



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:16 AM UTC

PDB ID : 4ZSE / pdb_00004zse
Title : Crystal structure of EGFR 696-1022 T790M/V948R, crystal form II
Authors : Yan, X.E.; Yun, C.H.
Deposited on : 2015-05-13
Resolution : 1.97 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

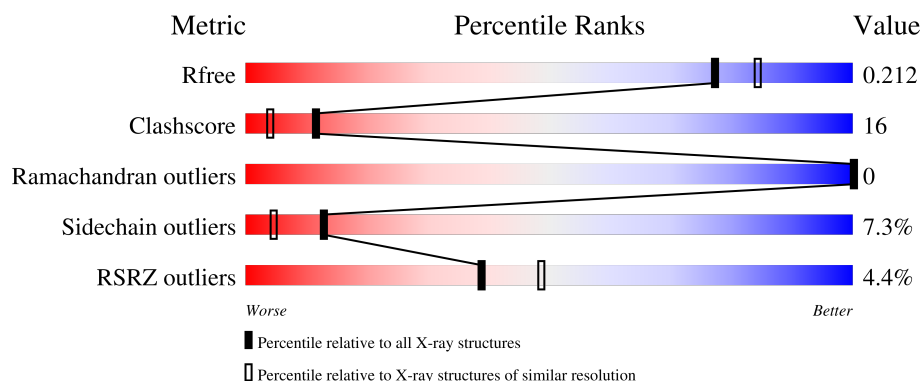
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	331	5% 67% 20% • • 10%
1	B	331	4% 68% 22% • 5%
1	C	331	4% 66% 21% • 9%
1	D	331	4% 63% 23% 5% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10588 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.

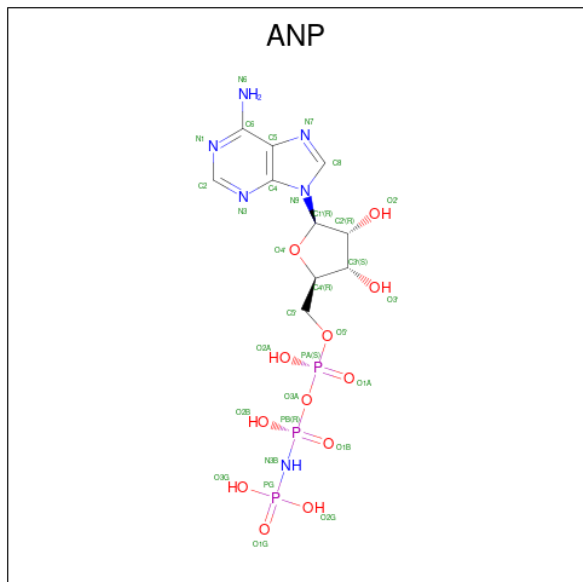
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	2	0
			2380	1526	405	429	20			
1	B	313	Total	C	N	O	S	0	3	0
			2507	1614	419	454	20			
1	C	301	Total	C	N	O	S	0	5	0
			2416	1556	406	434	20			
1	D	297	Total	C	N	O	S	0	0	0
			2355	1518	395	424	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	692	GLY	-	expression tag	UNP P00533
A	693	SER	-	expression tag	UNP P00533
A	694	THR	-	expression tag	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
B	692	GLY	-	expression tag	UNP P00533
B	693	SER	-	expression tag	UNP P00533
B	694	THR	-	expression tag	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
B	948	ARG	VAL	engineered mutation	UNP P00533
C	692	GLY	-	expression tag	UNP P00533
C	693	SER	-	expression tag	UNP P00533
C	694	THR	-	expression tag	UNP P00533
C	790	MET	THR	engineered mutation	UNP P00533
C	948	ARG	VAL	engineered mutation	UNP P00533
D	692	GLY	-	expression tag	UNP P00533
D	693	SER	-	expression tag	UNP P00533
D	694	THR	-	expression tag	UNP P00533
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

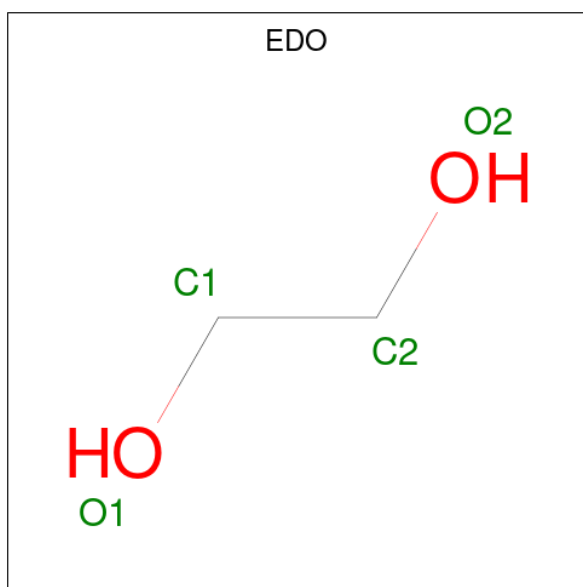


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



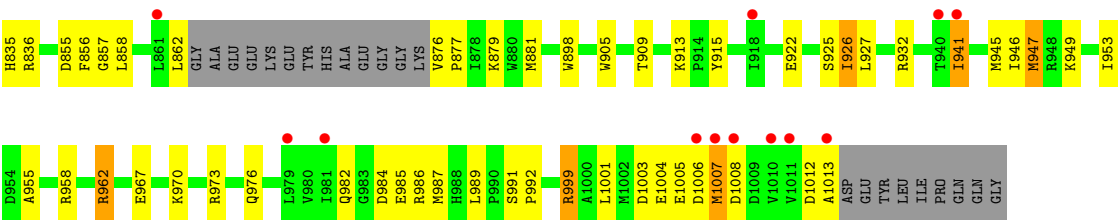
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

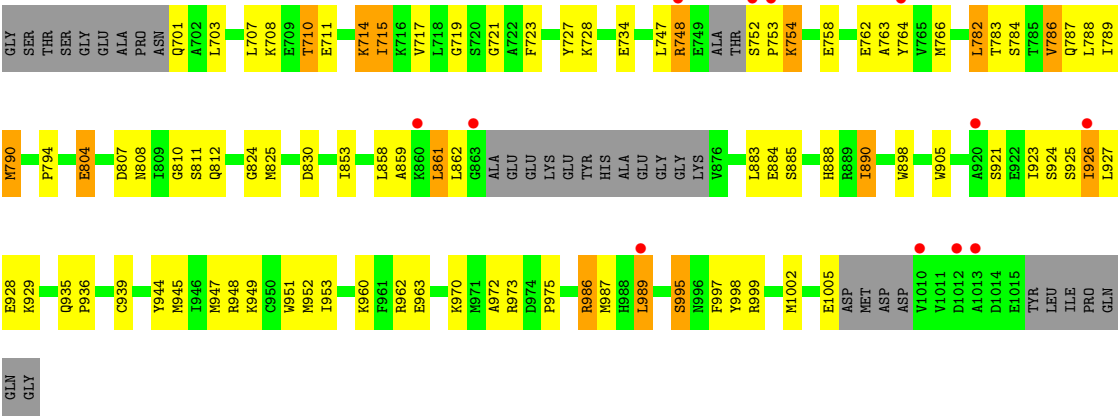
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	193	Total	O	0	0
			193	193		
5	B	256	Total	O	0	0
			256	256		
5	C	184	Total	O	0	0
			184	184		
5	D	165	Total	O	0	0
			165	165		

- Molecule 1: Epidermal growth factor receptor





• Molecule 1: Epidermal growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.82Å 102.32Å 86.75Å 90.00° 101.24° 90.00°	Depositor
Resolution (Å)	23.86 – 1.97 23.86 – 1.97	Depositor EDS
% Data completeness (in resolution range)	93.8 (23.86-1.97) 94.3 (23.86-1.97)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.190 , 0.213 0.194 , 0.212	Depositor DCC
R_{free} test set	4123 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10588	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EDO, 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	1.14	3/2439 (0.1%)	1.01	11/3300 (0.3%)
1	B	1.19	8/2570 (0.3%)	1.03	10/3479 (0.3%)
1	C	1.13	6/2483 (0.2%)	0.98	6/3360 (0.2%)
1	D	1.07	0/2404	0.97	4/3253 (0.1%)
All	All	1.13	17/9896 (0.2%)	1.00	31/13392 (0.2%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	759[A]	ILE	N-CA	-6.66	1.38	1.46
1	B	759[B]	ILE	N-CA	-6.66	1.38	1.46
1	A	790[A]	MET	CA-C	-6.63	1.44	1.52
1	A	790[B]	MET	CA-C	-6.63	1.44	1.52
1	C	776[A]	ARG	N-CA	-6.56	1.38	1.45
1	C	776[B]	ARG	N-CA	-6.56	1.38	1.45
1	C	769[A]	VAL	N-CA	-6.36	1.39	1.46
1	C	769[B]	VAL	N-CA	-6.36	1.39	1.46
1	B	790[A]	MET	N-CA	-6.31	1.37	1.45
1	B	790[B]	MET	N-CA	-6.31	1.37	1.45
1	B	1006	ASP	C-O	-5.95	1.16	1.24
1	B	812[A]	GLN	N-CA	-5.89	1.39	1.46
1	B	812[B]	GLN	N-CA	-5.89	1.39	1.46
1	C	776[A]	ARG	CA-C	-5.79	1.45	1.52
1	C	776[B]	ARG	CA-C	-5.79	1.45	1.52
1	A	936	PRO	C-O	-5.62	1.20	1.24
1	B	1007	MET	C-O	-5.50	1.17	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	784	SER	N-CA-C	-8.20	102.35	111.28
1	B	711	GLU	N-CA-C	8.03	121.14	111.82
1	C	723	PHE	N-CA-C	7.88	119.95	111.36
1	D	858	LEU	N-CA-C	-7.27	103.35	111.28
1	A	723	PHE	N-CA-C	7.24	119.25	111.36
1	A	783	THR	N-CA-C	-6.98	98.91	109.79
1	D	754	LYS	N-CA-C	6.85	120.62	109.59
1	C	778	LEU	N-CA-C	6.54	118.49	111.36
1	B	758	GLU	CA-C-N	6.39	128.62	120.56
1	B	758	GLU	C-N-CA	6.39	128.62	120.56
1	A	986	ARG	N-CA-C	6.38	118.31	111.36
1	C	711	GLU	N-CA-C	5.83	119.66	112.54
1	A	1001	LEU	N-CA-C	5.78	117.66	111.36
1	B	738	VAL	N-CA-C	5.71	117.39	109.80
1	A	715	ILE	N-CA-C	5.68	119.20	113.47
1	C	769[A]	VAL	CA-C-O	-5.54	113.94	120.76
1	C	769[B]	VAL	CA-C-O	-5.54	113.94	120.76
1	C	1001	LEU	N-CA-C	5.52	117.10	111.14
1	A	806	LYS	CA-C-N	-5.50	113.85	122.65
1	A	806	LYS	C-N-CA	-5.50	113.85	122.65
1	B	723	PHE	N-CA-C	5.40	118.08	111.82
1	D	939	CYS	N-CA-C	5.32	117.94	109.96
1	B	737	LYS	N-CA-C	5.28	117.11	111.36
1	B	784	SER	N-CA-C	-5.25	105.67	111.71
1	B	790[A]	MET	N-CA-C	5.24	116.95	109.14
1	B	790[B]	MET	N-CA-C	5.24	116.95	109.14
1	A	835	HIS	N-CA-C	5.19	116.75	111.14
1	A	806	LYS	N-CA-C	5.17	116.92	111.28
1	A	936	PRO	O-C-N	5.16	123.58	121.15
1	B	715	ILE	N-CA-C	5.16	115.99	111.56
1	D	715	ILE	N-CA-C	5.02	116.44	111.67

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	2380	0	2404	71	0
1	B	2507	0	2532	70	0
1	C	2416	0	2447	84	0
1	D	2355	0	2372	96	0
2	A	31	0	13	2	0
2	B	31	0	13	4	0
2	C	31	0	13	2	0
2	D	31	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	C	4	0	6	0	0
5	A	193	0	0	16	0
5	B	256	0	0	13	0
5	C	184	0	0	10	0
5	D	165	0	0	25	0
All	All	10588	0	9813	314	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 16.

All (314) 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:D:752:SER:CB	1:D:753:PRO:HD3	1.72	1.20
1:D:810:GLY:HA3	5:D:4101:HOH:O	1.50	1.09
1:B:698:ALA:CB	1:B:699:PRO:HD2	1.83	1.08
1:D:747:LEU:HD22	1:D:862:LEU:HD11	1.11	1.06
1:D:752:SER:HB3	1:D:753:PRO:HD3	1.15	1.06
1:C:713:LYS:HE3	5:C:3199:HOH:O	1.55	1.06
1:D:905:TRP:HB2	1:D:947:MET:CE	1.92	0.98
1:A:783:THR:HB	5:A:1318:HOH:O	1.61	0.97
1:D:752:SER:HB3	1:D:753:PRO:CD	1.93	0.97
1:C:946:ILE:HD11	1:C:967:GLU:OE1	1.63	0.97
1:B:698:ALA:HB1	1:B:699:PRO:HD2	1.46	0.94
1:D:701:GLN:HA	5:D:4218:HOH:O	1.69	0.93
1:D:905:TRP:HB2	1:D:947:MET:HE1	1.51	0.93
1:B:850:HIS:CE1	1:B:1007:MET:HE1	2.03	0.93
1:D:763:ALA:HA	1:D:766:MET:HE3	1.50	0.93
1:D:905:TRP:CB	1:D:947:MET:HE1	1.99	0.92
1:C:1003:ASP:OD1	1:C:1007:MET:HE3	1.68	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:700:ASN:ND2	1:C:701:GLN:H	1.69	0.91
1:C:999:ARG:HG2	1:C:999:ARG:HH21	1.34	0.90
1:D:752:SER:CB	1:D:753:PRO:CD	2.49	0.90
1:D:947:MET:HE2	1:D:951:TRP:CH2	2.06	0.89
1:D:747:LEU:HD22	1:D:862:LEU:CD1	2.02	0.88
1:A:790[A]:MET:HE2	5:A:1247:HOH:O	1.72	0.88
1:D:701:GLN:HG2	1:D:764:TYR:CD2	2.07	0.88
1:B:812[B]:GLN:HG2	5:B:2189:HOH:O	1.73	0.87
1:B:698:ALA:HB3	1:B:699:PRO:HD2	1.57	0.87
1:D:734:GLU:HG2	5:D:4135:HOH:O	1.73	0.87
1:B:698:ALA:CB	1:B:699:PRO:CD	2.51	0.86
1:B:698:ALA:HB1	1:B:699:PRO:CD	2.06	0.86
5:A:1293:HOH:O	1:C:716:LYS:HE3	1.75	0.85
1:B:810:GLY:HA3	5:B:2189:HOH:O	1.75	0.85
1:A:748:ARG:HD3	5:A:1230:HOH:O	1.76	0.85
1:D:714:LYS:HE3	1:D:787:GLN:OE1	1.80	0.81
1:B:850:HIS:ND1	1:B:1007:MET:HE1	1.95	0.80
1:C:999:ARG:HG2	1:C:999:ARG:NH2	1.94	0.79
1:D:947:MET:HE2	1:D:951:TRP:HH2	1.45	0.79
1:B:723:PHE:HD2	5:B:2193:HOH:O	1.64	0.78
1:A:833:LEU:HD13	1:A:856:PHE:CZ	2.19	0.77
1:B:941:ILE:O	1:B:945:MET:HG3	1.84	0.77
1:C:719:GLY:HA3	2:C:3001:ANP:H4'	1.66	0.76
1:D:808:ASN:HB3	5:D:4212:HOH:O	1.86	0.76
1:C:766[B]:MET:HE1	1:C:856:PHE:CE1	2.19	0.76
1:C:932:ARG:HH22	1:C:953:ILE:HD11	1.49	0.75
1:B:836:ARG:HD3	1:B:891:TYR:CG	2.23	0.74
1:C:1005:GLU:O	1:C:1007:MET:SD	2.46	0.74
1:D:905:TRP:CD1	1:D:947:MET:HE1	2.23	0.73
1:D:747:LEU:HD12	1:D:786:VAL:CG2	2.20	0.71
1:A:849:GLN:HG2	5:A:1351:HOH:O	1.91	0.71
1:D:812:GLN:HG2	1:D:989:LEU:HD13	1.71	0.71
1:A:991[B]:SER:OG	1:A:992:PRO:HD2	1.91	0.71
1:D:747:LEU:HD12	1:D:786:VAL:HG22	1.72	0.71
1:D:701:GLN:HG2	1:D:764:TYR:CE2	2.26	0.70
1:C:962:ARG:HG2	5:C:3149:HOH:O	1.91	0.70
1:D:763:ALA:HA	1:D:766:MET:CE	2.22	0.68
1:D:970:LYS:HE2	5:D:4244:HOH:O	1.94	0.68
1:A:737:LYS:CD	1:D:804:GLU:OE2	2.43	0.67
1:A:857:GLY:HA2	5:A:1251:HOH:O	1.95	0.66
1:B:734:GLU:HA	5:B:2110:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:790:MET:HE3	5:D:4190:HOH:O	1.95	0.66
1:C:807:ASP:HB2	5:C:3158:HOH:O	1.96	0.65
1:A:980:VAL:HG23	1:A:980:VAL:O	1.96	0.65
1:A:949:LYS:HD2	1:A:959:PRO:HG3	1.78	0.65
1:B:988:HIS:O	1:B:991:SER:HB2	1.97	0.65
1:D:752:SER:OG	1:D:753:PRO:HD3	1.95	0.65
1:A:960:LYS:HD3	5:A:1289:HOH:O	1.97	0.64
1:A:995:SER:O	1:A:999:ARG:HG3	1.97	0.64
1:B:850:HIS:CG	1:B:1007:MET:HE1	2.32	0.64
1:A:751:THR:HB	1:A:756:ASN:OD1	1.98	0.64
1:D:905:TRP:CG	1:D:947:MET:HE1	2.33	0.64
1:C:766[B]:MET:CE	1:C:856:PHE:CE1	2.80	0.64
1:A:935:GLN:HB2	1:A:944:TYR:CD2	2.33	0.63
1:A:960:LYS:HB2	1:A:963:GLU:HG3	1.81	0.63
1:C:984:ASP:HA	1:C:987:MET:HG2	1.80	0.63
1:A:944:TYR:CZ	1:A:948:ARG:HD3	2.33	0.63
1:C:991:SER:HB2	1:C:992:PRO:HD2	1.81	0.62
1:D:970:LYS:HA	1:D:973:ARG:NH1	2.14	0.62
1:D:905:TRP:CB	1:D:947:MET:CE	2.66	0.62
1:D:945:MET:HE3	1:D:945:MET:HA	1.81	0.62
1:D:960:LYS:HB2	1:D:963:GLU:HG3	1.82	0.62
1:A:790[B]:MET:HE2	2:A:1101:ANP:N6	2.15	0.62
1:B:746:GLU:OE1	1:B:785:THR:HG21	2.00	0.62
1:A:756:ASN:HA	1:A:759:ILE:HG13	1.81	0.61
1:B:919:PRO:HG2	1:B:922:GLU:OE1	2.00	0.61
1:A:855:ASP:CB	1:A:858:LEU:HD12	2.31	0.61
1:A:855:ASP:OD1	1:A:858:LEU:CD1	2.49	0.61
1:A:943:VAL:HG22	1:A:971:MET:CE	2.31	0.60
1:C:946:ILE:CD1	1:C:967:GLU:OE1	2.44	0.60
1:D:812:GLN:CG	1:D:989:LEU:HD13	2.31	0.60
1:A:926:ILE:HA	1:A:929:LYS:HE3	1.82	0.60
1:C:705:ARG:HD3	1:C:707:LEU:HD21	1.84	0.59
1:A:790[B]:MET:HE2	2:A:1101:ANP:HN61	1.65	0.59
1:D:719:GLY:HA3	2:D:4001:ANP:H4'	1.84	0.59
1:C:1008:ASP:CB	5:C:3148:HOH:O	2.50	0.59
1:A:732:ILE:HD12	1:A:732:ILE:N	2.18	0.59
1:D:944:TYR:CZ	1:D:948:ARG:HD3	2.37	0.59
1:D:703:LEU:HB2	5:D:4218:HOH:O	2.03	0.59
1:B:790[A]:MET:HE2	2:B:2001:ANP:HN61	1.67	0.59
1:C:999:ARG:CG	1:C:1007:MET:HE1	2.32	0.59
1:D:734:GLU:CD	5:D:4120:HOH:O	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:972:ALA:O	1:D:975:PRO:HD3	2.02	0.58
1:A:855:ASP:OD1	1:A:858:LEU:HD11	2.03	0.58
1:B:1013:ALA:HA	1:C:1006:ASP:HB2	1.85	0.58
1:D:783:THR:HG21	5:D:4199:HOH:O	2.02	0.58
1:B:963:GLU:O	1:B:967:GLU:HG3	2.03	0.58
1:C:762:GLU:OE1	1:C:766[B]:MET:HE3	2.04	0.58
1:C:955:ALA:O	1:C:958:ARG:HG3	2.04	0.58
1:A:766:MET:O	1:A:769:VAL:HG22	2.04	0.58
1:C:707:LEU:HD22	1:C:711:GLU:CD	2.30	0.57
1:B:723:PHE:HE2	5:B:2159:HOH:O	1.87	0.57
1:D:786:VAL:HG13	5:D:4153:HOH:O	2.05	0.57
1:B:766:MET:O	1:B:769:VAL:HG22	2.04	0.57
1:C:992:PRO:HG2	5:C:3192:HOH:O	2.05	0.57
1:D:748:ARG:O	1:D:862:LEU:HD22	2.05	0.57
1:A:935:GLN:HB2	1:A:944:TYR:CE2	2.39	0.56
1:D:995:SER:O	1:D:999:ARG:HG3	2.06	0.56
1:C:999:ARG:HG3	1:C:1007:MET:HE1	1.88	0.56
1:A:807:ASP:O	1:A:987:MET:HE1	2.05	0.56
1:D:905:TRP:HB2	1:D:947:MET:HE3	1.86	0.56
1:A:819:VAL:HG12	1:A:823:LYS:HE3	1.89	0.55
1:C:769[B]:VAL:HG13	1:C:827:TYR:HE2	1.70	0.55
1:B:879:LYS:HG2	1:B:915:TYR:HD1	1.71	0.55
1:D:949:LYS:HA	1:D:952:MET:HE2	1.88	0.55
1:D:986:ARG:NH1	5:D:4103:HOH:O	2.39	0.55
1:B:745:LYS:HB2	1:B:790[B]:MET:HE1	1.89	0.55
1:C:766[B]:MET:SD	1:C:856:PHE:CD1	2.99	0.55
1:D:788:LEU:C	1:D:789:ILE:HD12	2.32	0.55
1:A:705:ARG:NH2	1:A:711:GLU:OE1	2.39	0.55
1:B:919:PRO:HG2	1:B:922:GLU:CD	2.32	0.54
1:A:985:GLU:HG2	1:A:986:ARG:N	2.23	0.54
1:A:788:LEU:C	1:A:789:ILE:HD12	2.32	0.54
1:C:700:ASN:ND2	1:C:701:GLN:N	2.48	0.54
1:A:829:GLU:HG3	1:A:893:HIS:CG	2.43	0.54
1:A:943:VAL:HG22	1:A:971:MET:HE1	1.89	0.53
1:A:971:MET:HE2	1:A:978:TYR:CD2	2.44	0.53
1:D:883:LEU:HD23	1:D:953:ILE:HD12	1.91	0.53
1:C:762:GLU:HG3	1:C:766[B]:MET:HE3	1.91	0.53
1:B:714:LYS:HE3	1:B:787:GLN:OE1	2.09	0.52
1:C:999:ARG:HH21	1:C:999:ARG:CG	2.12	0.52
1:B:719:GLY:HA3	2:B:2001:ANP:H4'	1.92	0.52
1:D:734:GLU:HB3	5:D:4120:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:905:TRP:CA	1:D:947:MET:HE1	2.40	0.51
1:A:844:LEU:HD21	5:A:1238:HOH:O	2.09	0.51
1:C:835:HIS:O	1:C:836:ARG:HB2	2.09	0.51
1:C:985:GLU:HG2	1:C:986:ARG:N	2.25	0.51
1:A:995:SER:HB3	5:A:1351:HOH:O	2.09	0.51
1:B:926:ILE:HD12	1:B:931:GLU:HB2	1.93	0.51
1:C:984:ASP:HA	1:C:987:MET:CG	2.40	0.51
1:C:877:PRO:O	1:C:881:MET:HG3	2.09	0.51
1:D:734:GLU:CB	5:D:4120:HOH:O	2.59	0.51
1:D:923:ILE:O	1:D:926:ILE:HG13	2.10	0.51
1:B:699:PRO:HB3	5:B:2289:HOH:O	2.10	0.50
1:A:855:ASP:HB3	1:A:858:LEU:HD12	1.93	0.50
1:C:932:ARG:NH2	1:C:953:ILE:HD11	2.23	0.50
1:B:833:LEU:HD13	1:B:856:PHE:CZ	2.46	0.50
1:D:723:PHE:CE1	1:D:859:ALA:HA	2.47	0.50
1:D:747:LEU:HD12	1:D:786:VAL:HG21	1.93	0.50
1:A:790[B]:MET:HE3	5:A:1224:HOH:O	2.11	0.50
1:C:999:ARG:HD2	1:C:1007:MET:HE1	1.94	0.50
1:D:905:TRP:HD1	1:D:947:MET:HE1	1.76	0.50
1:A:943:VAL:CG2	1:A:971:MET:HE1	2.41	0.49
1:D:949:LYS:CB	1:D:952:MET:HE2	2.41	0.49
1:C:769[B]:VAL:HG13	1:C:827:TYR:CE2	2.47	0.49
1:D:925:SER:O	1:D:929:LYS:HG3	2.11	0.49
1:A:833:LEU:HB3	1:A:856:PHE:CE2	2.47	0.49
1:B:923:ILE:HG22	1:B:927:LEU:HD22	1.94	0.49
1:C:762:GLU:OE1	1:C:766[B]:MET:CE	2.60	0.49
1:D:754:LYS:HD3	1:D:758:GLU:HG2	1.95	0.49
1:D:949:LYS:O	1:D:952:MET:HG3	2.13	0.49
1:C:700:ASN:CG	1:C:701:GLN:H	2.20	0.49
1:C:898:TRP:CD1	1:C:898:TRP:C	2.91	0.49
1:A:943:VAL:CG2	1:A:971:MET:CE	2.91	0.48
1:B:823:LYS:HA	1:B:965:ILE:HD11	1.95	0.48
1:D:789:ILE:HD12	1:D:789:ILE:N	2.28	0.48
1:B:726:VAL:CG2	2:B:2001:ANP:H5'1	2.42	0.48
1:B:855:ASP:HA	1:B:858:LEU:HD13	1.94	0.48
1:B:931:GLU:O	1:B:932:ARG:HD3	2.14	0.48
1:C:812:GLN:HE22	1:C:1013:ALA:N	2.11	0.48
1:A:971:MET:HE2	1:A:978:TYR:HB3	1.96	0.48
1:C:806:LYS:O	1:C:807:ASP:HB2	2.14	0.48
1:D:786:VAL:CG1	5:D:4153:HOH:O	2.60	0.48
1:D:924:SER:HB3	5:D:4110:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:723:PHE:HZ	1:C:862:LEU:C	2.22	0.48
1:B:810:GLY:CA	5:B:2189:HOH:O	2.47	0.48
1:A:751:THR:CB	1:A:756:ASN:OD1	2.60	0.47
1:D:762:GLU:OE2	1:D:861:LEU:CD1	2.63	0.47
1:D:790:MET:CE	5:D:4190:HOH:O	2.55	0.47
1:D:949:LYS:HG2	1:D:952:MET:HE2	1.95	0.47
1:D:960:LYS:HD2	5:D:4105:HOH:O	2.14	0.47
1:A:857:GLY:CA	5:A:1251:HOH:O	2.57	0.47
1:C:788:LEU:C	1:C:789:ILE:HD12	2.39	0.47
1:B:790[A]:MET:HE1	1:B:854:THR:OG1	2.14	0.47
1:B:771:ASN:CG	1:B:772:PRO:HD2	2.39	0.47
1:A:960:LYS:HD2	1:A:960:LYS:HA	1.68	0.47
1:A:1005:GLU:HG3	5:A:1208:HOH:O	2.15	0.47
1:B:942:ASP:HA	1:B:945:MET:HE2	1.97	0.46
1:C:827:TYR:HB2	5:C:3255:HOH:O	2.14	0.46
1:A:941:ILE:HD11	1:A:945:MET:SD	2.55	0.46
1:D:707:LEU:HD22	1:D:711:GLU:CD	2.41	0.46
1:C:707:LEU:HD22	1:C:711:GLU:OE2	2.15	0.46
1:C:766[B]:MET:SD	1:C:857:GLY:HA3	2.56	0.46
1:A:949:LYS:O	1:A:952:MET:HG2	2.16	0.46
1:B:811:SER:OG	1:B:975:PRO:HB2	2.16	0.46
1:D:808:ASN:CB	5:D:4212:HOH:O	2.53	0.46
1:D:884:GLU:HG2	1:D:885:SER:N	2.30	0.46
1:C:905:TRP:HB2	1:C:947:MET:CE	2.46	0.46
1:B:905:TRP:HB2	1:B:947:MET:HE3	1.97	0.46
1:C:879:LYS:HG2	1:C:915:TYR:CD1	2.51	0.46
1:A:855:ASP:CG	1:A:858:LEU:CD1	2.89	0.46
1:B:879:LYS:HG2	1:B:915:TYR:CD1	2.50	0.45
1:B:755:ALA:O	1:B:759[A]:ILE:HG12	2.16	0.45
1:C:945:MET:O	1:C:949:LYS:HG3	2.16	0.45
1:D:715:ILE:HD11	1:D:728:LYS:HE3	1.98	0.45
1:D:808:ASN:ND2	5:D:4111:HOH:O	2.49	0.45
1:C:705:ARG:HE	1:C:707:LEU:CD2	2.28	0.45
1:B:788:LEU:C	1:B:789:ILE:HD12	2.42	0.45
1:D:811:SER:OG	1:D:975:PRO:HB2	2.15	0.45
1:A:924:SER:O	1:A:928:GLU:HG3	2.17	0.45
1:B:769:VAL:HG23	1:B:769:VAL:O	2.17	0.45
1:B:812[B]:GLN:CG	5:B:2189:HOH:O	2.47	0.45
1:B:1005:GLU:HG3	1:C:1004:GLU:OE2	2.17	0.45
1:C:716:LYS:NZ	5:C:3101:HOH:O	2.37	0.45
1:C:1012:ASP:CB	5:C:3262:HOH:O	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:ILE:O	1:A:945:MET:HG3	2.17	0.45
1:B:835:HIS:O	1:B:836:ARG:HB2	2.17	0.45
1:B:769:VAL:HG21	5:B:2133:HOH:O	2.17	0.45
1:B:772:PRO:O	1:B:852:LYS:HE3	2.16	0.44
1:B:812[B]:GLN:NE2	5:B:2109:HOH:O	2.43	0.44
1:D:883:LEU:CD2	1:D:953:ILE:HD12	2.47	0.44
1:D:883:LEU:HB3	5:D:4178:HOH:O	2.18	0.44
1:A:977:ARG:HD2	5:A:1358:HOH:O	2.15	0.44
1:B:1001:LEU:HD21	1:C:742:VAL:HG12	1.98	0.44
1:D:723:PHE:HB3	1:D:862:LEU:CD1	2.47	0.44
1:D:898:TRP:CD1	1:D:898:TRP:C	2.95	0.44
1:A:783:THR:OG1	1:A:785:THR:O	2.30	0.44
1:D:949:LYS:CA	1:D:952:MET:HE2	2.46	0.44
1:B:790[A]:MET:HE2	2:B:2001:ANP:N6	2.32	0.44
1:B:850:HIS:CE1	1:B:1007:MET:CE	2.89	0.44
1:A:971:MET:CE	1:A:978:TYR:CD2	3.01	0.44
1:B:970:LYS:HA	1:B:973:ARG:NH1	2.32	0.44
1:A:980:VAL:O	1:A:980:VAL:CG2	2.62	0.44
1:B:708:LYS:O	1:B:711:GLU:HB2	2.18	0.44
1:C:905:TRP:CD1	1:C:947:MET:HE1	2.53	0.44
1:B:785:THR:HG23	1:B:787:GLN:HG3	2.00	0.44
1:D:807:ASP:C	5:D:4154:HOH:O	2.61	0.44
1:B:970:LYS:O	1:B:973:ARG:HB2	2.18	0.43
1:C:905:TRP:CB	1:C:947:MET:HE1	2.48	0.43
1:C:1003:ASP:CG	1:C:1007:MET:HE3	2.41	0.43
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.52	0.43
1:A:855:ASP:CA	1:A:858:LEU:HD12	2.48	0.43
1:C:766[B]:MET:SD	1:C:856:PHE:CE1	3.11	0.43
1:C:999:ARG:NH2	5:C:3108:HOH:O	2.41	0.43
1:D:747:LEU:HB2	1:D:786:VAL:HG13	2.00	0.43
1:B:991:SER:HA	1:B:992:PRO:HD3	1.85	0.43
1:A:789:ILE:HD12	1:A:789:ILE:N	2.33	0.43
1:C:922:GLU:O	1:C:926:ILE:HG23	2.17	0.43
1:D:1002:MET:HE2	5:D:4185:HOH:O	2.17	0.43
1:B:1006:ASP:CG	5:B:2108:HOH:O	2.62	0.43
1:C:700:ASN:HD22	1:C:701:GLN:H	1.59	0.43
1:B:952:MET:HE3	1:B:957:SER:HB3	2.00	0.43
1:C:932:ARG:NH2	1:C:953:ILE:CD1	2.82	0.43
1:D:721:GLY:HA3	5:D:4157:HOH:O	2.18	0.43
1:B:1001:LEU:HD13	1:C:740:ILE:HG21	2.00	0.42
1:C:941:ILE:HG23	1:C:945:MET:HE3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:ARG:HD3	1:D:997:PHE:CG	2.54	0.42
1:C:726:VAL:CG2	2:C:3001:ANP:H5'1	2.49	0.42
1:D:825:MET:HG2	1:D:853:ILE:HD11	2.00	0.42
1:D:717:VAL:HG22	1:D:727:TYR:CE2	2.54	0.42
1:D:707:LEU:HD23	1:D:707:LEU:HA	1.89	0.42
1:D:710:THR:HB	5:D:4194:HOH:O	2.19	0.42
1:D:888:HIS:HB2	1:D:890:ILE:HG23	2.01	0.42
1:A:832:ARG:NH1	5:A:1210:HOH:O	2.53	0.42
1:B:748:ARG:HG3	1:D:830:ASP:HA	2.02	0.42
1:A:905:TRP:HD1	1:A:947:MET:HE1	1.84	0.41
1:A:944:TYR:OH	1:A:948:ARG:HD3	2.19	0.41
1:B:723:PHE:CD2	5:B:2193:HOH:O	2.52	0.41
1:A:971:MET:HG2	1:A:978:TYR:CG	2.56	0.41
1:B:942:ASP:HA	1:B:945:MET:CE	2.50	0.41
1:C:905:TRP:HB2	1:C:947:MET:HE1	2.01	0.41
1:C:970:LYS:O	1:C:973:ARG:HB2	2.20	0.41
1:B:771:ASN:HA	1:B:772:PRO:HD3	1.90	0.41
1:B:926:ILE:HG13	1:B:927:LEU:N	2.34	0.41
1:D:794:PRO:HD2	5:D:4185:HOH:O	2.19	0.41
1:C:855:ASP:OD1	1:C:858:LEU:HD12	2.20	0.41
1:D:708:LYS:O	1:D:711:GLU:HB2	2.20	0.41
1:D:782:LEU:HD12	1:D:782:LEU:HA	1.77	0.41
5:A:1293:HOH:O	1:C:716:LYS:CE	2.50	0.41
1:C:700:ASN:CG	1:C:701:GLN:N	2.79	0.41
1:C:705:ARG:HD3	1:C:707:LEU:CD2	2.51	0.41
1:C:766[A]:MET:HE2	1:C:777:LEU:HD22	2.02	0.41
1:C:1003:ASP:OD1	1:C:1007:MET:CE	2.53	0.41
1:D:883:LEU:CD2	1:D:953:ILE:CD1	2.98	0.41
1:D:944:TYR:O	1:D:948:ARG:HG2	2.21	0.41
1:A:849:GLN:CG	5:A:1351:HOH:O	2.62	0.40
1:A:905:TRP:HB2	1:A:947:MET:HE3	2.03	0.40
1:A:923:ILE:HG22	1:A:927:LEU:HD22	2.03	0.40
1:A:945:MET:HE2	1:A:945:MET:HB3	1.91	0.40
1:C:766[B]:MET:CE	1:C:856:PHE:HE1	2.33	0.40
1:C:905:TRP:O	1:C:909:THR:HG23	2.22	0.40
1:C:962:ARG:HE	1:C:962:ARG:HB3	1.69	0.40
1:C:999:ARG:CD	1:C:1007:MET:HE1	2.50	0.40
1:D:824:GLY:HA3	1:D:853:ILE:HD12	2.03	0.40
1:D:701:GLN:CG	1:D:764:TYR:CE2	3.02	0.40
1:A:995:SER:H	1:A:995:SER:HG	1.57	0.40
1:B:754:LYS:HB2	1:B:759[A]:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:769:VAL:CG2	1:B:776:ARG:HA	2.52	0.40
5:B:2214:HOH:O	1:C:700:ASN:HB2	2.21	0.40
1:C:879:LYS:NZ	5:C:3124:HOH:O	2.53	0.40
1:A:908:MET:HG3	1:A:939:CYS:SG	2.61	0.40
1:B:813:TYR:CZ	1:B:990:PRO:HG2	2.55	0.40
1:D:935:GLN:HA	1:D:936:PRO:HD3	1.93	0.40
1:C:999:ARG:NH2	1:C:999:ARG:CG	2.70	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	295/331 (89%)	291 (99%)	4 (1%)	0	100	100
1	B	312/331 (94%)	307 (98%)	5 (2%)	0	100	100
1	C	302/331 (91%)	299 (99%)	3 (1%)	0	100	100
1	D	289/331 (87%)	284 (98%)	5 (2%)	0	100	100
All	All	1198/1324 (90%)	1181 (99%)	17 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/290 (90%)	244 (94%)	17 (6%)	15	6
1	B	274/290 (94%)	255 (93%)	19 (7%)	14	5
1	C	265/290 (91%)	245 (92%)	20 (8%)	12	4
1	D	255/290 (88%)	234 (92%)	21 (8%)	10	3
All	All	1055/1160 (91%)	978 (93%)	77 (7%)	13	4

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	706	ILE
1	A	720	SER
1	A	752	SER
1	A	754	LYS
1	A	759	ILE
1	A	782	LEU
1	A	783	THR
1	A	785	THR
1	A	786	VAL
1	A	806	LYS
1	A	927	LEU
1	A	941	ILE
1	A	949	LYS
1	A	986	ARG
1	A	991[A]	SER
1	A	991[B]	SER
1	A	995	SER
1	B	700	ASN
1	B	713	LYS
1	B	716	LYS
1	B	760	LEU
1	B	785	THR
1	B	786	VAL
1	B	876	VAL
1	B	926	ILE
1	B	927	LEU
1	B	929	LYS
1	B	931	GLU
1	B	952	MET
1	B	973	ARG
1	B	985	GLU
1	B	1001	LEU
1	B	1007	MET

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Mol	Chain	Res	Type
1	B	1009	ASP
1	B	1010	VAL
1	B	1012	ASP
1	C	701	GLN
1	C	714	LYS
1	C	749	GLU
1	C	782	LEU
1	C	783	THR
1	C	804	GLU
1	C	806	LYS
1	C	876	VAL
1	C	913	LYS
1	C	925	SER
1	C	926	ILE
1	C	927	LEU
1	C	941	ILE
1	C	947	MET
1	C	962	ARG
1	C	976	GLN
1	C	982	GLN
1	C	989	LEU
1	C	999	ARG
1	C	1007	MET
1	D	710	THR
1	D	714	LYS
1	D	748	ARG
1	D	782	LEU
1	D	784	SER
1	D	786	VAL
1	D	790	MET
1	D	804	GLU
1	D	861	LEU
1	D	890	ILE
1	D	921	SER
1	D	926	ILE
1	D	927	LEU
1	D	928	GLU
1	D	962	ARG
1	D	986	ARG
1	D	987	MET
1	D	989	LEU
1	D	995	SER

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Mol	Chain	Res	Type
1	D	998	TYR
1	D	1005	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	771	ASN
1	A	812	GLN
1	A	826	ASN
1	A	888	HIS
1	C	700	ASN
1	C	701	GLN
1	C	805	HIS
1	C	812	GLN
1	D	808	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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	EDO	C	3003	-	3,3,3	0.31	0	2,2,2	0.62	0
2	ANP	A	1101	3	33,33,33	2.08	11 (33%)	45,52,52	2.04	14 (31%)
2	ANP	D	4001	3	33,33,33	1.95	10 (30%)	45,52,52	2.06	14 (31%)
2	ANP	C	3001	3	33,33,33	1.95	11 (33%)	45,52,52	2.19	15 (33%)
2	ANP	B	2001	3	33,33,33	2.02	10 (30%)	45,52,52	1.97	14 (31%)

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	EDO	C	3003	-	-	1/1/1/1	-
2	ANP	A	1101	3	-	3/18/38/38	0/3/3/3
2	ANP	D	4001	3	-	3/18/38/38	0/3/3/3
2	ANP	C	3001	3	-	7/18/38/38	0/3/3/3
2	ANP	B	2001	3	-	9/18/38/38	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	ANP	PB-O2B	-4.76	1.44	1.56
2	D	4001	ANP	PB-O2B	-4.66	1.44	1.56
2	B	2001	ANP	PB-O2B	-4.19	1.45	1.56
2	A	1101	ANP	PG-O2G	-4.16	1.45	1.56
2	C	3001	ANP	PB-O2B	-4.15	1.45	1.56
2	C	3001	ANP	C5-N7	-4.00	1.31	1.39
2	D	4001	ANP	PG-O3G	-3.97	1.46	1.56
2	B	2001	ANP	PB-O1B	-3.97	1.40	1.46
2	A	1101	ANP	C5-N7	-3.93	1.31	1.39
2	D	4001	ANP	C5-N7	-3.81	1.32	1.39
2	C	3001	ANP	PG-O2G	-3.76	1.46	1.56
2	B	2001	ANP	PG-O3G	-3.73	1.46	1.56
2	B	2001	ANP	C5-N7	-3.72	1.32	1.39
2	B	2001	ANP	C8-N9	-3.34	1.31	1.37
2	B	2001	ANP	C5-C4	-3.32	1.33	1.39
2	D	4001	ANP	C5-C4	-3.28	1.33	1.39
2	A	1101	ANP	C5-C4	-3.28	1.33	1.39
2	D	4001	ANP	C8-N9	-3.22	1.32	1.37
2	C	3001	ANP	C5-C4	-3.20	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3001	ANP	PA-O3A	-3.14	1.56	1.59
2	C	3001	ANP	C8-N9	-3.14	1.32	1.37
2	A	1101	ANP	C8-N9	-3.14	1.32	1.37
2	B	2001	ANP	C5-C6	-3.04	1.32	1.41
2	D	4001	ANP	C5-C6	-2.97	1.32	1.41
2	A	1101	ANP	C4-N9	-2.91	1.31	1.37
2	A	1101	ANP	C5-C6	-2.79	1.33	1.41
2	A	1101	ANP	PG-N3B	-2.78	1.56	1.63
2	B	2001	ANP	C4-N9	-2.78	1.31	1.37
2	C	3001	ANP	C5-C6	-2.74	1.33	1.41
2	C	3001	ANP	C2-N1	2.62	1.38	1.33
2	D	4001	ANP	C4-N9	-2.57	1.32	1.37
2	A	1101	ANP	C2-N1	2.46	1.38	1.33
2	B	2001	ANP	C2-N1	2.45	1.38	1.33
2	B	2001	ANP	PA-O2A	-2.44	1.44	1.55
2	D	4001	ANP	C2-N1	2.42	1.38	1.33
2	C	3001	ANP	C4-N9	-2.41	1.32	1.37
2	A	1101	ANP	PA-O2A	-2.39	1.44	1.55
2	A	1101	ANP	C2-N3	2.24	1.37	1.33
2	C	3001	ANP	PA-O2A	-2.21	1.45	1.55
2	D	4001	ANP	C2-N3	2.20	1.37	1.33
2	C	3001	ANP	C2-N3	2.20	1.37	1.33
2	D	4001	ANP	PA-O2A	-2.10	1.45	1.55

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4001	ANP	N3-C2-N1	-6.66	118.51	128.58
2	B	2001	ANP	N3-C2-N1	-6.59	118.61	128.58
2	A	1101	ANP	N3-C2-N1	-6.58	118.62	128.58
2	C	3001	ANP	N3-C2-N1	-6.04	119.44	128.58
2	C	3001	ANP	O1B-PB-N3B	-4.85	104.62	111.77
2	C	3001	ANP	C5-C4-N3	-4.67	120.28	126.72
2	D	4001	ANP	O2B-PB-O1B	4.46	119.44	109.87
2	D	4001	ANP	C5-C4-N3	-4.42	120.64	126.72
2	A	1101	ANP	C5-C4-N3	-4.38	120.69	126.72
2	C	3001	ANP	O2B-PB-O1B	4.21	118.89	109.87
2	A	1101	ANP	O2B-PB-O1B	4.14	118.75	109.87
2	B	2001	ANP	N9-C8-N7	-4.04	108.20	113.94
2	A	1101	ANP	N9-C8-N7	-3.92	108.38	113.94
2	B	2001	ANP	C5-C4-N3	-3.89	121.35	126.72
2	C	3001	ANP	N9-C8-N7	-3.62	108.81	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4001	ANP	N9-C8-N7	-3.51	108.95	113.94
2	C	3001	ANP	O3G-PG-O1G	-3.38	104.98	113.45
2	B	2001	ANP	O2B-PB-O1B	3.35	117.05	109.87
2	D	4001	ANP	C2-N3-C4	3.27	119.81	111.83
2	A	1101	ANP	C2-N3-C4	3.25	119.77	111.83
2	C	3001	ANP	C5-N7-C8	3.12	108.36	103.45
2	C	3001	ANP	C2-N3-C4	3.09	119.39	111.83
2	B	2001	ANP	C2-N3-C4	3.05	119.29	111.83
2	A	1101	ANP	C5-N7-C8	3.02	108.19	103.45
2	A	1101	ANP	O1B-PB-N3B	-2.99	107.37	111.77
2	B	2001	ANP	C5-N7-C8	2.97	108.12	103.45
2	A	1101	ANP	C4-C5-N7	-2.79	107.39	110.58
2	C	3001	ANP	C4-C5-N7	-2.79	107.39	110.58
2	C	3001	ANP	C6-C5-C4	2.79	120.98	117.18
2	B	2001	ANP	C4-C5-N7	-2.73	107.47	110.58
2	D	4001	ANP	C5-N7-C8	2.72	107.73	103.45
2	A	1101	ANP	C6-C5-C4	2.70	120.86	117.18
2	C	3001	ANP	O2G-PG-O1G	2.67	120.14	113.45
2	B	2001	ANP	O1B-PB-N3B	-2.62	107.92	111.77
2	D	4001	ANP	C5-C6-N6	-2.60	116.84	123.29
2	D	4001	ANP	C4-C5-N7	-2.57	107.65	110.58
2	C	3001	ANP	N3-C4-N9	2.49	131.40	127.17
2	D	4001	ANP	C6-C5-C4	2.49	120.57	117.18
2	D	4001	ANP	C5-C4-N9	2.45	108.48	105.81
2	D	4001	ANP	O1B-PB-N3B	-2.42	108.20	111.77
2	A	1101	ANP	C5-C6-N6	-2.41	117.31	123.29
2	B	2001	ANP	C5-C6-N6	-2.39	117.36	123.29
2	D	4001	ANP	O3G-PG-O1G	2.39	119.44	113.45
2	A	1101	ANP	C5-C4-N9	2.39	108.42	105.81
2	C	3001	ANP	C5-C6-N6	-2.38	117.40	123.29
2	C	3001	ANP	C5-C4-N9	2.30	108.31	105.81
2	B	2001	ANP	C6-C5-C4	2.23	120.23	117.18
2	D	4001	ANP	O4'-C1'-N9	-2.23	103.81	108.09
2	A	1101	ANP	N3-C4-N9	2.19	130.89	127.17
2	D	4001	ANP	N3-C4-N9	2.19	130.88	127.17
2	B	2001	ANP	C5-C4-N9	2.18	108.18	105.81
2	B	2001	ANP	C4-N9-C8	2.17	108.02	105.74
2	C	3001	ANP	O1G-PG-N3B	-2.14	108.61	111.77
2	A	1101	ANP	O2G-PG-O1G	2.12	118.76	113.45
2	B	2001	ANP	O2G-PG-O1G	-2.11	108.17	113.45
2	A	1101	ANP	O3G-PG-O1G	-2.10	108.19	113.45
2	B	2001	ANP	O3G-PG-O1G	2.08	118.67	113.45

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	ANP	PB-N3B-PG-O1G
2	A	1101	ANP	PA-O3A-PB-O2B
2	A	1101	ANP	C5'-O5'-PA-O2A
2	B	2001	ANP	PG-N3B-PB-O3A
2	B	2001	ANP	PA-O3A-PB-O2B
2	B	2001	ANP	C5'-O5'-PA-O1A
2	B	2001	ANP	C5'-O5'-PA-O3A
2	C	3001	ANP	PB-N3B-PG-O1G
2	C	3001	ANP	PA-O3A-PB-O2B
2	C	3001	ANP	C5'-O5'-PA-O2A
2	D	4001	ANP	PG-N3B-PB-O3A
2	B	2001	ANP	O4'-C4'-C5'-O5'
2	B	2001	ANP	C3'-C4'-C5'-O5'
2	C	3001	ANP	PG-N3B-PB-O3A
2	B	2001	ANP	C5'-O5'-PA-O2A
2	C	3001	ANP	C5'-O5'-PA-O3A
4	C	3003	EDO	O1-C1-C2-O2
2	B	2001	ANP	PG-N3B-PB-O1B
2	D	4001	ANP	PA-O3A-PB-O2B
2	C	3001	ANP	C3'-C4'-C5'-O5'
2	B	2001	ANP	PA-O3A-PB-O1B
2	C	3001	ANP	PA-O3A-PB-O1B
2	D	4001	ANP	PA-O3A-PB-O1B

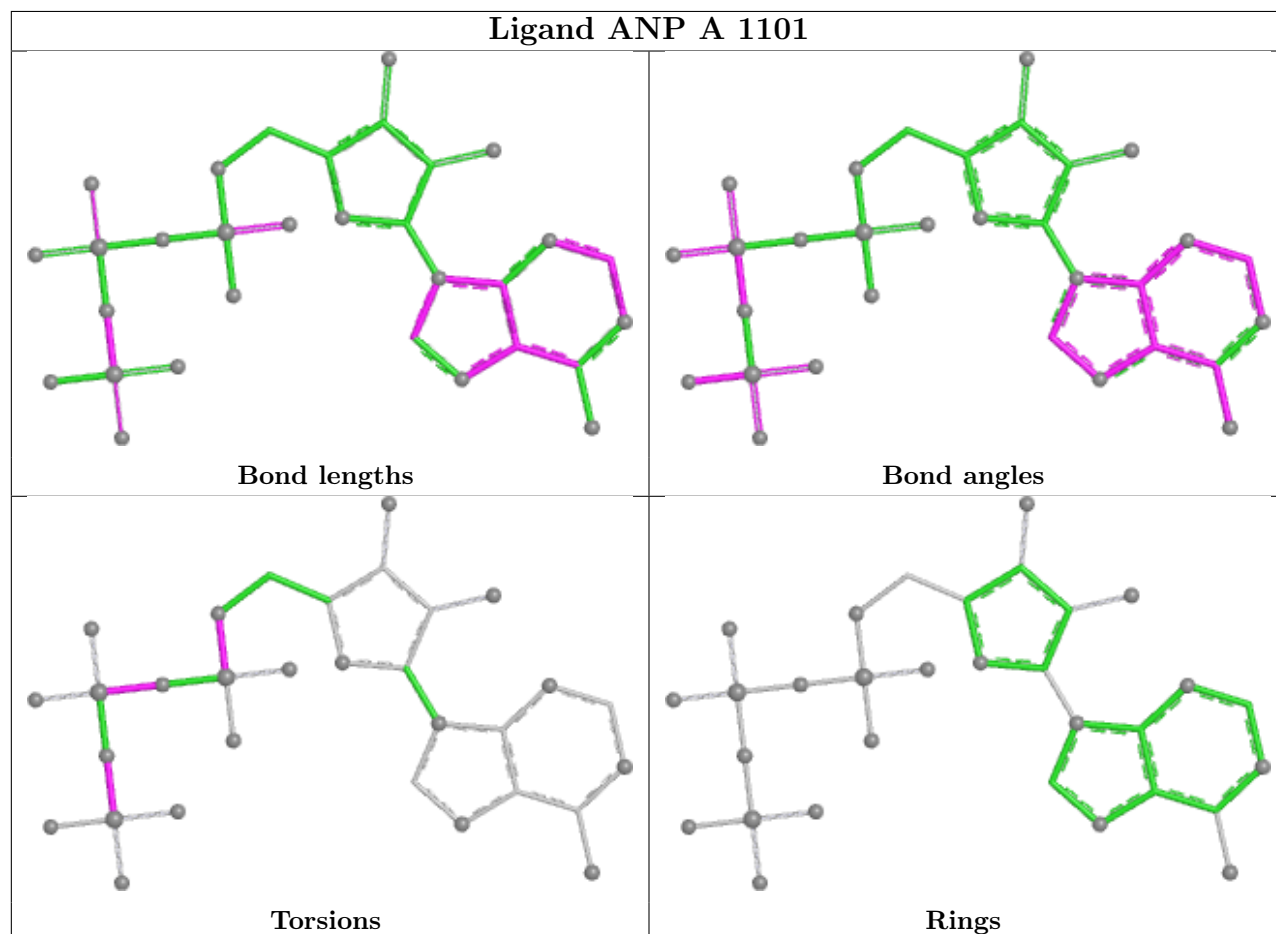
There are no ring outliers.

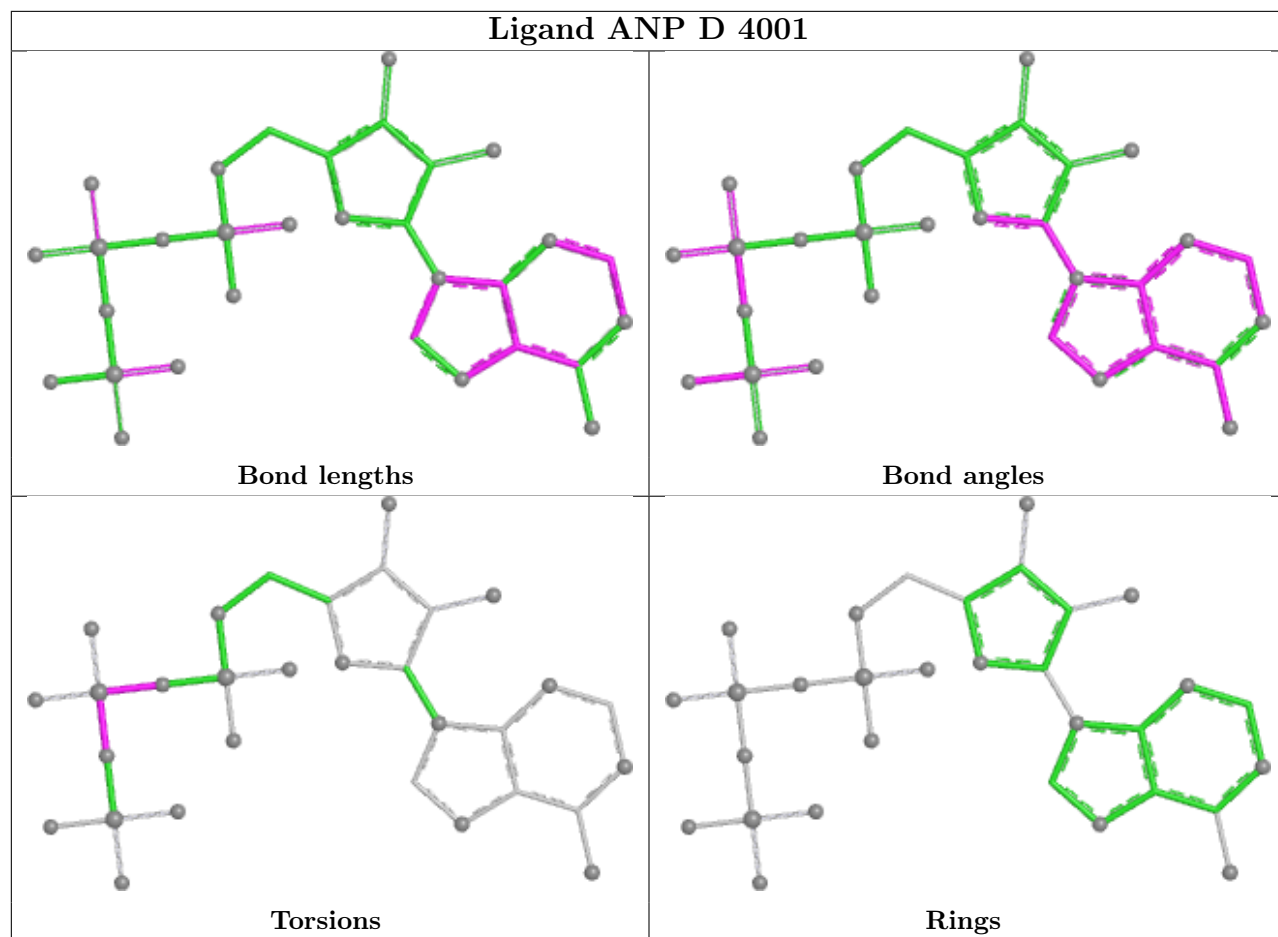
4 monomers are involved in 9 short contacts:

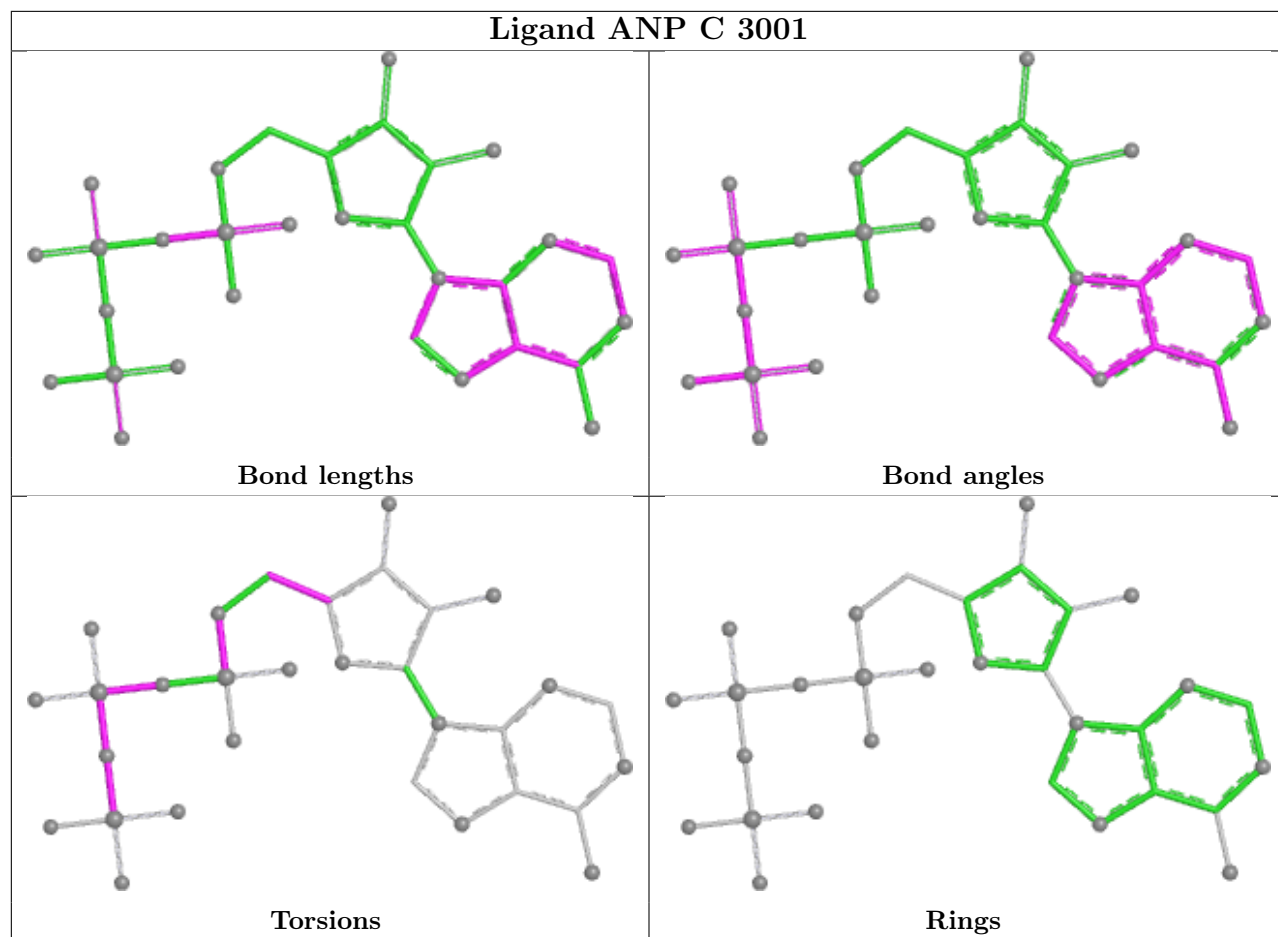
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	ANP	2	0
2	D	4001	ANP	1	0
2	C	3001	ANP	2	0
2	B	2001	ANP	4	0

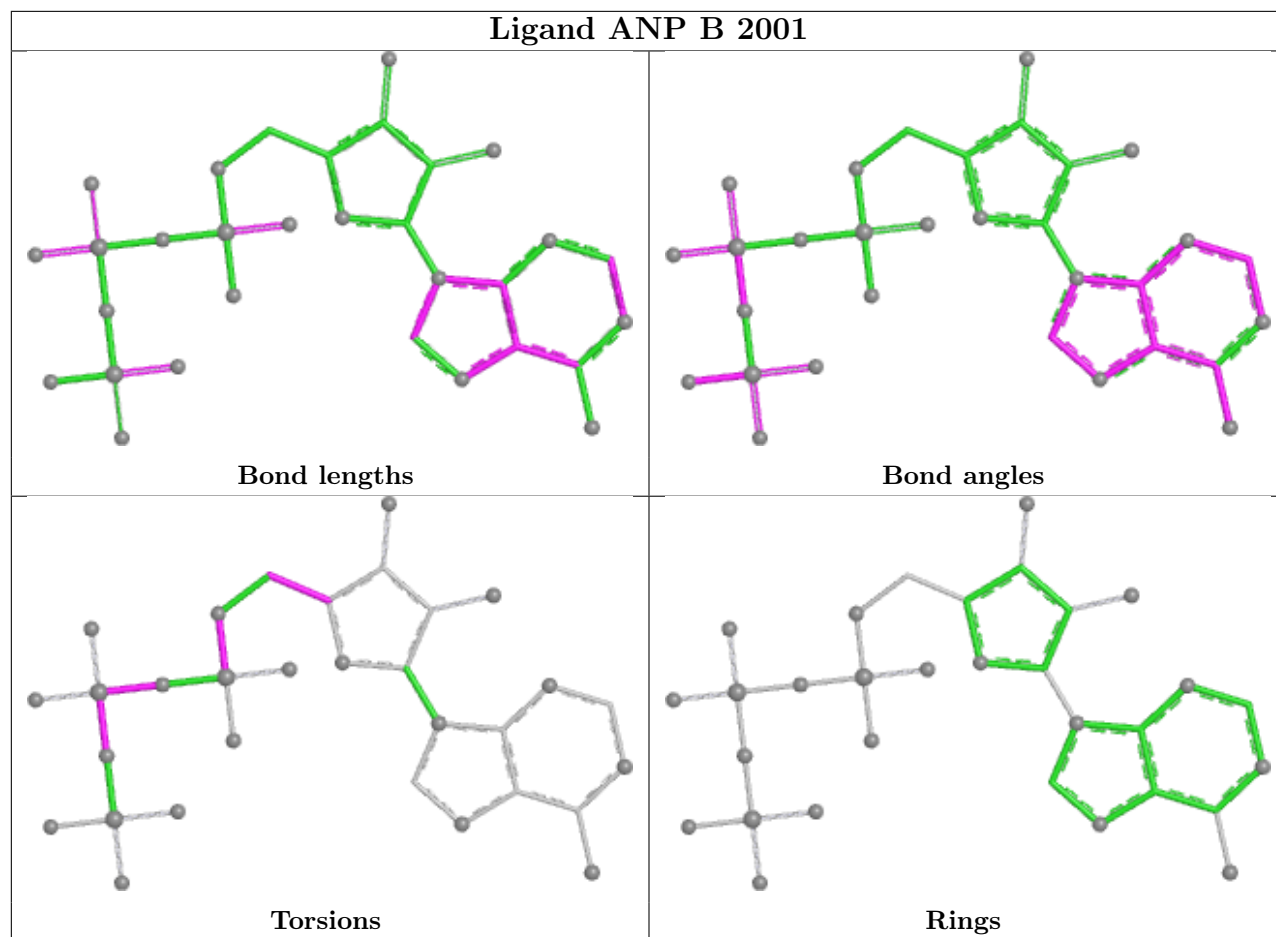
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	297/331 (89%)	0.16	15 (5%)	33 43	12, 26, 60, 78	3 (1%)
1	B	313/331 (94%)	0.04	12 (3%)	44 54	13, 25, 47, 72	5 (1%)
1	C	301/331 (90%)	0.39	14 (4%)	36 46	11, 30, 51, 66	19 (6%)
1	D	297/331 (89%)	0.24	12 (4%)	42 52	15, 30, 51, 73	1 (0%)
All	All	1208/1324 (91%)	0.21	53 (4%)	39 49	11, 28, 52, 78	28 (2%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1006	ASP	5.6
1	C	1011	VAL	4.5
1	A	751	THR	4.5
1	A	755	ALA	4.2
1	A	753	PRO	4.2
1	B	1013	ALA	3.9
1	D	1013	ALA	3.9
1	A	750	ALA	3.8
1	A	807	ASP	3.7
1	A	752	SER	3.4
1	B	699	PRO	3.2
1	B	1022	GLY	3.1
1	A	1007	MET	3.0
1	B	1011	VAL	3.0
1	D	753	PRO	3.0
1	A	861	LEU	2.8
1	C	979	LEU	2.8
1	D	748	ARG	2.8
1	A	991[A]	SER	2.7
1	A	988	HIS	2.7
1	C	700	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	861	LEU	2.7
1	B	698	ALA	2.6
1	B	750	ALA	2.6
1	C	918	ILE	2.6
1	A	699	PRO	2.6
1	A	785	THR	2.6
1	A	783	THR	2.6
1	A	756	ASN	2.5
1	C	722	ALA	2.5
1	C	940	THR	2.5
1	B	784	SER	2.5
1	C	1007	MET	2.5
1	B	1008	ASP	2.5
1	C	1013	ALA	2.5
1	B	1009	ASP	2.4
1	C	1008	ASP	2.4
1	D	752	SER	2.4
1	B	1010	VAL	2.3
1	D	1010	VAL	2.3
1	B	751	THR	2.3
1	D	920	ALA	2.3
1	D	989	LEU	2.3
1	D	764	TYR	2.2
1	D	926	ILE	2.2
1	D	863	GLY	2.2
1	C	941	ILE	2.1
1	A	782	LEU	2.1
1	D	860	LYS	2.1
1	B	723	PHE	2.1
1	C	981	ILE	2.1
1	D	1012	ASP	2.1
1	C	1010	VAL	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](#)

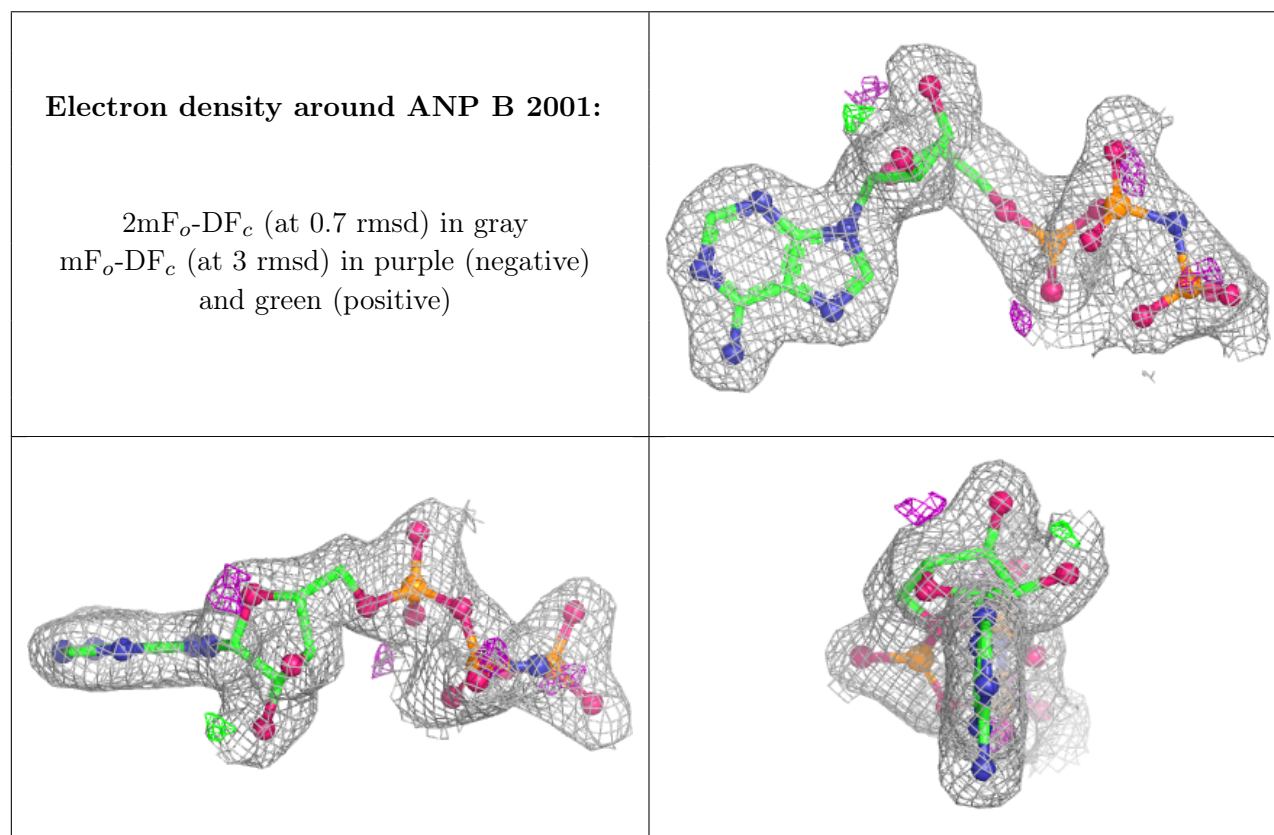
There are no oligosaccharides in this entry.

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.

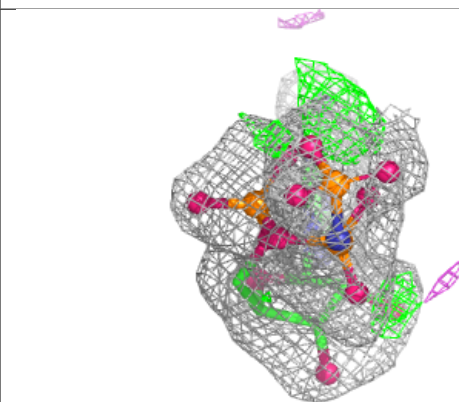
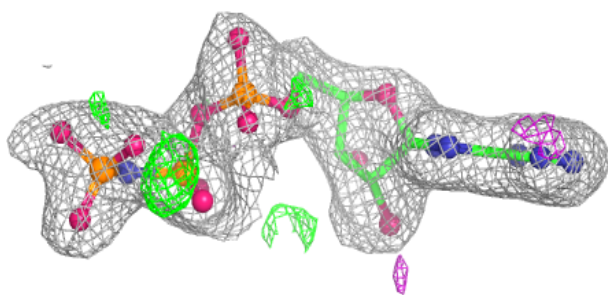
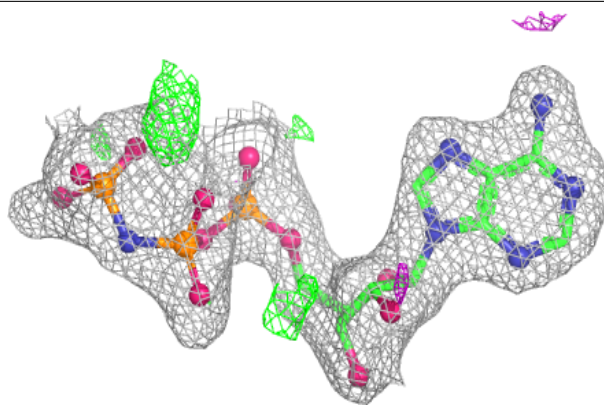
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	C	3003	4/4	0.90	0.10	39,39,41,52	0
3	MG	D	4002	1/1	0.92	0.06	27,27,27,27	0
2	ANP	B	2001	31/31	0.95	0.07	19,27,34,36	0
2	ANP	D	4001	31/31	0.95	0.07	19,28,35,43	0
2	ANP	C	3001	31/31	0.96	0.06	17,28,34,38	0
2	ANP	A	1101	31/31	0.96	0.06	12,22,29,35	0
3	MG	A	1102	1/1	0.97	0.04	24,24,24,24	0
3	MG	C	3002	1/1	0.97	0.05	35,35,35,35	0
3	MG	B	2002	1/1	0.98	0.07	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.

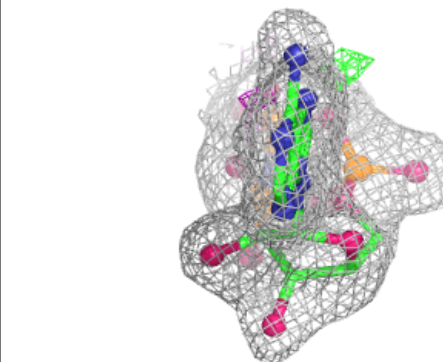
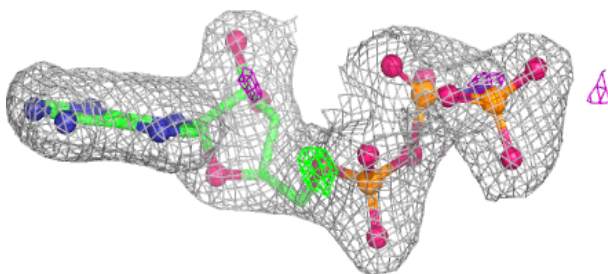
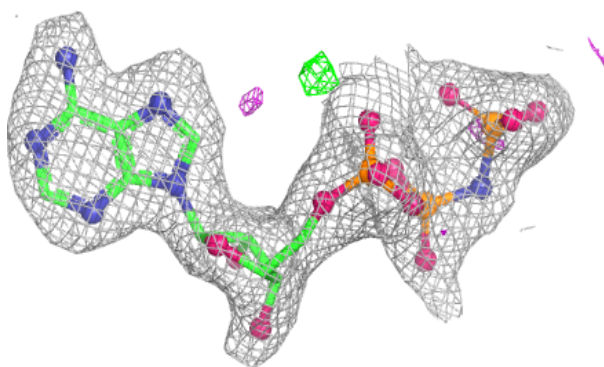


Electron density around ANP D 4001:

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

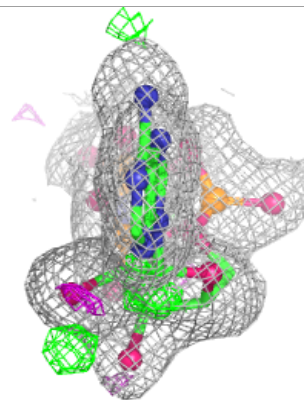
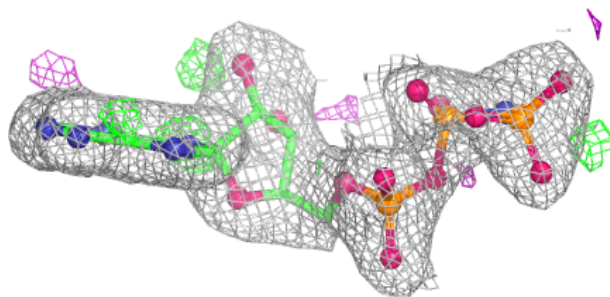
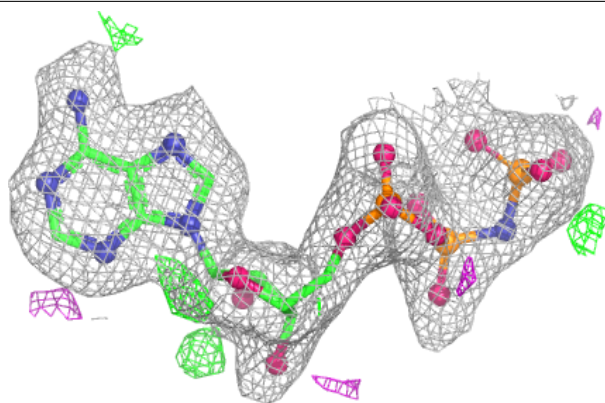
**Electron density around ANP C 3001:**

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



Electron density around ANP A 1101:

$2mF_o-DF_c$ (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.