Full wwPDB X-ray Structure Validation Report (i)

Feb 22, 2024 – 02:34 AM EST

PDB ID	:	4RH3
Title	:	AMPPCP-bound structure of human platelet phosphofructokinase in an R-state, crystal form II
Authors	:	Kloos, M.
Deposited on	:	2014-10-01
Resolution	:	3.02 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:

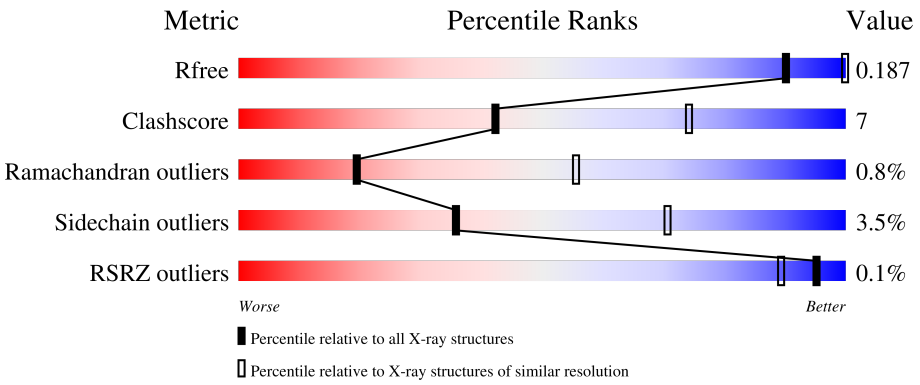
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.02 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	743	82% 15% • •
1	B	743	80% 17% • •
1	C	743	83% 15% • •
1	D	743	82% 15% • •

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	B	803	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22487 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP-dependent 6-phosphofructokinase, platelet type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	731	5582	3500	989	1054	39	0	0	0
1	B	731	5582	3500	989	1054	39	0	0	0
1	C	731	5582	3500	989	1054	39	0	0	0
1	D	731	5582	3500	989	1054	39	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	VAL	-	expression tag	UNP Q01813
A	21	PRO	-	expression tag	UNP Q01813
A	22	ASP	-	expression tag	UNP Q01813
A	23	PRO	-	expression tag	UNP Q01813
A	24	THR	-	expression tag	UNP Q01813
A	25	SER	-	expression tag	UNP Q01813
B	20	VAL	-	expression tag	UNP Q01813
B	21	PRO	-	expression tag	UNP Q01813
B	22	ASP	-	expression tag	UNP Q01813
B	23	PRO	-	expression tag	UNP Q01813
B	24	THR	-	expression tag	UNP Q01813
B	25	SER	-	expression tag	UNP Q01813
C	20	VAL	-	expression tag	UNP Q01813
C	21	PRO	-	expression tag	UNP Q01813
C	22	ASP	-	expression tag	UNP Q01813
C	23	PRO	-	expression tag	UNP Q01813
C	24	THR	-	expression tag	UNP Q01813
C	25	SER	-	expression tag	UNP Q01813
D	20	VAL	-	expression tag	UNP Q01813
D	21	PRO	-	expression tag	UNP Q01813
D	22	ASP	-	expression tag	UNP Q01813

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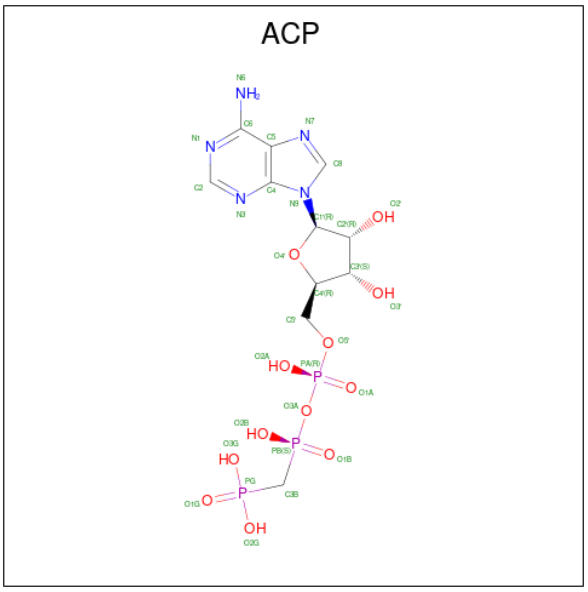
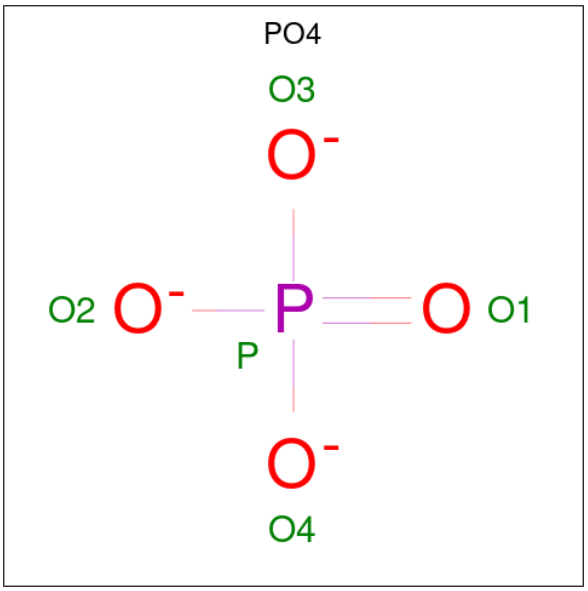
Chain	Residue	Modelled	Actual	Comment	Reference
D	23	PRO	-	expression tag	UNP Q01813
D	24	THR	-	expression tag	UNP Q01813
D	25	SER	-	expression tag	UNP Q01813

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	11	5	12	3	0	0
			Total	C	N	O	P		
2	B	1	31	11	5	12	3	0	0
			Total	C	N	O	P		
2	C	1	31	11	5	12	3	0	0
			Total	C	N	O	P		
2	D	1	31	11	5	12	3	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



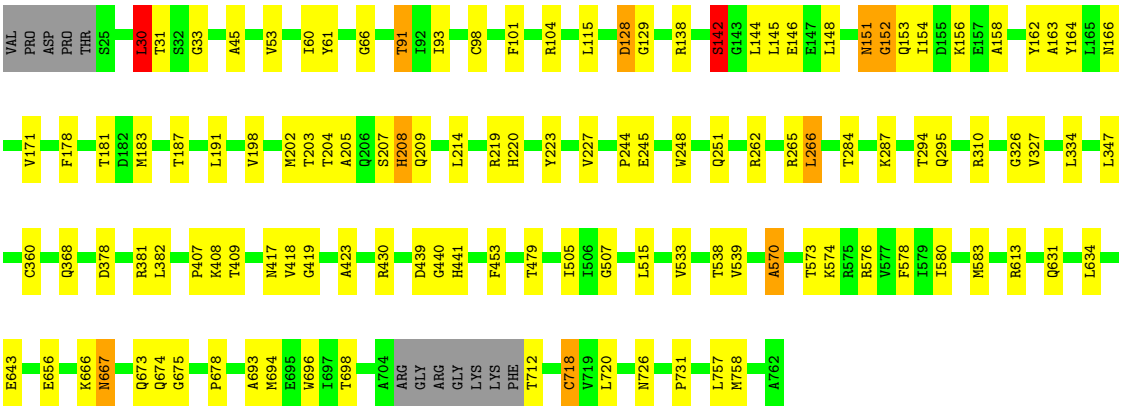
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	A	1	5	4	1	0	0
			Total	O	P		
3	A	1	5	4	1	0	0
			Total	O	P		
3	B	1	5	4	1	0	0
			Total	O	P		
3	B	1	5	4	1	0	0
			Total	O	P		
3	C	1	5	4	1	0	0
			Total	O	P		
3	C	1	5	4	1	0	0
			Total	O	P		
3	D	1	5	4	1	0	0

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.

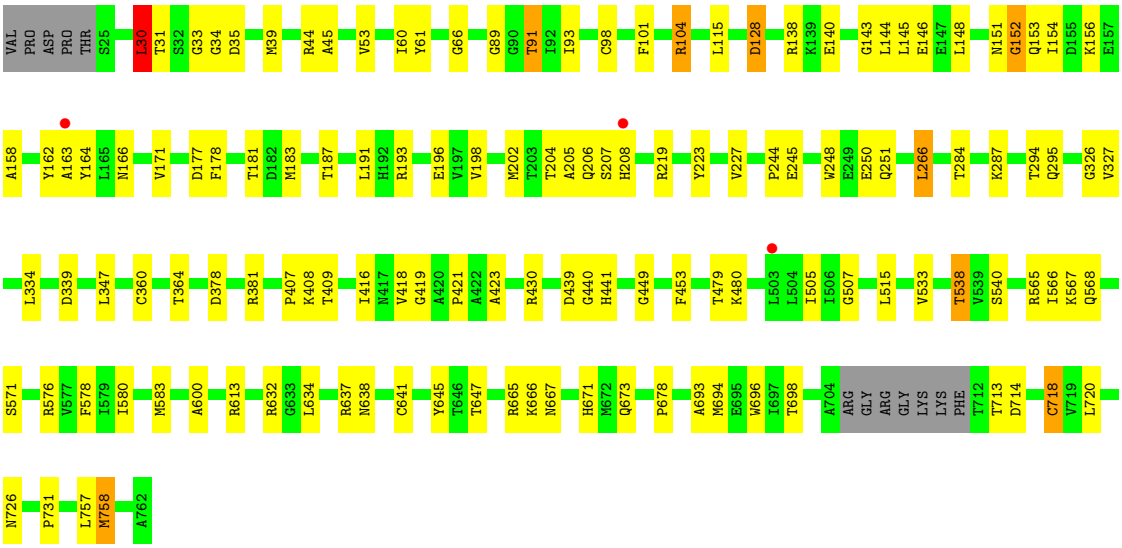
• Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

Chain A:



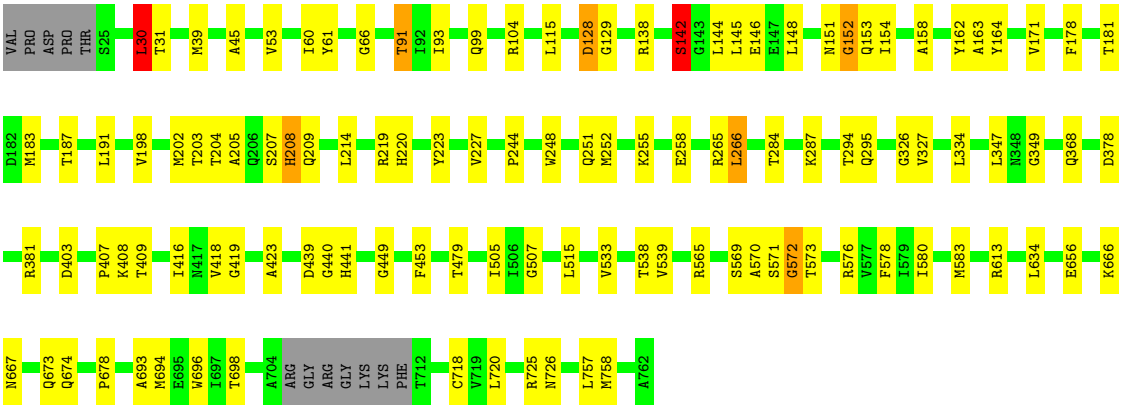
• Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

Chain B:



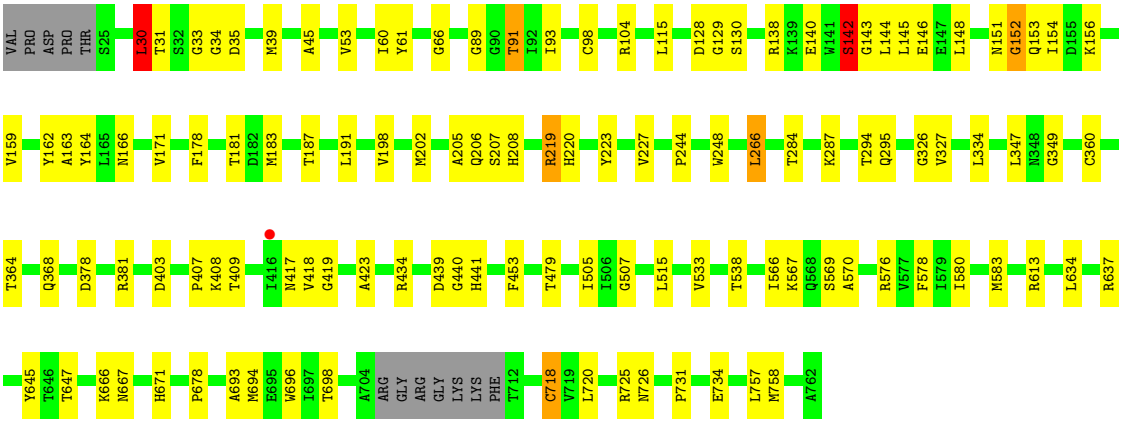
• Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

Chain C:



- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	132.91Å 132.91Å 397.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.90 – 3.02 46.90 – 3.02	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.90-3.02) 99.9 (46.90-3.02)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.146 , 0.187 0.144 , 0.187	Depositor DCC
R_{free} test set	4036 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	71.9	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 27.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.459 for -h,-k,l	Xtriage
Reported twinning fraction	0.511 for H, K, L 0.489 for -h,-k,l	Depositor
Outliers	0 of 80705 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22487	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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: PO4, ACP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.67	0/5671	0.77	3/7661 (0.0%)
1	B	0.63	0/5671	0.77	6/7661 (0.1%)
1	C	0.62	0/5671	0.76	3/7661 (0.0%)
1	D	0.60	0/5671	0.76	3/7661 (0.0%)
All	All	0.63	0/22684	0.76	15/30644 (0.0%)

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	2
1	C	0	2
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	128	ASP	CB-CG-OD1	8.18	125.66	118.30
1	C	565	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	D	35	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	B	30	LEU	CA-CB-CG	6.41	130.03	115.30
1	A	30	LEU	CA-CB-CG	6.13	129.41	115.30
1	C	30	LEU	CA-CB-CG	6.06	129.23	115.30
1	D	30	LEU	CA-CB-CG	5.96	129.01	115.30
1	B	104	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	D	219	ARG	NE-CZ-NH1	5.74	123.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	430	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	128	ASP	CB-CA-C	-5.35	99.71	110.40
1	B	339	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	262	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	44	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	35	ASP	CB-CG-OD2	-5.03	113.77	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	SER	Peptide
1	A	570	ALA	Peptide
1	C	142	SER	Peptide
1	C	572	GLY	Peptide
1	D	142	SER	Peptide

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	5582	0	5606	84	0
1	B	5582	0	5606	90	0
1	C	5582	0	5606	77	2
1	D	5582	0	5606	79	2
2	A	31	0	14	5	0
2	B	31	0	14	7	0
2	C	31	0	14	6	0
2	D	31	0	14	6	0
3	A	10	0	0	1	0
3	B	10	0	0	2	0
3	C	10	0	0	0	0
3	D	5	0	0	1	0
All	All	22487	0	22480	312	2

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 7.

All (312) 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:162:TYR:O	1:B:164:TYR:N	1.83	1.10
1:C:162:TYR:O	1:C:164:TYR:N	1.83	1.10
1:D:162:TYR:O	1:D:164:TYR:N	1.83	1.10
1:A:162:TYR:O	1:A:164:TYR:N	1.84	1.10
1:B:104:ARG:NH2	1:B:146:GLU:OE1	2.03	0.91
1:C:104:ARG:NH2	1:C:146:GLU:OE1	2.03	0.90
1:D:104:ARG:NH2	1:D:146:GLU:OE1	2.04	0.90
1:A:104:ARG:NH2	1:A:146:GLU:OE1	2.04	0.90
1:A:570:ALA:HA	1:B:421:PRO:HG2	1.57	0.84
1:C:128:ASP:HB2	2:C:800:ACP:O1G	1.78	0.83
1:A:203:THR:HG21	1:B:89:GLY:HA3	1.61	0.83
1:A:203:THR:CG2	1:B:89:GLY:C	2.50	0.79
1:A:205:ALA:HB3	1:A:266:LEU:HD23	1.67	0.76
1:C:203:THR:CG2	1:D:89:GLY:C	2.55	0.75
1:A:570:ALA:HA	1:B:421:PRO:CG	2.18	0.73
1:C:128:ASP:CB	2:C:800:ACP:O1G	2.36	0.73
1:C:207:SER:HB2	1:C:208:HIS:ND1	2.03	0.73
1:B:33:GLY:HA3	2:B:802:ACP:O2B	1.89	0.72
1:A:203:THR:HG21	1:B:89:GLY:CA	2.18	0.72
1:C:162:TYR:C	1:C:164:TYR:H	1.91	0.72
1:D:583:MET:HE2	1:D:671:HIS:HA	1.71	0.72
1:A:417:ASN:HB3	1:A:479:THR:CG2	2.19	0.71
1:D:417:ASN:HB3	1:D:479:THR:CG2	2.20	0.71
1:C:205:ALA:HB3	1:C:266:LEU:HD23	1.71	0.71
1:A:207:SER:HB2	1:A:208:HIS:ND1	2.05	0.70
1:C:203:THR:HG21	1:D:89:GLY:HA3	1.74	0.69
1:C:191:LEU:HD22	1:C:227:VAL:HG11	1.74	0.69
1:D:580:ILE:HD12	1:D:634:LEU:HD11	1.74	0.69
1:A:191:LEU:HD22	1:A:227:VAL:HG11	1.76	0.68
1:B:583:MET:HE2	1:B:671:HIS:HA	1.75	0.67
1:D:191:LEU:HD22	1:D:227:VAL:HG11	1.77	0.67
1:B:580:ILE:HD12	1:B:634:LEU:HD11	1.77	0.67
1:C:378:ASP:OD1	1:C:381:ARG:NH2	2.29	0.66
1:A:417:ASN:HB3	1:A:479:THR:HG22	1.78	0.66
1:A:580:ILE:HD12	1:A:634:LEU:HD11	1.78	0.66
1:B:378:ASP:OD1	1:B:381:ARG:NH2	2.29	0.66
1:D:162:TYR:C	1:D:164:TYR:H	1.94	0.65
1:B:191:LEU:HD22	1:B:227:VAL:HG11	1.77	0.65
1:D:378:ASP:OD1	1:D:381:ARG:NH2	2.30	0.65
1:D:566:ILE:HG21	1:D:580:ILE:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:580:ILE:HD12	1:C:634:LEU:HD11	1.79	0.64
1:A:378:ASP:OD1	1:A:381:ARG:NH2	2.30	0.64
1:D:417:ASN:HB3	1:D:479:THR:HG22	1.78	0.64
1:A:244:PRO:HB2	1:A:248:TRP:CD1	2.32	0.64
1:B:162:TYR:C	1:B:164:TYR:H	1.93	0.64
1:A:203:THR:HG21	1:B:89:GLY:C	2.18	0.63
1:B:713:THR:OG1	1:B:714:ASP:N	2.31	0.63
1:A:203:THR:HG23	1:B:89:GLY:O	1.99	0.63
1:B:566:ILE:HG21	1:B:580:ILE:HD11	1.80	0.63
1:D:98:CYS:N	2:D:800:ACP:O3'	2.29	0.63
1:B:583:MET:CE	1:B:671:HIS:HA	2.29	0.63
1:D:583:MET:CE	1:D:671:HIS:HA	2.28	0.62
1:D:439:ASP:OD2	1:D:698:THR:HG21	2.00	0.62
1:B:98:CYS:N	2:B:802:ACP:O3'	2.29	0.62
1:D:244:PRO:HB2	1:D:248:TRP:CD1	2.35	0.62
1:C:203:THR:HG21	1:D:89:GLY:CA	2.29	0.62
1:B:439:ASP:OD2	1:B:698:THR:HG21	2.00	0.61
1:A:294:THR:HG22	1:A:295:GLN:HE21	1.64	0.61
1:C:53:VAL:O	1:C:53:VAL:HG12	2.01	0.61
1:C:294:THR:HG22	1:C:295:GLN:HE21	1.64	0.61
1:B:294:THR:HG22	1:B:295:GLN:HE21	1.66	0.60
1:A:439:ASP:OD2	1:A:698:THR:HG21	2.00	0.60
1:B:244:PRO:HB2	1:B:248:TRP:CD1	2.35	0.60
1:A:98:CYS:N	2:A:800:ACP:O3'	2.33	0.59
1:A:198:VAL:O	1:A:202:MET:HG3	2.03	0.59
1:C:439:ASP:OD2	1:C:698:THR:HG21	2.01	0.59
1:A:573:THR:OG1	1:B:480:LYS:HE2	2.03	0.59
1:A:53:VAL:HG12	1:A:53:VAL:O	2.03	0.59
1:C:128:ASP:CG	2:C:800:ACP:O1G	2.41	0.58
1:C:244:PRO:HB2	1:C:248:TRP:CD1	2.37	0.58
1:C:209:GLN:HA	1:C:265:ARG:O	2.02	0.58
1:A:408:LYS:HB2	1:A:440:GLY:HA3	1.86	0.58
1:A:209:GLN:HA	1:A:265:ARG:O	2.03	0.58
1:D:294:THR:HG22	1:D:295:GLN:HE21	1.67	0.58
1:A:191:LEU:HD22	1:A:227:VAL:CG1	2.34	0.58
1:A:423:ALA:HB1	1:A:678:PRO:HB3	1.86	0.58
1:C:203:THR:HG21	1:D:89:GLY:C	2.23	0.58
1:C:191:LEU:HD22	1:C:227:VAL:CG1	2.34	0.57
1:B:645:TYR:CE2	1:C:656:GLU:HG2	2.38	0.57
1:D:53:VAL:HG12	1:D:53:VAL:O	2.03	0.57
1:D:198:VAL:O	1:D:202:MET:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:VAL:HG12	1:B:53:VAL:O	2.04	0.57
1:C:203:THR:HG23	1:D:89:GLY:O	2.04	0.57
1:B:198:VAL:O	1:B:202:MET:HG3	2.04	0.57
1:B:128:ASP:HB2	2:B:802:ACP:O3G	2.05	0.57
1:C:198:VAL:O	1:C:202:MET:HG3	2.05	0.57
1:D:191:LEU:HD22	1:D:227:VAL:CG1	2.35	0.57
1:D:408:LYS:HB2	1:D:440:GLY:HA3	1.85	0.56
1:C:408:LYS:HB2	1:C:440:GLY:HA3	1.88	0.56
1:A:441:HIS:NE2	1:A:698:THR:HG22	2.21	0.56
1:A:418:VAL:O	1:A:507:GLY:HA3	2.06	0.56
1:C:441:HIS:NE2	1:C:698:THR:HG22	2.21	0.56
1:A:162:TYR:C	1:A:164:TYR:H	1.97	0.55
1:A:539:VAL:HG11	1:A:674:GLN:HA	1.89	0.55
1:B:191:LEU:HD22	1:B:227:VAL:CG1	2.37	0.55
1:D:441:HIS:NE2	1:D:698:THR:HG22	2.22	0.55
1:D:434:ARG:NH1	3:D:801:PO4:O2	2.39	0.55
1:D:418:VAL:O	1:D:507:GLY:HA3	2.07	0.54
1:D:30:LEU:HB3	1:D:60:ILE:HB	1.90	0.54
1:D:423:ALA:HB1	1:D:678:PRO:HB3	1.89	0.54
1:B:441:HIS:NE2	1:B:698:THR:HG22	2.23	0.54
1:B:128:ASP:OD1	1:B:177:ASP:HB3	2.06	0.54
1:B:408:LYS:HB2	1:B:440:GLY:HA3	1.90	0.54
1:A:203:THR:HG23	1:B:89:GLY:C	2.27	0.54
1:A:208:HIS:ND1	1:A:208:HIS:N	2.56	0.54
1:A:573:THR:HG23	1:B:480:LYS:NZ	2.23	0.53
1:A:533:VAL:HB	1:A:696:TRP:CZ3	2.44	0.53
1:A:142:SER:HA	1:A:144:LEU:HB2	1.90	0.53
1:A:144:LEU:HD12	1:A:144:LEU:H	1.74	0.53
1:B:430:ARG:HH22	3:B:803:PO4:P	2.31	0.53
1:B:533:VAL:HB	1:B:696:TRP:CZ3	2.44	0.53
1:C:423:ALA:HB1	1:C:678:PRO:HB3	1.90	0.53
1:C:30:LEU:HB3	1:C:60:ILE:HB	1.91	0.52
1:C:208:HIS:ND1	1:C:208:HIS:N	2.57	0.52
1:C:61:TYR:O	1:C:66:GLY:HA3	2.10	0.52
1:D:580:ILE:HD12	1:D:634:LEU:CD1	2.39	0.52
1:D:533:VAL:HB	1:D:696:TRP:CZ3	2.44	0.52
1:A:30:LEU:HB3	1:A:60:ILE:HB	1.91	0.52
1:C:539:VAL:HG11	1:C:674:GLN:HA	1.92	0.52
1:A:151:ASN:OD1	1:A:151:ASN:N	2.43	0.52
1:A:656:GLU:HG2	1:D:645:TYR:CE2	2.45	0.52
1:B:61:TYR:O	1:B:66:GLY:HA3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:ILE:HD12	1:B:634:LEU:CD1	2.40	0.52
1:A:574:LYS:HB3	1:A:631:GLN:O	2.10	0.51
1:C:142:SER:HA	1:C:144:LEU:HB2	1.90	0.51
1:A:53:VAL:HG11	1:A:334:LEU:HD12	1.92	0.51
1:D:142:SER:HA	1:D:144:LEU:HB2	1.93	0.51
1:B:418:VAL:O	1:B:507:GLY:HA3	2.11	0.51
1:B:177:ASP:OD2	2:B:802:ACP:O1G	2.28	0.51
1:B:205:ALA:HB3	1:B:266:LEU:HD23	1.92	0.51
1:A:573:THR:HG23	1:B:480:LYS:HZ1	1.75	0.51
1:B:423:ALA:HB1	1:B:678:PRO:HB3	1.93	0.51
1:A:61:TYR:O	1:A:66:GLY:HA3	2.10	0.51
1:C:183:MET:HE1	1:C:187:THR:HB	1.93	0.51
1:C:418:VAL:O	1:C:507:GLY:HA3	2.10	0.51
1:C:666:LYS:C	1:C:667:ASN:HD22	2.13	0.51
1:B:91:THR:HG22	1:B:93:ILE:H	1.76	0.51
1:A:419:GLY:O	1:A:479:THR:HB	2.11	0.50
1:D:162:TYR:C	1:D:164:TYR:N	2.60	0.50
1:C:91:THR:HG22	1:C:93:ILE:H	1.76	0.50
1:D:205:ALA:HB3	1:D:266:LEU:HD23	1.92	0.50
1:C:569:SER:O	1:C:570:ALA:C	2.47	0.50
1:C:580:ILE:HD12	1:C:634:LEU:CD1	2.42	0.50
1:C:205:ALA:HB1	1:C:266:LEU:CB	2.42	0.50
1:B:30:LEU:HB3	1:B:60:ILE:HB	1.92	0.50
1:B:430:ARG:HH12	3:B:803:PO4:P	2.35	0.50
1:D:91:THR:HG22	1:D:93:ILE:H	1.75	0.50
1:C:533:VAL:HB	1:C:696:TRP:CZ3	2.47	0.50
1:A:91:THR:HG22	1:A:93:ILE:H	1.76	0.49
1:C:693:ALA:HB2	1:C:720:LEU:HD23	1.95	0.49
1:A:417:ASN:HB3	1:A:479:THR:HG23	1.92	0.49
1:B:566:ILE:HD13	1:B:580:ILE:HD11	1.94	0.49
1:D:61:TYR:O	1:D:66:GLY:HA3	2.11	0.49
1:A:580:ILE:HD12	1:A:634:LEU:CD1	2.42	0.49
1:A:31:THR:CB	1:A:91:THR:HG21	2.43	0.49
1:B:53:VAL:HG11	1:B:334:LEU:HD12	1.95	0.49
1:B:183:MET:HE1	1:B:187:THR:HB	1.94	0.49
2:C:800:ACP:O2A	2:C:800:ACP:O3G	2.31	0.49
1:C:129:GLY:N	2:C:800:ACP:O1B	2.45	0.48
1:D:417:ASN:HB3	1:D:479:THR:HG23	1.92	0.48
1:B:183:MET:CE	1:B:187:THR:HB	2.43	0.48
1:C:53:VAL:HG11	1:C:334:LEU:HD12	1.94	0.48
1:D:223:TYR:CE2	1:D:227:VAL:HG21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:GLY:O	1:D:479:THR:HB	2.13	0.48
1:A:284:THR:OG1	1:A:287:LYS:HB2	2.14	0.48
1:D:569:SER:O	1:D:570:ALA:C	2.52	0.48
1:B:693:ALA:HB2	1:B:720:LEU:HD23	1.96	0.48
1:A:310:ARG:HB2	1:B:204:THR:HG21	1.95	0.48
1:D:33:GLY:O	1:D:34:GLY:C	2.52	0.48
1:A:223:TYR:CE2	1:A:227:VAL:HG21	2.49	0.47
1:C:284:THR:OG1	1:C:287:LYS:HB2	2.14	0.47
1:D:129:GLY:HA3	2:D:800:ACP:O2A	2.13	0.47
1:B:140:GLU:O	1:B:143:GLY:N	2.46	0.47
1:B:223:TYR:CE2	1:B:227:VAL:HG21	2.50	0.47
1:D:183:MET:CE	1:D:187:THR:HB	2.44	0.47
1:A:693:ALA:HB2	1:A:720:LEU:HD23	1.97	0.47
1:A:183:MET:CE	1:A:187:THR:HB	2.44	0.47
1:C:223:TYR:CE2	1:C:227:VAL:HG21	2.49	0.47
1:A:53:VAL:HG11	1:A:334:LEU:CD1	2.45	0.47
1:A:220:HIS:HB3	1:A:368:GLN:HE22	1.79	0.47
1:B:31:THR:CG2	1:B:39:MET:SD	3.03	0.47
1:B:101:PHE:HD2	2:B:802:ACP:H8	1.79	0.47
1:B:171:VAL:HG11	1:B:178:PHE:HB2	1.97	0.47
1:C:151:ASN:O	1:C:152:GLY:C	2.53	0.47
1:C:171:VAL:HG11	1:C:178:PHE:HB2	1.96	0.47
1:C:726:ASN:OD1	1:C:726:ASN:N	2.48	0.47
1:D:53:VAL:HG11	1:D:334:LEU:HD12	1.96	0.47
1:D:220:HIS:HB3	1:D:368:GLN:HE22	1.79	0.47
1:D:726:ASN:N	1:D:726:ASN:OD1	2.46	0.47
1:B:284:THR:OG1	1:B:287:LYS:HB2	2.15	0.47
1:C:220:HIS:HB3	1:C:368:GLN:HE22	1.80	0.47
1:A:183:MET:HE1	1:A:187:THR:HB	1.96	0.47
1:D:171:VAL:HG11	1:D:178:PHE:HB2	1.97	0.47
1:B:726:ASN:N	1:B:726:ASN:OD1	2.47	0.46
1:C:45:ALA:HB3	1:C:326:GLY:HA3	1.96	0.46
1:C:31:THR:CB	1:C:91:THR:HG21	2.45	0.46
1:C:128:ASP:OD2	2:C:800:ACP:O1G	2.33	0.46
1:C:183:MET:CE	1:C:187:THR:HB	2.46	0.46
1:B:31:THR:CB	1:B:91:THR:HG21	2.45	0.46
1:B:193:ARG:NH1	1:B:196:GLU:OE1	2.48	0.46
1:B:205:ALA:HB1	1:B:266:LEU:HB3	1.97	0.46
1:C:115:LEU:HD11	1:C:144:LEU:HD22	1.97	0.46
1:D:205:ALA:HB1	1:D:266:LEU:HB3	1.97	0.46
1:C:203:THR:HG23	1:D:89:GLY:C	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ALA:HB1	1:C:266:LEU:HB2	1.98	0.46
1:A:726:ASN:OD1	1:A:726:ASN:N	2.49	0.46
1:C:207:SER:HB2	1:C:208:HIS:CE1	2.50	0.46
1:A:45:ALA:HB3	1:A:326:GLY:HA3	1.98	0.46
1:C:576:ARG:HD2	1:C:578:PHE:CE1	2.51	0.46
1:A:128:ASP:C	1:A:128:ASP:OD1	2.54	0.45
1:D:31:THR:CB	1:D:91:THR:HG21	2.46	0.45
1:B:98:CYS:HB3	2:B:802:ACP:O2'	2.16	0.45
1:D:566:ILE:HD13	1:D:580:ILE:HD11	1.97	0.45
1:D:666:LYS:C	1:D:667:ASN:HD22	2.18	0.45
3:A:802:PO4:O2	1:B:665:ARG:NE	2.37	0.45
1:D:284:THR:OG1	1:D:287:LYS:HB2	2.15	0.45
1:D:693:ALA:HB2	1:D:720:LEU:HD23	1.96	0.45
1:A:153:GLN:OE1	1:A:154:ILE:N	2.48	0.45
1:A:33:GLY:HA3	2:A:800:ACP:O2B	2.17	0.45
1:A:666:LYS:C	1:A:667:ASN:HD22	2.19	0.45
1:B:666:LYS:C	1:B:667:ASN:HD22	2.18	0.45
1:B:115:LEU:HD11	1:B:144:LEU:HD22	1.98	0.45
1:C:53:VAL:HG11	1:C:334:LEU:CD1	2.47	0.45
1:D:45:ALA:HB3	1:D:326:GLY:HA3	1.98	0.45
1:A:151:ASN:O	1:A:152:GLY:C	2.55	0.44
1:A:31:THR:HB	1:A:91:THR:HG21	1.99	0.44
1:A:207:SER:CB	1:A:208:HIS:ND1	2.75	0.44
1:C:153:GLN:OE1	1:C:154:ILE:N	2.49	0.44
1:A:207:SER:HB2	1:A:208:HIS:CE1	2.52	0.44
1:C:207:SER:CB	1:C:208:HIS:ND1	2.75	0.44
1:D:31:THR:CG2	1:D:39:MET:SD	3.05	0.44
1:A:171:VAL:HG11	1:A:178:PHE:HB2	1.99	0.44
1:B:33:GLY:O	1:B:34:GLY:C	2.56	0.44
1:B:327:VAL:HG21	1:B:757:LEU:HD22	2.00	0.44
1:B:567:LYS:HD2	1:B:634:LEU:HD22	2.00	0.44
1:D:153:GLN:OE1	1:D:154:ILE:N	2.50	0.44
1:D:327:VAL:HG21	1:D:757:LEU:HD22	1.99	0.44
1:D:129:GLY:H	2:D:800:ACP:C3B	2.30	0.43
1:D:151:ASN:O	1:D:152:GLY:C	2.56	0.43
1:A:198:VAL:HG22	1:A:214:LEU:CD1	2.48	0.43
1:B:505:ILE:HD12	1:B:515:LEU:HD21	2.01	0.43
1:C:349:GLY:HA3	1:C:725:ARG:HD3	2.00	0.43
1:A:178:PHE:CE2	1:A:360:CYS:HB3	2.53	0.43
1:C:198:VAL:HG22	1:C:214:LEU:CD1	2.48	0.43
1:C:694:MET:O	1:C:698:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:SER:OG	1:B:632:ARG:NH1	2.43	0.43
1:D:53:VAL:HG11	1:D:334:LEU:CD1	2.48	0.43
2:B:802:ACP:C4'	2:B:802:ACP:O2A	2.67	0.43
1:A:675:GLY:C	1:B:565:ARG:HD3	2.38	0.43
1:C:31:THR:HB	1:C:91:THR:HG21	2.01	0.43
1:C:327:VAL:HG21	1:C:757:LEU:HD22	2.00	0.43
1:D:130:SER:OG	2:D:800:ACP:O1B	2.16	0.43
1:B:45:ALA:HB3	1:B:326:GLY:HA3	1.99	0.43
1:C:158:ALA:O	1:C:162:TYR:HB2	2.19	0.43
1:D:128:ASP:OD1	2:D:800:ACP:C3B	2.67	0.43
1:A:505:ILE:HD12	1:A:515:LEU:HD21	2.01	0.42
1:D:183:MET:HE1	1:D:187:THR:HB	2.00	0.42
1:B:694:MET:O	1:B:698:THR:HG23	2.19	0.42
1:C:91:THR:HG22	1:C:93:ILE:HG12	2.01	0.42
1:A:327:VAL:HG21	1:A:757:LEU:HD22	2.01	0.42
1:A:158:ALA:O	1:A:162:TYR:HB2	2.19	0.42
1:A:115:LEU:HD11	1:A:144:LEU:CD2	2.49	0.42
1:B:53:VAL:HG11	1:B:334:LEU:CD1	2.49	0.42
1:A:91:THR:HG22	1:A:93:ILE:HG12	2.01	0.42
1:B:91:THR:HG22	1:B:93:ILE:HG12	2.02	0.42
1:D:637:ARG:HD3	1:D:647:THR:OG1	2.19	0.42
1:B:153:GLN:OE1	1:B:154:ILE:N	2.52	0.42
1:A:583:MET:HG3	1:A:673:GLN:OE1	2.20	0.42
1:D:140:GLU:O	1:D:143:GLY:N	2.52	0.42
1:D:718:CYS:HB3	1:D:731:PRO:HA	2.02	0.42
1:A:378:ASP:O	1:A:382:LEU:HG	2.19	0.41
1:A:718:CYS:HB3	1:A:731:PRO:HA	2.02	0.41
1:B:158:ALA:O	1:B:162:TYR:HB2	2.20	0.41
1:B:576:ARG:HD2	1:B:578:PHE:CE1	2.55	0.41
1:C:205:ALA:HB1	1:C:266:LEU:HB3	2.03	0.41
1:D:91:THR:HG22	1:D:93:ILE:HG12	2.02	0.41
1:D:115:LEU:HD11	1:D:144:LEU:HD22	2.00	0.41
1:D:31:THR:HB	1:D:91:THR:HG21	2.02	0.41
1:D:576:ARG:HD2	1:D:578:PHE:CE1	2.55	0.41
1:A:576:ARG:HD2	1:A:578:PHE:CE1	2.55	0.41
1:B:637:ARG:HD3	1:B:647:THR:OG1	2.21	0.41
1:B:638:ASN:HB3	1:B:641:CYS:HB3	2.03	0.41
1:D:360:CYS:O	1:D:364:THR:HG23	2.21	0.41
2:A:800:ACP:O1A	2:A:800:ACP:C4'	2.68	0.41
1:C:252:MET:O	1:C:255:LYS:HB3	2.21	0.41
1:C:416:ILE:HD11	1:C:449:GLY:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:ALA:HB1	1:C:573:THR:HB	2.03	0.41
1:D:159:VAL:O	1:D:162:TYR:HD1	2.04	0.41
1:D:349:GLY:HA3	1:D:725:ARG:HD3	2.02	0.41
1:A:694:MET:O	1:A:698:THR:HG23	2.20	0.41
1:B:360:CYS:O	1:B:364:THR:HG23	2.20	0.41
1:B:600:ALA:HB3	1:B:758:MET:HE1	2.03	0.41
1:C:583:MET:H	1:C:673:GLN:HE22	1.67	0.41
1:D:129:GLY:H	2:D:800:ACP:H3B2	1.86	0.41
1:D:567:LYS:HD2	1:D:634:LEU:HD22	2.02	0.41
1:B:266:LEU:CD1	1:B:266:LEU:C	2.90	0.41
1:B:419:GLY:O	1:B:479:THR:HG23	2.21	0.41
1:C:571:SER:HA	1:C:572:GLY:HA2	1.77	0.41
1:D:694:MET:O	1:D:698:THR:HG23	2.20	0.41
1:B:538:THR:HB	1:B:540:SER:H	1.85	0.41
1:A:205:ALA:HB1	1:A:266:LEU:CB	2.51	0.40
1:B:416:ILE:HD11	1:B:449:GLY:C	2.41	0.40
1:C:31:THR:CG2	1:C:39:MET:SD	3.09	0.40
1:B:583:MET:HG3	1:B:673:GLN:OE1	2.22	0.40
1:A:101:PHE:O	2:A:800:ACP:H2	2.22	0.40
1:B:151:ASN:O	1:B:152:GLY:C	2.59	0.40
1:B:718:CYS:HB3	1:B:731:PRO:HA	2.03	0.40
1:B:31:THR:HB	1:B:91:THR:HG21	2.03	0.40
1:C:505:ILE:HD12	1:C:515:LEU:HD21	2.04	0.40
1:D:505:ILE:HD12	1:D:515:LEU:HD21	2.03	0.40
1:A:129:GLY:O	2:A:800:ACP:C8	2.70	0.40
1:C:419:GLY:O	1:C:479:THR:HG23	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:THR:O	1:D:734:GLU:OE1[5_7107]	2.11	0.09
1:C:294:THR:CG2	1:D:734:GLU:OE2[5_7107]	2.16	0.04

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	727/743 (98%)	687 (94%)	34 (5%)	6 (1%)	19	55
1	B	727/743 (98%)	682 (94%)	39 (5%)	6 (1%)	19	55
1	C	727/743 (98%)	685 (94%)	37 (5%)	5 (1%)	22	59
1	D	727/743 (98%)	682 (94%)	38 (5%)	7 (1%)	15	50
All	All	2908/2972 (98%)	2736 (94%)	148 (5%)	24 (1%)	19	55

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	SER
1	A	163	ALA
1	B	163	ALA
1	C	142	SER
1	C	163	ALA
1	D	142	SER
1	D	163	ALA
1	A	152	GLY
1	A	407	PRO
1	A	409	THR
1	B	152	GLY
1	B	207	SER
1	B	407	PRO
1	B	409	THR
1	C	152	GLY
1	C	407	PRO
1	C	409	THR
1	D	152	GLY
1	D	207	SER
1	D	407	PRO
1	D	409	THR
1	A	245	GLU
1	B	206	GLN
1	D	206	GLN

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	589/599 (98%)	565 (96%)	24 (4%)	30	66
1	B	589/599 (98%)	568 (96%)	21 (4%)	35	69
1	C	589/599 (98%)	569 (97%)	20 (3%)	37	72
1	D	589/599 (98%)	571 (97%)	18 (3%)	40	74
All	All	2356/2396 (98%)	2273 (96%)	83 (4%)	36	70

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	91	THR
1	A	128	ASP
1	A	138	ARG
1	A	145	LEU
1	A	148	LEU
1	A	151	ASN
1	A	156	LYS
1	A	166	ASN
1	A	181	THR
1	A	204	THR
1	A	208	HIS
1	A	219	ARG
1	A	251	GLN
1	A	266	LEU
1	A	347	LEU
1	A	453	PHE
1	A	538	THR
1	A	613	ARG
1	A	643	GLU
1	A	667	ASN
1	A	712	THR
1	A	718	CYS
1	A	758	MET

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Mol	Chain	Res	Type
1	B	30	LEU
1	B	91	THR
1	B	138	ARG
1	B	145	LEU
1	B	148	LEU
1	B	156	LYS
1	B	166	ASN
1	B	181	THR
1	B	208	HIS
1	B	219	ARG
1	B	245	GLU
1	B	250	GLU
1	B	251	GLN
1	B	266	LEU
1	B	347	LEU
1	B	453	PHE
1	B	538	THR
1	B	568	GLN
1	B	613	ARG
1	B	718	CYS
1	B	758	MET
1	C	30	LEU
1	C	91	THR
1	C	99	GLN
1	C	138	ARG
1	C	145	LEU
1	C	148	LEU
1	C	181	THR
1	C	204	THR
1	C	208	HIS
1	C	219	ARG
1	C	251	GLN
1	C	258	GLU
1	C	266	LEU
1	C	347	LEU
1	C	403	ASP
1	C	453	PHE
1	C	538	THR
1	C	613	ARG
1	C	718	CYS
1	C	758	MET
1	D	30	LEU

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Mol	Chain	Res	Type
1	D	91	THR
1	D	138	ARG
1	D	145	LEU
1	D	148	LEU
1	D	156	LYS
1	D	166	ASN
1	D	181	THR
1	D	208	HIS
1	D	219	ARG
1	D	266	LEU
1	D	347	LEU
1	D	403	ASP
1	D	453	PHE
1	D	538	THR
1	D	613	ARG
1	D	718	CYS
1	D	758	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	GLN
1	A	405	GLN
1	A	616	GLN
1	A	644	ASN
1	B	295	GLN
1	B	405	GLN
1	B	616	GLN
1	B	671	HIS
1	B	749	GLN
1	C	295	GLN
1	C	405	GLN
1	C	644	ASN
1	D	295	GLN
1	D	405	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)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACP	D	800	-	27,33,33	0.63	0	32,52,52	1.07	3 (9%)
3	PO4	C	802	-	4,4,4	0.74	0	6,6,6	0.80	0
3	PO4	B	803	-	4,4,4	1.19	0	6,6,6	0.64	0
3	PO4	D	801	-	4,4,4	0.72	0	6,6,6	1.21	0
2	ACP	B	802	-	27,33,33	1.29	1 (3%)	32,52,52	1.62	7 (21%)
3	PO4	B	801	-	4,4,4	0.79	0	6,6,6	1.24	0
2	ACP	C	800	-	27,33,33	2.62	1 (3%)	32,52,52	1.02	3 (9%)
3	PO4	A	802	-	4,4,4	0.99	0	6,6,6	1.60	1 (16%)
3	PO4	C	801	-	4,4,4	0.75	0	6,6,6	1.63	2 (33%)
3	PO4	A	801	-	4,4,4	0.74	0	6,6,6	1.37	1 (16%)
2	ACP	A	800	-	27,33,33	1.04	1 (3%)	32,52,52	1.60	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACP	D	800	-	-	6/15/38/38	0/3/3/3
2	ACP	B	802	-	-	5/15/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACP	C	800	-	-	2/15/38/38	0/3/3/3
2	ACP	A	800	-	-	4/15/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	800	ACP	PB-O3A	13.23	1.73	1.58
2	B	802	ACP	PB-O3A	4.95	1.63	1.58
2	A	800	ACP	PB-O3A	3.58	1.62	1.58

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	800	ACP	O1B-PB-C3B	4.76	121.66	109.07
2	A	800	ACP	PB-O3A-PA	-3.80	120.50	132.56
2	A	800	ACP	O5'-C5'-C4'	3.70	121.72	108.99
2	B	802	ACP	C1'-N9-C4	3.59	132.94	126.64
3	A	802	PO4	O2-P-O1	-3.41	98.41	110.89
2	B	802	ACP	O5'-C5'-C4'	3.27	120.25	108.99
2	C	800	ACP	O1B-PB-C3B	3.15	117.40	109.07
2	B	802	ACP	O1B-PB-C3B	3.01	117.03	109.07
2	D	800	ACP	O1B-PB-C3B	2.92	116.80	109.07
3	C	801	PO4	O3-P-O2	2.62	116.39	107.97
2	D	800	ACP	O5'-PA-O1A	2.55	119.05	109.07
2	B	802	ACP	PA-O5'-C5'	-2.51	106.96	121.68
2	B	802	ACP	O2A-PA-O5'	-2.50	96.12	107.75
3	C	801	PO4	O2-P-O1	-2.47	101.87	110.89
3	A	801	PO4	O3-P-O2	2.47	115.89	107.97
2	B	802	ACP	C3'-C2'-C1'	2.45	104.67	100.98
2	A	800	ACP	C5-C6-N6	2.42	124.03	120.35
2	C	800	ACP	PB-O3A-PA	2.41	140.21	132.56
2	D	800	ACP	C5-C6-N6	2.39	123.99	120.35
2	A	800	ACP	C3'-C2'-C1'	2.39	104.57	100.98
2	B	802	ACP	O2B-PB-O1B	-2.34	102.25	110.07
2	C	800	ACP	C5-C6-N6	2.06	123.47	120.35

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	ACP	PB-C3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
2	A	800	ACP	PB-C3B-PG-O2G
2	A	800	ACP	PB-C3B-PG-O3G
2	A	800	ACP	C4'-C5'-O5'-PA
2	B	802	ACP	C5'-O5'-PA-O1A
2	B	802	ACP	C5'-O5'-PA-O3A
2	B	802	ACP	C3'-C4'-C5'-O5'
2	D	800	ACP	C5'-O5'-PA-O3A
2	B	802	ACP	O4'-C4'-C5'-O5'
2	B	802	ACP	C4'-C5'-O5'-PA
2	D	800	ACP	C4'-C5'-O5'-PA
2	D	800	ACP	C5'-O5'-PA-O1A
2	C	800	ACP	PB-C3B-PG-O2G
2	D	800	ACP	PB-C3B-PG-O2G
2	D	800	ACP	PB-C3B-PG-O3G
2	C	800	ACP	PB-C3B-PG-O1G
2	D	800	ACP	PB-C3B-PG-O1G

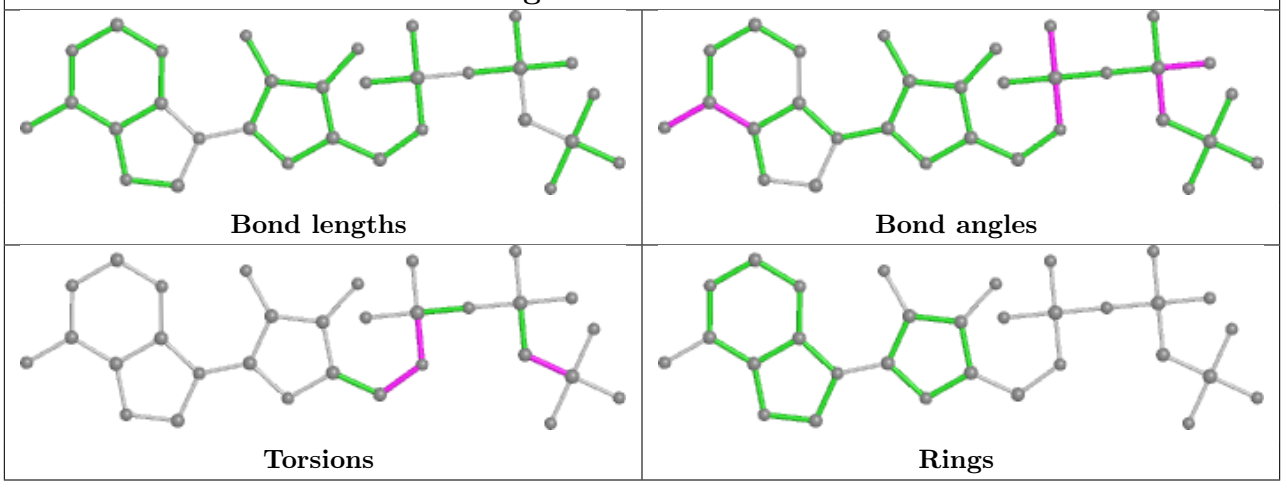
There are no ring outliers.

7 monomers are involved in 28 short contacts:

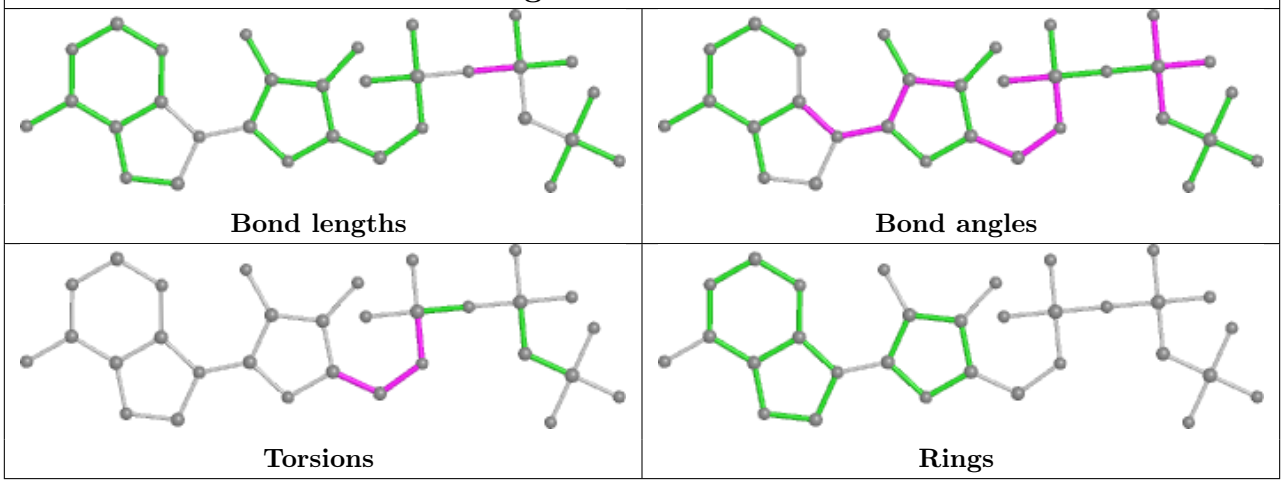
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	800	ACP	6	0
3	B	803	PO4	2	0
3	D	801	PO4	1	0
2	B	802	ACP	7	0
2	C	800	ACP	6	0
3	A	802	PO4	1	0
2	A	800	ACP	5	0

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.

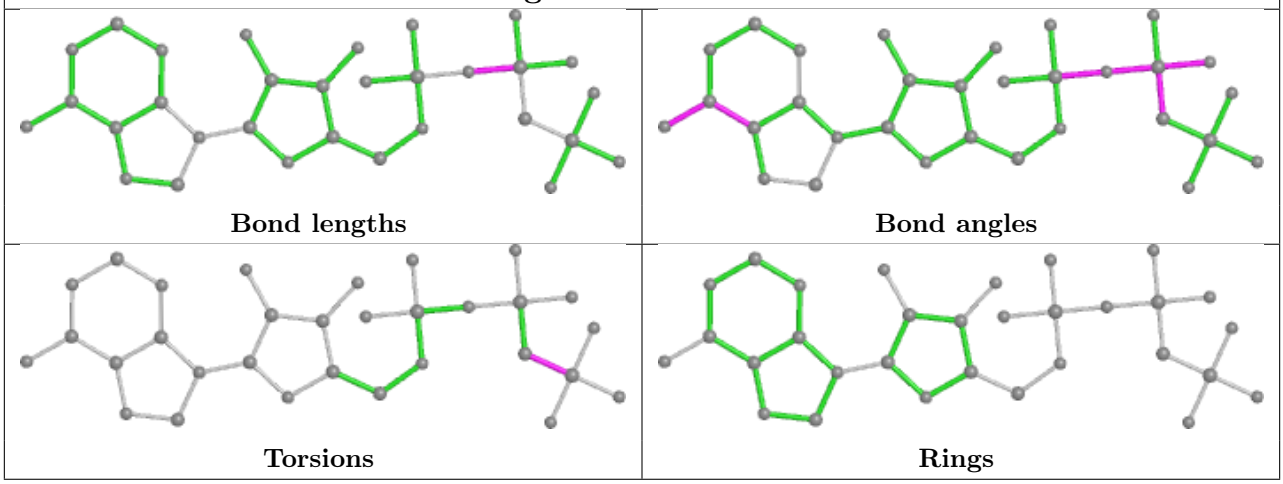
Ligand ACP D 800

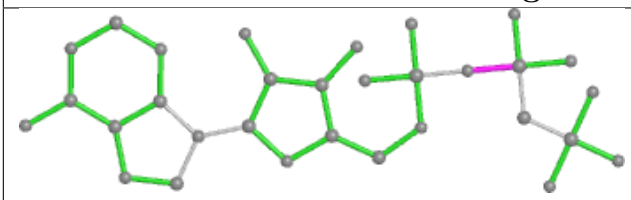
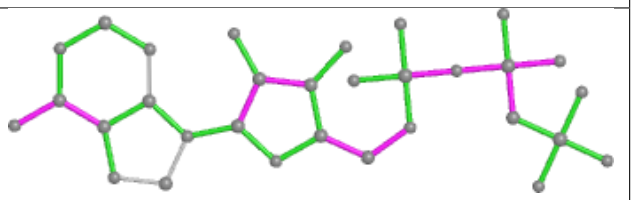
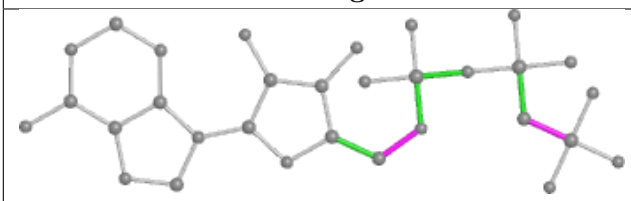
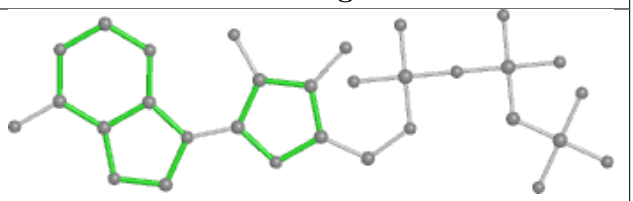


Ligand ACP B 802



Ligand ACP C 800



Ligand ACP A 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	731/743 (98%)	-0.55	0 100 100	37, 68, 111, 178	0
1	B	731/743 (98%)	-0.51	3 (0%) 92 78	33, 72, 118, 153	0
1	C	731/743 (98%)	-0.53	0 100 100	45, 76, 115, 157	0
1	D	731/743 (98%)	-0.48	1 (0%) 95 89	41, 81, 132, 178	0
All	All	2924/2972 (98%)	-0.52	4 (0%) 95 89	33, 74, 121, 178	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	163	ALA	2.5
1	B	208	HIS	2.4
1	D	416	ILE	2.3
1	B	503	LEU	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

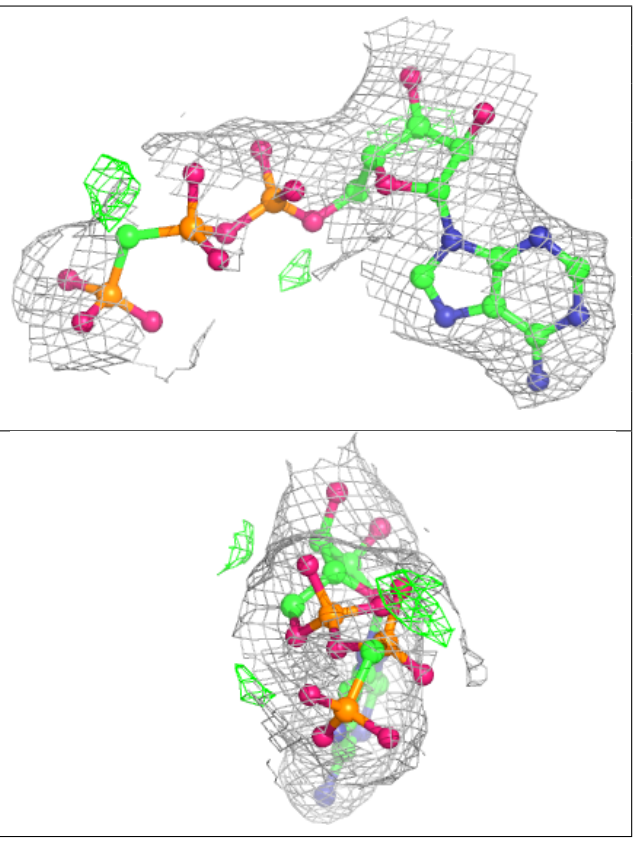
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACP	A	800	31/31	0.96	0.14	58,70,103,125	0
3	PO4	B	801	5/5	0.96	0.10	80,90,105,110	0
2	ACP	D	800	31/31	0.97	0.14	58,73,92,99	0
2	ACP	C	800	31/31	0.97	0.13	58,76,103,130	0
3	PO4	C	802	5/5	0.97	0.15	57,63,65,73	0
3	PO4	D	801	5/5	0.97	0.12	69,78,84,95	0
2	ACP	B	802	31/31	0.98	0.15	49,63,77,79	0
3	PO4	B	803	5/5	0.98	0.14	61,67,76,81	0
3	PO4	C	801	5/5	0.98	0.12	65,68,71,78	0
3	PO4	A	801	5/5	0.98	0.13	49,53,56,58	0
3	PO4	A	802	5/5	0.98	0.17	48,48,54,64	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.

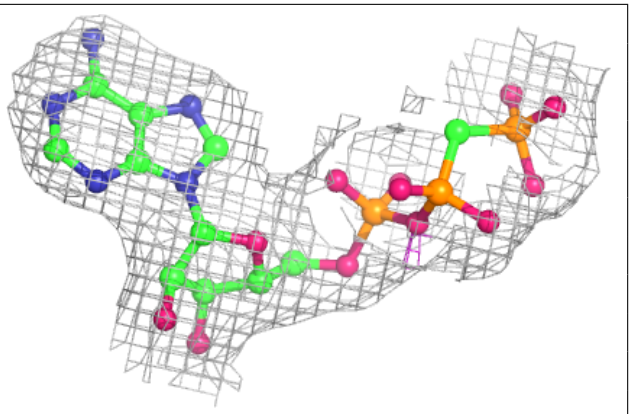
Electron density around ACP A 800:

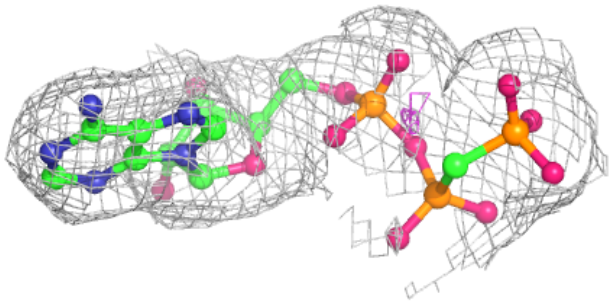
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

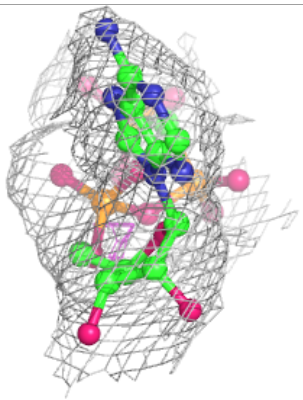


Electron density around ACP D 800:

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







Electron density around ACP C 800:

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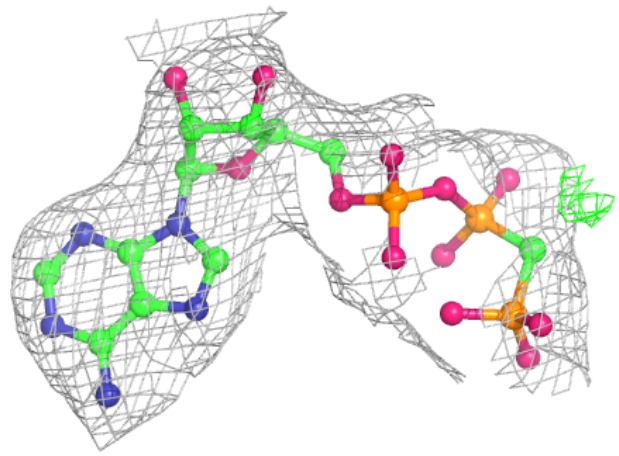
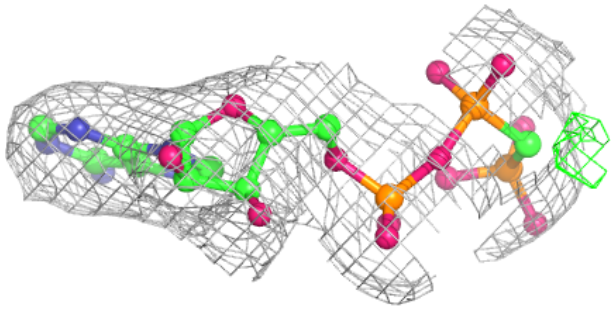
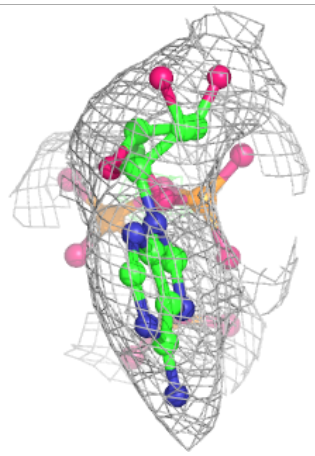
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

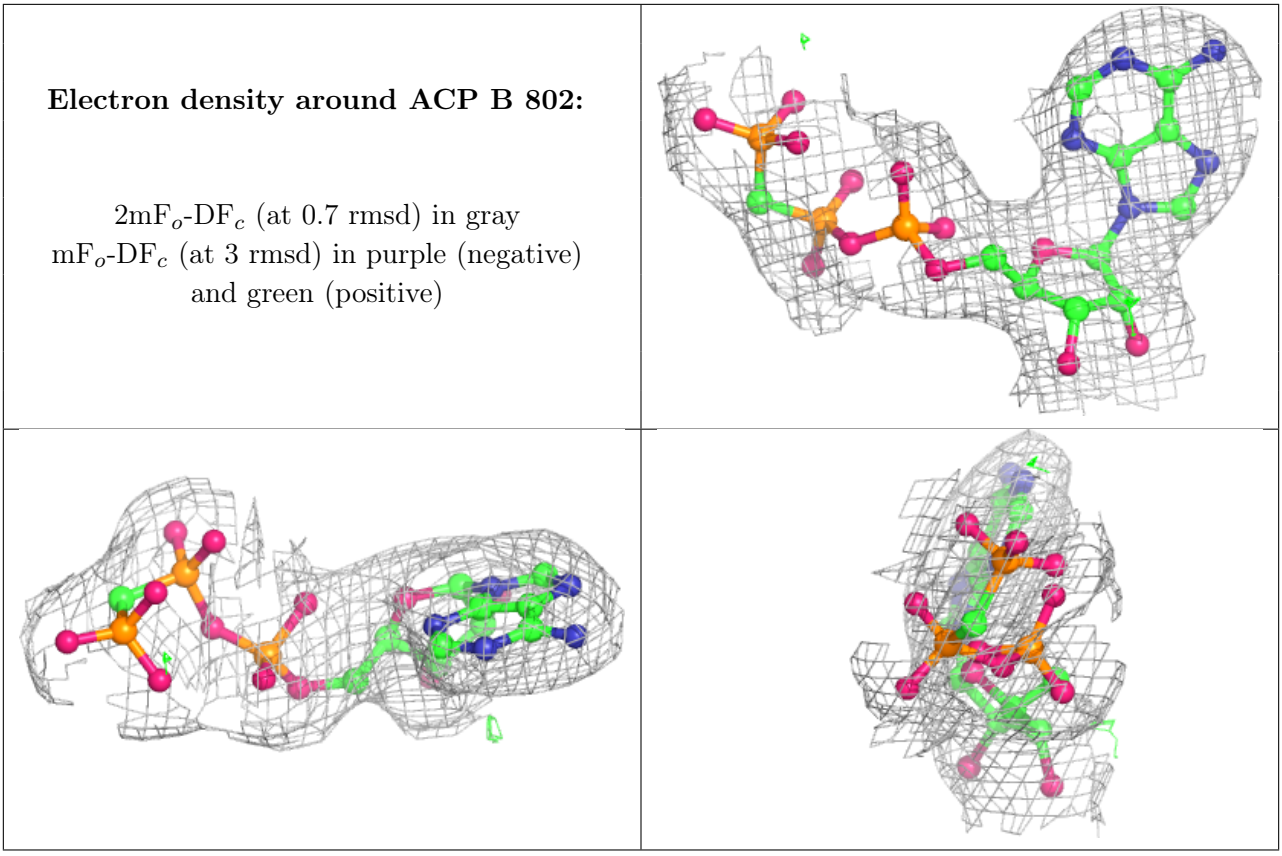






Electron density around ACP B 802:

$2mF_o$-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.