Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2025 – 02:27 PM JST

PDB ID	:	8YPY
Title	:	Crystal strcuture of human phosphoribosyl pyrophosphate synthetase2 (PRPS2) in complex with ligands
Authors	:	Zhang, L.; Zhang, L.
Deposited on	:	2024-03-18
Resolution	:	2.74 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

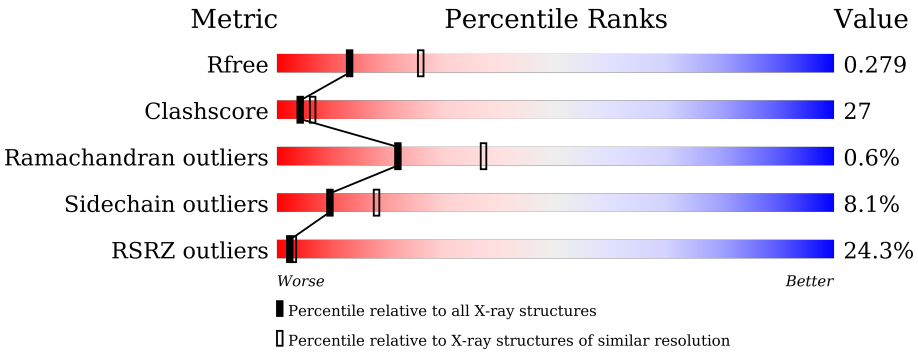
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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}	164625	1649 (2.76-2.72)
Clashscore	180529	1744 (2.76-2.72)
Ramachandran outliers	177936	1710 (2.76-2.72)
Sidechain outliers	177891	1711 (2.76-2.72)
RSRZ outliers	164620	1649 (2.76-2.72)

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	321	12% 60% 30% 5%
1	B	321	22% 56% 31% 5% 8%
1	C	321	29% 46% 41% 8%
1	D	321	39% 47% 38% 7% 7%
1	E	321	25% 53% 36% 7%
1	F	321	10% 61% 29% 5%

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
2	APC	D	1001	-	-	X	-
2	APC	E	1001	-	-	X	-
3	HSX	A	1002	-	X	-	-
3	HSX	D	1002	-	-	X	-
3	HSX	F	2001	-	X	-	-
5	PO4	A	1005	-	X	X	-
5	PO4	A	1006	-	X	-	-
5	PO4	A	1007	-	X	-	-
5	PO4	F	2003	-	X	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14222 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.

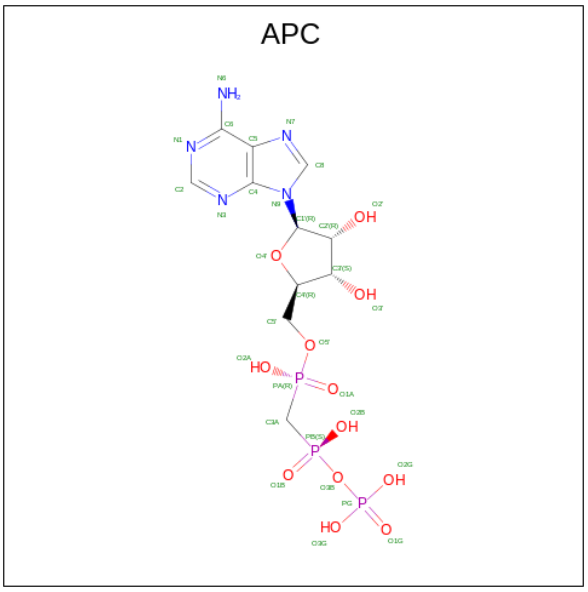
- Molecule 1 is a protein called Isoform 2 of Ribose-phosphate pyrophosphokinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2355	1475	416	449	15			
1	B	296	Total	C	N	O	S	0	0	0
			2251	1414	395	427	15			
1	C	294	Total	C	N	O	S	0	0	0
			2232	1402	390	425	15			
1	D	298	Total	C	N	O	S	0	0	0
			2265	1423	396	431	15			
1	E	299	Total	C	N	O	S	0	0	0
			2276	1429	400	432	15			
1	F	308	Total	C	N	O	S	0	0	0
			2351	1473	415	448	15			

There are 6 discrepancies between the modelled and reference sequences:

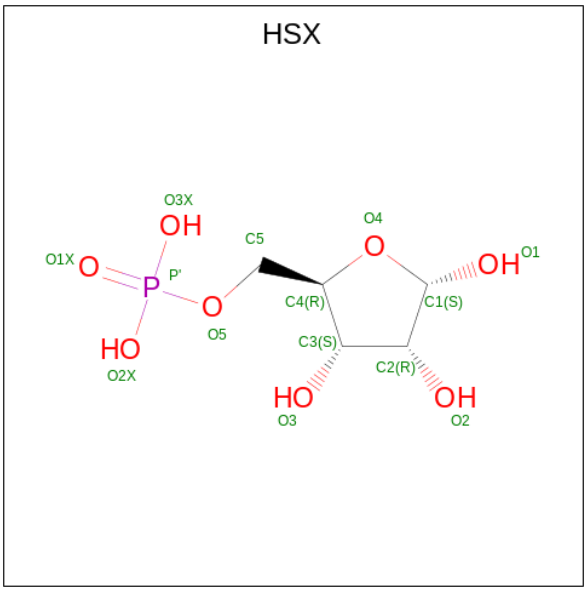
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P11908
B	1	SER	-	expression tag	UNP P11908
C	1	SER	-	expression tag	UNP P11908
D	1	SER	-	expression tag	UNP P11908
E	1	SER	-	expression tag	UNP P11908
F	1	SER	-	expression tag	UNP P11908

- Molecule 2 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is 5-O-phosphono-alpha-D-ribofuranose (three-letter code: HSX) (formula: $C_5H_{11}O_8P$).

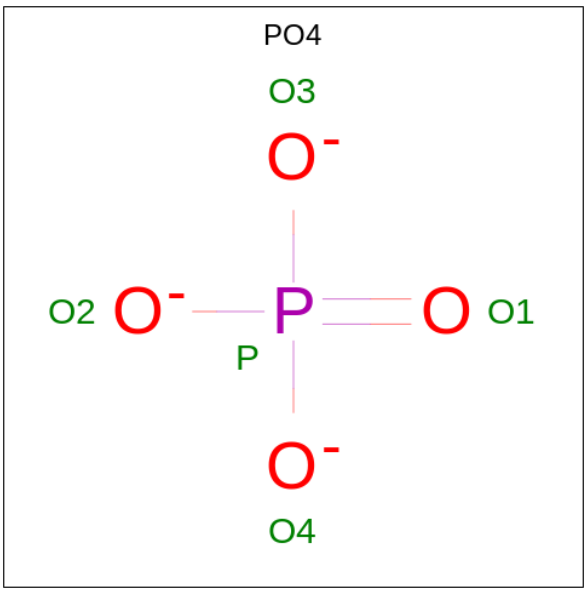


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 14 5 8 1	0	0
3	B	1	Total C O P 14 5 8 1	0	0
3	C	1	Total C O P 14 5 8 1	0	0
3	D	1	Total C O P 14 5 8 1	0	0
3	E	1	Total C O P 14 5 8 1	0	0
3	F	1	Total C O P 14 5 8 1	0	0

- Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cd 1 1	0	0
4	B	1	Total Cd 1 1	0	0
4	C	1	Total Cd 1 1	0	0
4	D	1	Total Cd 1 1	0	0
4	E	1	Total Cd 1 1	0	0
4	F	1	Total Cd 1 1	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0
5	F	1	Total O P 5 4 1	0	0

- Molecule 6 is water.

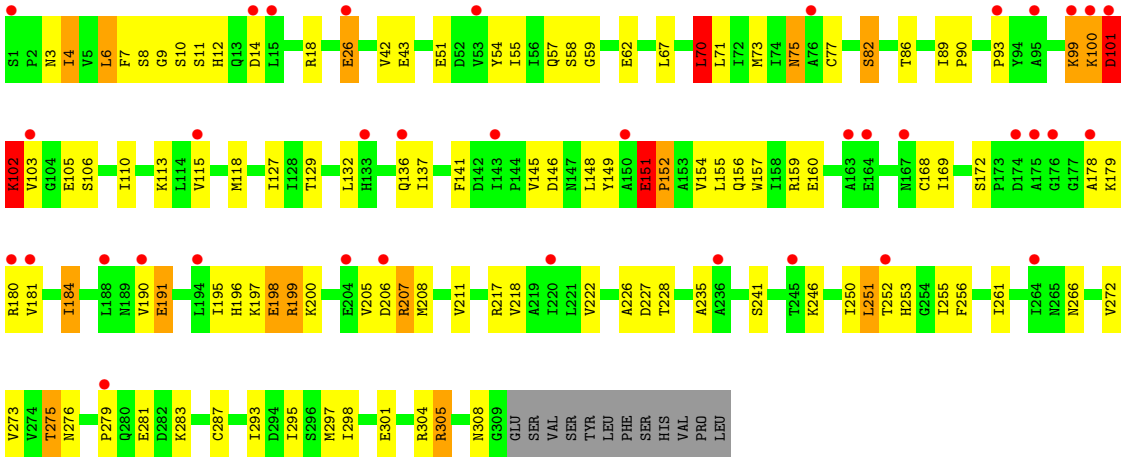
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	61	Total O 61 61	0	0
6	B	32	Total O 32 32	0	0
6	C	6	Total O 6 6	0	0
6	D	8	Total O 8 8	0	0
6	E	25	Total O 25 25	0	0
6	F	59	Total O 59 59	0	0

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.

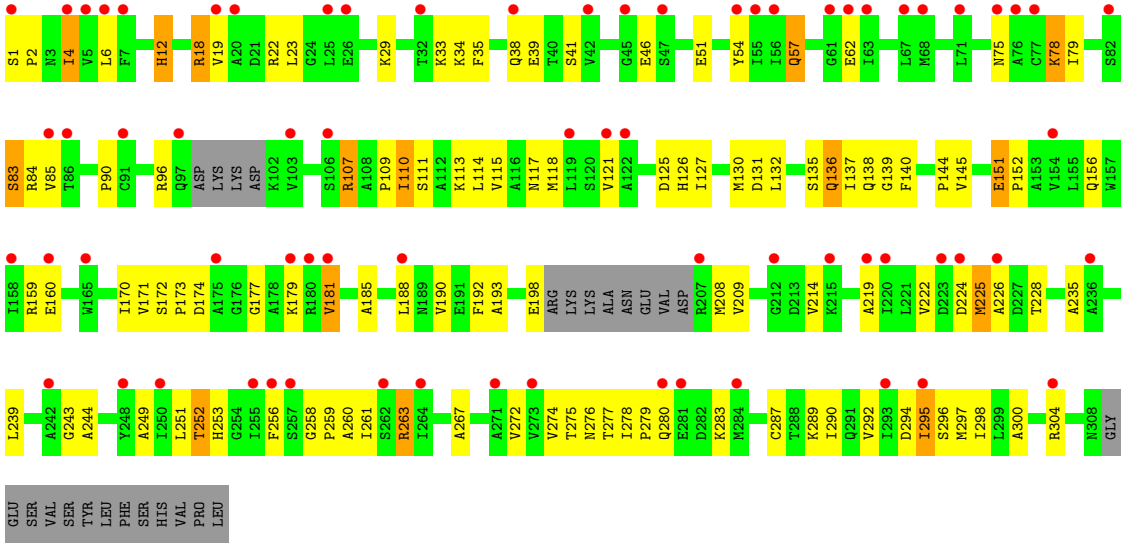
• Molecule 1: Isoform 2 of Ribose-phosphate pyrophosphokinase 2

Chain A:



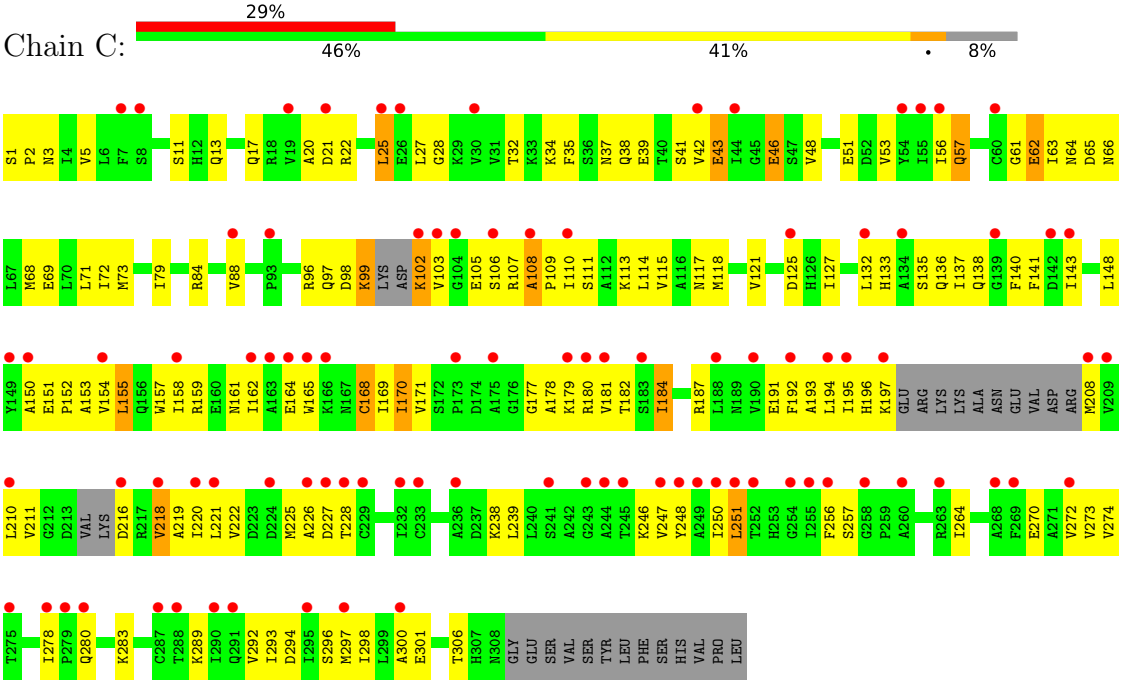
• Molecule 1: Isoform 2 of Ribose-phosphate pyrophosphokinase 2

Chain B:



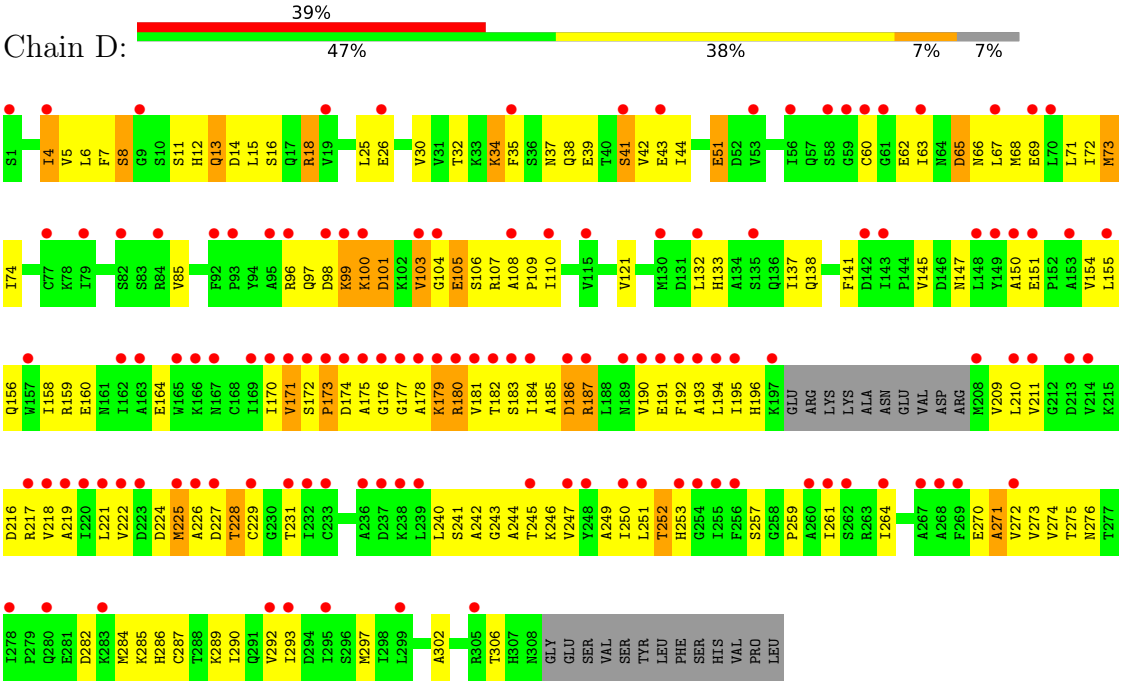
• Molecule 1: Isoform 2 of Ribose-phosphate pyrophosphokinase 2

Chain C:



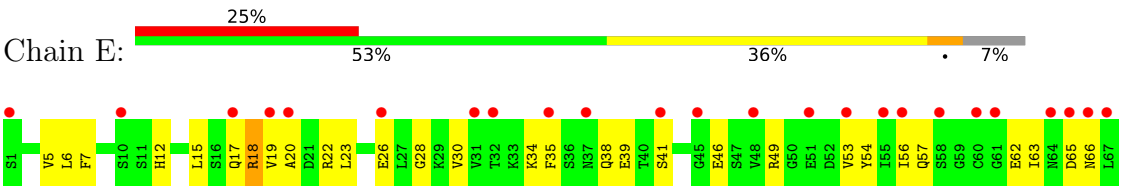
• Molecule 1: Isoform 2 of Ribose-phosphate pyrophosphokinase 2

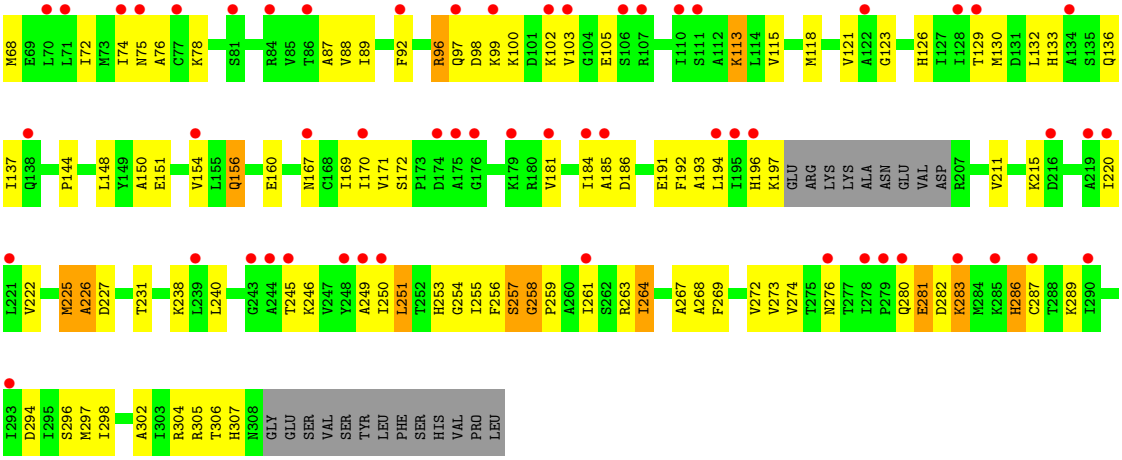
Chain D:



• Molecule 1: Isoform 2 of Ribose-phosphate pyrophosphokinase 2

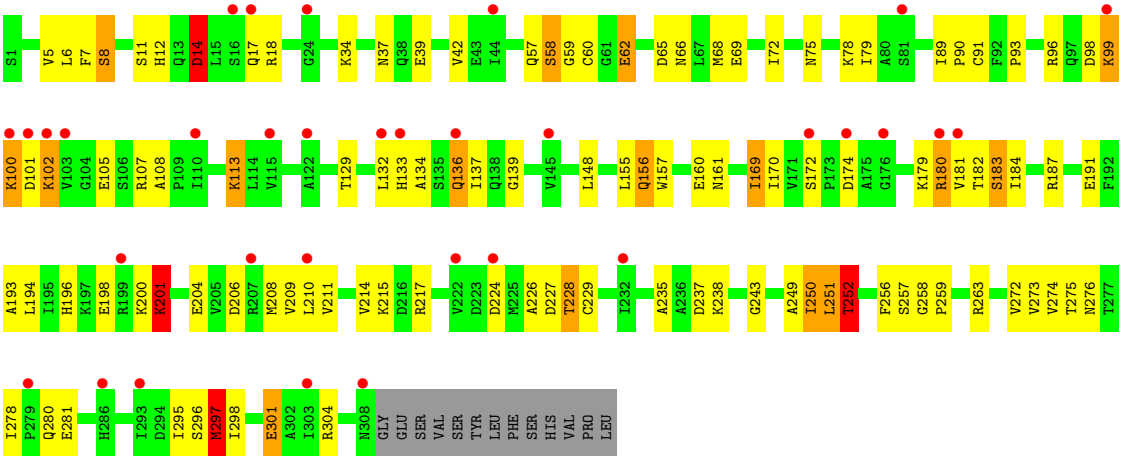
Chain E:





• Molecule 1: Isoform 2 of Ribose-phosphate pyrophosphokinase 2

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.70Å 73.60Å 170.50Å 90.00° 94.44° 90.00°	Depositor
Resolution (Å)	46.91 – 2.74 46.91 – 2.74	Depositor EDS
% Data completeness (in resolution range)	88.0 (46.91-2.74) 87.9 (46.91-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.272 , 0.286 0.268 , 0.279	Depositor DCC
R_{free} test set	3153 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	14222	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.93% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: APC, HSX, CD, PO4

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	1.26	18/2387 (0.8%)	0.99	7/3229 (0.2%)
1	B	1.18	4/2281 (0.2%)	0.92	1/3087 (0.0%)
1	C	0.99	4/2261 (0.2%)	0.95	0/3059
1	D	1.00	4/2296 (0.2%)	0.89	0/3108
1	E	1.12	2/2307 (0.1%)	0.91	2/3122 (0.1%)
1	F	1.39	22/2383 (0.9%)	0.99	4/3224 (0.1%)
All	All	1.17	54/13915 (0.4%)	0.94	14/18829 (0.1%)

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	62	GLU	CD-OE1	-9.41	1.15	1.25
1	F	62	GLU	CD-OE2	-8.51	1.16	1.25
1	A	151	GLU	CD-OE2	-8.41	1.16	1.25
1	A	152	PRO	C-O	-7.32	1.08	1.23
1	F	58	SER	CA-CB	-6.82	1.42	1.52
1	C	108	ALA	C-N	-6.48	1.22	1.34
1	A	8	SER	CB-OG	-6.47	1.33	1.42
1	F	62	GLU	C-O	-6.35	1.11	1.23
1	F	256	PHE	C-O	-6.32	1.11	1.23
1	B	151	GLU	CD-OE1	-6.25	1.18	1.25
1	F	8	SER	CB-OG	-6.20	1.34	1.42
1	A	6	LEU	C-O	-6.12	1.11	1.23
1	F	59	GLY	C-O	-6.07	1.14	1.23
1	D	51	GLU	CD-OE2	-6.03	1.19	1.25
1	F	237	ASP	C-O	-6.00	1.11	1.23
1	A	272	VAL	C-O	-5.95	1.12	1.23
1	D	105	GLU	CD-OE1	-5.86	1.19	1.25
1	F	201	LYS	N-CA	-5.82	1.34	1.46
1	F	252	THR	C-O	-5.81	1.12	1.23
1	F	37	ASN	C-O	-5.77	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	GLU	CD-OE1	-5.76	1.19	1.25
1	E	105	GLU	CG-CD	-5.71	1.43	1.51
1	A	195	ILE	C-O	-5.70	1.12	1.23
1	A	198	GLU	CD-OE2	-5.68	1.19	1.25
1	A	179	LYS	C-O	-5.66	1.12	1.23
1	F	42	VAL	C-O	-5.66	1.12	1.23
1	A	8	SER	C-O	-5.65	1.12	1.23
1	F	250	ILE	C-O	-5.48	1.12	1.23
1	B	151	GLU	CD-OE2	-5.47	1.19	1.25
1	F	14	ASP	CB-CG	-5.47	1.40	1.51
1	D	5	VAL	C-O	-5.47	1.12	1.23
1	B	110	ILE	C-O	-5.46	1.12	1.23
1	A	151	GLU	CD-OE1	-5.42	1.19	1.25
1	F	301	GLU	CD-OE1	-5.40	1.19	1.25
1	F	258	GLY	C-O	-5.36	1.15	1.23
1	F	58	SER	CB-OG	-5.34	1.35	1.42
1	A	253	HIS	CE1-NE2	-5.30	1.20	1.32
1	F	39	GLU	CD-OE2	-5.28	1.19	1.25
1	F	297	MET	C-O	-5.26	1.13	1.23
1	F	228	THR	C-O	-5.26	1.13	1.23
1	A	184	ILE	C-O	-5.25	1.13	1.23
1	C	51	GLU	CD-OE1	-5.24	1.19	1.25
1	A	7	PHE	C-O	-5.20	1.13	1.23
1	B	243	GLY	C-N	-5.17	1.22	1.34
1	E	254	GLY	C-O	-5.14	1.15	1.23
1	F	34	LYS	C-O	-5.13	1.13	1.23
1	C	43	GLU	C-O	-5.13	1.13	1.23
1	A	70	LEU	C-O	-5.13	1.13	1.23
1	D	253	HIS	C-N	-5.12	1.23	1.33
1	A	241	SER	CB-OG	-5.11	1.35	1.42
1	F	7	PHE	C-O	-5.09	1.13	1.23
1	C	62	GLU	CD-OE2	-5.05	1.20	1.25
1	A	253	HIS	C-O	-5.02	1.13	1.23
1	A	11	SER	CB-OG	-5.01	1.35	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	101	ASP	C-N-CA	-8.08	101.50	121.70
1	A	197	LYS	CB-CA-C	-7.28	95.84	110.40
1	A	305	ARG	CG-CD-NE	7.20	126.92	111.80
1	A	199	ARG	C-N-CA	-6.89	104.47	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	174	ASP	CB-CG-OD2	6.88	124.50	118.30
1	F	102	LYS	C-N-CA	-6.38	105.75	121.70
1	F	174	ASP	CB-CG-OD1	6.20	123.88	118.30
1	E	100	LYS	N-CA-C	-5.56	95.98	111.00
1	A	305	ARG	CB-CA-C	-5.54	99.32	110.40
1	A	154	VAL	CA-CB-CG1	5.53	119.19	110.90
1	F	174	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	E	226	ALA	N-CA-CB	-5.48	102.42	110.10
1	A	146	ASP	CB-CA-C	-5.37	99.66	110.40
1	F	100	LYS	C-N-CA	5.16	134.59	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2355	0	2403	85	0
1	B	2251	0	2292	118	0
1	C	2232	0	2270	173	0
1	D	2265	0	2309	184	0
1	E	2276	0	2325	144	0
1	F	2351	0	2401	88	0
2	A	62	0	28	6	0
2	C	62	0	28	8	0
2	D	31	0	14	12	0
2	E	31	0	14	14	0
3	A	14	0	0	1	0
3	B	14	0	0	1	0
3	C	14	0	0	0	0
3	D	14	0	0	6	0
3	E	14	0	0	2	0
3	F	14	0	0	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	15	0	0	2	0
5	D	5	0	0	1	0
5	F	5	0	0	2	0
6	A	61	0	0	8	0
6	B	32	0	0	2	1
6	C	6	0	0	0	0
6	D	8	0	0	0	0
6	E	25	0	0	4	0
6	F	59	0	0	3	1
All	All	14222	0	14084	757	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (757) 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:E:226:ALA:HB2	1:E:251:LEU:CD1	1.33	1.55
1:C:99:LYS:CB	1:C:107:ARG:NH2	1.70	1.49
1:C:99:LYS:HB2	1:C:107:ARG:NH2	1.12	1.43
1:D:34:LYS:NZ	1:D:38:GLN:NE2	1.62	1.40
1:D:177:GLY:O	1:D:180:ARG:HB3	1.27	1.35
1:A:101:ASP:O	1:A:103:VAL:N	1.58	1.34
1:C:99:LYS:CA	1:C:107:ARG:NH2	1.93	1.32
1:E:274:VAL:HG21	1:E:280:GLN:NE2	1.44	1.30
1:E:226:ALA:CB	1:E:251:LEU:CD1	2.09	1.28
1:C:99:LYS:HB2	1:C:107:ARG:CZ	1.66	1.26
1:E:226:ALA:CB	1:E:251:LEU:HD11	1.63	1.24
2:E:1001:APC:O3G	1:F:179:LYS:CE	1.86	1.23
1:D:171:VAL:O	1:D:221:LEU:HA	1.39	1.21
1:E:35:PHE:CE2	1:E:41:SER:OG	1.89	1.20
1:B:34:LYS:HE2	1:B:38:GLN:O	1.42	1.19
1:F:201:LYS:CD	1:F:204:GLU:HG3	1.72	1.19
1:F:201:LYS:HD2	1:F:204:GLU:CG	1.74	1.18
1:F:96:ARG:NH2	1:F:227:ASP:OD2	1.76	1.16
1:D:171:VAL:HG13	1:D:193:ALA:O	1.42	1.15
2:E:1001:APC:O3G	1:F:179:LYS:HE3	0.99	1.14
1:E:133:HIS:NE2	2:E:1001:APC:H3A2	1.62	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LYS:HA	1:C:107:ARG:NH2	1.52	1.12
1:A:169:ILE:HD11	1:A:217:ARG:HD2	1.30	1.12
1:C:62:GLU:HG2	1:C:65:ASP:OD2	1.47	1.12
1:E:259:PRO:O	1:E:263:ARG:HG3	1.48	1.12
1:A:169:ILE:HD11	1:A:217:ARG:CD	1.78	1.11
1:E:226:ALA:HB2	1:E:251:LEU:HD13	1.18	1.10
1:B:4:ILE:HD11	1:B:6:LEU:HD21	1.10	1.07
1:C:168:CYS:HB2	1:C:218:VAL:HG23	1.07	1.06
1:C:168:CYS:CB	1:C:218:VAL:HG23	1.84	1.06
1:B:4:ILE:HD11	1:B:6:LEU:CD2	1.86	1.06
1:E:274:VAL:CG2	1:E:280:GLN:NE2	2.18	1.05
1:D:96:ARG:HH21	2:D:1001:APC:C5	1.70	1.04
1:D:96:ARG:NH2	2:D:1001:APC:C5	2.20	1.04
1:F:102:LYS:HB3	1:F:105:GLU:O	1.57	1.04
1:C:102:LYS:HG2	1:C:103:VAL:H	1.23	1.03
1:D:171:VAL:CG1	1:D:193:ALA:O	2.06	1.03
1:D:227:ASP:OD1	1:D:257:SER:OG	1.78	1.02
1:E:226:ALA:HB2	1:E:251:LEU:HD11	1.06	1.02
1:C:99:LYS:HA	1:C:107:ARG:HH22	1.09	1.01
1:B:156:GLN:O	1:B:160:GLU:HG3	1.60	1.01
1:D:180:ARG:O	1:D:184:ILE:HD12	1.60	1.01
1:F:201:LYS:CD	1:F:204:GLU:CG	2.33	1.00
1:C:168:CYS:HB2	1:C:218:VAL:CG2	1.90	1.00
1:D:121:VAL:HG11	1:E:121:VAL:HG11	1.44	0.98
1:D:177:GLY:O	1:D:180:ARG:CB	2.11	0.98
1:D:173:PRO:HB3	1:D:231:THR:CG2	1.94	0.97
1:A:180:ARG:HD3	5:A:1005:PO4:O4	1.64	0.96
1:C:22:ARG:HE	1:C:296:SER:HB2	1.29	0.96
1:C:102:LYS:CG	1:C:103:VAL:H	1.76	0.96
1:C:96:ARG:NE	1:C:225:MET:HE1	1.80	0.95
1:E:274:VAL:HG21	1:E:280:GLN:HE22	1.14	0.95
1:D:180:ARG:NH2	1:D:224:ASP:HB3	1.82	0.95
1:C:246:LYS:HD3	1:C:270:GLU:HG3	1.48	0.94
1:D:97:GLN:HE21	1:D:99:LYS:HB3	1.34	0.93
1:E:170:ILE:HG22	1:E:181:VAL:HG13	1.51	0.93
1:F:301:GLU:OE2	1:F:304:ARG:NH2	2.01	0.93
1:D:37:ASN:O	1:D:38:GLN:HB2	1.66	0.92
1:F:99:LYS:HG3	1:F:107:ARG:HD2	1.49	0.92
1:A:101:ASP:O	1:A:102:LYS:C	1.96	0.92
1:D:96:ARG:NE	1:D:225:MET:SD	2.42	0.91
1:C:102:LYS:HG2	1:C:103:VAL:N	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:VAL:CG2	1:E:280:GLN:HE21	1.82	0.91
1:C:246:LYS:HD3	1:C:270:GLU:CG	2.00	0.91
1:C:42:VAL:HG11	1:C:73:MET:HG2	1.51	0.91
1:C:168:CYS:CB	1:C:218:VAL:CG2	2.48	0.89
1:E:113:LYS:HE2	1:F:139:GLY:O	1.73	0.89
1:F:89:ILE:O	1:F:129:THR:OG1	1.89	0.89
1:D:178:ALA:O	1:D:180:ARG:N	2.05	0.89
1:D:100:LYS:HB2	1:D:100:LYS:NZ	1.87	0.89
1:C:141:PHE:HB3	1:C:143:ILE:HG22	1.54	0.89
1:D:96:ARG:NH2	2:D:1001:APC:C6	2.36	0.88
1:F:102:LYS:CB	1:F:105:GLU:O	2.22	0.88
1:D:34:LYS:NZ	1:D:38:GLN:HE21	1.69	0.88
1:D:173:PRO:CB	1:D:231:THR:CG2	2.52	0.88
1:E:99:LYS:H	2:E:1001:APC:H3'	1.40	0.87
1:D:171:VAL:HG13	1:D:193:ALA:C	1.95	0.86
1:B:259:PRO:O	1:B:263:ARG:CG	2.23	0.86
1:B:256:PHE:CB	1:B:283:LYS:HE2	2.05	0.85
1:E:89:ILE:O	1:E:129:THR:HG23	1.77	0.85
1:E:98:ASP:HA	2:E:1001:APC:O2'	1.75	0.85
1:B:172:SER:HB3	1:B:181:VAL:HG11	1.59	0.85
1:D:8:SER:OG	1:D:16:SER:OG	1.93	0.85
1:B:256:PHE:HB2	1:B:283:LYS:HE2	1.59	0.84
1:F:208:MET:HE3	1:F:235:ALA:HA	1.58	0.84
1:C:211:VAL:HG12	1:D:211:VAL:HG12	1.58	0.84
1:C:62:GLU:CG	1:C:65:ASP:OD2	2.23	0.84
1:B:34:LYS:HE2	1:B:38:GLN:C	1.98	0.84
1:C:208:MET:O	1:C:238:LYS:HE2	1.78	0.84
1:E:133:HIS:CD2	2:E:1001:APC:H3A2	2.13	0.84
1:E:133:HIS:NE2	2:E:1001:APC:C3A	2.41	0.83
1:E:170:ILE:HD13	1:E:185:ALA:HA	1.61	0.83
1:B:34:LYS:CE	1:B:38:GLN:O	2.26	0.83
1:D:180:ARG:HH21	1:D:224:ASP:HB3	1.43	0.82
1:E:130:MET:HE1	1:E:150:ALA:HB2	1.60	0.82
1:F:201:LYS:HD3	1:F:204:GLU:HG3	1.59	0.82
1:F:201:LYS:HD2	1:F:204:GLU:HG3	1.41	0.82
1:A:200:LYS:HD2	1:A:206:ASP:OD1	1.78	0.82
1:C:37:ASN:O	1:C:38:GLN:HB2	1.79	0.82
1:E:227:ASP:OD1	1:E:255:ILE:CG2	2.28	0.82
1:C:34:LYS:CE	1:C:38:GLN:HE21	1.92	0.82
1:C:96:ARG:CD	1:C:225:MET:HE1	2.10	0.82
1:A:169:ILE:HD11	1:A:217:ARG:HD3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ILE:CD1	1:C:191:GLU:O	2.29	0.81
1:D:173:PRO:HB3	1:D:231:THR:HG22	1.60	0.81
1:F:136:GLN:NE2	1:F:136:GLN:H	1.78	0.81
1:C:169:ILE:HD11	1:C:192:PHE:HA	1.62	0.81
1:D:97:GLN:HG2	1:D:99:LYS:H	1.46	0.80
1:B:79:ILE:HD12	1:C:110:ILE:HG22	1.64	0.80
1:B:267:ALA:O	1:B:289:LYS:NZ	2.15	0.80
1:D:96:ARG:NH2	2:D:1001:APC:N7	2.30	0.80
1:D:18:ARG:HG3	1:D:18:ARG:HH11	1.46	0.80
1:C:169:ILE:HD12	1:C:191:GLU:O	1.81	0.80
1:E:35:PHE:HE2	1:E:41:SER:OG	1.56	0.80
1:B:33:LYS:O	1:B:41:SER:HB3	1.83	0.79
1:B:107:ARG:NH2	1:C:43:GLU:OE2	2.14	0.79
1:F:201:LYS:HD2	1:F:204:GLU:HG2	1.64	0.79
1:E:98:ASP:OD1	2:E:1001:APC:O2'	2.00	0.79
1:C:96:ARG:NE	1:C:225:MET:CE	2.45	0.79
1:C:96:ARG:CZ	1:C:225:MET:HE3	2.11	0.79
1:B:35:PHE:CD2	2:C:1002:APC:N6	2.50	0.79
1:C:133:HIS:NE2	2:C:1002:APC:O1B	2.14	0.79
1:F:250:ILE:HG12	1:F:273:VAL:HB	1.63	0.79
1:E:227:ASP:OD1	1:E:255:ILE:HG21	1.84	0.78
1:D:96:ARG:HH21	2:D:1001:APC:C6	1.94	0.78
1:A:26:GLU:OE2	6:A:1101:HOH:O	2.00	0.78
1:A:115:VAL:HA	1:A:118:MET:HE2	1.63	0.78
1:B:198:GLU:OE1	1:B:209:VAL:HG21	1.84	0.77
1:E:98:ASP:HA	2:E:1001:APC:C2'	2.13	0.77
1:E:226:ALA:HB3	1:E:251:LEU:CD1	2.14	0.77
1:C:180:ARG:O	1:C:184:ILE:HG13	1.85	0.77
6:E:1119:HOH:O	1:F:108:ALA:CB	2.32	0.77
1:B:185:ALA:HB1	1:B:190:VAL:O	1.84	0.77
1:C:34:LYS:HE3	1:C:38:GLN:HE21	1.49	0.77
1:B:259:PRO:O	1:B:263:ARG:HG3	1.85	0.76
1:F:201:LYS:HD3	1:F:204:GLU:CG	2.14	0.76
3:F:2001:HSX:O3X	3:F:2001:HSX:O3	2.04	0.76
1:D:108:ALA:O	1:D:110:ILE:N	2.19	0.76
2:A:1001:APC:H3'	2:A:1001:APC:N3	2.00	0.75
1:B:294:ASP:OD1	1:B:296:SER:OG	2.03	0.75
1:D:245:THR:HG22	1:D:246:LYS:HG3	1.67	0.75
1:D:97:GLN:NE2	1:D:99:LYS:HB3	2.01	0.75
1:D:249:ALA:HB3	1:D:272:VAL:HG22	1.68	0.75
3:D:1002:HSX:O3X	3:D:1002:HSX:O3	2.05	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:VAL:CG1	1:D:193:ALA:C	2.55	0.75
1:B:275:THR:CG2	1:B:295:ILE:HG12	2.17	0.75
1:D:39:GLU:OE1	2:E:1001:APC:N6	2.17	0.75
1:D:228:THR:CB	3:D:1002:HSX:O3	2.35	0.74
1:D:42:VAL:O	1:D:43:GLU:HG2	1.87	0.74
1:D:99:LYS:HE3	1:D:107:ARG:H	1.52	0.74
1:B:260:ALA:HA	1:B:263:ARG:HG3	1.70	0.73
1:D:34:LYS:HZ2	1:D:38:GLN:NE2	1.81	0.73
1:E:34:LYS:HE2	1:E:38:GLN:O	1.88	0.73
1:B:115:VAL:HA	1:B:118:MET:HE2	1.70	0.73
2:A:1004:APC:H2'	1:F:98:ASP:OD1	1.88	0.73
1:A:12:HIS:HD2	6:A:1132:HOH:O	1.69	0.73
1:C:187:ARG:HH12	1:D:103:VAL:HG23	1.53	0.73
1:B:259:PRO:O	1:B:263:ARG:HG2	1.88	0.73
1:E:171:VAL:HA	1:E:193:ALA:O	1.89	0.73
1:B:172:SER:HB3	1:B:181:VAL:CG1	2.18	0.73
1:D:186:ASP:OD1	1:D:186:ASP:N	2.21	0.72
1:F:200:LYS:HE2	1:F:206:ASP:OD1	1.87	0.72
1:D:63:ILE:CD1	1:E:39:GLU:HG3	2.19	0.72
1:D:155:LEU:O	1:D:159:ARG:HG3	1.90	0.72
6:E:1119:HOH:O	1:F:108:ALA:HB2	1.89	0.72
1:C:148:LEU:HD13	1:C:298:ILE:HG22	1.70	0.71
1:E:156:GLN:O	1:E:160:GLU:HG3	1.90	0.71
1:E:281:GLU:N	1:E:281:GLU:CD	2.43	0.71
1:E:170:ILE:CG2	1:E:181:VAL:HG13	2.18	0.71
1:E:226:ALA:CB	1:E:251:LEU:HD13	2.02	0.71
1:A:99:LYS:HE3	1:A:106:SER:HA	1.71	0.71
1:C:192:PHE:HZ	1:D:194:LEU:HD11	1.55	0.71
1:D:228:THR:OG1	3:D:1002:HSX:O3	2.08	0.71
1:D:228:THR:HB	3:D:1002:HSX:O3	1.91	0.71
1:E:280:GLN:O	1:E:283:LYS:N	2.16	0.71
1:D:110:ILE:HG21	1:E:75:ASN:O	1.90	0.70
1:A:102:LYS:O	1:A:105:GLU:O	2.07	0.70
1:F:297:MET:N	1:F:297:MET:SD	2.59	0.70
1:D:282:ASP:O	1:D:285:LYS:HG2	1.90	0.70
1:A:110:ILE:CD1	1:F:79:ILE:HD12	2.22	0.70
1:E:274:VAL:HG23	1:E:280:GLN:HE21	1.56	0.70
1:C:39:GLU:OE1	2:C:1001:APC:N6	2.24	0.70
1:A:273:VAL:HG12	1:A:293:ILE:HD12	1.72	0.70
1:C:102:LYS:CG	1:C:103:VAL:N	2.45	0.69
1:E:132:LEU:HD13	1:E:137:ILE:HB	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ARG:NE	1:C:296:SER:HB2	2.06	0.69
1:C:196:HIS:HE1	1:D:186:ASP:OD2	1.74	0.69
1:D:63:ILE:CD1	1:E:39:GLU:CG	2.70	0.69
1:A:226:ALA:HB2	1:A:251:LEU:HG	1.74	0.69
1:C:169:ILE:CD1	1:C:192:PHE:HA	2.23	0.69
1:F:201:LYS:CD	1:F:204:GLU:HG2	2.17	0.69
1:C:99:LYS:HB2	1:C:107:ARG:NE	2.08	0.69
1:B:127:ILE:HB	1:B:145:VAL:HG22	1.75	0.69
1:E:231:THR:HB	3:E:1002:HSX:O3	1.93	0.69
1:F:226:ALA:HB2	1:F:251:LEU:HD22	1.75	0.69
1:A:10:SER:H	1:A:57:GLN:HE22	1.41	0.68
1:B:170:ILE:HG22	1:B:181:VAL:HB	1.72	0.68
1:D:284:MET:SD	1:D:290:ILE:HG22	2.32	0.68
1:E:281:GLU:N	1:E:281:GLU:OE1	2.25	0.68
1:C:158:ILE:HD12	1:C:162:ILE:HD12	1.75	0.68
1:D:250:ILE:HD13	1:D:273:VAL:HB	1.75	0.68
1:C:168:CYS:HB3	1:C:218:VAL:CG2	2.21	0.68
1:F:208:MET:CE	1:F:235:ALA:HA	2.23	0.68
1:E:191:GLU:OE2	1:F:209:VAL:HG11	1.94	0.68
2:A:1001:APC:H8	6:A:1139:HOH:O	1.93	0.68
1:B:276:ASN:OD1	1:B:295:ILE:HG13	1.94	0.68
1:C:20:ALA:HB1	1:C:25:LEU:O	1.94	0.68
1:D:178:ALA:C	1:D:180:ARG:H	1.96	0.68
1:B:57:GLN:HA	1:B:57:GLN:NE2	2.08	0.68
1:B:4:ILE:CD1	1:B:6:LEU:CD2	2.70	0.67
1:C:178:ALA:CB	1:D:175:ALA:HB1	2.23	0.67
1:F:58:SER:HB2	1:F:90:PRO:HG2	1.77	0.67
1:C:256:PHE:O	1:C:283:LYS:NZ	2.28	0.67
1:C:219:ALA:HB3	1:C:247:VAL:HG12	1.77	0.67
1:F:14:ASP:O	1:F:18:ARG:HG3	1.95	0.67
1:C:96:ARG:CZ	1:C:225:MET:CE	2.73	0.67
1:D:18:ARG:HG3	1:D:18:ARG:NH1	2.08	0.67
1:B:35:PHE:CE2	2:C:1002:APC:C6	2.78	0.66
1:C:274:VAL:HG23	1:C:292:VAL:HG22	1.76	0.66
1:E:98:ASP:HA	2:E:1001:APC:H2'	1.76	0.66
1:A:156:GLN:O	1:A:160:GLU:HG3	1.96	0.66
1:F:201:LYS:CE	1:F:204:GLU:HG3	2.26	0.66
1:E:196:HIS:CE1	1:F:182:THR:HG23	2.30	0.66
1:F:68:MET:HE2	1:F:72:ILE:HD11	1.77	0.66
1:C:195:ILE:CG1	1:C:210:LEU:HD23	2.26	0.66
1:B:132:LEU:HD13	1:B:137:ILE:HB	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:CYS:O	1:A:82:SER:OG	2.13	0.65
1:B:121:VAL:CG1	1:C:117:ASN:HB3	2.26	0.65
1:F:133:HIS:ND1	1:F:224:ASP:OD2	2.24	0.65
1:B:4:ILE:CD1	1:B:6:LEU:HD21	2.06	0.65
1:D:100:LYS:HB2	1:D:100:LYS:HZ3	1.61	0.65
1:F:201:LYS:HD2	1:F:204:GLU:CB	2.27	0.65
1:A:152:PRO:O	1:A:156:GLN:HG3	1.97	0.65
1:B:107:ARG:HG3	1:B:107:ARG:HH11	1.62	0.64
1:E:170:ILE:HD13	1:E:185:ALA:CA	2.26	0.64
1:D:178:ALA:C	1:D:180:ARG:N	2.47	0.64
1:E:62:GLU:HG2	1:E:65:ASP:OD2	1.97	0.64
1:E:154:VAL:HG13	1:E:250:ILE:HG21	1.79	0.64
1:B:171:VAL:HG22	1:B:193:ALA:HB3	1.80	0.64
1:C:178:ALA:HB1	1:D:175:ALA:HB1	1.77	0.64
1:C:169:ILE:HD11	1:C:192:PHE:CA	2.26	0.64
1:A:169:ILE:CD1	1:A:217:ARG:HD3	2.27	0.64
1:C:63:ILE:HG13	1:C:64:ASN:N	2.10	0.64
1:B:275:THR:HG21	1:B:295:ILE:HG12	1.79	0.64
1:D:285:LYS:HG3	1:D:286:HIS:HD2	1.62	0.64
1:E:197:LYS:NZ	1:E:231:THR:OG1	2.24	0.64
1:D:171:VAL:O	1:D:221:LEU:CA	2.32	0.64
1:C:34:LYS:HE3	1:C:38:GLN:NE2	2.12	0.63
1:C:187:ARG:NH1	1:D:103:VAL:HG23	2.13	0.63
1:D:228:THR:O	1:D:229:CYS:HB2	1.99	0.63
1:E:226:ALA:HB3	1:E:251:LEU:HD11	1.75	0.63
1:E:261:ILE:HD11	1:E:283:LYS:HG2	1.80	0.63
1:B:39:GLU:HG2	1:C:63:ILE:HD11	1.80	0.63
1:A:148:LEU:HD13	1:A:298:ILE:HG22	1.81	0.63
1:C:37:ASN:O	1:C:38:GLN:CB	2.46	0.63
1:C:192:PHE:CZ	1:D:194:LEU:HD11	2.33	0.63
1:D:182:THR:O	1:D:186:ASP:OD1	2.17	0.63
1:F:148:LEU:HD13	1:F:298:ILE:HG22	1.79	0.63
1:E:78:LYS:HD3	1:E:123:GLY:HA3	1.81	0.63
1:B:35:PHE:HD2	2:C:1002:APC:N6	1.97	0.62
1:A:184:ILE:HD11	5:A:1005:PO4:O3	1.99	0.62
1:A:252:THR:HA	1:A:275:THR:HG23	1.80	0.62
1:C:158:ILE:HD11	1:C:250:ILE:CD1	2.29	0.62
1:D:63:ILE:HD11	1:E:39:GLU:HA	1.80	0.62
1:D:100:LYS:HB2	1:D:100:LYS:HZ2	1.64	0.62
1:F:208:MET:HE3	1:F:235:ALA:CA	2.28	0.62
1:B:159:ARG:NH2	6:B:2103:HOH:O	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:ARG:HD3	1:E:225:MET:SD	2.39	0.62
2:A:1001:APC:O1G	1:B:179:LYS:HE2	2.00	0.62
1:B:35:PHE:CD2	2:C:1002:APC:C6	2.83	0.62
1:D:173:PRO:CB	1:D:231:THR:HG22	2.23	0.62
1:B:208:MET:HE1	1:B:235:ALA:HA	1.82	0.62
1:C:125:ASP:C	1:C:143:ILE:HD11	2.20	0.62
1:B:256:PHE:HB3	1:B:283:LYS:HE2	1.80	0.61
1:D:171:VAL:HG12	1:D:193:ALA:O	1.99	0.61
1:E:259:PRO:HB2	1:E:263:ARG:HE	1.64	0.61
1:D:34:LYS:CE	1:D:38:GLN:NE2	2.59	0.61
1:D:284:MET:SD	1:D:290:ILE:CG2	2.88	0.61
1:A:9:GLY:HA3	1:A:57:GLN:NE2	2.15	0.61
1:F:136:GLN:H	1:F:136:GLN:HE21	1.48	0.61
1:C:168:CYS:HB2	1:C:218:VAL:O	2.00	0.61
1:A:42:VAL:HG11	1:A:73:MET:HB3	1.81	0.61
1:C:63:ILE:CG1	1:C:64:ASN:N	2.63	0.61
1:C:138:GLN:OE1	1:D:106:SER:OG	2.17	0.61
1:C:182:THR:HG23	1:D:196:HIS:CD2	2.36	0.61
1:C:272:VAL:HG13	1:C:272:VAL:O	1.99	0.61
1:A:181:VAL:HG12	1:A:222:VAL:HG22	1.83	0.61
1:D:99:LYS:HB2	1:D:107:ARG:HB2	1.83	0.61
1:E:35:PHE:CD2	1:E:41:SER:OG	2.53	0.61
1:D:173:PRO:CB	1:D:231:THR:HG21	2.30	0.60
1:A:149:TYR:O	6:A:1102:HOH:O	2.16	0.60
1:D:96:ARG:NH2	2:D:1001:APC:N6	2.48	0.60
1:D:285:LYS:HG3	1:D:286:HIS:CD2	2.36	0.60
1:F:113:LYS:HD2	1:F:113:LYS:O	2.01	0.60
1:C:195:ILE:HG13	1:C:210:LEU:HD23	1.82	0.60
1:D:217:ARG:HA	1:D:217:ARG:NE	2.15	0.60
1:D:171:VAL:HG12	1:D:194:LEU:HA	1.82	0.60
1:F:132:LEU:HD13	1:F:137:ILE:HB	1.82	0.60
1:B:275:THR:HG22	1:B:295:ILE:HG12	1.82	0.60
1:C:5:VAL:HB	1:C:53:VAL:HG22	1.82	0.60
1:C:62:GLU:OE2	1:C:62:GLU:HA	2.00	0.60
1:A:256:PHE:HB2	1:A:283:LYS:HE2	1.84	0.60
2:A:1004:APC:H3A2	1:F:133:HIS:NE2	2.17	0.60
1:D:183:SER:O	1:D:187:ARG:HG2	2.02	0.60
2:E:1001:APC:H2'	2:E:1001:APC:N3	2.16	0.60
1:F:156:GLN:O	1:F:160:GLU:HG3	2.02	0.60
1:A:110:ILE:HD13	1:F:79:ILE:HD12	1.84	0.59
1:F:57:GLN:NE2	1:F:69:GLU:OE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ILE:CD1	1:A:217:ARG:CD	2.68	0.59
1:D:252:THR:O	1:D:275:THR:OG1	2.17	0.59
1:B:170:ILE:O	1:B:192:PHE:HB2	2.02	0.59
1:B:294:ASP:CG	1:B:296:SER:HG	2.04	0.59
1:D:156:GLN:O	1:D:160:GLU:HG3	2.02	0.59
1:D:178:ALA:HA	1:D:181:VAL:HG22	1.84	0.59
1:D:217:ARG:O	1:D:244:ALA:HA	2.02	0.59
1:B:274:VAL:O	1:B:292:VAL:HA	2.02	0.59
1:C:218:VAL:HG23	1:C:218:VAL:O	2.02	0.59
1:C:133:HIS:HE2	2:C:1002:APC:PB	2.24	0.59
1:D:240:LEU:O	1:D:242:ALA:N	2.36	0.59
1:F:62:GLU:HG2	1:F:65:ASP:OD2	2.03	0.59
1:B:131:ASP:OD2	1:B:252:THR:HG21	2.03	0.59
1:D:225:MET:O	1:D:225:MET:HG2	2.02	0.59
1:F:200:LYS:CE	1:F:206:ASP:OD1	2.51	0.59
1:D:63:ILE:HD13	1:E:39:GLU:HG3	1.84	0.58
1:D:170:ILE:HD12	1:D:185:ALA:HA	1.83	0.58
1:D:99:LYS:CB	1:D:107:ARG:HB2	2.34	0.58
1:A:200:LYS:HE3	1:A:205:VAL:HA	1.85	0.58
1:B:75:ASN:HD22	1:C:114:LEU:HD13	1.68	0.58
1:E:170:ILE:HG22	1:E:181:VAL:CG1	2.31	0.58
1:C:158:ILE:HD11	1:C:250:ILE:HD11	1.85	0.58
1:D:8:SER:OG	1:D:16:SER:CB	2.51	0.58
1:D:264:ILE:O	1:D:289:LYS:HE3	2.04	0.58
1:A:132:LEU:HD13	1:A:137:ILE:HB	1.85	0.58
1:C:103:VAL:HG12	1:C:103:VAL:O	2.03	0.58
1:D:216:ASP:N	1:D:243:GLY:O	2.37	0.58
1:E:211:VAL:HG12	1:F:211:VAL:HG12	1.86	0.58
1:E:78:LYS:HD3	1:E:123:GLY:CA	2.34	0.57
1:F:60:CYS:O	1:F:66:ASN:ND2	2.35	0.57
1:A:304:ARG:HD2	6:A:1135:HOH:O	2.04	0.57
1:B:256:PHE:O	1:B:283:LYS:HE2	2.03	0.57
1:C:127:ILE:HD12	1:C:141:PHE:CE2	2.39	0.57
1:A:266:ASN:ND2	6:A:1103:HOH:O	2.17	0.57
1:B:18:ARG:O	1:B:22:ARG:HG3	2.05	0.57
1:E:249:ALA:HB2	1:E:269:PHE:CE1	2.39	0.57
1:B:1:SER:H2	1:B:2:PRO:HD2	1.69	0.57
1:C:63:ILE:O	1:C:64:ASN:C	2.38	0.57
1:C:171:VAL:O	1:C:221:LEU:HA	2.05	0.57
1:D:62:GLU:O	1:D:62:GLU:HG3	2.05	0.57
1:C:157:TRP:CH2	1:C:273:VAL:HG21	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ILE:CD1	1:E:39:GLU:HG2	2.35	0.56
1:D:96:ARG:HH22	2:D:1001:APC:C5	2.16	0.56
1:B:33:LYS:HG3	1:B:34:LYS:N	2.20	0.56
1:C:246:LYS:CD	1:C:270:GLU:HG3	2.26	0.56
1:E:280:GLN:O	1:E:282:ASP:N	2.39	0.56
3:F:2001:HSX:C5	6:F:2122:HOH:O	2.52	0.56
1:C:111:SER:O	1:C:115:VAL:HG23	2.04	0.56
1:C:182:THR:HG23	1:D:196:HIS:NE2	2.21	0.56
1:F:183:SER:O	1:F:187:ARG:HG3	2.05	0.56
1:B:4:ILE:CD1	1:B:23:LEU:HD13	2.36	0.56
1:E:22:ARG:HD2	1:E:296:SER:HB2	1.88	0.56
1:E:7:PHE:CD1	1:E:30:VAL:HG22	2.40	0.56
1:C:296:SER:O	1:C:300:ALA:HB2	2.06	0.56
1:C:141:PHE:CB	1:C:143:ILE:HG22	2.33	0.55
1:D:110:ILE:CG2	1:E:75:ASN:O	2.54	0.55
1:A:196:HIS:HA	6:A:1120:HOH:O	2.04	0.55
1:B:1:SER:N	1:B:2:PRO:CD	2.69	0.55
1:E:264:ILE:HD11	1:E:287:CYS:SG	2.46	0.55
1:F:93:PRO:HA	5:F:2003:PO4:O3	2.05	0.55
1:C:136:GLN:OE1	1:C:136:GLN:N	2.37	0.55
3:F:2001:HSX:P'	3:F:2001:HSX:C3	2.94	0.55
1:B:113:LYS:HD2	1:B:113:LYS:O	2.06	0.55
1:D:99:LYS:HE3	1:D:107:ARG:N	2.21	0.55
1:B:135:SER:O	1:B:138:GLN:HG3	2.07	0.55
1:D:164:GLU:OE1	1:D:164:GLU:N	2.38	0.55
1:E:68:MET:HG3	1:E:72:ILE:HD12	1.88	0.55
1:C:196:HIS:CE1	1:D:186:ASP:OD2	2.57	0.55
1:A:301:GLU:HG3	6:A:1123:HOH:O	2.07	0.55
1:E:172:SER:HB3	1:E:181:VAL:HG21	1.89	0.55
6:E:1119:HOH:O	1:F:108:ALA:HB1	1.99	0.55
1:C:184:ILE:HD12	1:C:222:VAL:HG11	1.89	0.54
1:E:34:LYS:NZ	1:E:38:GLN:HE21	2.05	0.54
1:E:98:ASP:HA	2:E:1001:APC:HO2'	1.72	0.54
1:C:32:THR:HG21	1:C:69:GLU:CD	2.26	0.54
1:C:170:ILE:HG22	1:C:181:VAL:HB	1.89	0.54
1:E:18:ARG:O	1:E:22:ARG:HG3	2.07	0.54
1:C:69:GLU:O	1:C:73:MET:HG3	2.07	0.54
1:A:198:GLU:OE2	1:A:207:ARG:HG2	2.07	0.54
1:A:208:MET:HE1	1:A:235:ALA:HA	1.90	0.54
1:B:249:ALA:HB3	1:B:272:VAL:HG22	1.90	0.54
1:B:295:ILE:HG22	1:B:298:ILE:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:VAL:C	1:D:43:GLU:HG2	2.26	0.54
1:F:210:LEU:HB2	1:F:238:LYS:HE3	1.89	0.54
1:E:68:MET:CE	1:E:72:ILE:HD11	2.37	0.54
1:F:198:GLU:OE2	1:F:209:VAL:HG21	2.07	0.54
1:C:35:PHE:CE2	1:C:41:SER:HB2	2.43	0.54
1:D:30:VAL:HG22	1:D:44:ILE:HA	1.89	0.54
1:E:78:LYS:HD3	1:E:123:GLY:O	2.08	0.54
1:E:245:THR:OG1	1:E:246:LYS:HG3	2.07	0.54
1:E:62:GLU:O	1:E:66:ASN:ND2	2.41	0.53
1:E:256:PHE:HB2	1:E:283:LYS:HD3	1.89	0.53
1:A:67:LEU:O	1:A:71:LEU:HG	2.07	0.53
1:E:129:THR:HG22	1:E:130:MET:H	1.74	0.53
1:A:89:ILE:O	1:A:129:THR:HG23	2.09	0.53
1:E:15:LEU:O	1:E:19:VAL:HG22	2.08	0.53
1:C:169:ILE:O	1:C:169:ILE:HG23	2.06	0.53
1:F:172:SER:HB3	1:F:194:LEU:HD13	1.89	0.53
1:D:63:ILE:HD11	1:E:39:GLU:CA	2.39	0.53
1:D:133:HIS:NE2	2:D:1001:APC:O1B	2.30	0.53
1:D:227:ASP:OD1	1:D:257:SER:CB	2.56	0.53
2:C:1001:APC:H3'	2:C:1001:APC:N3	2.24	0.53
1:A:276:ASN:OD1	1:A:295:ILE:HG13	2.08	0.53
1:D:173:PRO:HB3	1:D:231:THR:HG23	1.89	0.53
1:E:184:ILE:HD11	1:E:222:VAL:HG21	1.91	0.53
1:A:136:GLN:HB2	1:B:136:GLN:HG3	1.92	0.52
1:C:219:ALA:O	1:C:247:VAL:HA	2.09	0.52
1:E:269:PHE:O	1:E:289:LYS:HE2	2.08	0.52
1:C:171:VAL:HA	1:C:193:ALA:O	2.09	0.52
1:C:34:LYS:CE	1:C:38:GLN:NE2	2.69	0.52
1:D:7:PHE:CE1	1:D:30:VAL:HG23	2.44	0.52
1:D:97:GLN:HG3	1:D:98:ASP:H	1.73	0.52
1:D:217:ARG:O	1:D:244:ALA:CA	2.58	0.52
1:C:195:ILE:HG12	1:C:210:LEU:HD23	1.90	0.52
1:F:251:LEU:HB2	1:F:274:VAL:HG12	1.89	0.52
1:E:280:GLN:O	1:E:281:GLU:C	2.48	0.52
1:F:180:ARG:NH2	6:F:2103:HOH:O	2.36	0.52
1:C:57:GLN:OE1	1:C:66:ASN:HB3	2.10	0.52
1:A:14:ASP:O	1:A:18:ARG:HG3	2.10	0.52
3:A:1002:HSX:C3	3:A:1002:HSX:O3X	2.58	0.52
1:B:151:GLU:O	1:B:152:PRO:C	2.44	0.52
1:C:170:ILE:CG2	1:C:181:VAL:HB	2.39	0.52
1:B:57:GLN:NE2	1:B:57:GLN:CA	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ILE:CD1	1:A:217:ARG:HH11	2.22	0.51
1:C:118:MET:HA	1:C:121:VAL:HG12	1.90	0.51
1:C:132:LEU:HD13	1:C:137:ILE:HB	1.92	0.51
1:C:192:PHE:HE2	1:C:194:LEU:HD22	1.76	0.51
1:E:302:ALA:O	1:E:306:THR:HG23	2.10	0.51
1:A:70:LEU:O	1:A:70:LEU:HD23	2.10	0.51
1:D:34:LYS:HE3	1:D:65:ASP:OD2	2.11	0.51
1:B:156:GLN:OE1	6:B:2101:HOH:O	2.18	0.51
1:D:183:SER:O	1:D:187:ARG:CG	2.59	0.51
1:E:257:SER:O	1:E:258:GLY:C	2.48	0.51
1:D:222:VAL:HG12	1:D:250:ILE:HB	1.92	0.51
1:B:109:PRO:O	1:B:109:PRO:HG2	2.11	0.51
1:C:125:ASP:O	1:C:143:ILE:HD11	2.11	0.51
1:D:180:ARG:O	1:D:184:ILE:CD1	2.48	0.51
1:E:7:PHE:HD1	1:E:30:VAL:CG2	2.24	0.51
1:B:256:PHE:O	1:B:283:LYS:CE	2.59	0.51
1:D:13:GLN:HG3	1:D:13:GLN:O	2.09	0.51
1:E:103:VAL:CG2	1:F:187:ARG:HH12	2.24	0.51
1:F:276:ASN:OD1	1:F:295:ILE:HG13	2.11	0.50
1:B:109:PRO:HG3	1:B:140:PHE:HZ	1.76	0.50
1:B:110:ILE:O	1:B:110:ILE:HG13	2.10	0.50
1:C:17:GLN:NE2	1:C:21:ASP:OD1	2.45	0.50
1:D:99:LYS:HB2	1:D:107:ARG:CD	2.42	0.50
1:F:157:TRP:O	1:F:161:ASN:HB2	2.12	0.50
1:E:7:PHE:CD1	1:E:30:VAL:CG2	2.94	0.50
1:D:104:GLY:O	1:D:105:GLU:HB3	2.11	0.50
1:D:302:ALA:O	1:D:306:THR:HG23	2.11	0.50
1:E:170:ILE:CD1	1:E:185:ALA:HA	2.38	0.50
1:E:227:ASP:OD1	1:E:255:ILE:HG22	2.10	0.50
1:A:308:ASN:OD1	1:A:308:ASN:N	2.44	0.50
1:B:121:VAL:HG11	1:C:117:ASN:HB3	1.93	0.50
1:E:286:HIS:ND1	1:E:286:HIS:N	2.59	0.50
1:B:251:LEU:O	1:B:274:VAL:HA	2.12	0.50
1:B:117:ASN:HB3	1:C:121:VAL:HG21	1.94	0.49
1:D:175:ALA:O	1:D:178:ALA:N	2.41	0.49
1:D:222:VAL:O	1:D:222:VAL:HG23	2.12	0.49
1:A:3:ASN:HB2	1:A:51:GLU:OE2	2.12	0.49
1:A:172:SER:HB2	1:A:181:VAL:HG11	1.95	0.49
1:C:32:THR:HG21	1:C:69:GLU:OE2	2.12	0.49
1:C:105:GLU:HA	1:D:147:ASN:O	2.12	0.49
1:A:199:ARG:O	1:A:200:LYS:C	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:THR:HG22	1:D:293:ILE:HB	1.94	0.49
1:A:190:VAL:HG12	1:A:191:GLU:H	1.77	0.49
1:C:178:ALA:HB3	1:D:175:ALA:HB1	1.92	0.49
1:D:63:ILE:HD11	1:E:39:GLU:CG	2.43	0.49
1:E:62:GLU:CG	1:E:65:ASP:OD2	2.60	0.49
1:E:68:MET:HE3	1:E:72:ILE:HD11	1.94	0.49
1:A:10:SER:H	1:A:57:GLN:NE2	2.08	0.49
1:A:58:SER:HB2	1:A:90:PRO:HG2	1.94	0.49
1:B:12:HIS:CD2	1:B:279:PRO:HD3	2.48	0.49
1:C:153:ALA:HB1	1:C:293:ILE:HG21	1.93	0.49
1:A:127:ILE:HB	1:A:145:VAL:HG22	1.94	0.49
1:C:96:ARG:CG	1:C:225:MET:HE1	2.42	0.49
1:D:74:ILE:HG23	1:D:85:VAL:HG11	1.94	0.49
1:A:55:ILE:HD13	1:A:73:MET:HG3	1.95	0.49
1:B:1:SER:N	1:B:2:PRO:HD2	2.28	0.49
1:D:264:ILE:HG22	1:D:289:LYS:HD2	1.94	0.49
1:E:253:HIS:HA	6:E:1104:HOH:O	2.13	0.49
1:B:107:ARG:HG3	1:B:107:ARG:NH1	2.27	0.49
1:B:111:SER:O	1:B:115:VAL:HG23	2.12	0.49
1:C:84:ARG:HH22	1:C:306:THR:HG22	1.76	0.49
1:B:12:HIS:CG	1:B:279:PRO:HD3	2.47	0.49
1:E:12:HIS:CD2	1:E:15:LEU:HB3	2.48	0.49
1:C:157:TRP:CE3	1:C:158:ILE:HD13	2.48	0.48
1:D:39:GLU:HG3	1:E:63:ILE:HD12	1.95	0.48
1:E:28:GLY:HA2	1:E:46:GLU:OE1	2.14	0.48
1:E:78:LYS:CD	1:E:123:GLY:O	2.60	0.48
1:E:126:HIS:CE1	1:E:144:PRO:HB2	2.48	0.48
1:F:75:ASN:ND2	6:F:2104:HOH:O	2.46	0.48
1:B:170:ILE:O	1:B:192:PHE:CB	2.62	0.48
1:A:252:THR:HA	1:A:275:THR:CG2	2.42	0.48
1:A:261:ILE:HD11	1:A:283:LYS:HD2	1.94	0.48
1:B:198:GLU:HG2	1:B:209:VAL:HG23	1.95	0.48
1:C:151:GLU:O	1:C:152:PRO:C	2.49	0.48
1:D:240:LEU:O	1:D:241:SER:C	2.50	0.48
1:D:217:ARG:O	1:D:244:ALA:HB1	2.14	0.48
1:F:169:ILE:HG22	1:F:217:ARG:HB3	1.95	0.48
1:C:107:ARG:O	1:C:108:ALA:C	2.52	0.48
1:C:158:ILE:O	1:C:159:ARG:C	2.45	0.48
1:D:219:ALA:HB3	1:D:247:VAL:HG22	1.95	0.48
1:D:35:PHE:CE2	1:D:41:SER:HB2	2.49	0.48
1:C:157:TRP:CZ2	1:C:273:VAL:HG21	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:ARG:HE	1:D:218:VAL:H	1.63	0.47
1:A:54:TYR:CD2	1:A:86:THR:HB	2.49	0.47
1:C:221:LEU:HD11	1:C:239:LEU:HD12	1.96	0.47
1:D:11:SER:HB2	1:D:60:CYS:SG	2.54	0.47
1:D:261:ILE:HG23	1:D:287:CYS:HB2	1.95	0.47
1:C:22:ARG:NH2	1:C:294:ASP:OD2	2.47	0.47
1:D:228:THR:OG1	3:D:1002:HSX:C3	2.62	0.47
1:D:155:LEU:CD2	1:D:184:ILE:HG23	2.44	0.47
1:F:249:ALA:HB3	1:F:272:VAL:HG22	1.96	0.47
1:D:228:THR:HG1	3:D:1002:HSX:C3	2.27	0.47
1:D:99:LYS:HB2	1:D:107:ARG:HD2	1.97	0.47
2:D:1001:APC:H3'	2:D:1001:APC:N3	2.30	0.47
1:E:72:ILE:O	1:E:76:ALA:HB2	2.15	0.47
1:E:272:VAL:O	1:E:272:VAL:HG12	2.15	0.47
1:B:109:PRO:HG3	1:B:140:PHE:CZ	2.50	0.47
1:D:63:ILE:HD12	1:E:39:GLU:HG2	1.97	0.47
1:E:96:ARG:CD	1:E:225:MET:SD	3.02	0.47
1:A:273:VAL:HG12	1:A:293:ILE:CD1	2.43	0.47
1:C:227:ASP:OD1	1:C:257:SER:HB3	2.14	0.47
1:D:151:GLU:O	1:D:155:LEU:HG	2.15	0.47
1:C:278:ILE:O	1:C:280:GLN:HG2	2.15	0.46
1:F:102:LYS:HA	1:F:102:LYS:HD2	1.53	0.46
1:B:34:LYS:HE2	1:B:38:GLN:CA	2.44	0.46
1:D:251:LEU:O	1:D:274:VAL:HA	2.15	0.46
1:A:12:HIS:CG	1:A:279:PRO:HD3	2.51	0.46
1:D:217:ARG:O	1:D:244:ALA:CB	2.63	0.46
1:E:150:ALA:O	1:E:154:VAL:HG23	2.15	0.46
1:C:220:ILE:HG12	1:C:248:TYR:HB2	1.98	0.46
1:C:226:ALA:HB2	1:C:251:LEU:HD13	1.96	0.46
1:A:155:LEU:O	1:A:159:ARG:HG3	2.16	0.46
1:C:264:ILE:O	1:C:289:LYS:HE3	2.15	0.46
1:D:97:GLN:CG	1:D:98:ASP:N	2.79	0.46
1:D:99:LYS:HB2	1:D:99:LYS:HE2	1.57	0.46
1:F:250:ILE:HA	1:F:273:VAL:O	2.16	0.46
2:A:1004:APC:H3'	2:A:1004:APC:N3	2.30	0.46
1:B:96:ARG:HD3	1:B:225:MET:CE	2.46	0.46
1:C:159:ARG:HA	1:C:165:TRP:CD1	2.51	0.46
1:E:250:ILE:HG12	1:E:273:VAL:CG2	2.45	0.46
1:F:102:LYS:HB2	1:F:105:GLU:O	2.14	0.46
1:F:252:THR:HA	1:F:275:THR:HG23	1.96	0.46
1:A:250:ILE:HG12	1:A:273:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:GLU:HA	1:D:154:VAL:HG22	1.98	0.46
1:D:173:PRO:CG	1:D:231:THR:HG22	2.45	0.46
1:F:155:LEU:HD21	1:F:184:ILE:HG23	1.97	0.46
1:D:6:LEU:HD12	1:D:6:LEU:HA	1.72	0.46
1:E:5:VAL:HB	1:E:53:VAL:HA	1.98	0.46
1:A:70:LEU:HD23	1:A:70:LEU:C	2.36	0.46
1:E:186:ASP:OD1	1:F:196:HIS:HE1	1.99	0.46
1:F:136:GLN:NE2	1:F:136:GLN:N	2.58	0.46
1:F:215:LYS:HA	1:F:243:GLY:O	2.16	0.46
1:B:188:LEU:O	1:B:190:VAL:HG13	2.16	0.45
1:C:135:SER:O	1:C:138:GLN:HG3	2.16	0.45
1:D:155:LEU:HD21	1:D:184:ILE:HG23	1.97	0.45
1:E:259:PRO:HB2	1:E:263:ARG:NE	2.30	0.45
1:F:228:THR:O	1:F:229:CYS:HB2	2.15	0.45
1:C:297:MET:O	1:C:301:GLU:HB2	2.16	0.45
1:E:129:THR:HG22	1:E:130:MET:N	2.30	0.45
1:A:4:ILE:HD13	1:A:4:ILE:HG21	1.58	0.45
1:F:169:ILE:HD11	1:F:193:ALA:HB2	1.98	0.45
1:A:190:VAL:HG12	1:A:191:GLU:N	2.32	0.45
1:B:51:GLU:O	1:B:83:SER:HB2	2.17	0.45
1:C:62:GLU:CG	1:C:65:ASP:CG	2.84	0.45
1:C:181:VAL:HG23	1:C:182:THR:H	1.81	0.45
1:D:7:PHE:HB3	1:D:73:MET:HE2	1.99	0.45
1:D:150:ALA:HB3	1:D:252:THR:CG2	2.46	0.45
1:D:190:VAL:HG12	1:D:191:GLU:O	2.16	0.45
1:B:29:LYS:N	1:B:46:GLU:OE1	2.44	0.45
1:C:178:ALA:HB1	1:D:175:ALA:CB	2.46	0.45
1:D:66:ASN:HA	1:D:69:GLU:HG2	1.99	0.45
1:D:97:GLN:O	2:D:1001:APC:O3'	2.28	0.45
1:E:238:LYS:O	1:E:238:LYS:HG3	2.15	0.45
1:E:297:MET:CE	1:E:304:ARG:HH22	2.30	0.45
1:A:10:SER:N	1:A:57:GLN:NE2	2.65	0.45
1:E:17:GLN:O	1:E:20:ALA:HB3	2.16	0.45
1:E:54:TYR:OH	1:E:307:HIS:HB2	2.16	0.45
1:A:70:LEU:C	1:A:70:LEU:CD2	2.85	0.44
1:C:274:VAL:O	1:C:292:VAL:HA	2.17	0.44
1:D:98:ASP:HA	2:D:1001:APC:O3'	2.16	0.44
1:D:4:ILE:HD13	1:D:4:ILE:HG21	1.57	0.44
1:D:158:ILE:O	1:D:160:GLU:N	2.50	0.44
1:A:261:ILE:HG23	1:A:287:CYS:HB2	1.99	0.44
1:B:19:VAL:HA	1:B:22:ARG:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:ILE:HD11	1:E:87:ALA:HB2	1.99	0.44
1:F:78:LYS:O	1:F:78:LYS:HG3	2.17	0.44
1:E:170:ILE:HG22	1:E:181:VAL:HG22	1.99	0.44
1:B:6:LEU:HD13	1:B:54:TYR:HB2	1.99	0.44
1:C:177:GLY:O	1:C:180:ARG:N	2.50	0.44
1:D:240:LEU:C	1:D:242:ALA:N	2.69	0.44
1:E:249:ALA:HB3	1:E:272:VAL:HG22	1.99	0.44
1:E:297:MET:HE1	1:E:304:ARG:HH22	1.83	0.44
1:D:67:LEU:O	1:D:71:LEU:HG	2.17	0.44
1:E:56:ILE:HA	1:E:88:VAL:HB	1.99	0.44
1:E:194:LEU:HD21	1:F:194:LEU:HD21	1.98	0.44
1:A:6:LEU:HD23	1:A:6:LEU:HA	1.63	0.44
1:B:224:ASP:OD1	1:B:225:MET:HG3	2.17	0.44
1:A:151:GLU:CB	1:A:152:PRO:HD3	2.48	0.44
1:D:132:LEU:HD13	1:D:137:ILE:HB	2.00	0.44
1:A:157:TRP:CH2	1:A:273:VAL:HG21	2.53	0.44
1:B:170:ILE:O	1:B:192:PHE:HA	2.18	0.44
1:B:181:VAL:HG12	1:B:222:VAL:HG22	2.00	0.44
1:E:92:PHE:HB2	1:E:129:THR:HG21	1.99	0.44
1:C:169:ILE:HD12	1:C:170:ILE:H	1.83	0.43
1:B:39:GLU:HG2	1:C:63:ILE:CD1	2.46	0.43
1:B:278:ILE:O	1:B:280:GLN:HG2	2.17	0.43
1:C:109:PRO:HG2	1:C:140:PHE:CZ	2.52	0.43
1:E:225:MET:HA	1:E:253:HIS:O	2.18	0.43
1:F:11:SER:OG	1:F:57:GLN:OE1	2.25	0.43
1:B:225:MET:HB3	1:B:253:HIS:HB2	2.00	0.43
1:B:287:CYS:SG	1:B:290:ILE:HG13	2.58	0.43
1:C:250:ILE:HG12	1:C:273:VAL:HB	1.99	0.43
1:D:100:LYS:HB3	1:D:101:ASP:H	1.44	0.43
1:D:226:ALA:HB2	1:D:251:LEU:HG	1.99	0.43
1:D:251:LEU:HB2	1:D:274:VAL:HG12	2.00	0.43
5:D:1004:PO4:O1	1:E:39:GLU:OE2	2.35	0.43
1:E:280:GLN:N	1:E:281:GLU:OE1	2.51	0.43
1:A:252:THR:O	1:A:275:THR:HG23	2.17	0.43
1:C:63:ILE:HD13	1:C:63:ILE:HG21	1.68	0.43
1:A:6:LEU:HD23	1:A:54:TYR:HB2	2.01	0.43
1:A:168:CYS:O	1:A:169:ILE:HD13	2.19	0.43
1:B:84:ARG:CG	1:B:85:VAL:N	2.82	0.43
1:C:27:LEU:HD23	1:C:27:LEU:HA	1.44	0.43
1:C:150:ALA:O	1:C:153:ALA:HB3	2.18	0.43
1:E:171:VAL:HG12	1:E:172:SER:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:SER:N	1:A:57:GLN:HE22	2.14	0.43
1:B:226:ALA:HB2	1:B:251:LEU:HG	1.99	0.43
1:C:68:MET:O	1:C:68:MET:HG3	2.17	0.43
1:C:99:LYS:HG3	1:C:102:LYS:NZ	2.34	0.43
1:F:259:PRO:O	1:F:263:ARG:HG3	2.18	0.43
3:F:2001:HSX:C3	3:F:2001:HSX:O2X	2.67	0.43
1:A:59:GLY:HA3	1:A:93:PRO:HG3	2.01	0.43
1:E:148:LEU:HD13	1:E:298:ILE:HG22	2.01	0.43
1:A:218:VAL:HG22	1:A:246:LYS:HB2	2.00	0.43
1:C:5:VAL:HG11	1:C:48:VAL:HG12	2.00	0.43
1:C:99:LYS:HG3	1:C:102:LYS:HE3	2.00	0.43
1:D:173:PRO:O	1:D:195:ILE:HG22	2.18	0.43
1:D:173:PRO:HB2	1:D:231:THR:HG21	1.99	0.43
1:E:191:GLU:HG3	1:E:192:PHE:N	2.34	0.43
1:E:196:HIS:CE1	1:F:182:THR:CG2	3.02	0.43
1:F:99:LYS:HE2	1:F:99:LYS:HB2	1.61	0.43
1:A:155:LEU:HD21	1:A:184:ILE:HG23	2.01	0.43
1:B:172:SER:CB	1:B:181:VAL:HG11	2.40	0.43
1:B:181:VAL:HG12	1:B:222:VAL:CG2	2.48	0.43
1:C:154:VAL:HG13	1:C:250:ILE:HG21	2.01	0.43
1:D:192:PHE:CD1	1:D:192:PHE:C	2.92	0.43
1:E:250:ILE:HG12	1:E:273:VAL:HB	2.01	0.43
1:E:274:VAL:CG2	1:E:280:GLN:HE22	2.01	0.42
3:E:1002:HSX:O2X	3:E:1002:HSX:C3	2.67	0.42
1:B:177:GLY:O	1:B:181:VAL:HG13	2.18	0.42
1:D:18:ARG:NH1	1:D:18:ARG:CG	2.73	0.42
1:B:170:ILE:O	1:B:192:PHE:CA	2.67	0.42
1:B:300:ALA:O	1:B:304:ARG:HG3	2.19	0.42
1:D:179:LYS:HB2	1:D:179:LYS:HE3	1.47	0.42
1:B:214:VAL:CG1	1:B:244:ALA:HB2	2.50	0.42
1:B:219:ALA:HB1	1:B:239:LEU:HD13	2.01	0.42
1:C:22:ARG:HE	1:C:296:SER:CB	2.15	0.42
1:F:170:ILE:HG22	1:F:181:VAL:HB	2.01	0.42
1:B:78:LYS:NZ	1:B:125:ASP:OD1	2.49	0.42
1:C:1:SER:HB2	1:C:2:PRO:HD3	2.02	0.42
1:C:162:ILE:HG22	1:C:165:TRP:N	2.35	0.42
1:C:197:LYS:HD3	1:C:197:LYS:C	2.40	0.42
1:E:68:MET:HG3	1:E:72:ILE:CD1	2.48	0.42
1:E:267:ALA:O	1:E:289:LYS:NZ	2.52	0.42
1:B:126:HIS:CE1	1:B:144:PRO:HB2	2.54	0.42
1:D:209:VAL:HG22	1:D:210:LEU:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:VAL:HA	1:E:118:MET:HE2	2.01	0.42
1:C:155:LEU:HD12	1:C:155:LEU:HA	1.77	0.42
1:D:97:GLN:O	2:D:1001:APC:H3'	2.19	0.42
1:F:278:ILE:O	1:F:280:GLN:HG2	2.20	0.42
1:C:274:VAL:HG23	1:C:292:VAL:CG2	2.48	0.42
1:D:32:THR:HG21	1:D:69:GLU:OE1	2.20	0.42
1:D:184:ILE:HD13	1:D:222:VAL:HG21	2.01	0.42
1:D:270:GLU:O	1:D:271:ALA:HB2	2.19	0.42
1:A:75:ASN:HD22	1:A:75:ASN:C	2.22	0.42
1:D:178:ALA:HA	1:D:181:VAL:CG2	2.48	0.42
1:D:222:VAL:HA	1:D:250:ILE:O	2.20	0.42
1:B:114:LEU:CD2	1:C:72:ILE:HG12	2.50	0.42
1:C:71:LEU:HD11	1:C:118:MET:HE3	2.02	0.42
1:C:226:ALA:HB2	1:C:251:LEU:HD22	2.00	0.42
1:D:138:GLN:HG2	1:D:145:VAL:HB	2.02	0.42
1:C:34:LYS:NZ	1:C:38:GLN:HE21	2.17	0.41
1:C:56:ILE:HG12	1:C:88:VAL:HB	2.02	0.41
1:E:68:MET:O	1:E:72:ILE:HD12	2.20	0.41
1:F:201:LYS:HE2	1:F:204:GLU:HG3	2.02	0.41
1:A:252:THR:O	1:A:252:THR:HG22	2.19	0.41
1:B:90:PRO:HB2	1:B:277:THR:HB	2.02	0.41
1:C:157:TRP:O	1:C:161:ASN:HB2	2.20	0.41
2:E:1001:APC:C2'	2:E:1001:APC:N3	2.84	0.41
1:F:214:VAL:O	1:F:214:VAL:HG23	2.20	0.41
1:B:4:ILE:HD11	1:B:23:LEU:HD13	2.01	0.41
1:C:28:GLY:HA2	1:C:46:GLU:OE2	2.20	0.41
1:C:218:VAL:CG2	1:C:218:VAL:O	2.68	0.41
1:C:62:GLU:HG3	1:C:65:ASP:CG	2.40	0.41
1:C:155:LEU:HD11	1:C:184:ILE:HG22	2.01	0.41
1:C:168:CYS:CB	1:C:218:VAL:HG22	2.43	0.41
1:E:12:HIS:NE2	1:E:276:ASN:O	2.40	0.41
1:A:141:PHE:CD1	1:A:145:VAL:HG21	2.56	0.41
1:B:297:MET:O	1:B:297:MET:HG3	2.20	0.41
1:C:57:GLN:HE21	1:C:57:GLN:HB2	1.67	0.41
1:D:12:HIS:CE1	1:D:14:ASP:HB3	2.56	0.41
1:E:34:LYS:HZ1	1:E:38:GLN:NE2	2.19	0.41
1:E:57:GLN:O	1:E:89:ILE:HA	2.20	0.41
1:A:227:ASP:HA	1:A:255:ILE:HB	2.01	0.41
1:B:272:VAL:O	1:B:290:ILE:HA	2.21	0.41
1:E:34:LYS:HZ3	1:E:38:GLN:HE21	1.69	0.41
1:F:134:ALA:HB1	1:F:136:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ALA:HA	1:A:181:VAL:HG22	2.02	0.41
1:B:256:PHE:CE2	1:B:290:ILE:HD13	2.56	0.41
1:B:261:ILE:HD11	1:B:283:LYS:HB3	2.02	0.41
1:A:99:LYS:HB3	1:A:100:LYS:H	1.74	0.41
1:B:225:MET:HA	1:B:253:HIS:O	2.21	0.41
1:E:240:LEU:HD11	1:E:268:ALA:CB	2.51	0.41
1:A:252:THR:CA	1:A:275:THR:HG23	2.48	0.41
1:B:110:ILE:HD12	1:C:79:ILE:HG13	2.01	0.41
3:B:2001:HSX:O5	3:B:2001:HSX:C1	2.69	0.41
1:C:103:VAL:O	1:C:103:VAL:CG1	2.69	0.41
1:C:113:LYS:NZ	1:D:141:PHE:O	2.53	0.41
1:C:169:ILE:CD1	1:C:191:GLU:C	2.86	0.41
1:D:184:ILE:HD12	1:D:184:ILE:H	1.86	0.41
1:D:240:LEU:O	1:D:243:GLY:N	2.36	0.41
1:E:6:LEU:HD21	1:E:23:LEU:HD12	2.02	0.41
1:E:294:ASP:CG	1:E:296:SER:HG	2.23	0.41
1:F:17:GLN:O	1:F:17:GLN:HG3	2.21	0.41
1:F:182:THR:HG22	1:F:183:SER:N	2.35	0.41
3:F:2001:HSX:O3	3:F:2001:HSX:P'	2.78	0.41
1:C:208:MET:O	1:C:238:LYS:CE	2.60	0.41
1:C:211:VAL:HG12	1:D:211:VAL:CG1	2.39	0.41
1:A:113:LYS:HE2	1:B:139:GLY:O	2.21	0.40
1:B:113:LYS:HD2	1:B:113:LYS:HA	1.72	0.40
1:B:275:THR:HG22	1:B:295:ILE:CG1	2.50	0.40
1:C:157:TRP:HE3	1:C:158:ILE:HD13	1.84	0.40
1:D:15:LEU:O	1:D:18:ARG:HB2	2.22	0.40
1:D:172:SER:O	1:D:195:ILE:HB	2.21	0.40
1:F:91:CYS:SG	5:F:2003:PO4:O2	2.79	0.40
1:C:296:SER:O	1:C:300:ALA:CB	2.69	0.40
1:E:136:GLN:CD	1:E:136:GLN:H	2.24	0.40
1:E:154:VAL:CG1	1:E:250:ILE:HG21	2.49	0.40
1:B:295:ILE:HG13	1:B:295:ILE:H	1.67	0.40
1:D:15:LEU:HD22	1:D:276:ASN:O	2.21	0.40
1:E:226:ALA:HB3	1:E:251:LEU:HD12	2.01	0.40
1:B:172:SER:HA	1:B:173:PRO:HD3	1.80	0.40
1:B:258:GLY:HA3	1:B:259:PRO:HD2	1.92	0.40
1:C:164:GLU:O	1:C:165:TRP:C	2.60	0.40
1:D:68:MET:O	1:D:72:ILE:HG13	2.22	0.40
1:F:89:ILE:O	1:F:129:THR:CB	2.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:2120:HOH:O	6:F:2127:HOH:O[2_645]	2.13	0.07

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	307/321 (96%)	287 (94%)	17 (6%)	3 (1%)	13 23
1	B	290/321 (90%)	279 (96%)	11 (4%)	0	100 100
1	C	286/321 (89%)	264 (92%)	21 (7%)	1 (0%)	37 55
1	D	294/321 (92%)	275 (94%)	14 (5%)	5 (2%)	7 13
1	E	295/321 (92%)	274 (93%)	20 (7%)	1 (0%)	37 55
1	F	306/321 (95%)	287 (94%)	18 (6%)	1 (0%)	37 55
All	All	1778/1926 (92%)	1666 (94%)	101 (6%)	11 (1%)	22 37

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	LYS
1	F	101	ASP
1	D	176	GLY
1	E	258	GLY
1	A	100	LYS
1	D	173	PRO
1	D	180	ARG
1	D	271	ALA
1	D	109	PRO
1	A	99	LYS
1	C	61	GLY

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	259/271 (96%)	240 (93%)	19 (7%)	11 21
1	B	248/271 (92%)	232 (94%)	16 (6%)	14 25
1	C	246/271 (91%)	226 (92%)	20 (8%)	9 18
1	D	250/271 (92%)	224 (90%)	26 (10%)	5 10
1	E	251/271 (93%)	230 (92%)	21 (8%)	9 17
1	F	259/271 (96%)	238 (92%)	21 (8%)	9 18
All	All	1513/1626 (93%)	1390 (92%)	123 (8%)	9 18

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	26	GLU
1	A	43	GLU
1	A	62	GLU
1	A	70	LEU
1	A	75	ASN
1	A	82	SER
1	A	101	ASP
1	A	102	LYS
1	A	151	GLU
1	A	191	GLU
1	A	207	ARG
1	A	211	VAL
1	A	228	THR
1	A	251	LEU
1	A	275	THR
1	A	281	GLU
1	A	297	MET
1	A	305	ARG
1	B	4	ILE
1	B	12	HIS
1	B	18	ARG

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Mol	Chain	Res	Type
1	B	57	GLN
1	B	62	GLU
1	B	78	LYS
1	B	83	SER
1	B	107	ARG
1	B	130	MET
1	B	136	GLN
1	B	181	VAL
1	B	225	MET
1	B	228	THR
1	B	252	THR
1	B	263	ARG
1	B	295	ILE
1	C	3	ASN
1	C	11	SER
1	C	13	GLN
1	C	25	LEU
1	C	46	GLU
1	C	57	GLN
1	C	97	GLN
1	C	98	ASP
1	C	99	LYS
1	C	102	LYS
1	C	106	SER
1	C	155	LEU
1	C	168	CYS
1	C	170	ILE
1	C	179	LYS
1	C	184	ILE
1	C	216	ASP
1	C	218	VAL
1	C	228	THR
1	C	251	LEU
1	D	4	ILE
1	D	8	SER
1	D	13	GLN
1	D	18	ARG
1	D	25	LEU
1	D	26	GLU
1	D	34	LYS
1	D	41	SER
1	D	51	GLU

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Mol	Chain	Res	Type
1	D	65	ASP
1	D	73	MET
1	D	99	LYS
1	D	100	LYS
1	D	101	ASP
1	D	103	VAL
1	D	171	VAL
1	D	174	ASP
1	D	179	LYS
1	D	186	ASP
1	D	187	ARG
1	D	225	MET
1	D	228	THR
1	D	252	THR
1	D	259	PRO
1	D	292	VAL
1	D	297	MET
1	E	18	ARG
1	E	26	GLU
1	E	49	ARG
1	E	96	ARG
1	E	97	GLN
1	E	102	LYS
1	E	113	LYS
1	E	151	GLU
1	E	156	GLN
1	E	167	ASN
1	E	169	ILE
1	E	215	LYS
1	E	220	ILE
1	E	225	MET
1	E	251	LEU
1	E	257	SER
1	E	264	ILE
1	E	281	GLU
1	E	283	LYS
1	E	286	HIS
1	E	305	ARG
1	F	5	VAL
1	F	6	LEU
1	F	8	SER
1	F	12	HIS

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Mol	Chain	Res	Type
1	F	14	ASP
1	F	99	LYS
1	F	100	LYS
1	F	113	LYS
1	F	136	GLN
1	F	156	GLN
1	F	169	ILE
1	F	180	ARG
1	F	183	SER
1	F	191	GLU
1	F	201	LYS
1	F	251	LEU
1	F	252	THR
1	F	257	SER
1	F	281	GLU
1	F	296	SER
1	F	297	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	57	GLN
1	A	138	GLN
1	A	280	GLN
1	B	75	ASN
1	B	189	ASN
1	C	13	GLN
1	C	38	GLN
1	C	75	ASN
1	C	117	ASN
1	C	161	ASN
1	C	196	HIS
1	C	291	GLN
1	D	66	ASN
1	D	75	ASN
1	D	97	GLN
1	D	286	HIS
1	E	38	GLN
1	E	66	ASN
1	E	138	GLN
1	E	156	GLN

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Mol	Chain	Res	Type
1	E	280	GLN
1	F	75	ASN
1	F	136	GLN
1	F	234	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
5	PO4	F	2003	-	4,4,4	3.31	3 (75%)	6,6,6	3.39	5 (83%)
3	HSX	B	2001	-	14,14,14	1.37	2 (14%)	20,21,21	1.32	2 (10%)
3	HSX	C	1003	-	14,14,14	1.26	1 (7%)	20,21,21	1.01	1 (5%)
3	HSX	F	2001	-	14,14,14	2.34	9 (64%)	20,21,21	3.16	12 (60%)
3	HSX	E	1002	-	14,14,14	1.41	2 (14%)	20,21,21	1.84	9 (45%)
5	PO4	A	1006	-	4,4,4	2.03	2 (50%)	6,6,6	1.80	2 (33%)
2	APC	D	1001	-	27,33,33	2.21	9 (33%)	31,52,52	2.33	11 (35%)
5	PO4	A	1005	-	4,4,4	2.47	3 (75%)	6,6,6	1.40	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PO4	A	1007	-	4,4,4	2.75	3 (75%)	6,6,6	2.14	3 (50%)
2	APC	E	1001	-	27,33,33	1.28	4 (14%)	31,52,52	1.15	2 (6%)
3	HSX	D	1002	-	14,14,14	1.20	1 (7%)	20,21,21	1.12	2 (10%)
3	HSX	A	1002	-	14,14,14	2.04	8 (57%)	20,21,21	3.04	13 (65%)
2	APC	C	1002	-	27,33,33	2.21	8 (29%)	31,52,52	2.35	13 (41%)
2	APC	C	1001	-	27,33,33	2.29	9 (33%)	31,52,52	2.32	11 (35%)
5	PO4	D	1004	-	4,4,4	1.73	1 (25%)	6,6,6	1.33	1 (16%)
2	APC	A	1001	-	27,33,33	1.31	4 (14%)	31,52,52	1.44	5 (16%)
2	APC	A	1004	-	27,33,33	2.23	9 (33%)	31,52,52	2.35	10 (32%)

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	HSX	B	2001	-	-	0/6/22/22	0/1/1/1
3	HSX	C	1003	-	-	3/6/22/22	0/1/1/1
3	HSX	F	2001	-	-	6/6/22/22	0/1/1/1
3	HSX	E	1002	-	-	2/6/22/22	0/1/1/1
2	APC	D	1001	-	-	8/15/38/38	0/3/3/3
2	APC	E	1001	-	-	2/15/38/38	0/3/3/3
3	HSX	D	1002	-	-	2/6/22/22	0/1/1/1
3	HSX	A	1002	-	-	3/6/22/22	0/1/1/1
2	APC	C	1002	-	-	3/15/38/38	0/3/3/3
2	APC	C	1001	-	-	2/15/38/38	0/3/3/3
2	APC	A	1001	-	-	1/15/38/38	0/3/3/3
2	APC	A	1004	-	-	7/15/38/38	0/3/3/3

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1002	APC	C2-N3	5.02	1.40	1.32
2	D	1001	APC	C2-N3	5.00	1.40	1.32
2	C	1001	APC	C2-N3	4.97	1.40	1.32
2	A	1004	APC	C2-N3	4.83	1.39	1.32
5	F	2003	PO4	P-O1	-4.63	1.39	1.50
2	A	1004	APC	O4'-C1'	4.44	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	APC	O4'-C1'	4.41	1.47	1.41
2	C	1002	APC	O4'-C1'	4.31	1.47	1.41
2	D	1001	APC	O4'-C1'	4.29	1.47	1.41
2	C	1002	APC	PA-O5'	4.23	1.63	1.57
2	A	1004	APC	PB-O3B	3.96	1.62	1.58
2	C	1001	APC	PB-O3B	3.84	1.62	1.58
3	F	2001	HSX	P'-O5	-3.75	1.48	1.60
2	C	1001	APC	PA-O5'	3.71	1.62	1.57
2	C	1002	APC	PB-O2B	-3.62	1.47	1.56
2	A	1004	APC	PB-O2B	-3.61	1.47	1.56
5	A	1007	PO4	P-O3	-3.55	1.43	1.54
2	A	1001	APC	PB-O2B	-3.52	1.48	1.56
2	C	1001	APC	PA-O2A	-3.52	1.48	1.56
2	D	1001	APC	PB-O3B	3.49	1.62	1.58
2	D	1001	APC	PB-O2B	-3.43	1.48	1.56
2	C	1001	APC	PB-O2B	-3.42	1.48	1.56
2	C	1002	APC	PA-O2A	-3.39	1.48	1.56
5	F	2003	PO4	P-O2	-3.38	1.44	1.54
2	A	1004	APC	PA-O2A	-3.34	1.48	1.56
2	D	1001	APC	PA-O2A	-3.33	1.48	1.56
3	F	2001	HSX	P'-O3X	-3.27	1.42	1.54
3	C	1003	HSX	C1-C2	-3.22	1.49	1.52
5	F	2003	PO4	P-O4	-3.16	1.45	1.54
5	A	1007	PO4	P-O2	-3.13	1.45	1.54
2	D	1001	APC	C2-N1	3.12	1.39	1.33
5	A	1005	PO4	P-O2	-3.09	1.45	1.54
3	F	2001	HSX	P'-O2X	-3.05	1.43	1.54
2	C	1002	APC	C2-N1	3.05	1.39	1.33
2	C	1001	APC	C2-N1	3.03	1.39	1.33
2	A	1004	APC	C2-N1	3.03	1.39	1.33
2	E	1001	APC	PA-O2A	-2.93	1.49	1.56
3	A	1002	HSX	O4-C1	-2.88	1.39	1.43
5	A	1005	PO4	P-O3	-2.88	1.45	1.54
2	D	1001	APC	PA-O5'	2.85	1.61	1.57
2	E	1001	APC	PB-O2B	-2.76	1.49	1.56
3	A	1002	HSX	P'-O2X	-2.74	1.44	1.54
2	A	1001	APC	C8-N7	-2.73	1.29	1.34
3	F	2001	HSX	C3-C4	-2.72	1.46	1.53
3	F	2001	HSX	O3-C3	-2.71	1.36	1.43
3	F	2001	HSX	O4-C4	-2.71	1.38	1.45
2	C	1001	APC	C5-C4	-2.71	1.33	1.40
2	A	1004	APC	C5-C4	-2.69	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1004	APC	C6-C5	-2.65	1.33	1.43
2	C	1002	APC	C5-C4	-2.64	1.33	1.40
2	C	1002	APC	C6-C5	-2.63	1.33	1.43
2	D	1001	APC	C6-C5	-2.62	1.33	1.43
2	C	1001	APC	C6-C5	-2.61	1.33	1.43
2	A	1004	APC	PA-O5'	2.60	1.61	1.57
2	D	1001	APC	C5-C4	-2.60	1.34	1.40
3	A	1002	HSX	P'-O5	-2.40	1.52	1.60
2	E	1001	APC	C8-N7	-2.39	1.30	1.34
5	D	1004	PO4	P-O4	-2.38	1.47	1.54
3	A	1002	HSX	C1-C2	2.35	1.55	1.52
2	E	1001	APC	PG-O2G	-2.35	1.45	1.54
5	A	1006	PO4	P-O3	-2.27	1.47	1.54
2	A	1001	APC	PA-O2A	-2.26	1.51	1.56
3	F	2001	HSX	O5-C5	-2.26	1.36	1.44
3	A	1002	HSX	C3-C4	-2.25	1.47	1.53
5	A	1006	PO4	P-O4	-2.24	1.47	1.54
3	B	2001	HSX	O4-C1	-2.23	1.40	1.43
3	A	1002	HSX	O4-C4	-2.21	1.40	1.45
3	E	1002	HSX	O4-C4	-2.20	1.40	1.45
2	A	1001	APC	PB-O3B	2.19	1.60	1.58
3	E	1002	HSX	C3-C4	-2.17	1.47	1.53
3	F	2001	HSX	C1-C2	2.15	1.55	1.52
5	A	1005	PO4	P-O4	-2.14	1.48	1.54
3	D	1002	HSX	C1-C2	-2.13	1.50	1.52
5	A	1007	PO4	P-O1	-2.11	1.45	1.50
3	A	1002	HSX	P'-O1X	-2.05	1.43	1.50
3	A	1002	HSX	P'-O3X	-2.04	1.47	1.54
3	B	2001	HSX	O4-C4	-2.03	1.40	1.45
3	F	2001	HSX	C5-C4	-2.03	1.45	1.51

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	2001	HSX	O3-C3-C4	-7.98	87.96	111.05
3	A	1002	HSX	O1-C1-O4	-7.45	101.59	111.13
2	D	1001	APC	N3-C2-N1	-6.85	117.97	128.68
2	A	1004	APC	N3-C2-N1	-6.83	118.00	128.68
2	C	1001	APC	N3-C2-N1	-6.79	118.06	128.68
2	C	1002	APC	N3-C2-N1	-6.56	118.42	128.68
2	A	1004	APC	C1'-N9-C4	6.02	137.21	126.64
2	C	1001	APC	C1'-N9-C4	6.00	137.19	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1001	APC	C1'-N9-C4	5.90	137.01	126.64
5	F	2003	PO4	O4-P-O3	5.57	125.86	107.97
2	C	1002	APC	C1'-N9-C4	4.98	135.38	126.64
3	F	2001	HSX	O3X-P'-O5	-4.85	93.84	106.73
3	F	2001	HSX	O5-C5-C4	-4.45	93.66	108.99
2	C	1002	APC	PB-O3B-PG	-4.26	117.63	132.62
3	A	1002	HSX	O4-C1-C2	4.23	109.67	104.46
3	A	1002	HSX	O3-C3-C4	-4.18	98.97	111.05
2	A	1001	APC	PB-O3B-PG	4.18	147.32	132.62
3	A	1002	HSX	O2X-P'-O5	-3.92	96.30	106.73
5	F	2003	PO4	O3-P-O2	-3.89	95.49	107.97
3	B	2001	HSX	P'-O5-C5	-3.80	107.81	118.30
3	F	2001	HSX	O2-C2-C1	3.76	122.19	111.82
3	A	1002	HSX	O3X-P'-O2X	3.65	121.58	107.64
3	A	1002	HSX	C5-C4-C3	-3.51	102.02	115.18
5	A	1007	PO4	O3-P-O1	-3.48	98.17	110.89
3	F	2001	HSX	O3X-P'-O1X	3.45	124.18	110.68
3	A	1002	HSX	O2-C2-C1	3.42	121.26	111.82
3	F	2001	HSX	O2X-P'-O5	3.38	115.74	106.73
3	F	2001	HSX	C5-C4-C3	-3.36	102.58	115.18
2	E	1001	APC	PB-O3B-PG	3.20	143.88	132.62
3	F	2001	HSX	O5-P'-O1X	-3.15	97.64	106.47
5	F	2003	PO4	O3-P-O1	-3.13	99.45	110.89
5	A	1006	PO4	O3-P-O2	3.11	117.95	107.97
3	E	1002	HSX	C1-C2-C3	3.05	106.12	102.30
3	F	2001	HSX	O4-C4-C3	2.99	111.04	105.11
2	A	1004	APC	C2'-C3'-C4'	-2.98	96.85	102.64
2	C	1001	APC	C5-C6-N6	-2.97	115.83	120.35
2	C	1001	APC	O2A-PA-O1A	2.92	119.81	110.07
2	C	1002	APC	O2A-PA-O1A	2.92	119.80	110.07
2	C	1002	APC	O3B-PG-O1G	-2.89	95.15	111.19
5	A	1007	PO4	O4-P-O1	2.88	121.43	110.89
2	D	1001	APC	O2A-PA-O1A	2.87	119.64	110.07
2	C	1001	APC	O2B-PB-O1B	2.84	119.55	110.07
3	A	1002	HSX	C2-C3-C4	2.84	108.15	102.64
2	C	1001	APC	O3G-PG-O2G	2.84	118.48	107.64
2	C	1002	APC	O3G-PG-O2G	2.82	118.42	107.64
2	A	1001	APC	C1'-N9-C4	2.82	131.59	126.64
2	D	1001	APC	C5-C6-N6	-2.78	116.13	120.35
3	A	1002	HSX	O5-C5-C4	-2.76	99.51	108.99
2	A	1004	APC	O3G-PG-O2G	2.75	118.14	107.64
2	D	1001	APC	O3G-PG-O2G	2.75	118.14	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1004	APC	O2B-PB-O1B	2.74	119.21	110.07
2	C	1002	APC	O2B-PB-O1B	2.74	119.21	110.07
3	F	2001	HSX	O4-C1-C2	2.73	107.82	104.46
3	E	1002	HSX	O1-C1-O4	-2.72	107.66	111.13
2	A	1004	APC	C5-C6-N6	-2.71	116.23	120.35
2	D	1001	APC	O2B-PB-O1B	2.70	119.09	110.07
2	A	1004	APC	O2A-PA-O1A	2.68	119.01	110.07
3	D	1002	HSX	O3X-P'-O2X	2.67	117.84	107.64
2	C	1002	APC	C5-C6-N6	-2.66	116.31	120.35
2	C	1001	APC	O3G-PG-O3B	-2.65	95.73	104.64
3	E	1002	HSX	O3X-P'-O2X	2.64	117.72	107.64
2	C	1001	APC	PB-O3B-PG	-2.62	123.41	132.62
3	A	1002	HSX	O3X-P'-O5	-2.61	99.80	106.73
2	A	1004	APC	O2G-PG-O3B	-2.60	95.90	104.64
2	C	1002	APC	C2'-C3'-C4'	-2.60	97.60	102.64
2	D	1001	APC	O2G-PG-O3B	-2.56	96.05	104.64
2	D	1001	APC	O3B-PG-O1G	-2.51	97.27	111.19
3	E	1002	HSX	C5-C4-C3	-2.48	105.88	115.18
5	D	1004	PO4	O4-P-O1	-2.48	101.83	110.89
2	A	1004	APC	O3B-PG-O1G	-2.42	97.74	111.19
2	A	1001	APC	O2A-PA-O1A	2.42	118.16	110.07
2	D	1001	APC	PB-O3B-PG	-2.41	124.14	132.62
2	C	1002	APC	O4'-C4'-C3'	-2.37	100.43	105.11
3	C	1003	HSX	O2-C2-C1	-2.37	105.29	111.82
3	E	1002	HSX	O5-P'-O1X	-2.30	100.03	106.47
2	C	1002	APC	O2G-PG-O3B	-2.30	96.93	104.64
5	F	2003	PO4	O2-P-O1	2.30	119.29	110.89
3	A	1002	HSX	O4-C4-C3	2.29	109.65	105.11
2	D	1001	APC	C2'-C3'-C4'	-2.28	98.21	102.64
3	E	1002	HSX	O3-C3-C4	-2.27	104.47	111.05
3	A	1002	HSX	O5-P'-O1X	2.26	112.81	106.47
2	A	1001	APC	O4'-C1'-C2'	-2.26	103.63	106.93
3	E	1002	HSX	O2X-P'-O1X	2.25	119.47	110.68
2	C	1001	APC	O3B-PG-O1G	-2.24	98.76	111.19
3	D	1002	HSX	O2X-P'-O5	-2.23	100.81	106.73
5	A	1006	PO4	O2-P-O1	-2.19	102.89	110.89
5	A	1007	PO4	O4-P-O3	2.16	114.92	107.97
3	F	2001	HSX	O1-C1-O4	-2.16	108.36	111.13
2	A	1004	APC	PB-O3B-PG	-2.16	125.02	132.62
3	E	1002	HSX	O5-C5-C4	-2.15	101.60	108.99
3	E	1002	HSX	C2-C3-C4	-2.14	98.49	102.64
2	A	1001	APC	C5-C6-N6	2.13	123.58	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1002	HSX	P'-O5-C5	2.13	124.15	118.30
5	F	2003	PO4	O4-P-O1	-2.08	103.29	110.89
3	B	2001	HSX	C5-C4-C3	-2.08	107.40	115.18
2	C	1002	APC	O3G-PG-O1G	2.06	118.74	110.68
3	F	2001	HSX	C2-C3-C4	2.04	106.61	102.64
2	C	1001	APC	O2G-PG-O3B	-2.04	97.81	104.64
2	E	1001	APC	C5-C6-N6	2.04	123.45	120.35
2	C	1002	APC	O2G-PG-O1G	2.03	118.64	110.68
2	C	1001	APC	O3G-PG-O1G	2.03	118.62	110.68
5	A	1005	PO4	O2-P-O1	2.02	118.30	110.89
2	D	1001	APC	O2G-PG-O1G	2.01	118.54	110.68

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1004	APC	PA-C3A-PB-O1B
2	A	1004	APC	PA-C3A-PB-O2B
2	A	1004	APC	PA-C3A-PB-O3B
2	A	1004	APC	PB-C3A-PA-O1A
2	A	1004	APC	C5'-O5'-PA-O1A
2	C	1001	APC	PB-O3B-PG-O3G
2	C	1002	APC	C5'-O5'-PA-O1A
2	D	1001	APC	PA-C3A-PB-O1B
2	D	1001	APC	PA-C3A-PB-O2B
3	C	1003	HSX	O4-C4-C5-O5
3	C	1003	HSX	C4-C5-O5-P'
3	D	1002	HSX	C4-C5-O5-P'
3	F	2001	HSX	O4-C4-C5-O5
3	F	2001	HSX	C5-O5-P'-O1X
3	F	2001	HSX	C5-O5-P'-O2X
3	F	2001	HSX	C5-O5-P'-O3X
2	D	1001	APC	C5'-O5'-PA-O1A
2	A	1001	APC	O4'-C4'-C5'-O5'
2	C	1002	APC	O4'-C4'-C5'-O5'
2	D	1001	APC	O4'-C4'-C5'-O5'
2	D	1001	APC	C3'-C4'-C5'-O5'
3	F	2001	HSX	C3-C4-C5-O5
3	C	1003	HSX	C3-C4-C5-O5
2	E	1001	APC	C5'-O5'-PA-C3A
3	F	2001	HSX	C4-C5-O5-P'
3	A	1002	HSX	O4-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
2	E	1001	APC	C3'-C4'-C5'-O5'
2	D	1001	APC	PA-C3A-PB-O3B
3	A	1002	HSX	C4-C5-O5-P'
2	C	1001	APC	C5'-O5'-PA-C3A
2	D	1001	APC	PB-C3A-PA-O1A
3	A	1002	HSX	C3-C4-C5-O5
2	A	1004	APC	C5'-O5'-PA-O2A
2	C	1002	APC	C5'-O5'-PA-O2A
2	D	1001	APC	C5'-O5'-PA-O2A
3	D	1002	HSX	O4-C4-C5-O5
3	E	1002	HSX	O4-C4-C5-O5
3	E	1002	HSX	C4-C5-O5-P'
2	A	1004	APC	O4'-C4'-C5'-O5'

There are no ring outliers.

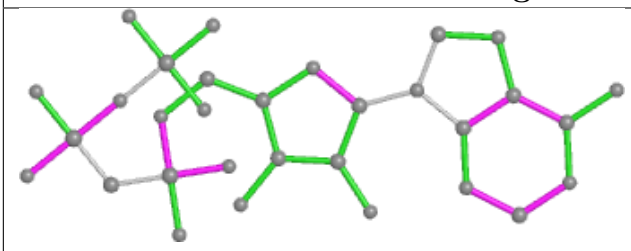
14 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	2003	PO4	2	0
3	B	2001	HSX	1	0
3	F	2001	HSX	5	0
3	E	1002	HSX	2	0
2	D	1001	APC	12	0
5	A	1005	PO4	2	0
2	E	1001	APC	14	0
3	D	1002	HSX	6	0
3	A	1002	HSX	1	0
2	C	1002	APC	6	0
2	C	1001	APC	2	0
5	D	1004	PO4	1	0
2	A	1001	APC	3	0
2	A	1004	APC	3	0

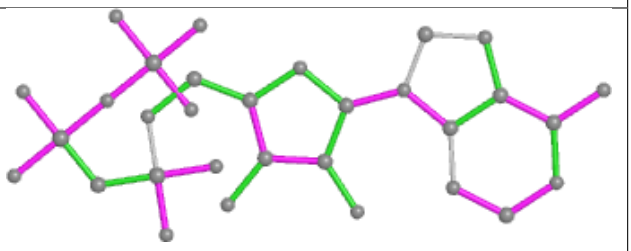
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

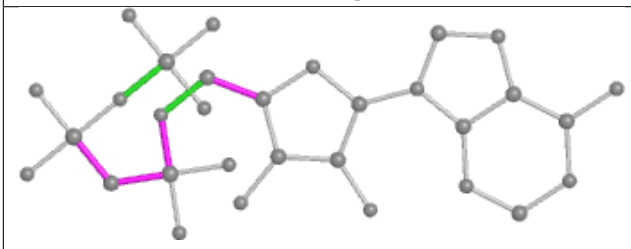
Ligand APC D 1001



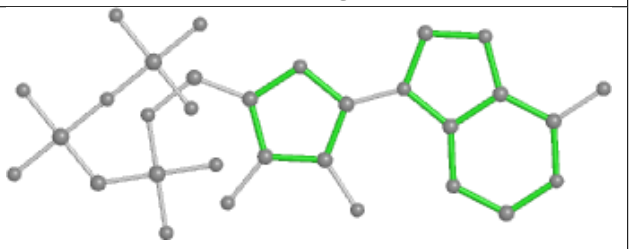
Bond lengths



Bond angles

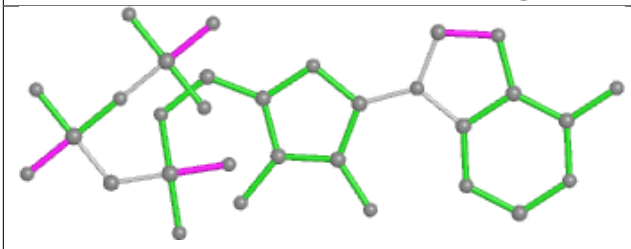


Torsions

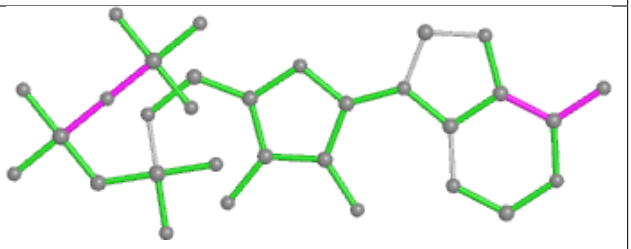


Rings

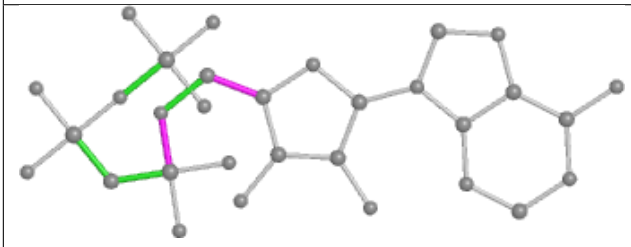
Ligand APC E 1001



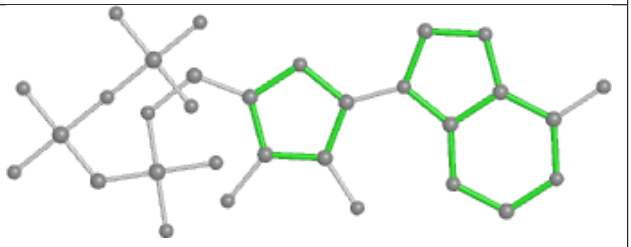
Bond lengths



Bond angles

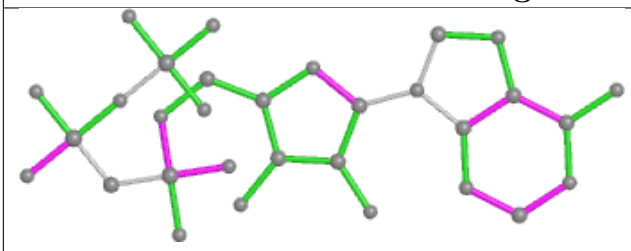


Torsions

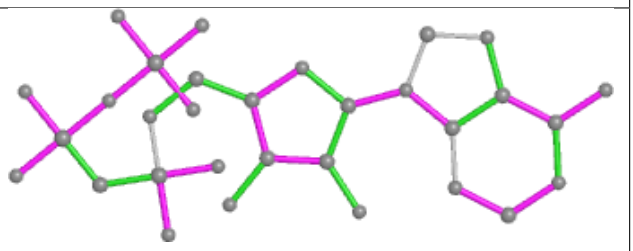


Rings

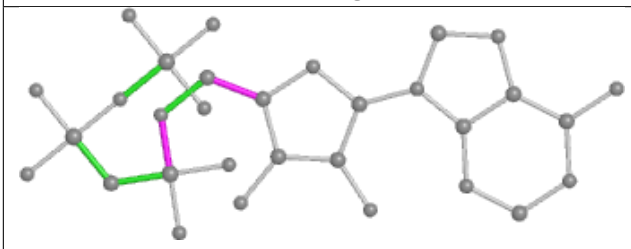
Ligand APC C 1002



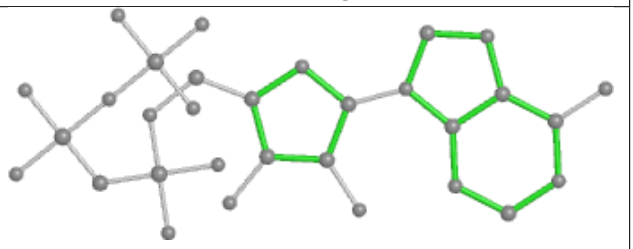
Bond lengths



Bond angles

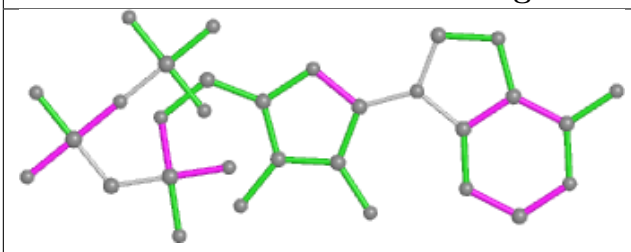


Torsions

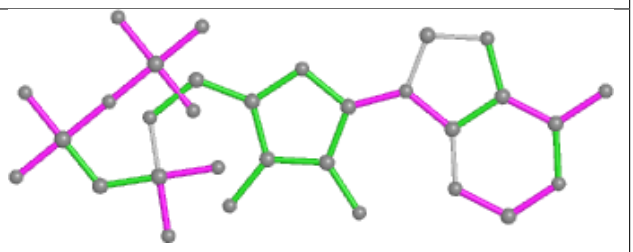


Rings

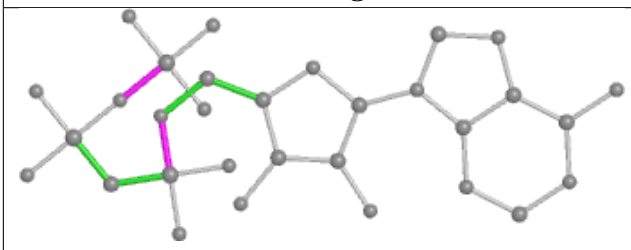
Ligand APC C 1001



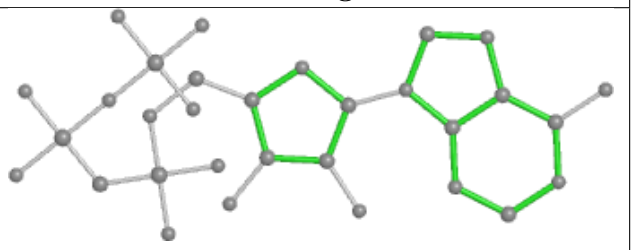
Bond lengths



Bond angles

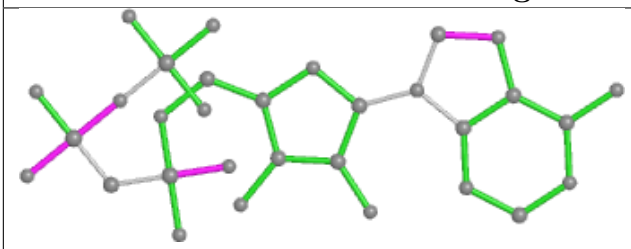


Torsions

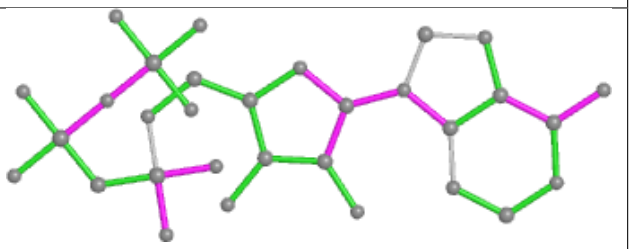


Rings

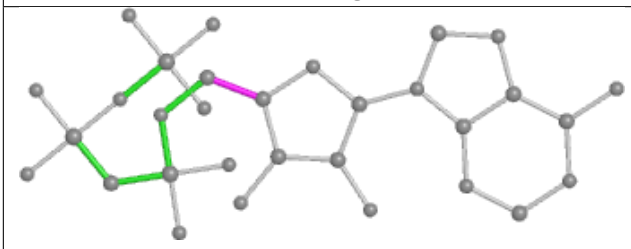
Ligand APC A 1001



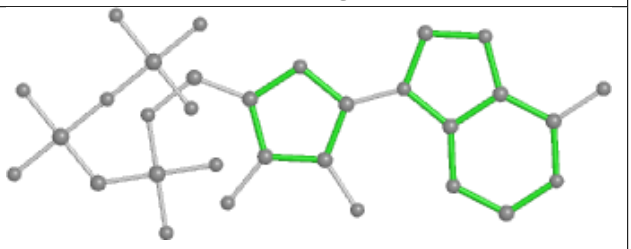
Bond lengths



Bond angles

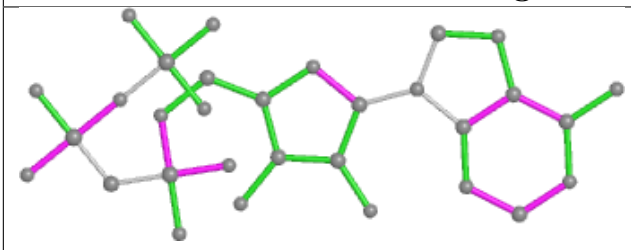


Torsions

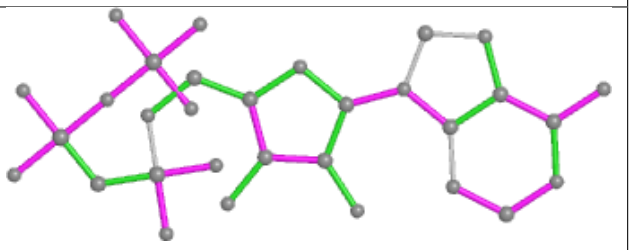


Rings

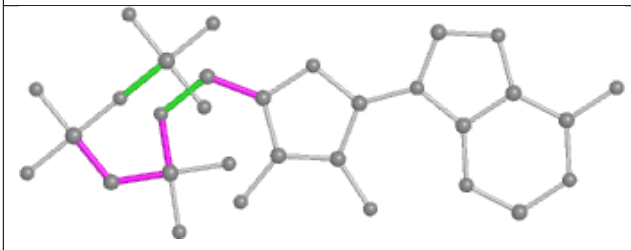
Ligand APC A 1004



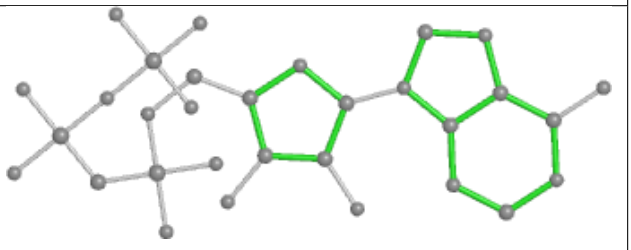
Bond lengths



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	309/321 (96%)	1.05	37 (11%) 10 12	16, 31, 52, 99	0
1	B	296/321 (92%)	1.40	70 (23%) 2 3	27, 47, 65, 78	0
1	C	294/321 (91%)	1.71	93 (31%) 1 1	35, 64, 88, 99	0
1	D	298/321 (92%)	1.94	125 (41%) 1 0	33, 66, 96, 113	0
1	E	299/321 (93%)	1.51	80 (26%) 2 2	30, 47, 69, 94	0
1	F	308/321 (95%)	0.90	33 (10%) 12 15	16, 30, 49, 98	0
All	All	1804/1926 (93%)	1.41	438 (24%) 2 3	16, 45, 85, 113	0

All (438) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	98	ASP	7.1
1	C	221	LEU	6.9
1	B	4	ILE	6.8
1	C	250	ILE	6.7
1	D	172	SER	6.2
1	D	268	ALA	6.2
1	C	249	ALA	5.8
1	C	154	VAL	5.5
1	B	97	GLN	5.4
1	E	181	VAL	5.3
1	D	179	LYS	5.3
1	A	175	ALA	5.3
1	E	174	ASP	5.1
1	D	251	LEU	5.0
1	D	173	PRO	5.0
1	C	248	TYR	4.9
1	D	184	ILE	4.8
1	D	236	ALA	4.8
1	D	103	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	254	GLY	4.8
1	D	150	ALA	4.7
1	D	95	ALA	4.6
1	B	154	VAL	4.5
1	C	268	ALA	4.5
1	D	267	ALA	4.5
1	E	290	ILE	4.5
1	C	192	PHE	4.5
1	D	197	LYS	4.5
1	E	66	ASN	4.5
1	D	295	ILE	4.5
1	D	225	MET	4.4
1	C	280	GLN	4.4
1	D	59	GLY	4.4
1	D	178	ALA	4.4
1	C	220	ILE	4.3
1	C	173	PRO	4.3
1	A	136	GLN	4.3
1	D	1	SER	4.2
1	C	103	VAL	4.2
1	B	175	ALA	4.2
1	C	175	ALA	4.1
1	B	19	VAL	4.1
1	D	174	ASP	4.1
1	C	300	ALA	4.1
1	D	171	VAL	4.1
1	D	9	GLY	4.1
1	C	226	ALA	4.1
1	A	176	GLY	4.0
1	E	220	ILE	4.0
1	D	193	ALA	3.9
1	B	304	ARG	3.9
1	C	188	LEU	3.9
1	D	58	SER	3.8
1	E	61	GLY	3.8
1	C	21	ASP	3.8
1	A	150	ALA	3.8
1	F	99	LYS	3.8
1	D	61	GLY	3.8
1	E	32	THR	3.8
1	C	88	VAL	3.8
1	E	99	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	250	ILE	3.7
1	E	175	ALA	3.7
1	D	142	ASP	3.7
1	E	293	ILE	3.7
1	C	8	SER	3.7
1	F	100	LYS	3.7
1	B	103	VAL	3.7
1	E	97	GLN	3.7
1	B	5	VAL	3.7
1	D	222	VAL	3.7
1	D	60	CYS	3.7
1	D	208	MET	3.7
1	A	1	SER	3.7
1	C	279	PRO	3.6
1	D	269	PHE	3.6
1	E	60	CYS	3.6
1	D	169	ILE	3.6
1	D	245	THR	3.6
1	C	134	ALA	3.6
1	E	179	LYS	3.6
1	C	224	ASP	3.6
1	C	208	MET	3.5
1	D	155	LEU	3.5
1	F	172	SER	3.5
1	C	255	ILE	3.5
1	D	194	LEU	3.5
1	E	20	ALA	3.5
1	E	81	SER	3.5
1	C	278	ILE	3.4
1	A	206	ASP	3.4
1	C	102	LYS	3.4
1	D	175	ALA	3.4
1	C	42	VAL	3.4
1	C	190	VAL	3.4
1	E	176	GLY	3.4
1	A	15	LEU	3.4
1	D	100	LYS	3.4
1	F	174	ASP	3.4
1	B	25	LEU	3.4
1	C	165	TRP	3.4
1	C	56	ILE	3.4
1	E	194	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	250	ILE	3.3
1	E	110	ILE	3.3
1	E	184	ILE	3.3
1	C	194	LEU	3.3
1	F	24	GLY	3.3
1	F	81	SER	3.3
1	F	101	ASP	3.3
1	B	280	GLN	3.3
1	A	167	ASN	3.3
1	B	32	THR	3.3
1	B	165	TRP	3.3
1	E	55	ILE	3.3
1	C	263	ARG	3.3
1	E	75	ASN	3.3
1	B	158	ILE	3.3
1	B	224	ASP	3.3
1	C	179	LYS	3.3
1	D	226	ALA	3.2
1	B	223	ASP	3.2
1	B	1	SER	3.2
1	D	237	ASP	3.2
1	F	199	ARG	3.2
1	C	163	ALA	3.2
1	B	67	LEU	3.2
1	A	95	ALA	3.2
1	C	108	ALA	3.2
1	D	221	LEU	3.2
1	E	17	GLN	3.2
1	A	174	ASP	3.2
1	D	223	ASP	3.2
1	D	26	GLU	3.1
1	D	151	GLU	3.1
1	C	143	ILE	3.1
1	F	16	SER	3.1
1	D	248	TYR	3.1
1	A	245	THR	3.1
1	C	275	THR	3.1
1	B	188	LEU	3.1
1	D	211	VAL	3.1
1	C	7	PHE	3.1
1	B	61	GLY	3.1
1	E	248	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	191	GLU	3.1
1	C	297	MET	3.1
1	B	26	GLU	3.0
1	B	71	LEU	3.0
1	F	286	HIS	3.0
1	A	236	ALA	3.0
1	F	181	VAL	3.0
1	D	130	MET	3.0
1	C	195	ILE	3.0
1	B	122	ALA	3.0
1	C	260	ALA	3.0
1	E	276	ASN	3.0
1	E	280	GLN	3.0
1	D	176	GLY	3.0
1	E	45	GLY	3.0
1	B	293	ILE	3.0
1	A	100	LYS	3.0
1	C	244	ALA	3.0
1	E	219	ALA	3.0
1	F	210	LEU	2.9
1	A	220	ILE	2.9
1	A	99	LYS	2.9
1	D	214	VAL	2.9
1	C	26	GLU	2.9
1	D	239	LEU	2.9
1	E	261	ILE	2.9
1	C	228	THR	2.9
1	D	149	TYR	2.9
1	D	210	LEU	2.9
1	D	135	SER	2.9
1	F	103	VAL	2.9
1	D	213	ASP	2.9
1	D	170	ILE	2.8
1	E	278	ILE	2.8
1	B	47	SER	2.8
1	C	150	ALA	2.8
1	D	167	ASN	2.8
1	E	107	ARG	2.8
1	D	165	TRP	2.8
1	D	261	ILE	2.8
1	C	229	CYS	2.8
1	D	247	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	19	VAL	2.8
1	D	227	ASP	2.8
1	D	4	ILE	2.8
1	D	293	ILE	2.8
1	A	103	VAL	2.8
1	A	181	VAL	2.8
1	D	92	PHE	2.8
1	A	194	LEU	2.8
1	D	262	SER	2.7
1	B	212	GLY	2.7
1	D	79	ILE	2.7
1	B	77	CYS	2.7
1	D	153	ALA	2.7
1	D	254	GLY	2.7
1	B	264	ILE	2.7
1	D	264	ILE	2.7
1	D	218	VAL	2.7
1	F	102	LYS	2.7
1	E	58	SER	2.7
1	D	177	GLY	2.7
1	E	196	HIS	2.7
1	C	55	ILE	2.7
1	D	278	ILE	2.7
1	B	281	GLU	2.7
1	C	269	PHE	2.7
1	E	35	PHE	2.7
1	C	216	ASP	2.6
1	E	167	ASN	2.6
1	D	238	LYS	2.6
1	C	272	VAL	2.6
1	A	252	THR	2.6
1	F	207	ARG	2.6
1	E	1	SER	2.6
1	C	162	ILE	2.6
1	C	19	VAL	2.6
1	F	279	PRO	2.6
1	E	244	ALA	2.6
1	E	10	SER	2.6
1	C	149	TYR	2.6
1	B	121	VAL	2.6
1	D	132	LEU	2.6
1	B	226	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	104	GLY	2.6
1	B	106	SER	2.6
1	C	142	ASP	2.6
1	B	119	LEU	2.6
1	D	70	LEU	2.6
1	B	76	ALA	2.6
1	B	271	ALA	2.6
1	D	108	ALA	2.6
1	C	245	THR	2.6
1	B	255	ILE	2.6
1	C	110	ILE	2.6
1	B	62	GLU	2.5
1	E	77	CYS	2.5
1	D	186	ASP	2.5
1	D	53	VAL	2.5
1	A	76	ALA	2.5
1	B	20	ALA	2.5
1	B	45	GLY	2.5
1	B	295	ILE	2.5
1	C	243	GLY	2.5
1	B	215	LYS	2.5
1	A	164	GLU	2.5
1	C	227	ASP	2.5
1	F	136	GLN	2.5
1	F	180	ARG	2.5
1	D	219	ALA	2.5
1	D	195	ILE	2.5
1	F	293	ILE	2.5
1	B	86	THR	2.5
1	D	43	GLU	2.5
1	A	279	PRO	2.5
1	B	248	TYR	2.5
1	D	96	ARG	2.5
1	D	272	VAL	2.5
1	B	284	MET	2.5
1	F	303	ILE	2.5
1	A	204	GLU	2.5
1	D	82	SER	2.5
1	F	17	GLN	2.5
1	C	197	LYS	2.5
1	D	260	ALA	2.5
1	F	308	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	44	ILE	2.5
1	D	110	ILE	2.5
1	E	185	ALA	2.4
1	B	56	ILE	2.4
1	C	125	ASP	2.4
1	C	158	ILE	2.4
1	D	231	THR	2.4
1	C	210	LEU	2.4
1	D	93	PRO	2.4
1	D	190	VAL	2.4
1	A	143	ILE	2.4
1	E	243	GLY	2.4
1	C	252	THR	2.4
1	E	129	THR	2.4
1	E	245	THR	2.4
1	E	26	GLU	2.4
1	B	179	LYS	2.4
1	D	157	TRP	2.4
1	D	253	HIS	2.4
1	E	56	ILE	2.4
1	D	182	THR	2.4
1	E	84	ARG	2.4
1	A	190	VAL	2.4
1	C	181	VAL	2.4
1	E	103	VAL	2.4
1	F	110	ILE	2.4
1	F	232	ILE	2.4
1	D	229	CYS	2.4
1	E	31	VAL	2.3
1	C	236	ALA	2.3
1	C	295	ILE	2.3
1	D	220	ILE	2.3
1	D	77	CYS	2.3
1	F	224	ASP	2.3
1	C	132	LEU	2.3
1	E	70	LEU	2.3
1	A	26	GLU	2.3
1	B	160	GLU	2.3
1	C	180	ARG	2.3
1	D	180	ARG	2.3
1	D	280	GLN	2.3
1	B	219	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	242	ALA	2.3
1	C	258	GLY	2.3
1	E	67	LEU	2.3
1	C	233	CYS	2.3
1	C	287	CYS	2.3
1	D	63	ILE	2.3
1	E	170	ILE	2.3
1	E	249	ALA	2.3
1	B	54	TYR	2.3
1	D	189	ASN	2.3
1	E	51	GLU	2.3
1	E	65	ASP	2.3
1	D	233	CYS	2.3
1	E	279	PRO	2.3
1	B	38	GLN	2.3
1	D	19	VAL	2.3
1	E	154	VAL	2.3
1	D	232	ILE	2.3
1	B	236	ALA	2.3
1	E	122	ALA	2.3
1	B	6	LEU	2.3
1	C	183	SER	2.3
1	B	68	MET	2.2
1	D	67	LEU	2.3
1	D	148	LEU	2.3
1	D	217	ARG	2.2
1	E	216	ASP	2.2
1	B	85	VAL	2.2
1	C	291	GLN	2.2
1	D	181	VAL	2.2
1	E	128	ILE	2.2
1	C	104	GLY	2.2
1	E	239	LEU	2.2
1	C	106	SER	2.2
1	E	37	ASN	2.2
1	E	287	CYS	2.2
1	D	256	PHE	2.2
1	C	166	LYS	2.2
1	D	166	LYS	2.2
1	C	251	LEU	2.2
1	E	221	LEU	2.2
1	F	132	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	54	TYR	2.2
1	F	133	HIS	2.2
1	B	181	VAL	2.2
1	C	30	VAL	2.2
1	D	115	VAL	2.2
1	D	292	VAL	2.2
1	B	55	ILE	2.2
1	B	63	ILE	2.2
1	B	220	ILE	2.2
1	E	195	ILE	2.2
1	D	299	LEU	2.2
1	A	180	ARG	2.2
1	B	262	SER	2.2
1	D	183	SER	2.2
1	A	101	ASP	2.2
1	A	115	VAL	2.2
1	C	232	ILE	2.2
1	D	35	PHE	2.2
1	E	53	VAL	2.2
1	D	283	LYS	2.2
1	E	102	LYS	2.2
1	D	84	ARG	2.2
1	D	187	ARG	2.2
1	C	93	PRO	2.1
1	E	86	THR	2.1
1	C	256	PHE	2.1
1	D	143	ILE	2.1
1	E	92	PHE	2.1
1	E	285	LYS	2.1
1	E	71	LEU	2.1
1	B	207	ARG	2.1
1	D	305	ARG	2.1
1	C	288	THR	2.1
1	D	41	SER	2.1
1	A	264	ILE	2.1
1	B	273	VAL	2.1
1	F	145	VAL	2.1
1	D	163	ALA	2.1
1	E	134	ALA	2.1
1	F	122	ALA	2.1
1	A	93	PRO	2.1
1	D	99	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	209	VAL	2.1
1	D	56	ILE	2.1
1	E	48	VAL	2.1
1	E	64	ASN	2.1
1	C	139	GLY	2.1
1	C	60	CYS	2.1
1	C	164	GLU	2.1
1	D	69	GLU	2.1
1	B	257	SER	2.1
1	C	290	ILE	2.1
1	E	250	ILE	2.1
1	C	247	VAL	2.1
1	F	115	VAL	2.1
1	F	222	VAL	2.1
1	B	75	ASN	2.1
1	F	176	GLY	2.1
1	E	74	ILE	2.0
1	A	53	VAL	2.0
1	B	7	PHE	2.0
1	B	42	VAL	2.0
1	B	82	SER	2.0
1	C	218	VAL	2.0
1	C	241	SER	2.0
1	E	41	SER	2.0
1	E	138	GLN	2.0
1	B	180	ARG	2.0
1	A	14	ASP	2.0
1	A	163	ALA	2.0
1	A	178	ALA	2.0
1	E	283	LYS	2.0
1	A	133	HIS	2.0
1	B	91	CYS	2.0
1	D	162	ILE	2.0
1	D	255	ILE	2.0
1	F	44	ILE	2.0
1	A	188	LEU	2.0
1	B	256	PHE	2.0
1	C	25	LEU	2.0
1	D	192	PHE	2.0
1	E	106	SER	2.0
1	E	111	SER	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)

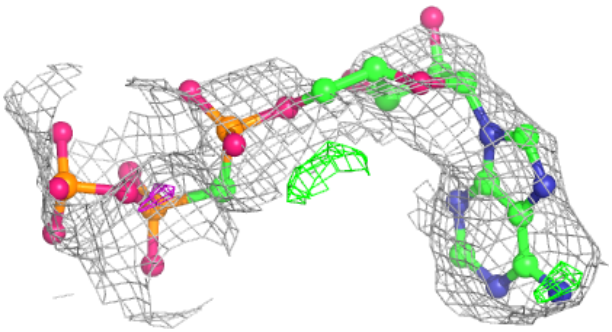
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

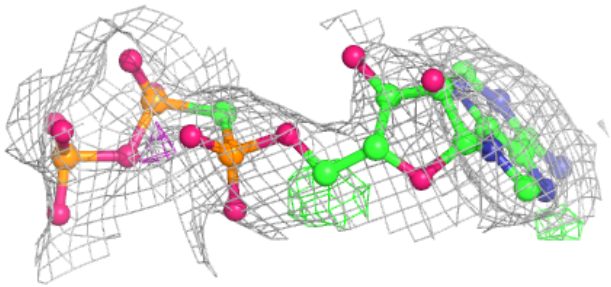
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HSX	D	1002	14/14	0.38	0.20	77,92,108,109	0
2	APC	C	1002	31/31	0.47	0.16	73,100,130,132	0
2	APC	D	1001	31/31	0.49	0.19	83,109,135,138	0
2	APC	C	1001	31/31	0.51	0.17	59,89,107,113	0
3	HSX	C	1003	14/14	0.54	0.20	79,93,107,118	0
5	PO4	A	1007	5/5	0.61	0.34	41,44,62,75	0
2	APC	E	1001	31/31	0.62	0.16	53,81,96,103	0
2	APC	A	1004	31/31	0.65	0.19	27,70,101,113	0
3	HSX	E	1002	14/14	0.70	0.15	55,60,106,118	0
2	APC	A	1001	31/31	0.70	0.17	29,64,96,99	0
3	HSX	A	1002	14/14	0.73	0.17	47,55,71,71	0
3	HSX	B	2001	14/14	0.74	0.17	57,74,88,88	0
5	PO4	F	2003	5/5	0.74	0.31	44,54,68,69	0
3	HSX	F	2001	14/14	0.75	0.15	47,55,71,71	0
5	PO4	D	1004	5/5	0.77	0.33	67,79,88,91	0
5	PO4	A	1005	5/5	0.83	0.22	46,54,56,79	0
5	PO4	A	1006	5/5	0.85	0.18	57,58,63,78	0
4	CD	F	2002	1/1	0.87	0.10	86,86,86,86	0
4	CD	A	1003	1/1	0.87	0.11	90,90,90,90	0
4	CD	D	1003	1/1	0.88	0.09	114,114,114,114	0
4	CD	E	1003	1/1	0.90	0.08	87,87,87,87	0
4	CD	B	2002	1/1	0.96	0.04	93,93,93,93	0
4	CD	C	1004	1/1	0.97	0.04	129,129,129,129	0

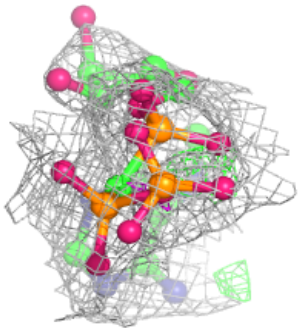
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around APC C 1002:

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

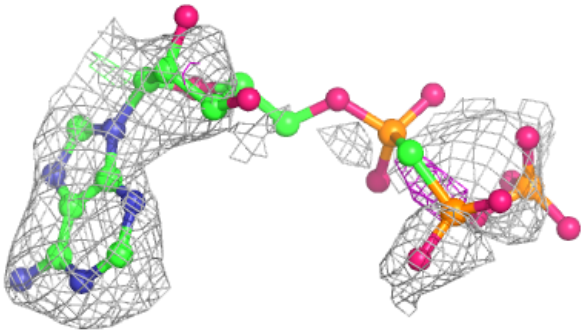


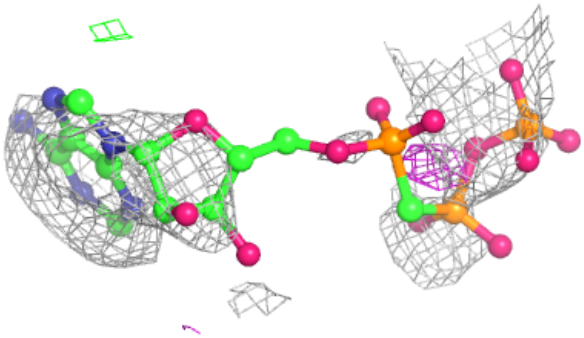


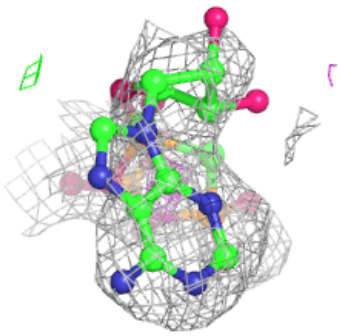


Electron density around APC D 1001:

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

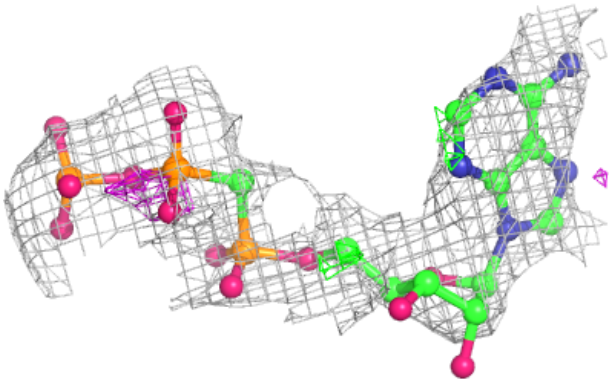


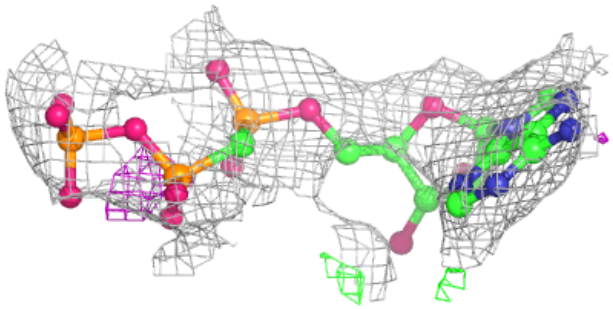


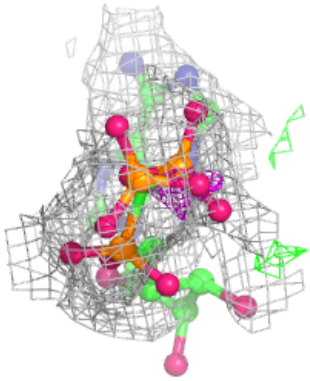


Electron density around APC C 1001:

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

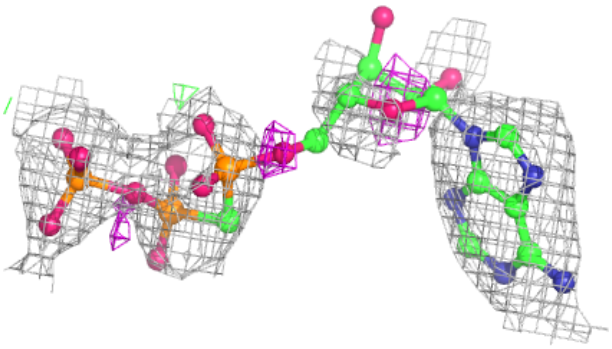


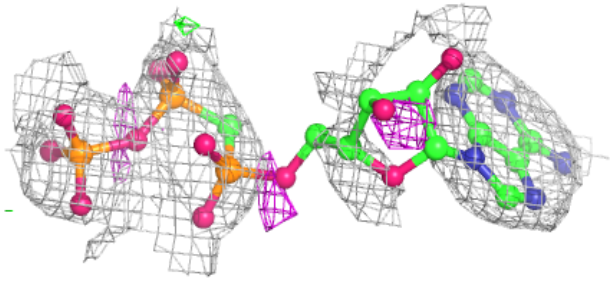


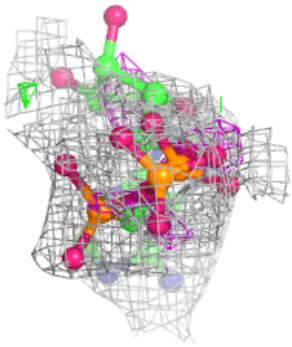


Electron density around APC E 1001:

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

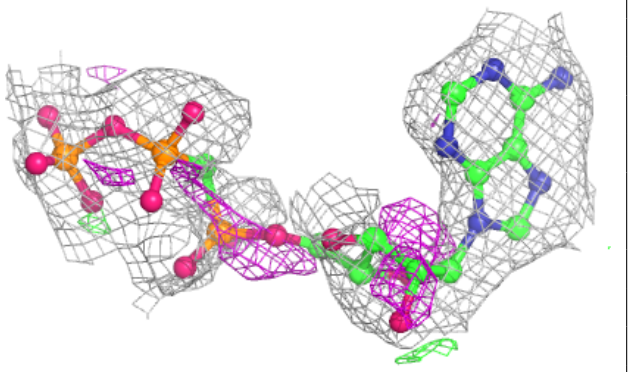


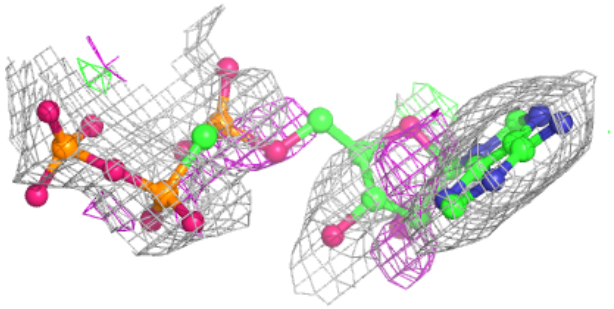


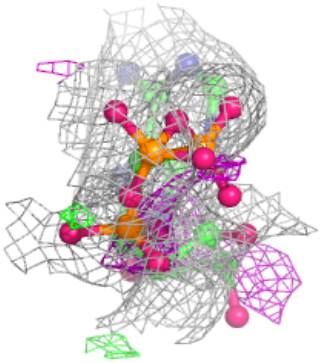


Electron density around APC A 1004:

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

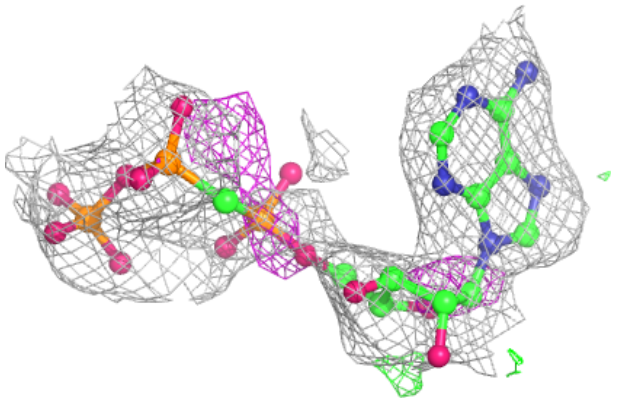


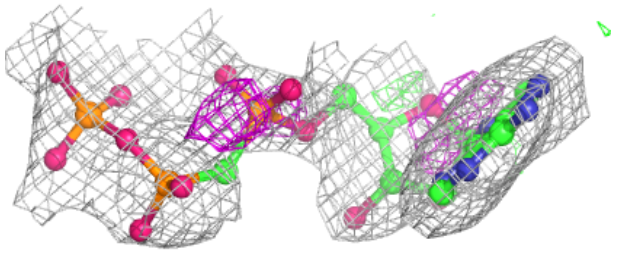


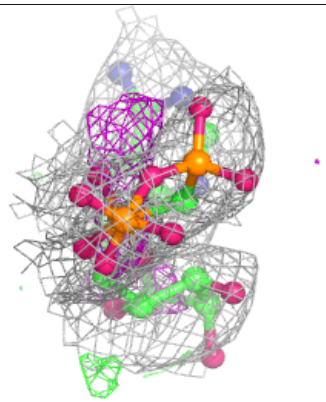


Electron density around APC A 1001:

$2mF_o$-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.