:ASP:OD1	2:B:884:TYR:OH	2.20	0.57
1:A:95:ARG:HD2	2:B:249:LEU:HD13	1.87	0.56
2:B:140:ILE:HG22	2:B:166:SER:HB3	1.86	0.56
2:B:925:PRO:HG2	2:B:992:HIS:CE1	2.40	0.56
1:A:567:PHE:HB3	1:A:580:ILE:HB	1.87	0.56
2:B:441:ASP:OD1	2:B:441:ASP:N	2.35	0.56
2:B:414:PRO:HB2	2:B:417:GLU:HG3	1.88	0.56
1:A:170:THR:O	2:B:888:LYS:NZ	2.37	0.55
1:A:481:ARG:HG2	1:A:483:ASP:H	1.71	0.55
1:A:1150:GLU:HB3	2:B:49:TYR:OH	2.05	0.55
1:A:288:ARG:HH12	3:X:17:DG:H21	1.52	0.55
1:A:939:HIS:CE1	1:A:941:ASP:HB3	2.41	0.55
3:X:35:DA:H2''	3:X:36:DG:C8	2.42	0.55
3:X:46:DT:H2''	3:X:47:DA:C8	2.41	0.55
1:A:268:ILE:HA	1:A:271:GLN:HG3	1.88	0.55
1:A:599:MET:HG2	1:A:609:VAL:HG11	1.89	0.55
2:B:495:ALA:HB1	2:B:500:GLU:HG3	1.89	0.54
1:A:748:ARG:NH1	2:B:357:ASP:OD2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ARG:NH1	1:A:835:ILE:O	2.40	0.54
1:A:298:ASP:HB3	1:A:301:LEU:HB2	1.90	0.54
2:B:990:ILE:HG13	2:B:1003:PRO:HG3	1.90	0.54
1:A:531:ASP:O	1:A:956:SER:OG	2.19	0.53
2:B:1009:PHE:HB2	2:B:1037:MET:HE3	1.91	0.53
1:A:523:THR:HA	1:A:877:LYS:HD3	1.89	0.53
2:B:488:LEU:HD13	2:B:508:TYR:HB2	1.91	0.53
2:B:928:THR:HG22	2:B:938:GLU:HG3	1.90	0.53
1:A:54:PRO:HB2	1:A:93:HIS:CE1	2.44	0.52
1:A:520:ASN:HB2	1:A:523:THR:HG23	1.91	0.52
1:A:551:GLU:O	1:A:555:ILE:HG13	2.10	0.52
1:A:366:ILE:HB	1:A:370:ASP:HB2	1.91	0.52
1:A:622:GLU:HG2	1:A:736:ARG:HB3	1.91	0.52
1:A:141:ILE:HD12	1:A:365:ILE:HD11	1.90	0.52
1:A:403:GLU:HA	1:A:432:ASN:HB2	1.91	0.52
1:A:214:GLU:HA	1:A:219:TYR:CD2	2.44	0.52
2:B:849:ARG:HG2	2:B:905:LYS:HG2	1.92	0.52
1:A:558:GLU:O	1:A:562:LEU:HG	2.10	0.51
1:A:1133:SER:HB3	1:A:1153:LEU:HD11	1.91	0.51
2:B:315:MET:HE2	2:B:666:TYR:HB3	1.91	0.51
2:B:36:ILE:HG23	2:B:66:PHE:HD2	1.75	0.51
2:B:829:LEU:HD22	2:B:889:LEU:HD13	1.93	0.51
2:B:658:PHE:HZ	2:B:684:ILE:HD12	1.76	0.51
1:A:230:LEU:HD12	1:A:271:GLN:HG2	1.93	0.51
1:A:1011:ARG:HD3	2:B:582:PRO:HB2	1.93	0.51
2:B:448:ARG:NH2	2:B:472:ASN:OD1	2.44	0.51
2:B:536:GLN:HB2	2:B:578:PHE:CE1	2.46	0.51
1:A:425:SER:OG	1:A:432:ASN:ND2	2.44	0.51
1:A:711:SER:N	1:A:751:GLU:OE2	2.32	0.51
2:B:825:ASP:HB3	2:B:871:LEU:HD11	1.92	0.51
1:A:1016:VAL:HG11	1:A:1200:GLN:HG3	1.92	0.50
2:B:98:LYS:HD2	2:B:555:MET:HG3	1.93	0.50
2:B:165:LEU:HD11	2:B:623:VAL:HG11	1.93	0.50
1:A:1120:LEU:O	1:A:1126:LYS:HD3	2.10	0.50
1:A:48:ILE:HD13	1:A:57:VAL:HG22	1.94	0.50
2:B:489:GLN:HG2	2:B:493:LYS:HE3	1.94	0.50
2:B:72:ALA:HA	2:B:190:LEU:HD13	1.93	0.49
2:B:960:VAL:HG22	2:B:1007:LEU:HB2	1.95	0.49
1:A:267:LEU:HD11	1:A:284:VAL:HG21	1.93	0.49
1:A:567:PHE:HA	1:A:568:LYS:HE3	1.95	0.49
1:A:500:ILE:HB	1:A:910:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:PHE:HB2	1:A:1222:TYR:CZ	2.48	0.48
2:B:730:LEU:O	2:B:734:THR:HG23	2.13	0.48
2:B:432:TYR:CE2	2:B:438:ILE:HD11	2.48	0.48
1:A:445:ARG:NH1	1:A:862:GLU:OE1	2.46	0.48
1:A:163:GLU:OE1	1:A:167:ARG:NH2	2.38	0.48
2:B:303:ILE:O	2:B:303:ILE:HG13	2.14	0.48
2:B:1115:MET:HB2	2:B:1144:LEU:HB2	1.95	0.48
1:A:763:ARG:NE	2:B:401:GLU:OE1	2.46	0.48
1:A:802:PRO:HA	1:A:875:LYS:HB2	1.95	0.48
1:A:622:GLU:H	1:A:622:GLU:CD	2.21	0.47
2:B:983:LEU:HD13	2:B:1088:LEU:HB3	1.96	0.47
1:A:1160:CYS:HB3	1:A:1171:LEU:HB3	1.96	0.47
1:A:901:THR:HB	1:A:939:HIS:HD2	1.79	0.47
2:B:531:ILE:HD12	2:B:532:ILE:HG13	1.96	0.47
1:A:975:LEU:HD22	2:B:767:PHE:HE1	1.80	0.47
2:B:9:ARG:O	2:B:12:SER:OG	2.20	0.47
1:A:183:GLN:NE2	1:A:822:TYR:OH	2.49	0.46
1:A:560:ARG:NH1	1:A:605:GLN:HB3	2.31	0.46
1:A:1105:ILE:HD12	1:A:1105:ILE:H	1.81	0.46
1:A:241:LEU:O	1:A:244:THR:OG1	2.21	0.46
1:A:945:HIS:C	1:A:947:ALA:H	2.22	0.46
1:A:1195:LYS:NZ	1:A:1198:GLU:HG3	2.30	0.46
1:A:77:ILE:HD13	1:A:106:ILE:HD13	1.97	0.46
2:B:933:ASN:O	2:B:933:ASN:ND2	2.49	0.46
2:B:912:ILE:HD13	2:B:997:LEU:HD11	1.97	0.46
2:B:1074:ARG:HG2	3:X:14:DC:H5"	1.98	0.46
1:A:976:GLU:CD	1:A:979:ARG:HH21	2.23	0.46
1:A:484:ILE:HD12	1:A:878:LEU:HB2	1.96	0.46
1:A:746:ARG:HA	1:A:749:GLN:HG2	1.97	0.46
1:A:1002:TYR:OH	2:B:586:ASP:OD2	2.30	0.46
2:B:128:THR:HG23	2:B:184:GLU:HG3	1.98	0.46
2:B:497:THR:HG22	2:B:559:GLU:HG2	1.96	0.46
2:B:713:LEU:O	2:B:716:VAL:HG22	2.15	0.45
1:A:226:ILE:HG12	1:A:319:LEU:HD11	1.98	0.45
1:A:531:ASP:OD2	1:A:887:HIS:N	2.49	0.45
1:A:803:VAL:HG22	1:A:877:LYS:HB2	1.98	0.45
1:A:813:PHE:HB2	1:A:815:MET:HE2	1.97	0.45
2:B:102:GLU:HG3	2:B:103:HIS:ND1	2.31	0.45
2:B:937:MET:HE2	2:B:1100:GLY:HA3	1.97	0.45
2:B:969:LEU:HB2	2:B:1008:TYR:HE1	1.82	0.45
1:A:623:VAL:O	1:A:627:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1201:ILE:HG13	1:A:1232:LEU:HD12	1.98	0.45
2:B:60:MET:HE2	2:B:60:MET:HB2	1.86	0.45
2:B:117:SER:O	2:B:120:THR:HG22	2.17	0.45
1:A:53:ASN:OD1	1:A:53:ASN:N	2.50	0.45
1:A:489:ASN:O	1:A:493:LYS:HG3	2.17	0.45
1:A:835:ILE:HG23	2:B:1015:MET:HE2	1.97	0.45
1:A:93:HIS:O	1:A:97:GLN:HG2	2.16	0.45
1:A:547:THR:HA	1:A:550:PHE:HD2	1.81	0.45
1:A:1085:THR:O	1:A:1089:LEU:HG	2.17	0.45
1:A:1139:LYS:HA	1:A:1142:TYR:O	2.17	0.45
1:A:371:LEU:HD12	1:A:371:LEU:HA	1.89	0.45
1:A:627:LEU:HA	1:A:627:LEU:HD12	1.82	0.45
1:A:724:MET:HE1	1:A:741:ARG:HG3	1.98	0.45
1:A:657:GLU:HB3	1:A:687:LEU:HD13	1.99	0.44
1:A:978:ILE:HA	2:B:747:TYR:OH	2.16	0.44
1:A:243:LEU:O	1:A:249:GLY:HA3	2.17	0.44
2:B:792:VAL:HG11	2:B:981:GLN:HA	1.98	0.44
1:A:229:VAL:HG21	1:A:319:LEU:HD13	1.99	0.44
1:A:392:GLU:CD	2:B:157:VAL:HG21	2.43	0.44
2:B:11:GLY:H	4:B:2161:ANP:HNB1	1.64	0.44
2:B:592:ASN:HD21	2:B:595:LEU:H	1.63	0.44
1:A:9:SER:HB3	1:A:11:TRP:H	1.83	0.44
1:A:732:GLY:O	1:A:736:ARG:HG3	2.17	0.44
2:B:716:VAL:O	2:B:716:VAL:HG23	2.17	0.44
1:A:851:MET:O	1:A:855:MET:HB2	2.17	0.44
2:B:772:VAL:HG11	2:B:1110:ILE:HG13	2.00	0.44
1:A:475:ASN:HD22	1:A:475:ASN:HA	1.57	0.44
1:A:753:THR:HG22	1:A:754:ALA:N	2.32	0.44
2:B:1084:GLU:HG2	2:B:1153:LEU:HD13	1.99	0.44
1:A:975:LEU:HD23	1:A:975:LEU:HA	1.88	0.43
2:B:95:LEU:HB2	2:B:554:MET:HE2	1.99	0.43
2:B:385:GLU:OE2	2:B:405:ARG:HD2	2.17	0.43
1:A:682:ASP:OD2	1:A:684:SER:OG	2.27	0.43
2:B:912:ILE:HG21	2:B:997:LEU:HD21	1.99	0.43
1:A:555:ILE:O	1:A:559:ILE:HG13	2.19	0.43
2:B:486:PHE:O	2:B:490:LYS:HG2	2.19	0.43
1:A:40:LEU:HG	1:A:405:LEU:HD23	2.01	0.43
1:A:595:ALA:O	1:A:599:MET:HG3	2.18	0.43
1:A:1161:LEU:HD23	1:A:1170:LEU:HA	2.00	0.43
2:B:946:VAL:HG21	2:B:996:TRP:HH2	1.84	0.43
1:A:44:MET:SD	1:A:62:VAL:HG21	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:MET:HE1	1:A:457:LYS:HZ2	1.83	0.43
1:A:975:LEU:HD22	2:B:767:PHE:CE1	2.53	0.43
2:B:957:LEU:HD23	2:B:989:SER:HB3	2.00	0.43
1:A:519:ASP:OD1	1:A:520:ASN:N	2.52	0.43
1:A:657:GLU:O	1:A:661:ILE:HG13	2.19	0.43
2:B:729:GLN:HG3	2:B:743:TRP:CD1	2.54	0.43
2:B:1086:ASP:OD2	2:B:1090:LYS:NZ	2.44	0.43
1:A:36:LYS:HB3	1:A:436:VAL:HB	2.00	0.43
2:B:1005:GLY:HA2	2:B:1085:PHE:CZ	2.54	0.43
2:B:311:ALA:HB1	2:B:663:ASP:O	2.18	0.43
2:B:774:GLN:NE2	2:B:1105:ASP:O	2.52	0.43
2:B:1040:LEU:HD12	2:B:1040:LEU:HA	1.83	0.43
1:A:702:ARG:HH22	2:B:427:ASP:CG	2.25	0.43
2:B:560:ILE:HA	2:B:560:ILE:HD12	1.76	0.43
1:A:583:ARG:HB2	1:A:786:ASP:OD1	2.19	0.42
1:A:610:TYR:CE1	1:A:779:ARG:HD2	2.53	0.42
2:B:267:LYS:HE3	2:B:267:LYS:HB2	1.87	0.42
2:B:308:LYS:HG2	2:B:309:GLN:N	2.34	0.42
2:B:10:SER:OG	4:B:2161:ANP:O1G	2.31	0.42
2:B:201:LYS:HA	2:B:227:HIS:O	2.19	0.42
1:A:844:PRO:HB3	1:A:848:LEU:HD23	2.00	0.42
1:A:864:LEU:HD12	1:A:864:LEU:HA	1.90	0.42
1:A:1138:ALA:HA	1:A:1152:LEU:CD1	2.48	0.42
2:B:541:TRP:O	2:B:545:ILE:HG12	2.18	0.42
1:A:408:GLU:OE1	1:A:797:LYS:HE2	2.20	0.42
1:A:730:MET:C	2:B:731:ARG:HD3	2.45	0.42
2:B:1130:CYS:SG	2:B:1131:GLN:N	2.92	0.42
1:A:711:SER:HB2	1:A:744:TYR:CE1	2.55	0.42
2:B:733:TRP:HB2	2:B:739:ILE:HD13	2.02	0.42
1:A:95:ARG:HG3	1:A:96:ARG:N	2.34	0.42
2:B:1152:ILE:O	2:B:1156:ILE:HG13	2.20	0.42
1:A:586:VAL:HG21	1:A:801:PHE:CD1	2.56	0.41
1:A:589:LEU:HD11	1:A:790:LEU:HD22	2.02	0.41
2:B:163:HIS:O	2:B:166:SER:OG	2.33	0.41
1:A:1193:LEU:HD13	1:A:1223:PHE:CZ	2.55	0.41
1:A:228:MET:HE2	1:A:228:MET:HB3	1.91	0.41
1:A:385:LYS:HE2	1:A:385:LYS:HB3	1.81	0.41
2:B:205:ILE:HD13	2:B:224:LEU:HD13	2.02	0.41
2:B:300:ARG:HA	2:B:301:PRO:HA	1.94	0.41
1:A:121:TYR:OH	2:B:122:GLN:NE2	2.53	0.41
1:A:1049:PHE:CD2	2:B:552:VAL:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1209:GLU:HA	1:A:1214:THR:O	2.20	0.41
1:A:287:LYS:HD2	1:A:287:LYS:N	2.36	0.41
1:A:898:ALA:HB1	1:A:926:ARG:HG3	2.02	0.41
2:B:404:PHE:CZ	2:B:430:GLU:HA	2.55	0.41
2:B:87:LEU:HD23	2:B:87:LEU:HA	1.88	0.41
2:B:953:LYS:NZ	2:B:1082:GLU:OE1	2.31	0.41
1:A:223:LYS:NZ	1:A:272:ASP:OD1	2.50	0.41
1:A:409:TYR:OH	1:A:417:GLU:OE1	2.30	0.41
3:X:52:DT:H2''	3:X:53:DT:OP2	2.20	0.41
1:A:63:VAL:HG11	1:A:109:LEU:HD13	2.01	0.41
1:A:589:LEU:O	1:A:793:ILE:HG13	2.21	0.41
1:A:998:LEU:HD23	1:A:998:LEU:HA	1.91	0.41
1:A:1056:THR:OG1	1:A:1057:ALA:N	2.52	0.41
2:B:41:ASP:OD1	2:B:41:ASP:N	2.52	0.41
1:A:659:SER:O	1:A:663:LEU:HG	2.21	0.41
1:A:995:ARG:NH1	2:B:752:SER:OG	2.54	0.41
2:B:126:MET:HE3	2:B:126:MET:HA	2.03	0.41
2:B:956:LEU:HD23	2:B:1002:THR:HB	2.03	0.41
1:A:166:ASP:HB3	1:A:837:PRO:HB3	2.02	0.40
2:B:1133:ASP:HB3	2:B:1136:LEU:HD22	2.03	0.40
3:X:17:DG:H2''	3:X:18:DC:C6	2.56	0.40
1:A:420:LEU:HA	1:A:423:VAL:HG22	2.03	0.40
1:A:1130:ILE:HB	1:A:1158:ILE:HB	2.03	0.40
2:B:308:LYS:HE2	2:B:308:LYS:HB3	1.87	0.40
2:B:769:ARG:O	2:B:771:GLU:N	2.52	0.40
1:A:213:ILE:HG22	1:A:219:TYR:CD1	2.56	0.40
1:A:640:ILE:HB	1:A:641:PRO:HD3	2.03	0.40
2:B:841:LEU:HD21	2:B:851:LEU:HD21	2.02	0.40
2:B:105:GLN:CD	2:B:105:GLN:H	2.30	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)
1:A:901:THR:OG1	2:B:756:ARG:NH1[2_545]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	1158/1232 (94%)	1120 (97%)	36 (3%)	2 (0%)	43	72
2	B	1149/1166 (98%)	1112 (97%)	36 (3%)	1 (0%)	48	77
All	All	2307/2398 (96%)	2232 (97%)	72 (3%)	3 (0%)	48	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	754	ALA
1	A	592	MET
2	B	923	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1013/1062 (95%)	957 (94%)	56 (6%)	19	51
2	B	1021/1029 (99%)	975 (96%)	46 (4%)	24	58
All	All	2034/2091 (97%)	1932 (95%)	102 (5%)	22	54

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	24	GLN
1	A	57	VAL

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Mol	Chain	Res	Type
1	A	87	GLN
1	A	96	ARG
1	A	117	LEU
1	A	234	LYS
1	A	236	LYS
1	A	261	LEU
1	A	292	VAL
1	A	295	ASP
1	A	316	LEU
1	A	371	LEU
1	A	414	LEU
1	A	425	SER
1	A	475	ASN
1	A	476	LYS
1	A	479	ARG
1	A	483	ASP
1	A	522	GLU
1	A	560	ARG
1	A	563	ILE
1	A	565	SER
1	A	568	LYS
1	A	574	LYS
1	A	575	LYS
1	A	577	HIS
1	A	583	ARG
1	A	622	GLU
1	A	627	LEU
1	A	659	SER
1	A	672	GLU
1	A	727	VAL
1	A	748	ARG
1	A	753	THR
1	A	781	LEU
1	A	789	ARG
1	A	797	LYS
1	A	852	LYS
1	A	853	LYS
1	A	854	LYS
1	A	855	MET
1	A	864	LEU
1	A	881	ILE
1	A	902	ASP

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Mol	Chain	Res	Type
1	A	928	ARG
1	A	970	GLU
1	A	1096	THR
1	A	1106	GLU
1	A	1152	LEU
1	A	1195	LYS
1	A	1198	GLU
1	A	1203	LEU
1	A	1206	LYS
1	A	1213	LYS
1	A	1225	ASP
2	B	16	LYS
2	B	33	LYS
2	B	54	THR
2	B	60	MET
2	B	125	ARG
2	B	157	VAL
2	B	179	GLN
2	B	181	LEU
2	B	207	VAL
2	B	219	ARG
2	B	223	GLN
2	B	242	TYR
2	B	250	GLU
2	B	261	ARG
2	B	332	HIS
2	B	337	GLU
2	B	445	LYS
2	B	454	PHE
2	B	456	SER
2	B	531	ILE
2	B	560	ILE
2	B	590	VAL
2	B	598	MET
2	B	620	GLU
2	B	719	LYS
2	B	772	VAL
2	B	840	ARG
2	B	887	GLU
2	B	914	LEU
2	B	932	LYS
2	B	937	MET

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Mol	Chain	Res	Type
2	B	957	LEU
2	B	964	SER
2	B	1017	GLN
2	B	1056	GLN
2	B	1068	LYS
2	B	1073	LEU
2	B	1076	ASP
2	B	1083	LYS
2	B	1085	PHE
2	B	1086	ASP
2	B	1127	LYS
2	B	1136	LEU
2	B	1138	GLU
2	B	1154	GLU
2	B	1157	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	87	GLN
1	A	93	HIS
1	A	183	GLN
1	A	270	HIS
1	A	383	ASN
1	A	402	HIS
1	A	475	ASN
1	A	579	ASN
1	A	638	GLN
1	A	819	ASN
1	A	887	HIS
1	A	912	GLN
1	A	939	HIS
2	B	122	GLN
2	B	450	GLN
2	B	463	GLN
2	B	592	ASN
2	B	694	HIS
2	B	729	GLN
2	B	812	HIS
2	B	933	ASN
2	B	1010	HIS

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Mol	Chain	Res	Type
2	B	1064	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	ANP	B	2161	5	32,33,33	0.92	4 (12%)	44,52,52	0.84	3 (6%)
6	SF4	B	2160	2	0,12,12	-	-	-		
4	ANP	A	2233	5	32,33,33	0.93	4 (12%)	44,52,52	0.82	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	B	2161	5	-	6/18/38/38	0/3/3/3
6	SF4	B	2160	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	A	2233	5	-	3/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2161	ANP	PG-O1G	2.67	1.50	1.46
4	A	2233	ANP	PG-O1G	2.57	1.50	1.46
4	A	2233	ANP	PG-N3B	2.42	1.69	1.63
4	A	2233	ANP	PB-O3A	-2.39	1.56	1.59
4	B	2161	ANP	PB-O1B	2.36	1.49	1.46
4	B	2161	ANP	PG-N3B	2.34	1.69	1.63
4	B	2161	ANP	PB-O3A	-2.12	1.56	1.59
4	A	2233	ANP	PB-O1B	2.09	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2233	ANP	PB-O3A-PA	-3.07	121.81	132.62
4	B	2161	ANP	PB-O3A-PA	-2.91	122.36	132.62
4	A	2233	ANP	O3G-PG-O1G	-2.63	106.84	113.45
4	B	2161	ANP	O1G-PG-N3B	-2.31	108.38	111.77
4	B	2161	ANP	O3G-PG-O1G	-2.10	108.18	113.45

There are no chirality outliers.

All (9) torsion outliers are listed below:

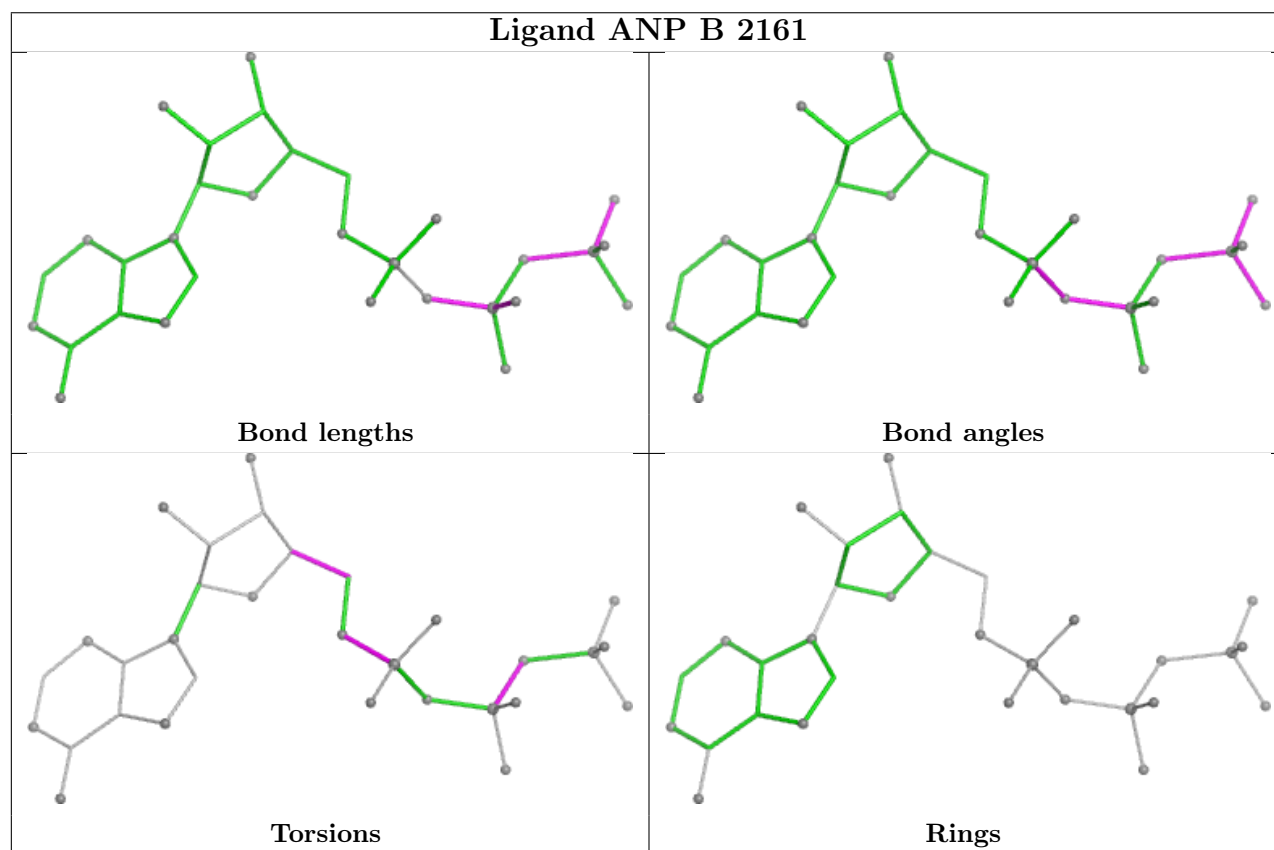
Mol	Chain	Res	Type	Atoms
4	A	2233	ANP	PB-N3B-PG-O1G
4	A	2233	ANP	PG-N3B-PB-O1B
4	A	2233	ANP	PG-N3B-PB-O3A
4	B	2161	ANP	PG-N3B-PB-O1B
4	B	2161	ANP	C5'-O5'-PA-O2A
4	B	2161	ANP	O4'-C4'-C5'-O5'
4	B	2161	ANP	C3'-C4'-C5'-O5'
4	B	2161	ANP	C5'-O5'-PA-O3A
4	B	2161	ANP	C5'-O5'-PA-O1A

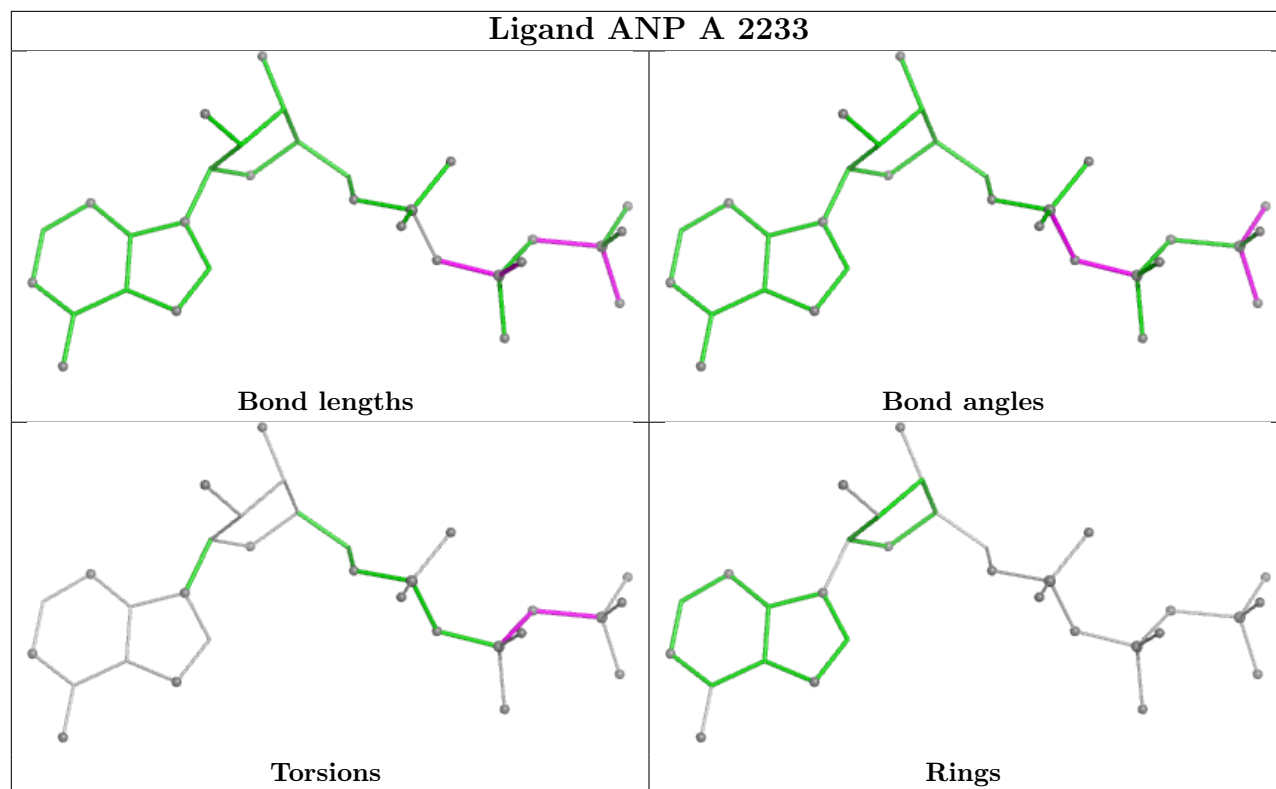
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2161	ANP	3	0
6	B	2160	SF4	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 [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 [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	1170/1232 (94%)	-0.17	11 (0%) 81 74	18, 48, 103, 129	0
2	B	1152/1166 (98%)	-0.29	3 (0%) 90 86	20, 48, 82, 122	1 (0%)
3	X	37/65 (56%)	0.81	3 (8%) 18 13	49, 122, 140, 153	0
All	All	2359/2463 (95%)	-0.21	17 (0%) 84 77	18, 48, 100, 153	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1148	ALA	3.1
1	A	1189	ALA	3.0
1	A	1230	LEU	2.9
1	A	1143	PRO	2.6
2	B	455	VAL	2.4
2	B	461	PHE	2.4
3	X	51	DT	2.3
1	A	1216	VAL	2.3
1	A	1098	GLU	2.3
1	A	1227	GLY	2.3
2	B	462	ALA	2.2
1	A	1178	ILE	2.1
3	X	48	DG	2.1
1	A	1232	LEU	2.1
1	A	1019	ILE	2.1
1	A	1142	TYR	2.1
3	X	8	DC	2.0

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

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

6.3 Carbohydrates [i](#)

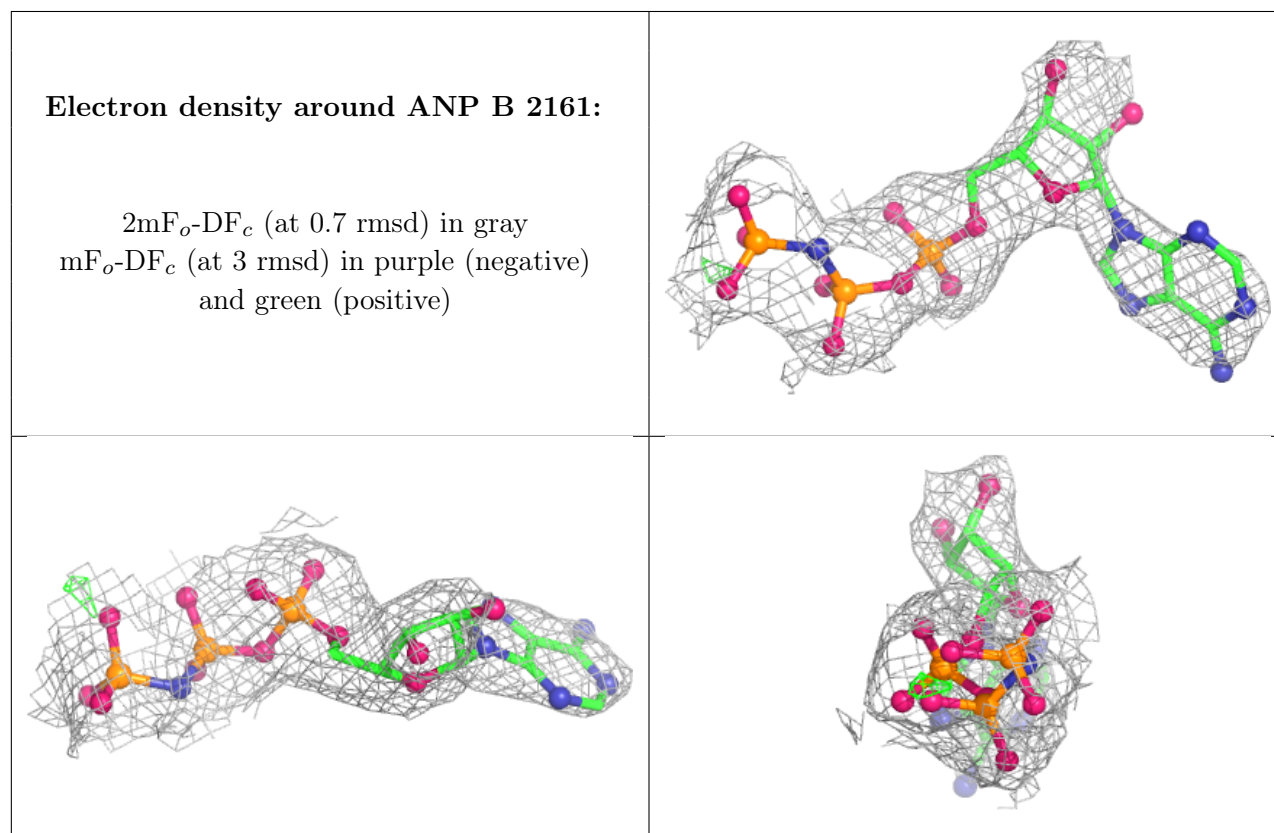
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

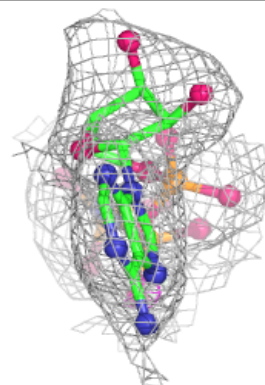
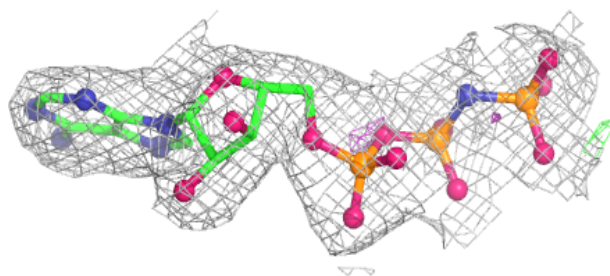
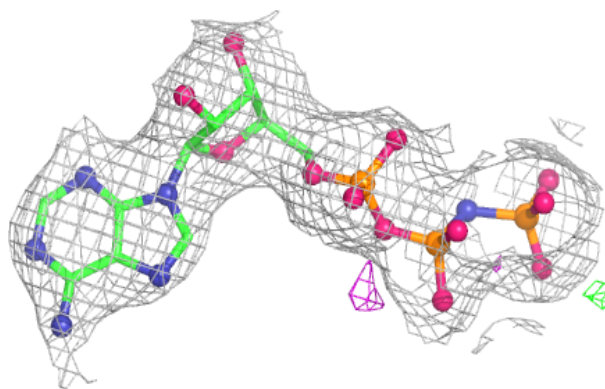
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ANP	B	2161	31/31	0.92	0.09	48,78,95,96	0
4	ANP	A	2233	31/31	0.95	0.07	37,50,61,67	0
5	MG	B	2162	1/1	0.96	0.06	65,65,65,65	0
6	SF4	B	2160	8/8	0.99	0.03	24,36,47,51	0
5	MG	A	2234	1/1	1.00	0.02	51,51,51,51	0

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 ANP A 2233:

$2mF_o-DF_c$ (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.