Full wwPDB X-ray Structure Validation Report (i)

Mar 13, 2024 – 06:52 PM JST

PDB ID	:	5X2A
Title	:	Crystal structure of EGFR 696-1022 T790M/V948R in complex with SKLB(3)
Authors	:	Yun, C.H.
Deposited on	:	2017-01-31
Resolution	:	1.85 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

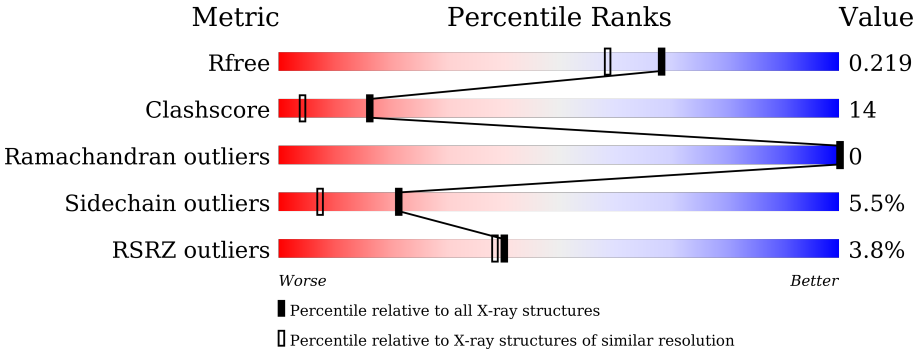
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.85 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}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 <=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% 66% 21% • 10%
1	B	331	2% 77% 18% • •
1	C	331	5% 72% 18% • 8%
1	D	331	2% 69% 17% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	B	1104	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11103 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
			Total	C	N	O	S			
1	A	297	2445	1578	417	430	20	0	9	0
1	B	322	2597	1669	437	471	20	0	9	0
1	C	303	2441	1567	414	441	19	0	4	0
1	D	297	2409	1551	413	426	19	0	3	0

There are 24 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	695	SER	-	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	695	SER	-	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	695	SER	-	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

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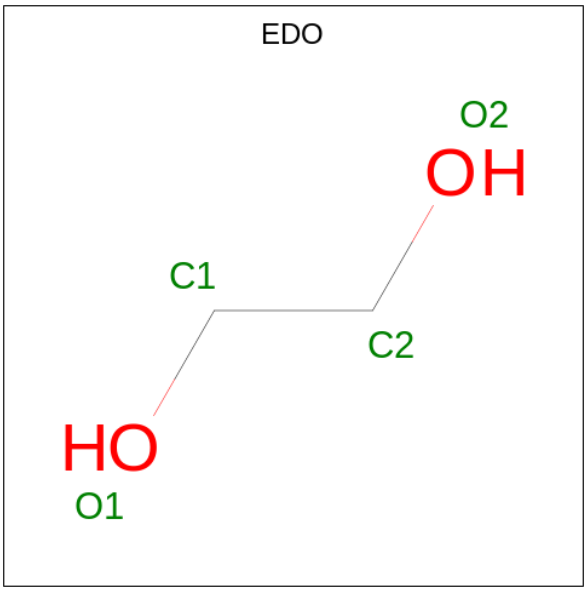
Chain	Residue	Modelled	Actual	Comment	Reference
D	695	SER	-	expression tag	UNP P00533
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	1	1	1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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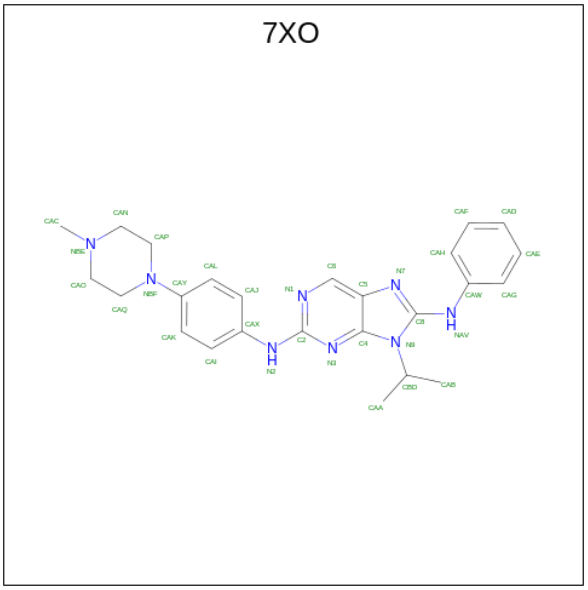
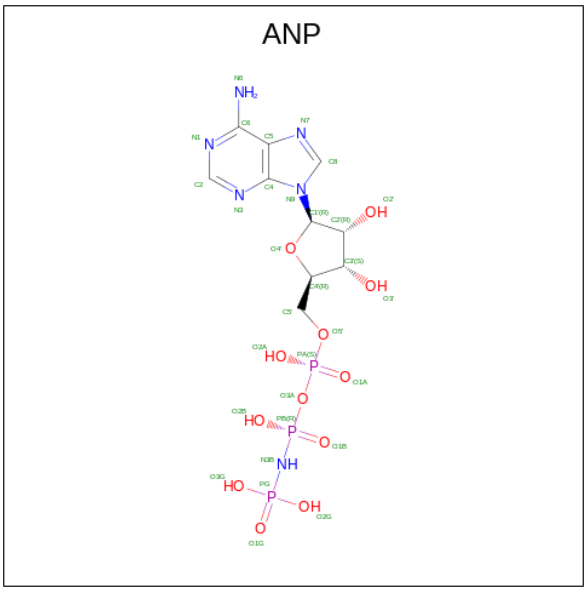
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	C	1	4	2	2	0	0
			Total	C	O		
3	C	1	4	2	2	0	0
			Total	C	O		
3	C	1	4	2	2	0	0

- Molecule 4 is N2-[4-(4-methylpiperazin-1-yl)phenyl]-N8-phenyl-9-propan-2-yl-purine-2,8-diamine (three-letter code: 7XO) (formula: $C_{25}H_{30}N_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
4	A	1	33	25	8	0	0
			Total	C	N		
4	B	1	13	11	2	0	0
			Total	C	N		
4	C	1	33	25	8	0	0

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	14	1	1	9	3	0	0
			Total	C	N	O	P		
5	B	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
5	D	1	31	10	6	12	3	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	1	1	1	0	0
			Total	Mg		
6	B	1	1	1	0	0
			Total	Mg		
6	D	2	2	2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	246	246	246	0	0
			Total	O		
7	B	317	317	317	0	0
			Total	O		
7	C	236	236	236	0	0

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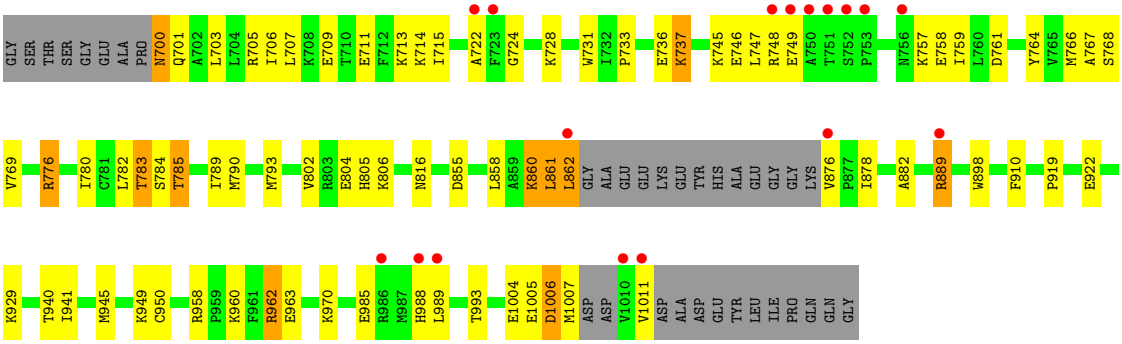
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	D	204	204	204	0	0

3 Residue-property plots (i)

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.

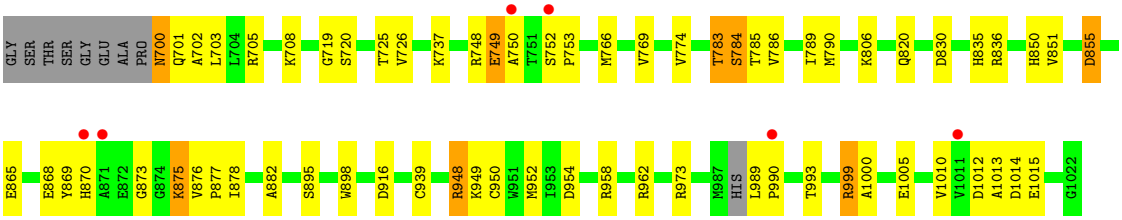
• Molecule 1: Epidermal growth factor receptor

Chain A:



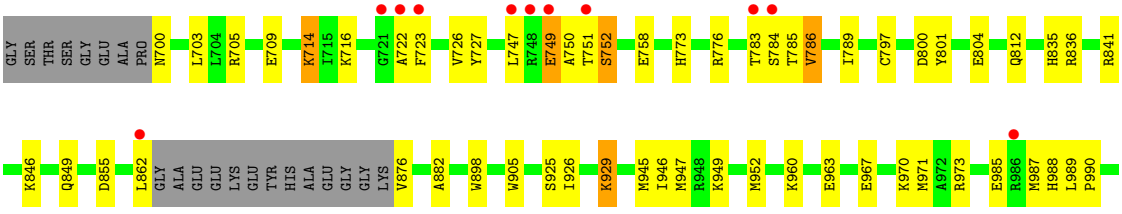
• Molecule 1: Epidermal growth factor receptor

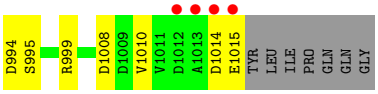
Chain B:



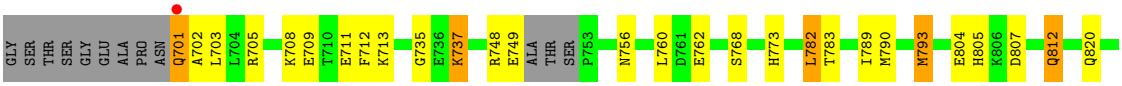
• Molecule 1: Epidermal growth factor receptor

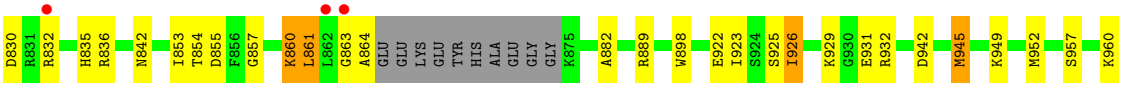
Chain C:

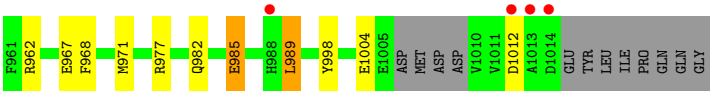




• Molecule 1: Epidermal growth factor receptor







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.19Å 103.97Å 87.15Å 90.00° 101.40° 90.00°	Depositor
Resolution (Å)	39.49 – 1.85 44.96 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.9 (39.49-1.85) 98.0 (44.96-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.173 , 0.219 0.174 , 0.219	Depositor DCC
R_{free} test set	5277 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	24.3	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11103	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 13.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, 7XO, CL, ANP, EDO

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	1.02	0/2526	0.95	1/3409 (0.0%)
1	B	1.05	1/2676 (0.0%)	0.92	5/3619 (0.1%)
1	C	1.01	1/2504 (0.0%)	0.87	1/3387 (0.0%)
1	D	0.99	0/2470	0.89	2/3333 (0.1%)
All	All	1.02	2/10176 (0.0%)	0.91	9/13748 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	895	SER	CA-CB	5.79	1.61	1.52
1	C	726	VAL	CB-CG1	5.08	1.63	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	846	LYS	CD-CE-NZ	-5.82	98.31	111.70
1	D	705	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	B	999	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	B	939	CYS	CA-CB-SG	-5.38	104.31	114.00
1	B	948	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	B	855	ASP	CB-CG-OD1	5.25	123.02	118.30
1	D	793	MET	CG-SD-CE	-5.20	91.88	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	973	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	776	ARG	NE-CZ-NH1	-5.05	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	790	MET	Mainchain

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	2445	0	2534	83	0
1	B	2597	0	2609	72	0
1	C	2441	0	2473	59	0
1	D	2409	0	2477	75	0
2	A	1	0	0	0	0
3	A	20	0	29	5	0
3	B	16	0	24	7	0
3	C	12	0	18	1	0
4	A	33	0	0	5	0
4	B	13	0	0	4	0
4	C	33	0	0	0	0
5	A	14	0	1	2	0
5	B	31	0	13	6	0
5	D	31	0	13	3	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	D	2	0	0	0	0
7	A	246	0	0	31	0
7	B	317	0	0	27	0
7	C	236	0	0	19	0
7	D	204	0	0	24	0
All	All	11103	0	10191	292	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 14.

All (292) 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:B:749[A]:GLU:HG3	7:D:1216:HOH:O	1.38	1.18
1:A:988:HIS:O	1:A:989:LEU:HD23	1.51	1.09
1:D:812:GLN:HG2	1:D:989:LEU:HD22	1.32	1.09
1:B:990:PRO:HG3	7:B:1493:HOH:O	1.51	1.06
1:C:812:GLN:HG2	1:C:989:LEU:HD22	1.35	1.02
1:D:854:THR:HG21	7:D:1206:HOH:O	1.56	1.02
1:C:723:PHE:CB	1:C:862:LEU:HD11	1.92	0.99
1:B:783:THR:HG22	1:B:784:SER:N	1.80	0.95
1:D:960:LYS:HE3	7:D:1290:HOH:O	1.67	0.93
1:A:962[A]:ARG:HH21	1:A:962[A]:ARG:HG3	1.32	0.92
1:B:783:THR:CG2	1:B:784:SER:H	1.81	0.92
1:B:749[A]:GLU:OE2	1:B:750:ALA:O	1.90	0.90
1:A:860:LYS:HB2	7:A:1213:HOH:O	1.70	0.90
1:A:766:MET:O	1:A:769[A]:VAL:HG22	1.69	0.90
1:A:747:LEU:HD13	1:A:862:LEU:HD21	1.54	0.88
1:D:945:MET:HE1	7:D:1365:HOH:O	1.72	0.87
1:B:783:THR:CG2	1:B:784:SER:N	2.37	0.87
1:B:870:HIS:HB2	7:B:1218:HOH:O	1.75	0.86
1:A:989:LEU:HD13	7:A:1374:HOH:O	1.74	0.86
1:A:714:LYS:HE2	7:A:1278:HOH:O	1.76	0.85
1:D:857:GLY:HA2	7:D:1236:HOH:O	1.75	0.85
1:D:853:ILE:HG23	7:D:1256:HOH:O	1.77	0.84
1:D:812:GLN:HG2	1:D:989:LEU:CD2	2.08	0.84
1:D:832[B]:ARG:CG	1:D:832[B]:ARG:HH11	1.93	0.82
1:C:723:PHE:CB	1:C:862:LEU:CD1	2.58	0.81
1:D:832[B]:ARG:HH11	1:D:832[B]:ARG:HG3	1.46	0.81
1:B:865:GLU:CG	1:B:868:GLU:OE1	2.30	0.80
1:A:962[A]:ARG:HG3	1:A:962[A]:ARG:NH2	1.93	0.80
1:B:1013:ALA:HB3	1:C:1008:ASP:OD2	1.81	0.80
1:A:861:LEU:C	1:A:862:LEU:HG	2.03	0.79
3:B:1104:EDO:C1	7:B:1210:HOH:O	2.29	0.79
1:C:747:LEU:HB2	1:C:786:VAL:HG13	1.65	0.79
1:D:860:LYS:HG2	1:D:861:LEU:N	1.97	0.78
1:D:701:GLN:NE2	1:D:701:GLN:N	2.30	0.78
1:B:1013:ALA:O	1:B:1014:ASP:HB2	1.82	0.78
1:B:783:THR:HG22	1:B:784:SER:H	1.40	0.77
1:B:783:THR:HB	7:B:1206:HOH:O	1.83	0.77
1:A:962[B]:ARG:HD3	7:A:1227:HOH:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1104:EDO:H11	7:B:1210:HOH:O	1.85	0.76
1:A:816:ASN:HD21	1:A:1011:VAL:H	1.31	0.75
1:A:701:GLN:HG3	7:A:1259:HOH:O	1.87	0.75
1:A:962[B]:ARG:NE	7:A:1203:HOH:O	2.21	0.74
1:B:790:MET:HB2	7:B:1445:HOH:O	1.88	0.74
1:C:705:ARG:HG3	1:C:705:ARG:HH11	1.53	0.74
1:D:923:ILE:HA	1:D:926:ILE:HD11	1.68	0.74
1:C:849[B]:GLN:HE21	1:C:990:PRO:HD2	1.53	0.74
1:B:750:ALA:HB3	1:B:753:PRO:HA	1.69	0.73
1:B:725[A]:THR:HG21	1:D:830:ASP:OD2	1.88	0.73
1:A:988:HIS:C	1:A:989:LEU:HD23	2.07	0.72
1:C:812:GLN:HG2	1:C:989:LEU:CD2	2.16	0.72
4:A:1107:7XO:CAB	5:A:1108:ANP:C5'	2.67	0.72
1:B:720:SER:CB	1:B:725[A]:THR:HG22	2.19	0.72
1:D:832[B]:ARG:HG3	1:D:832[B]:ARG:NH1	2.04	0.69
1:C:812:GLN:CG	1:C:989:LEU:HD22	2.18	0.69
7:A:1416:HOH:O	1:C:716:LYS:CD	2.41	0.69
1:A:769[A]:VAL:HG21	7:A:1256:HOH:O	1.93	0.68
1:A:705:ARG:HG2	1:A:707:LEU:CD2	2.24	0.68
1:D:854:THR:CG2	7:D:1206:HOH:O	2.24	0.68
1:B:989:LEU:CG	7:B:1478:HOH:O	2.41	0.68
1:A:793:MET:CE	7:A:1231:HOH:O	2.42	0.67
1:B:720:SER:HB3	1:B:725[A]:THR:HG22	1.75	0.67
1:A:705:ARG:HG2	1:A:707:LEU:HD23	1.76	0.67
1:D:923:ILE:HA	1:D:926:ILE:CD1	2.24	0.67
1:B:990:PRO:HD3	7:B:1375:HOH:O	1.93	0.67
1:B:725[A]:THR:CG2	1:D:830:ASP:OD2	2.42	0.67
1:B:989:LEU:N	7:B:1204:HOH:O	2.27	0.67
7:B:1338:HOH:O	1:C:773:HIS:HD2	1.77	0.66
1:A:876:VAL:N	7:A:1207:HOH:O	2.28	0.66
1:B:855:ASP:HB3	7:B:1367:HOH:O	1.95	0.65
1:B:750:ALA:O	1:B:753:PRO:HD3	1.97	0.65
1:C:960:LYS:HB2	1:C:963:GLU:HG3	1.79	0.65
1:D:701:GLN:N	1:D:701:GLN:CD	2.51	0.65
7:A:1416:HOH:O	1:C:716:LYS:HD3	1.95	0.65
1:A:737:LYS:HG3	1:D:804:GLU:OE2	1.97	0.64
1:C:999:ARG:NH2	7:C:1205:HOH:O	2.29	0.64
1:A:713[A]:LYS:NZ	7:A:1209:HOH:O	2.31	0.64
1:B:993:THR:HG21	7:C:1289:HOH:O	1.96	0.64
1:C:835:HIS:O	1:C:836:ARG:HB2	1.98	0.63
1:A:960:LYS:NZ	7:A:1211:HOH:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1107:7XO:CAC	7:A:1208:HOH:O	2.46	0.63
1:B:835:HIS:O	1:B:836:ARG:HB2	1.99	0.62
1:B:783:THR:HG23	1:B:784:SER:H	1.63	0.62
1:C:722:ALA:HB3	7:C:1271:HOH:O	1.99	0.62
1:B:749[A]:GLU:CD	1:B:750:ALA:O	2.38	0.62
1:B:820:GLN:NE2	1:B:851:VAL:H	1.98	0.62
1:D:949:LYS:HG2	1:D:952:MET:HE3	1.81	0.62
1:C:949:LYS:O	1:C:952:MET:HG3	2.00	0.61
1:B:1012:ASP:O	1:B:1015:GLU:HG3	2.00	0.61
1:A:701:GLN:HG2	1:A:764:TYR:CZ	2.36	0.61
1:C:714:LYS:HD3	1:C:727:TYR:CD1	2.36	0.60
1:D:842:ASN:O	1:D:854:THR:HG22	2.02	0.60
1:D:812:GLN:CG	1:D:989:LEU:HD22	2.21	0.60
1:C:709:GLU:OE2	1:C:784:SER:CB	2.50	0.60
4:B:1105:7XO:CAX	5:B:1106:ANP:H2	2.31	0.60
1:D:923:ILE:HD13	1:D:926:ILE:HD11	1.83	0.60
1:B:999:ARG:HD3	7:B:1365:HOH:O	2.00	0.59
1:A:962[B]:ARG:CD	7:A:1227:HOH:O	2.44	0.59
1:B:989:LEU:N	7:B:1210:HOH:O	2.34	0.59
1:C:973:ARG:HG2	7:C:1252:HOH:O	2.02	0.59
1:A:747:LEU:HD13	1:A:862:LEU:CD2	2.30	0.59
1:A:783:THR:HA	7:A:1210:HOH:O	2.02	0.59
1:C:700:ASN:HB3	1:C:703:LEU:HG	1.85	0.59
1:C:783:THR:HG21	7:C:1300:HOH:O	2.01	0.59
1:D:805:HIS:HB3	7:D:1214:HOH:O	2.03	0.58
1:B:720:SER:OG	1:B:725[A]:THR:HG22	2.03	0.58
1:C:849[B]:GLN:HE21	1:C:990:PRO:CD	2.17	0.58
1:B:785:THR:HG21	7:B:1266:HOH:O	2.03	0.58
1:D:737:LYS:HE2	7:D:1232:HOH:O	2.04	0.58
1:B:726:VAL:CG2	5:B:1106:ANP:H5'1	2.34	0.57
1:D:854:THR:HG23	1:D:855:ASP:OD2	2.04	0.57
1:B:820:GLN:HE22	1:B:851:VAL:H	1.52	0.57
1:C:705:ARG:HG3	1:C:705:ARG:NH1	2.17	0.57
1:D:782:LEU:HD12	7:D:1326:HOH:O	2.04	0.57
1:A:970:LYS:CE	3:A:1104:EDO:H12	2.34	0.57
1:C:1010:VAL:HA	7:C:1246:HOH:O	2.05	0.56
1:D:790[A]:MET:CE	7:D:1311:HOH:O	2.53	0.56
1:D:783:THR:HG21	7:D:1261:HOH:O	2.04	0.56
1:A:960:LYS:HG2	1:A:963:GLU:OE2	2.05	0.56
1:D:712:PHE:O	1:D:713:LYS:HE3	2.05	0.56
1:B:749[A]:GLU:OE2	1:B:750:ALA:C	2.44	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:970[B]:LYS:HE2	7:C:1214:HOH:O	2.05	0.55
1:C:841:ARG:HD2	7:C:1369:HOH:O	2.06	0.55
1:D:790[A]:MET:HE2	7:D:1311:HOH:O	2.05	0.55
1:B:916:ASP:OD1	3:B:1102:EDO:H11	2.06	0.55
1:A:970:LYS:HE3	3:A:1104:EDO:H12	1.88	0.55
1:C:970[B]:LYS:NZ	7:C:1214:HOH:O	2.39	0.55
1:B:700:ASN:ND2	1:B:702:ALA:H	2.05	0.55
1:C:709:GLU:HG3	1:C:783:THR:OG1	2.06	0.55
1:B:990:PRO:HG3	7:B:1375:HOH:O	2.07	0.54
1:D:832[C]:ARG:NH1	7:D:1216:HOH:O	2.40	0.54
1:D:949:LYS:HG2	1:D:952:MET:CE	2.37	0.54
1:D:835:HIS:O	1:D:836:ARG:HB2	2.08	0.54
4:B:1105:7XO:CAX	5:B:1106:ANP:C2	2.85	0.54
1:B:989:LEU:CG	1:B:990:PRO:CD	2.86	0.53
1:A:785:THR:CG2	1:A:785:THR:O	2.56	0.53
1:B:820:GLN:HE22	1:B:850:HIS:HA	1.73	0.53
1:C:1014:ASP:O	1:C:1015:GLU:CB	2.53	0.53
1:B:875:LYS:O	1:B:877:PRO:HD3	2.08	0.52
1:C:849[B]:GLN:NE2	1:C:990:PRO:HD2	2.23	0.52
1:D:762:GLU:OE2	1:D:860:LYS:HE3	2.09	0.52
1:C:785:THR:CB	7:C:1233:HOH:O	2.56	0.52
1:B:830:ASP:OD1	1:B:962[B]:ARG:NH1	2.42	0.52
1:D:748:ARG:O	1:D:749:GLU:C	2.48	0.52
3:B:1104:EDO:H12	7:B:1204:HOH:O	2.10	0.52
1:B:916:ASP:OD1	3:B:1102:EDO:C1	2.58	0.52
1:D:968:PHE:CD1	1:D:971:MET:CE	2.94	0.51
1:A:759:ILE:HD13	1:A:861:LEU:HD22	1.91	0.51
4:A:1107:7XO:N3	4:A:1107:7XO:CAI	2.72	0.51
1:C:800:ASP:O	1:C:804:GLU:HG3	2.11	0.51
1:A:782:LEU:C	7:A:1210:HOH:O	2.48	0.51
1:B:949:LYS:O	1:B:952[A]:MET:HG3	2.10	0.51
1:D:925:SER:O	1:D:929:LYS:HG3	2.10	0.51
1:A:745:LYS:HE3	4:A:1107:7XO:CAH	2.41	0.50
1:A:806:LYS:O	1:A:910:PHE:CD1	2.63	0.50
1:B:766:MET:O	1:B:769[A]:VAL:HG22	2.11	0.50
1:A:766:MET:O	1:A:769[A]:VAL:CG2	2.52	0.50
1:D:793:MET:CE	7:D:1235:HOH:O	2.59	0.50
1:A:737:LYS:CG	1:D:804:GLU:OE2	2.60	0.50
1:B:990:PRO:CG	7:B:1375:HOH:O	2.58	0.50
1:D:760:LEU:HD13	1:D:782:LEU:HD21	1.92	0.50
1:D:861:LEU:HD22	1:D:861:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:MET:HE1	7:A:1231:HOH:O	2.11	0.50
1:A:949:LYS:HE2	7:A:1344:HOH:O	2.11	0.50
1:A:985:GLU:HG3	7:A:1413:HOH:O	2.12	0.49
1:A:1006:ASP:HA	7:A:1237:HOH:O	2.11	0.49
1:C:722:ALA:HA	7:C:1396:HOH:O	2.11	0.49
1:C:749:GLU:OE1	1:C:750:ALA:O	2.30	0.49
1:A:962[A]:ARG:HH21	1:A:962[A]:ARG:CG	2.11	0.49
1:B:954:ASP:OD1	7:B:1201:HOH:O	2.20	0.49
1:A:941:ILE:O	1:A:945[B]:MET:HG3	2.12	0.49
1:D:889:ARG:NH1	7:D:1222:HOH:O	2.46	0.49
1:C:999:ARG:CZ	7:C:1205:HOH:O	2.61	0.49
1:C:789:ILE:HD12	1:C:789:ILE:N	2.27	0.49
1:A:767:ALA:O	1:A:776:ARG:HD2	2.13	0.49
1:B:769[A]:VAL:HG21	7:B:1285:HOH:O	2.13	0.49
1:A:941:ILE:HB	3:A:1105:EDO:H12	1.94	0.49
1:A:736:GLU:OE1	7:A:1201:HOH:O	2.20	0.48
1:B:700:ASN:C	1:B:700:ASN:HD22	2.16	0.48
1:D:790[A]:MET:HE2	5:D:1102:ANP:N6	2.28	0.48
1:B:949:LYS:O	1:B:952[B]:MET:HG2	2.13	0.48
5:D:1102:ANP:O2A	5:D:1102:ANP:O1B	2.30	0.48
1:D:985:GLU:CD	1:D:985:GLU:H	2.15	0.48
1:A:715:ILE:HD11	1:A:728:LYS:HE2	1.94	0.48
1:A:789:ILE:HD12	1:A:789:ILE:N	2.28	0.48
1:B:869:TYR:O	1:B:878:ILE:HD11	2.13	0.48
1:C:752:SER:N	7:C:1222:HOH:O	2.45	0.48
1:A:709:GLU:HG2	1:A:783:THR:CG2	2.44	0.48
1:C:801:TYR:OH	3:C:1102:EDO:H21	2.14	0.48
1:B:990:PRO:CD	7:B:1375:HOH:O	2.56	0.48
1:A:804:GLU:OE1	7:A:1202:HOH:O	2.20	0.48
1:C:905:TRP:CD1	1:C:947:MET:HE1	2.49	0.48
1:A:769[A]:VAL:HG23	1:A:776:ARG:HA	1.96	0.47
1:B:873:GLY:O	1:D:962:ARG:NH1	2.47	0.47
1:D:703:LEU:HD13	1:D:768:SER:HA	1.95	0.47
1:C:970[B]:LYS:CE	7:C:1214:HOH:O	2.62	0.47
1:A:993:THR:OG1	1:D:702:ALA:HA	2.15	0.47
1:D:922:GLU:O	1:D:926:ILE:HD13	2.15	0.47
1:A:805:HIS:HE1	1:D:735:GLY:O	1.97	0.47
1:C:995:SER:HB3	7:C:1205:HOH:O	2.13	0.47
1:C:905:TRP:HD1	1:C:947:MET:HE1	1.79	0.47
1:A:703:LEU:HD13	1:A:768:SER:HA	1.96	0.46
1:C:747:LEU:HG	1:C:786:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:968:PHE:CD1	1:D:971:MET:HE3	2.51	0.46
1:D:882:ALA:HA	1:D:898:TRP:CD2	2.50	0.46
1:A:705:ARG:HG2	1:A:707:LEU:HD21	1.97	0.46
1:D:793:MET:HE1	7:D:1235:HOH:O	2.15	0.46
1:B:876:VAL:HA	1:B:877:PRO:HD2	1.81	0.46
4:A:1107:7XO:N7	4:A:1107:7XO:CAG	2.78	0.46
1:B:990:PRO:HD3	7:B:1478:HOH:O	2.16	0.46
4:B:1105:7XO:CAP	7:B:1429:HOH:O	2.63	0.46
1:A:876:VAL:HG23	1:A:878:ILE:HG12	1.98	0.46
5:D:1102:ANP:O2B	5:D:1102:ANP:H5'2	2.15	0.46
7:A:1416:HOH:O	1:C:716:LYS:HD2	2.14	0.45
1:D:701:GLN:HG2	1:D:702:ALA:H	1.81	0.45
1:A:757:LYS:O	1:A:761:ASP:OD1	2.33	0.45
1:D:836:ARG:NH1	7:D:1213:HOH:O	2.36	0.45
1:A:706:ILE:HD13	1:A:780:ILE:HG22	1.98	0.45
1:A:876:VAL:CA	7:A:1207:HOH:O	2.63	0.45
1:D:773:HIS:CE1	1:D:820:GLN:HG2	2.51	0.45
1:B:726:VAL:HG21	5:B:1106:ANP:H5'1	1.97	0.45
1:C:985:GLU:H	1:C:985:GLU:CD	2.19	0.45
1:D:748:ARG:HG2	1:D:748:ARG:HH21	1.82	0.44
1:D:812:GLN:CG	1:D:989:LEU:CD2	2.89	0.44
1:A:919:PRO:HG2	1:A:922:GLU:OE2	2.18	0.44
1:A:940:THR:HA	3:A:1105:EDO:H21	1.99	0.44
1:A:962[B]:ARG:CZ	7:A:1203:HOH:O	2.64	0.44
4:B:1105:7XO:CAX	5:B:1106:ANP:N3	2.80	0.44
1:A:722:ALA:O	1:A:748[B]:ARG:NH2	2.43	0.44
7:B:1444:HOH:O	1:C:994:ASP:HB3	2.17	0.44
1:B:1000:ALA:HB2	1:C:776[A]:ARG:HH21	1.82	0.43
1:A:855:ASP:HA	1:A:858:LEU:HD13	1.99	0.43
1:B:806:LYS:HD3	7:B:1282:HOH:O	2.17	0.43
1:C:882:ALA:HA	1:C:898:TRP:CD2	2.52	0.43
1:A:941:ILE:HB	3:A:1105:EDO:C1	2.48	0.43
1:A:962[B]:ARG:CZ	7:A:1227:HOH:O	2.67	0.43
1:D:863:GLY:O	1:D:864:ALA:HB2	2.18	0.43
1:A:746:GLU:OE1	1:A:785:THR:HG21	2.18	0.43
1:B:769[B]:VAL:HG11	1:B:774:VAL:CG1	2.49	0.43
3:B:1104:EDO:C1	7:B:1223:HOH:O	2.66	0.43
1:C:750:ALA:CB	7:C:1364:HOH:O	2.66	0.43
1:A:802:VAL:O	1:A:806:LYS:HA	2.18	0.43
1:B:789:ILE:N	1:B:789:ILE:HD12	2.34	0.43
1:C:990:PRO:HD2	7:C:1243:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:LYS:O	1:A:806:LYS:HG3	2.18	0.43
1:C:752:SER:CB	7:C:1385:HOH:O	2.66	0.43
1:A:1004:GLU:HB2	1:D:1004:GLU:HB2	2.00	0.43
1:A:950:CYS:O	1:A:958:ARG:HD3	2.19	0.43
1:D:756:ASN:O	1:D:760:LEU:HB2	2.18	0.43
1:D:709:GLU:HG2	7:D:1261:HOH:O	2.18	0.43
1:A:746:GLU:OE2	7:A:1204:HOH:O	2.21	0.42
1:A:919:PRO:CG	1:A:922:GLU:OE2	2.67	0.42
1:D:790[B]:MET:HE3	7:D:1395:HOH:O	2.19	0.42
1:A:855:ASP:OD2	5:A:1108:ANP:O3G	2.37	0.42
1:C:750:ALA:HB1	7:C:1404:HOH:O	2.18	0.42
1:B:950:CYS:O	1:B:958:ARG:HD3	2.19	0.42
1:A:889:ARG:HD3	1:A:889:ARG:HA	1.54	0.42
1:A:724:GLY:HA2	1:A:748[A]:ARG:HG3	2.01	0.42
1:A:962[B]:ARG:NE	7:A:1227:HOH:O	2.52	0.42
1:B:1010:VAL:CB	7:B:1234:HOH:O	2.68	0.42
1:A:700:ASN:C	1:A:700:ASN:HD22	2.22	0.42
1:B:725[A]:THR:HG23	1:D:830:ASP:OD2	2.20	0.42
1:B:769[B]:VAL:HG11	1:B:774:VAL:HG11	2.02	0.42
1:B:990:PRO:CD	7:B:1478:HOH:O	2.67	0.42
1:D:737:LYS:HD3	1:D:737:LYS:HA	1.66	0.41
1:B:708:LYS:HB2	1:B:708:LYS:HE2	1.69	0.41
1:A:731:TRP:CH2	1:A:733:PRO:HG3	2.56	0.41
1:A:949:LYS:CE	7:A:1344:HOH:O	2.69	0.41
1:D:760:LEU:HD12	1:D:760:LEU:HA	1.85	0.41
1:D:805:HIS:ND1	7:D:1214:HOH:O	2.37	0.41
1:C:925:SER:O	1:C:929:LYS:HD3	2.21	0.41
1:B:700:ASN:HD22	1:B:701:GLN:N	2.18	0.41
1:D:1004:GLU:OE1	7:D:1201:HOH:O	2.21	0.41
1:C:723:PHE:CB	1:C:862:LEU:HD13	2.49	0.41
1:A:962[A]:ARG:NH2	1:A:962[A]:ARG:CG	2.69	0.41
1:C:970[B]:LYS:HE2	1:C:970[B]:LYS:HB2	1.58	0.41
1:D:789:ILE:N	1:D:789:ILE:HD12	2.35	0.41
1:D:807:ASP:HA	7:D:1270:HOH:O	2.19	0.41
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.56	0.41
1:C:963:GLU:O	1:C:967:GLU:HG3	2.20	0.41
1:D:737:LYS:CE	7:D:1232:HOH:O	2.66	0.41
1:D:967:GLU:O	1:D:971:MET:HG3	2.21	0.41
1:D:931:GLU:O	1:D:932:ARG:HD3	2.21	0.41
1:B:948:ARG:HG3	3:B:1103:EDO:H12	2.03	0.40
1:C:946:ILE:CD1	1:C:971:MET:CE	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:708:LYS:HB2	1:D:711:GLU:HG3	2.03	0.40
1:A:989:LEU:HD21	7:A:1305:HOH:O	2.21	0.40
1:C:898:TRP:CD1	1:C:898:TRP:C	2.94	0.40
1:B:719:GLY:HA3	5:B:1106:ANP:H4'	2.04	0.40
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.56	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	301/331 (91%)	292 (97%)	9 (3%)	0	100	100
1	B	327/331 (99%)	322 (98%)	5 (2%)	0	100	100
1	C	303/331 (92%)	299 (99%)	4 (1%)	0	100	100
1	D	293/331 (88%)	285 (97%)	8 (3%)	0	100	100
All	All	1224/1324 (92%)	1198 (98%)	26 (2%)	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	273/290 (94%)	255 (93%)	18 (7%)	16	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	279/290 (96%)	266 (95%)	13 (5%)	26	10
1	C	267/290 (92%)	253 (95%)	14 (5%)	23	8
1	D	266/290 (92%)	250 (94%)	16 (6%)	19	5
All	All	1085/1160 (94%)	1024 (94%)	61 (6%)	21	7

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	700	ASN
1	A	711	GLU
1	A	737	LYS
1	A	749	GLU
1	A	758	GLU
1	A	783	THR
1	A	784	SER
1	A	785	THR
1	A	860	LYS
1	A	861	LEU
1	A	862	LEU
1	A	889	ARG
1	A	962[A]	ARG
1	A	962[B]	ARG
1	A	962[C]	ARG
1	A	1005	GLU
1	A	1006	ASP
1	A	1007	MET
1	B	700	ASN
1	B	703	LEU
1	B	705	ARG
1	B	737	LYS
1	B	748	ARG
1	B	749[A]	GLU
1	B	749[B]	GLU
1	B	752	SER
1	B	783	THR
1	B	784	SER
1	B	786	VAL
1	B	875	LYS
1	B	1005	GLU
1	C	714	LYS
1	C	749	GLU

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Mol	Chain	Res	Type
1	C	751	THR
1	C	752	SER
1	C	758	GLU
1	C	786	VAL
1	C	797	CYS
1	C	855	ASP
1	C	876	VAL
1	C	926	ILE
1	C	929	LYS
1	C	945	MET
1	C	987	MET
1	C	988	HIS
1	D	701	GLN
1	D	737	LYS
1	D	782	LEU
1	D	812	GLN
1	D	860	LYS
1	D	861	LEU
1	D	926	ILE
1	D	942	ASP
1	D	945	MET
1	D	957	SER
1	D	977	ARG
1	D	982	GLN
1	D	985	GLU
1	D	989	LEU
1	D	998	TYR
1	D	1012	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	700	ASN
1	A	805	HIS
1	A	816	ASN
1	A	849	GLN
1	A	982	GLN
1	A	988	HIS
1	B	700	ASN
1	B	812	GLN
1	B	820	GLN
1	B	849	GLN

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Mol	Chain	Res	Type
1	C	773	HIS
1	C	812	GLN
1	C	976	GLN
1	D	701	GLN
1	D	976	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 5 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	B	1102	-	3,3,3	0.77	0	2,2,2	0.22	0
5	ANP	A	1108	6	12,13,33	3.24	4 (33%)	14,21,52	3.06	6 (42%)
3	EDO	A	1105	-	3,3,3	1.08	0	2,2,2	0.11	0
4	7XO	C	1104	-	33,37,37	1.13	3 (9%)	41,52,52	1.73	4 (9%)
3	EDO	C	1103	-	3,3,3	0.63	0	2,2,2	0.59	0
5	ANP	D	1102	6	29,33,33	2.12	8 (27%)	31,52,52	1.93	7 (22%)
3	EDO	B	1101	-	3,3,3	0.31	0	2,2,2	0.76	0
3	EDO	B	1103	-	3,3,3	1.07	0	2,2,2	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	C	1101	-	3,3,3	0.36	0	2,2,2	0.32	0
4	7XO	B	1105	-	14,14,37	0.41	0	18,18,52	1.35	2 (11%)
3	EDO	C	1102	-	3,3,3	1.08	0	2,2,2	0.53	0
3	EDO	A	1102	-	3,3,3	0.56	0	2,2,2	0.25	0
3	EDO	B	1104	-	3,3,3	0.32	0	2,2,2	0.60	0
4	7XO	A	1107	-	33,37,37	1.10	3 (9%)	41,52,52	1.59	6 (14%)
3	EDO	A	1106	-	3,3,3	0.58	0	2,2,2	0.21	0
3	EDO	A	1104	-	3,3,3	0.66	0	2,2,2	0.55	0
3	EDO	A	1103	-	3,3,3	0.55	0	2,2,2	0.34	0
5	ANP	B	1106	6	29,33,33	2.36	10 (34%)	31,52,52	2.09	7 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	1102	-	-	0/1/1/1	-
5	ANP	A	1108	6	-	2/11/15/38	-
3	EDO	A	1105	-	-	1/1/1/1	-
4	7XO	C	1104	-	-	1/14/26/26	0/5/5/5
3	EDO	C	1103	-	-	0/1/1/1	-
5	ANP	D	1102	6	-	7/14/38/38	0/3/3/3
3	EDO	B	1101	-	-	1/1/1/1	-
3	EDO	B	1103	-	-	0/1/1/1	-
3	EDO	C	1101	-	-	1/1/1/1	-
4	7XO	B	1105	-	-	4/4/14/26	0/2/2/5
3	EDO	C	1102	-	-	1/1/1/1	-
3	EDO	A	1102	-	-	0/1/1/1	-
3	EDO	B	1104	-	-	1/1/1/1	-
4	7XO	A	1107	-	-	2/14/26/26	0/5/5/5
3	EDO	A	1106	-	-	1/1/1/1	-
3	EDO	A	1104	-	-	1/1/1/1	-
3	EDO	A	1103	-	-	0/1/1/1	-
5	ANP	B	1106	6	-	5/14/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1108	ANP	PG-O1G	7.98	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1106	ANP	PG-N3B	-6.89	1.45	1.63
5	D	1102	ANP	PG-N3B	-5.80	1.48	1.63
5	B	1106	ANP	PB-O2B	-4.88	1.43	1.56
5	D	1102	ANP	PG-O2G	-4.46	1.44	1.56
5	A	1108	ANP	PB-O2B	-4.41	1.44	1.56
5	B	1106	ANP	PG-O2G	-4.33	1.45	1.56
5	A	1108	ANP	PG-O2G	-4.13	1.45	1.56
5	A	1108	ANP	PG-O3G	-3.90	1.46	1.56
5	D	1102	ANP	PB-O2B	-3.64	1.47	1.56
4	C	1104	7XO	CAX-N2	-3.57	1.32	1.40
4	A	1107	7XO	CAX-N2	-3.41	1.33	1.40
4	C	1104	7XO	CAW-NAV	-3.24	1.33	1.40
5	D	1102	ANP	C2-N3	3.21	1.37	1.32
5	B	1106	ANP	C2-N3	3.18	1.37	1.32
5	B	1106	ANP	C5-C4	-3.03	1.32	1.40
5	D	1102	ANP	C5-C4	-2.87	1.33	1.40
4	A	1107	7XO	CAW-NAV	-2.78	1.34	1.40
5	B	1106	ANP	C6-C5	-2.70	1.33	1.43
5	B	1106	ANP	O4'-C1'	-2.67	1.37	1.41
5	D	1102	ANP	C6-C5	-2.52	1.33	1.43
5	B	1106	ANP	C4-N3	-2.48	1.32	1.35
4	A	1107	7XO	C5-N7	-2.32	1.31	1.38
5	B	1106	ANP	C5-N7	-2.17	1.31	1.39
5	D	1102	ANP	C5-N7	-2.14	1.32	1.39
5	D	1102	ANP	C4-N3	-2.10	1.32	1.35
4	C	1104	7XO	C5-N7	-2.02	1.32	1.38
5	B	1106	ANP	O2'-C2'	-2.02	1.38	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1108	ANP	O1G-PG-N3B	-8.20	99.69	111.77
4	C	1104	7XO	N1-C2-N3	-7.19	119.57	126.52
5	B	1106	ANP	N3-C2-N1	-6.75	118.12	128.68
5	D	1102	ANP	N3-C2-N1	-6.52	118.49	128.68
4	A	1107	7XO	N1-C2-N3	-5.12	121.57	126.52
5	D	1102	ANP	O2B-PB-O1B	4.80	119.99	109.92
4	C	1104	7XO	C2-N3-C4	4.66	120.57	115.28
5	A	1108	ANP	O2B-PB-O1B	4.30	118.93	109.92
5	B	1106	ANP	O1G-PG-N3B	-4.22	105.55	111.77
4	B	1105	7XO	CAQ-NBF-CAP	4.03	120.42	111.52
5	A	1108	ANP	O2G-PG-O3G	3.99	118.26	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1106	ANP	O2B-PB-O1B	3.97	118.25	109.92
4	C	1104	7XO	C6-N1-C2	3.94	121.73	115.88
4	A	1107	7XO	C2-N3-C4	3.66	119.43	115.28
4	A	1107	7XO	C6-N1-C2	3.63	121.26	115.88
5	A	1108	ANP	O1B-PB-N3B	-3.59	106.48	111.77
5	D	1102	ANP	PB-O3A-PA	-3.58	120.02	132.62
5	B	1106	ANP	C1'-N9-C4	-3.51	120.47	126.64
4	C	1104	7XO	CAQ-NBF-CAP	3.06	118.28	111.52
4	B	1105	7XO	CAQ-CAO-NBE	-3.04	107.37	110.80
4	A	1107	7XO	CAC-NBE-CAN	-2.91	106.31	110.66
5	B	1106	ANP	PB-O3A-PA	-2.82	122.67	132.62
4	A	1107	7XO	CAC-NBE-CAO	-2.74	106.56	110.66
4	A	1107	7XO	CAQ-NBF-CAP	2.63	117.31	111.52
5	B	1106	ANP	C5-C6-N6	-2.52	116.52	120.35
5	A	1108	ANP	PB-O3A-PA	-2.51	123.77	132.62
5	A	1108	ANP	O2G-PG-O1G	-2.47	107.24	113.45
5	D	1102	ANP	O2G-PG-O1G	2.26	119.13	113.45
5	B	1106	ANP	C4-C5-N7	-2.20	107.11	109.40
5	D	1102	ANP	C2'-C3'-C4'	-2.10	98.56	102.64
5	D	1102	ANP	C5'-C4'-C3'	-2.07	107.44	115.18
5	D	1102	ANP	O2A-PA-O1A	2.04	122.34	112.24

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1108	ANP	PB-N3B-PG-O1G
5	B	1106	ANP	PG-N3B-PB-O1B
5	B	1106	ANP	C5'-O5'-PA-O1A
5	B	1106	ANP	C5'-O5'-PA-O3A
5	B	1106	ANP	O4'-C4'-C5'-O5'
5	D	1102	ANP	PG-N3B-PB-O1B
5	D	1102	ANP	C5'-O5'-PA-O1A
5	D	1102	ANP	C5'-O5'-PA-O2A
5	D	1102	ANP	C5'-O5'-PA-O3A
4	B	1105	7XO	CAL-CAY-NBF-CAQ
5	B	1106	ANP	C3'-C4'-C5'-O5'
5	D	1102	ANP	O4'-C4'-C5'-O5'
4	B	1105	7XO	CAL-CAY-NBF-CAP
4	B	1105	7XO	CAK-CAY-NBF-CAQ
4	B	1105	7XO	CAK-CAY-NBF-CAP
3	A	1106	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	1104	EDO	O1-C1-C2-O2
3	C	1101	EDO	O1-C1-C2-O2
5	A	1108	ANP	C5'-O5'-PA-O2A
5	D	1102	ANP	C3'-C4'-C5'-O5'
5	D	1102	ANP	PA-O3A-PB-O2B
3	B	1101	EDO	O1-C1-C2-O2
3	A	1104	EDO	O1-C1-C2-O2
3	A	1105	EDO	O1-C1-C2-O2
3	C	1102	EDO	O1-C1-C2-O2
4	A	1107	7XO	CAB-CBD-N9-C4
4	A	1107	7XO	CAA-CBD-N9-C4
4	C	1104	7XO	N3-C2-N2-CAX

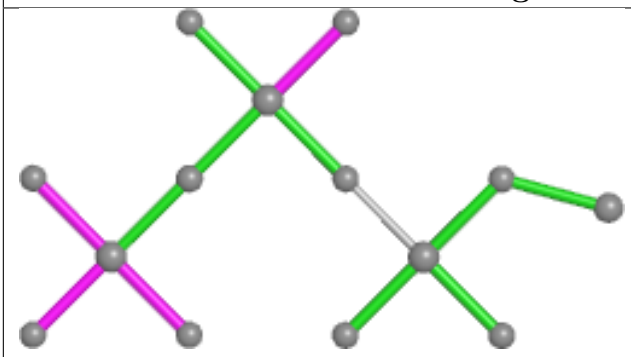
There are no ring outliers.

11 monomers are involved in 29 short contacts:

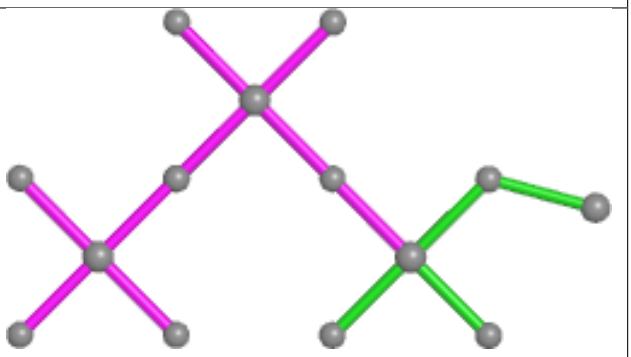
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1102	EDO	2	0
5	A	1108	ANP	2	0
3	A	1105	EDO	3	0
5	D	1102	ANP	3	0
3	B	1103	EDO	1	0
4	B	1105	7XO	4	0
3	C	1102	EDO	1	0
3	B	1104	EDO	4	0
4	A	1107	7XO	5	0
3	A	1104	EDO	2	0
5	B	1106	ANP	6	0

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.

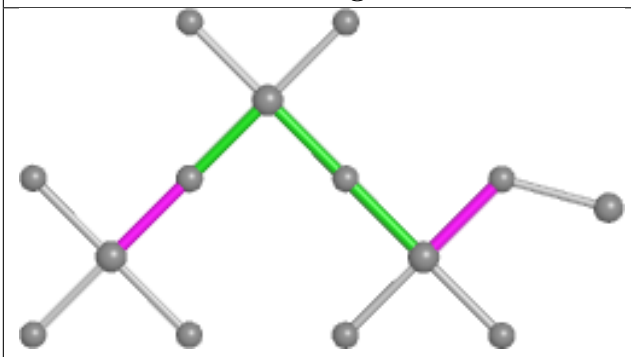
Ligand ANP A 1108



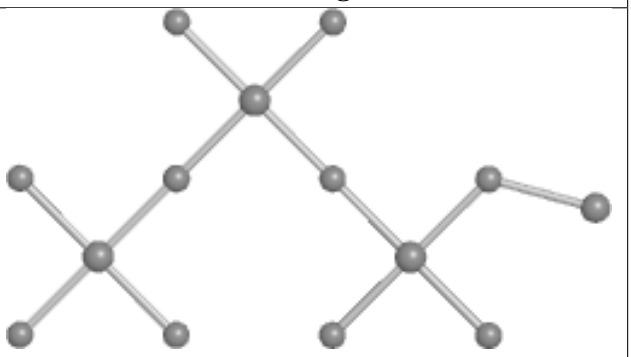
Bond lengths



Bond angles

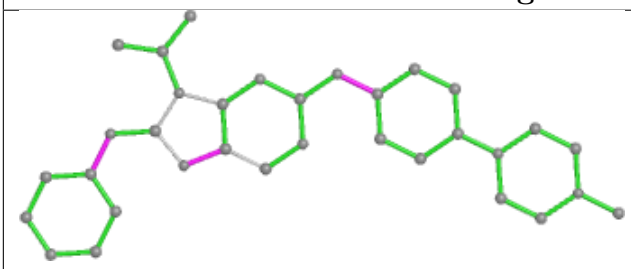


Torsions

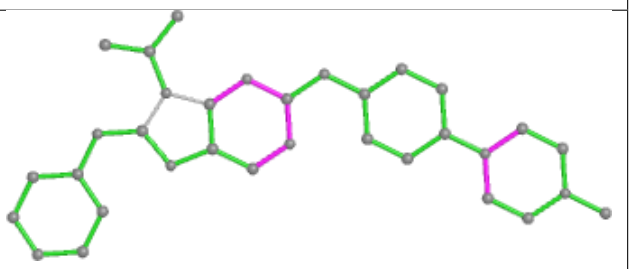


Rings

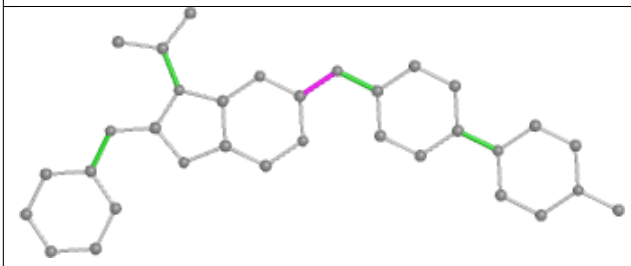
Ligand 7XO C 1104



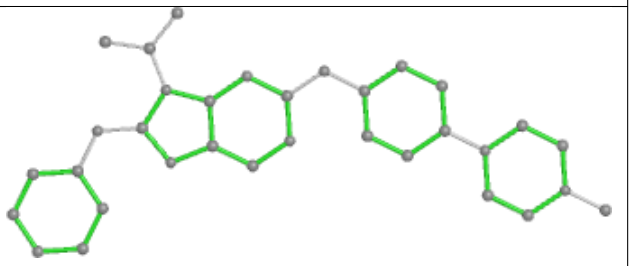
Bond lengths



Bond angles

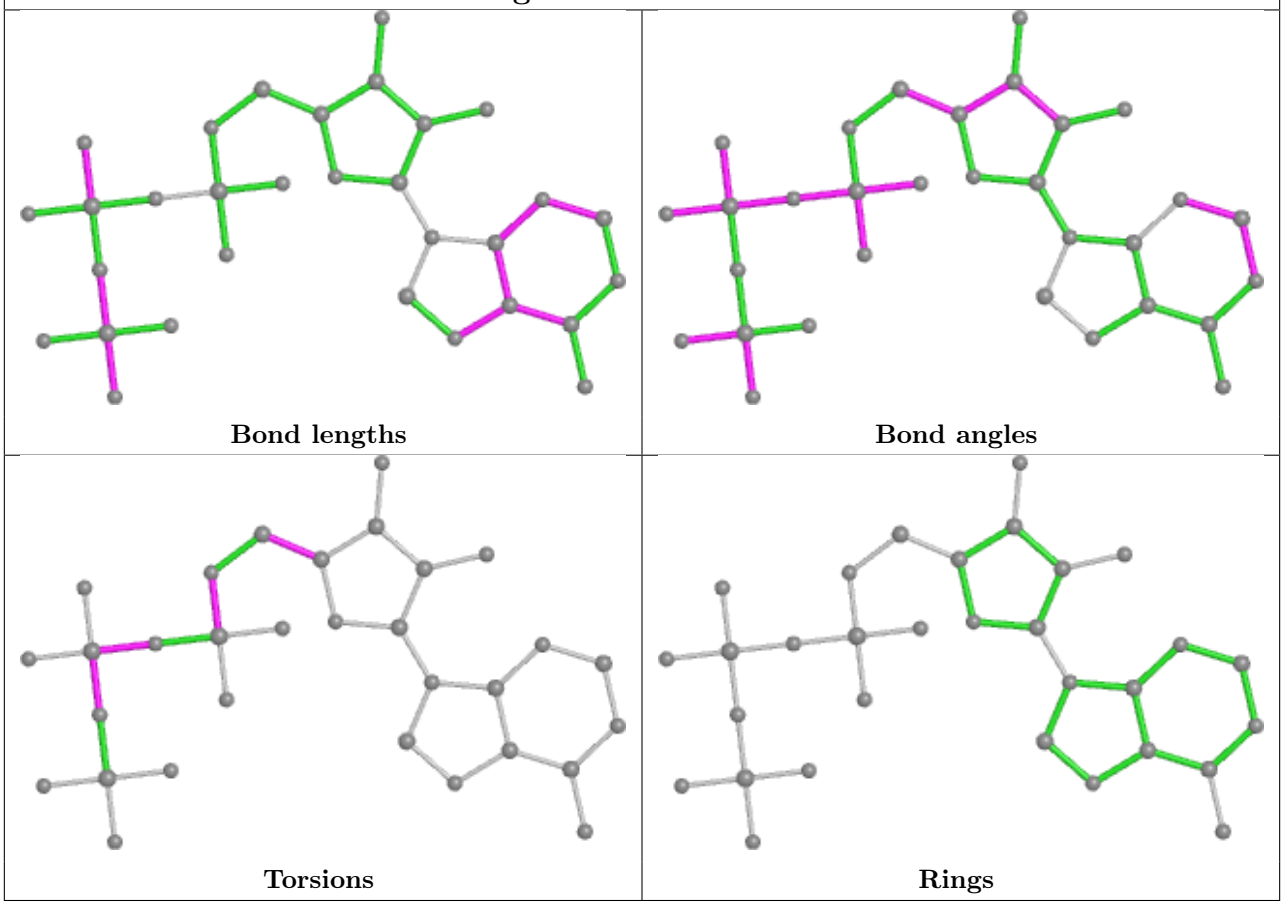


Torsions

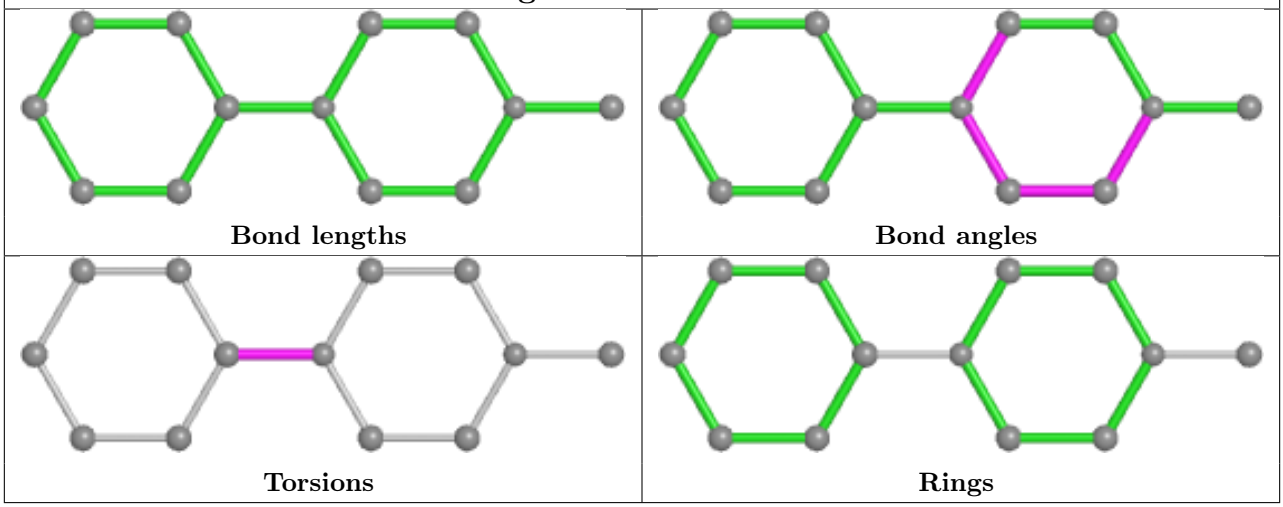


Rings

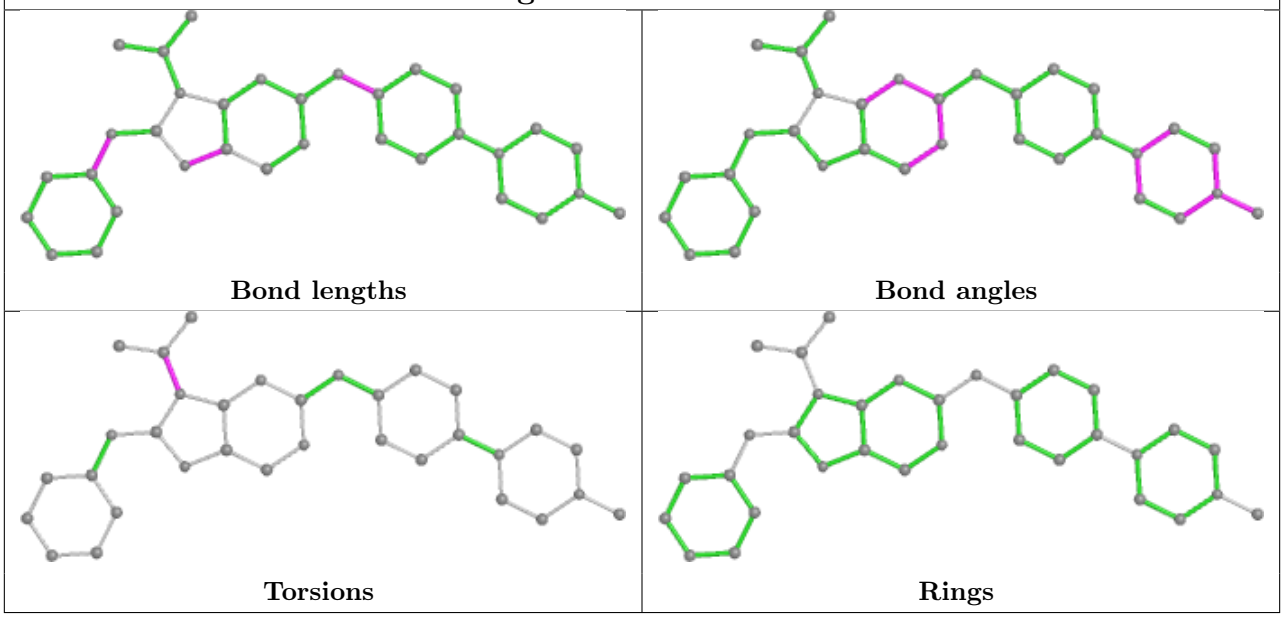
Ligand ANP D 1102



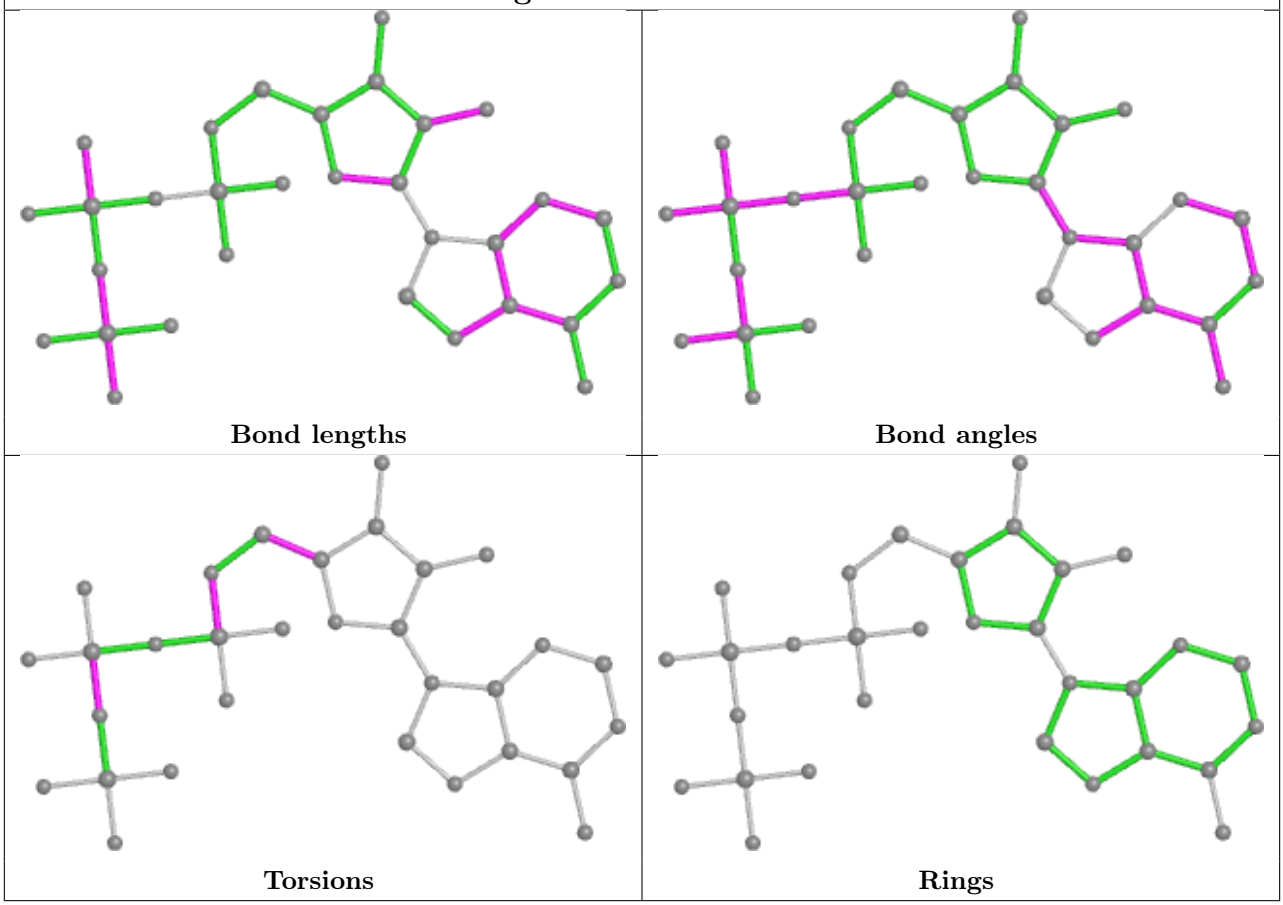
Ligand 7XO B 1105



Ligand 7XO A 1107



Ligand ANP B 1106



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	297/331 (89%)	-0.21	17 (5%)	23	23	13, 25, 55, 70	4 (1%)
1	B	322/331 (97%)	-0.22	6 (1%)	66	66	12, 24, 50, 63	12 (3%)
1	C	303/331 (91%)	-0.12	15 (4%)	28	27	14, 28, 53, 81	7 (2%)
1	D	297/331 (89%)	-0.13	8 (2%)	54	53	16, 31, 50, 74	5 (1%)
All	All	1219/1324 (92%)	-0.17	46 (3%)	40	38	12, 27, 52, 81	28 (2%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	723	PHE	10.3
1	C	722	ALA	7.3
1	A	862	LEU	5.9
1	A	723	PHE	5.2
1	B	750	ALA	4.8
1	D	1013	ALA	4.7
1	B	871	ALA	4.6
1	C	1015	GLU	4.5
1	A	752	SER	4.0
1	C	1014	ASP	3.8
1	C	783	THR	3.8
1	A	988	HIS	3.7
1	C	721	GLY	3.7
1	A	748[A]	ARG	3.6
1	A	986	ARG	3.4
1	C	748	ARG	3.4
1	B	752	SER	3.3
1	D	863	GLY	3.3
1	C	784	SER	3.2
1	C	1012	ASP	3.1
1	A	753	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	1014	ASP	3.0
1	B	870	HIS	2.9
1	C	986	ARG	2.8
1	D	701	GLN	2.8
1	C	749	GLU	2.8
1	D	832[A]	ARG	2.8
1	A	1010	VAL	2.8
1	B	990	PRO	2.8
1	A	1011	VAL	2.6
1	B	1011	VAL	2.6
1	A	751	THR	2.5
1	C	751	THR	2.5
1	A	749	GLU	2.5
1	C	862	LEU	2.5
1	D	1012	ASP	2.5
1	D	862	LEU	2.5
1	A	756	ASN	2.4
1	A	876	VAL	2.4
1	A	750	ALA	2.3
1	D	988	HIS	2.2
1	A	722	ALA	2.2
1	C	1013	ALA	2.2
1	A	889	ARG	2.1
1	A	989	LEU	2.1
1	C	747	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 monosaccharides in this entry.

6.4 Ligands (i)

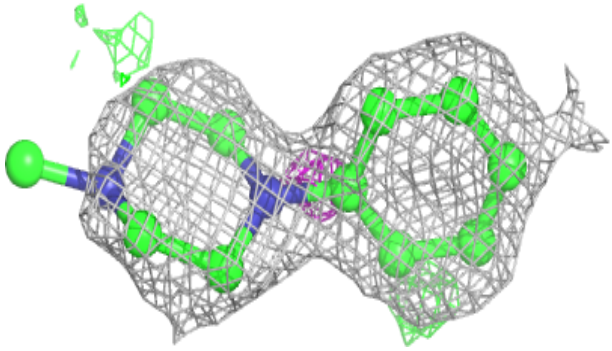
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

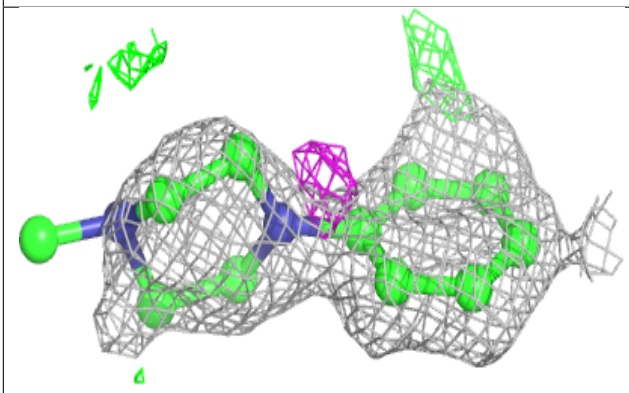
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	D	1101	1/1	0.23	0.22	54,54,54,54	0
3	EDO	B	1102	4/4	0.73	0.29	46,52,56,56	0
6	MG	D	1103	1/1	0.77	0.14	42,42,42,42	1
3	EDO	C	1102	4/4	0.80	0.19	37,39,43,44	0
3	EDO	C	1101	4/4	0.86	0.22	39,40,45,46	0
4	7XO	B	1105	13/33	0.86	0.16	26,46,65,71	0
3	EDO	B	1104	4/4	0.87	0.12	32,36,37,44	0
5	ANP	A	1108	14/31	0.87	0.22	23,34,39,39	14
6	MG	B	1107	1/1	0.89	0.24	32,32,32,32	1
3	EDO	C	1103	4/4	0.90	0.12	32,35,41,45	0
3	EDO	A	1106	4/4	0.90	0.20	37,37,51,53	0
6	MG	A	1109	1/1	0.91	0.32	31,31,31,31	1
5	ANP	B	1106	31/31	0.91	0.13	20,32,38,41	16
3	EDO	A	1103	4/4	0.92	0.12	28,35,40,44	0
5	ANP	D	1102	31/31	0.92	0.10	23,32,43,46	12
4	7XO	A	1107	33/33	0.92	0.13	16,31,48,53	0
3	EDO	B	1103	4/4	0.94	0.21	29,31,39,39	0
3	EDO	A	1104	4/4	0.94	0.17	40,48,49,51	0
4	7XO	C	1104	33/33	0.95	0.10	20,27,41,44	0
3	EDO	A	1105	4/4	0.95	0.18	21,24,31,34	0
3	EDO	B	1101	4/4	0.97	0.09	23,27,33,38	0
3	EDO	A	1102	4/4	0.99	0.05	23,27,28,31	0
2	CL	A	1101	1/1	1.00	0.07	35,35,35,35	0

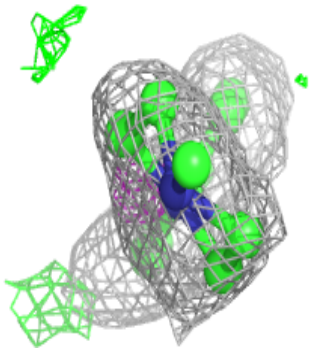
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7XO B 1105:

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

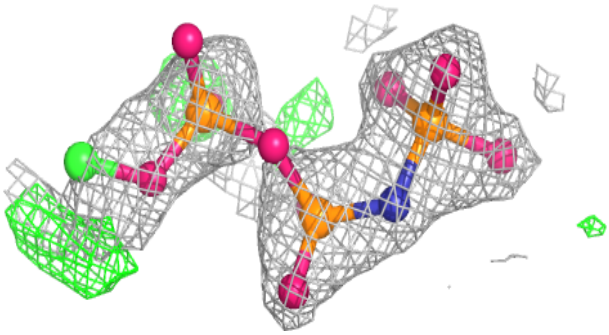


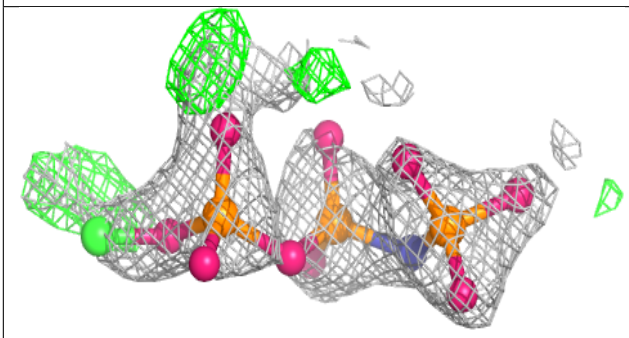


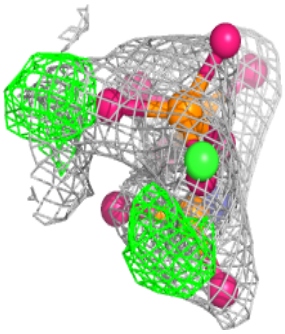


Electron density around ANP A 1108:

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

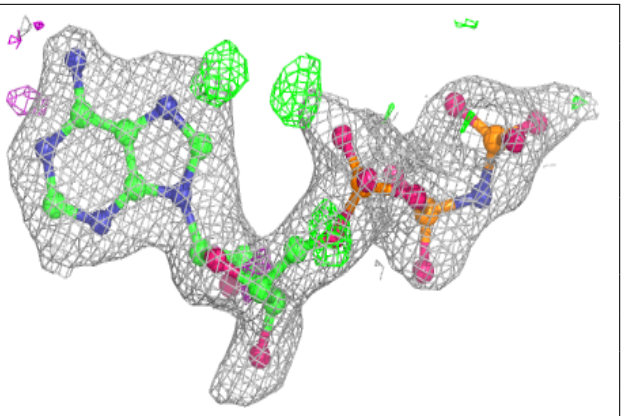


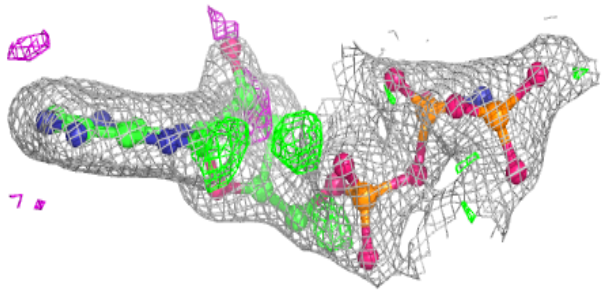


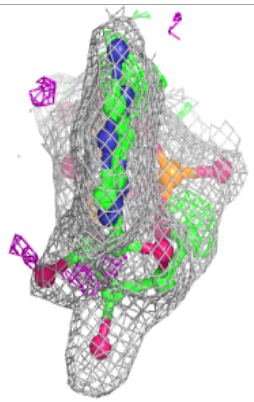


Electron density around ANP B 1106:

$2mF_o$-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 D 1102:

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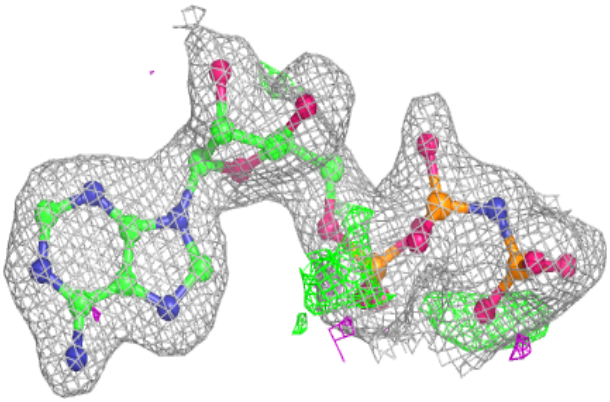
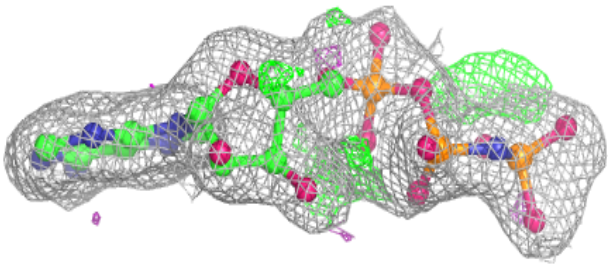
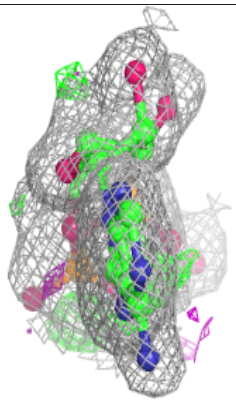
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

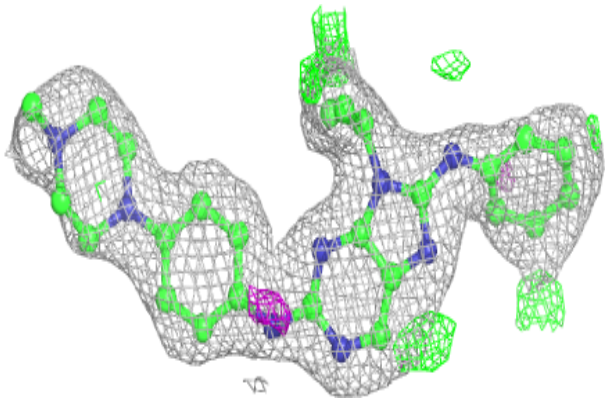


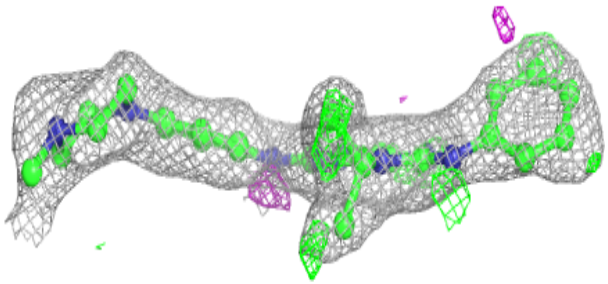


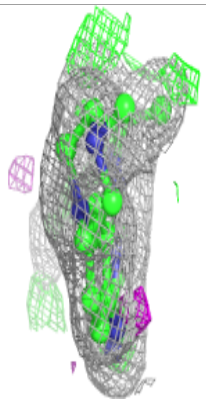


Electron density around 7XO A 1107:

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







Electron density around 7XO C 1104:

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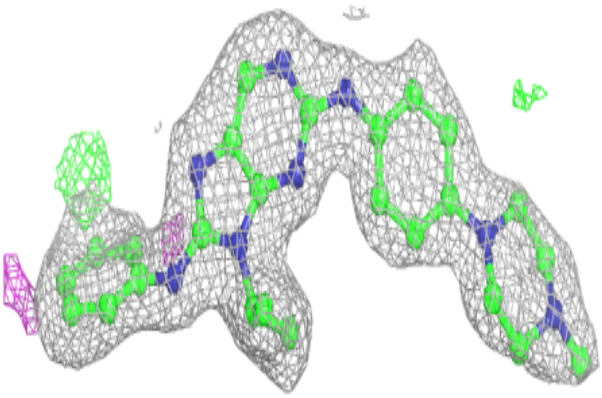
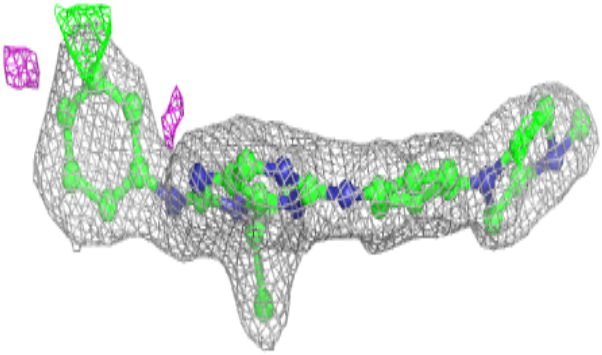
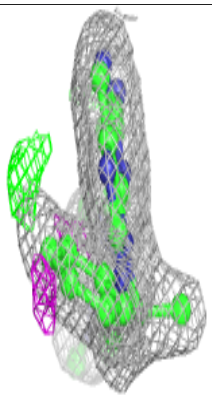
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.