



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:18 PM UTC

PDB ID : 8YPY / pdb_00008ypy
Title : Crystal structure 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:

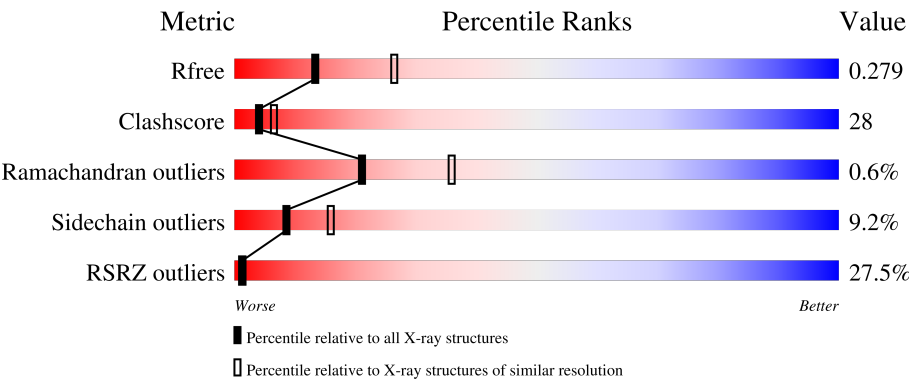
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance 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}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	321	13% 50%33%10% . .
1	B	321	26% 50%33%8% . 8%
1	C	321	32% 42%38%9% . 8%
1	D	321	44% 44%38%9% . 7%
1	E	321	28% 45%36%9% . 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	321	

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	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

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.

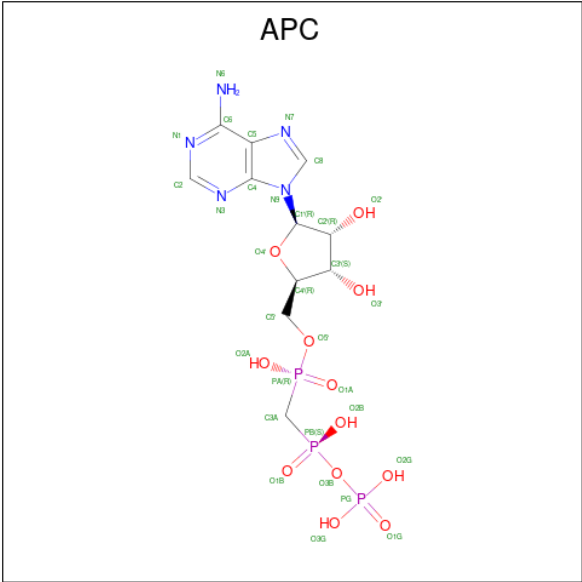
- Molecule 1 is a protein called Isoform 2 of Ribose-phosphate pyrophosphokinase 2.

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:

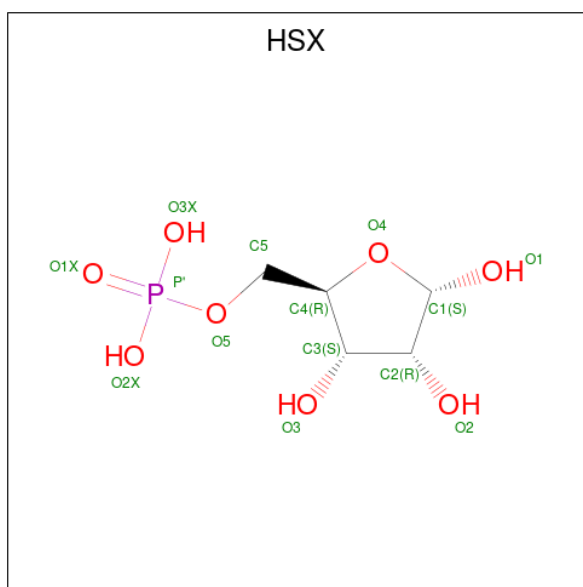
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P11908
B	1	SER	-	expression tag	UNP P11908
C	1	SER	-	expression tag	UNP P11908
D	1	SER	-	expression tag	UNP P11908
E	1	SER	-	expression tag	UNP P11908
F	1	SER	-	expression tag	UNP P11908

- Molecule 2 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: 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 (CCD ID: HSX) (formula: C₅H₁₁O₈P).

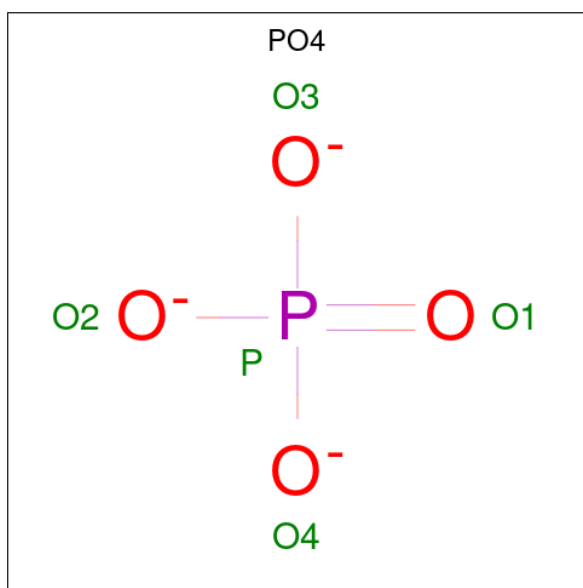


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			14	5	8	1		
3	B	1	Total	C	O	P	0	0
			14	5	8	1		
3	C	1	Total	C	O	P	0	0
			14	5	8	1		
3	D	1	Total	C	O	P	0	0
			14	5	8	1		
3	E	1	Total	C	O	P	0	0
			14	5	8	1		
3	F	1	Total	C	O	P	0	0
			14	5	8	1		

- Molecule 4 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

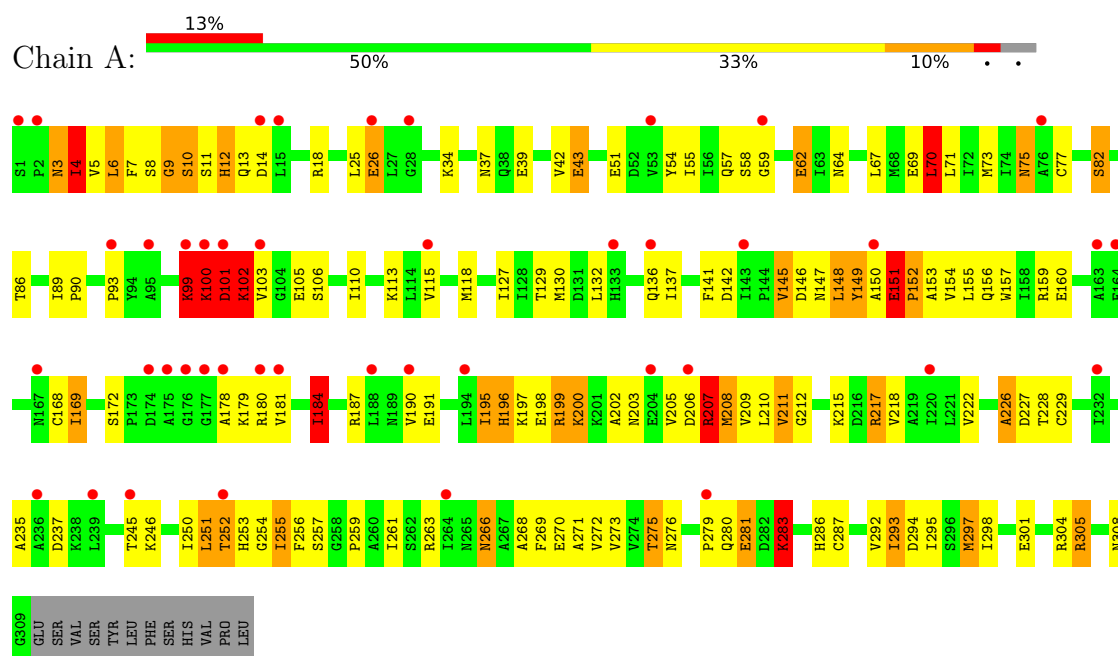
- Molecule 6 is water.

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

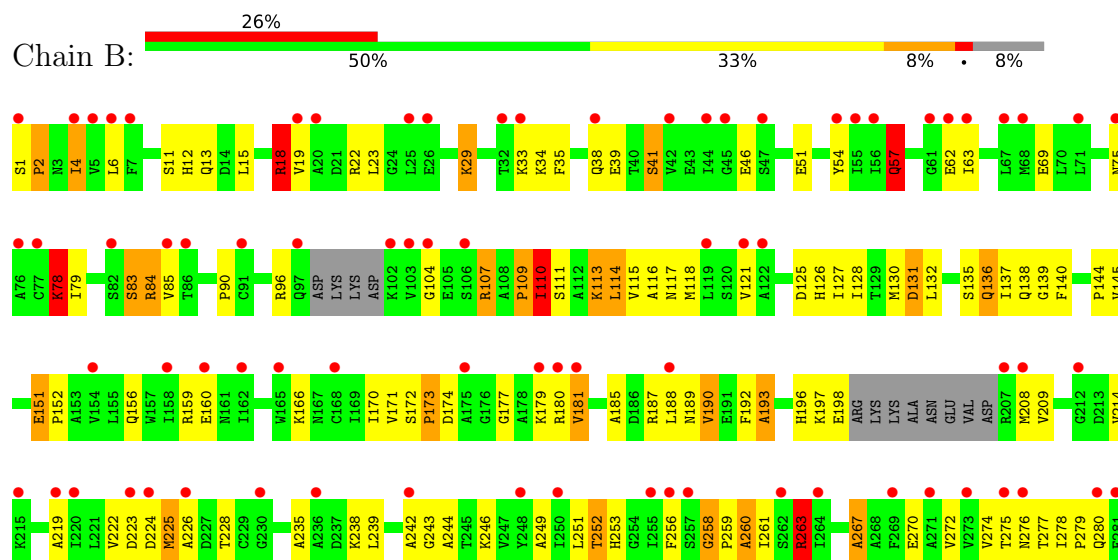
3 Residue-property plots

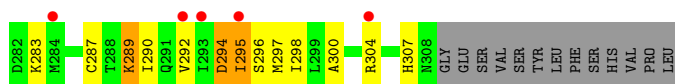
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

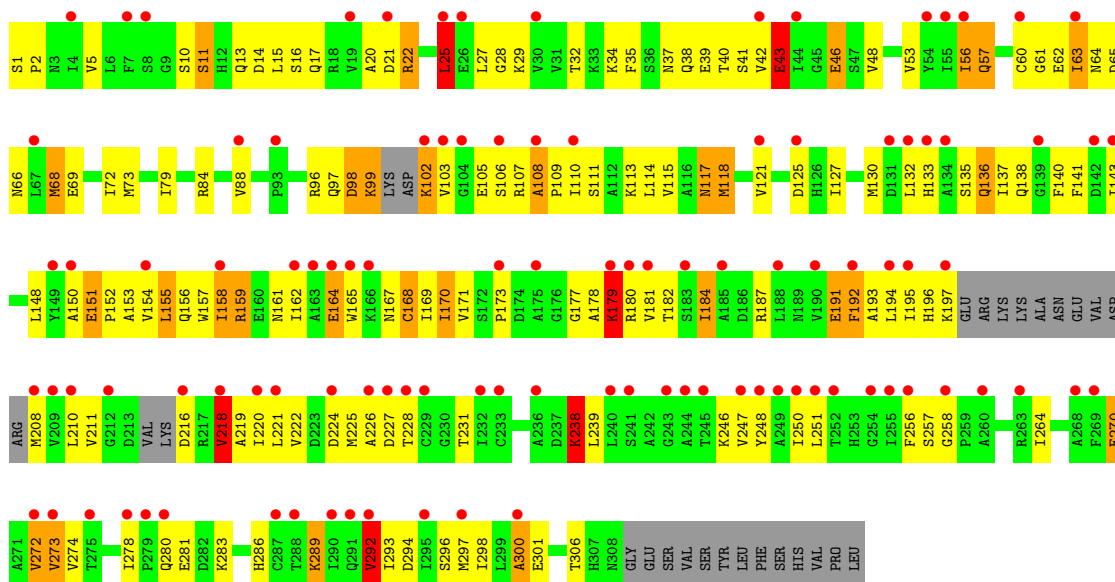


• Molecule 1: Isoform 2 of Ribose-phosphate pyrophosphokinase 2

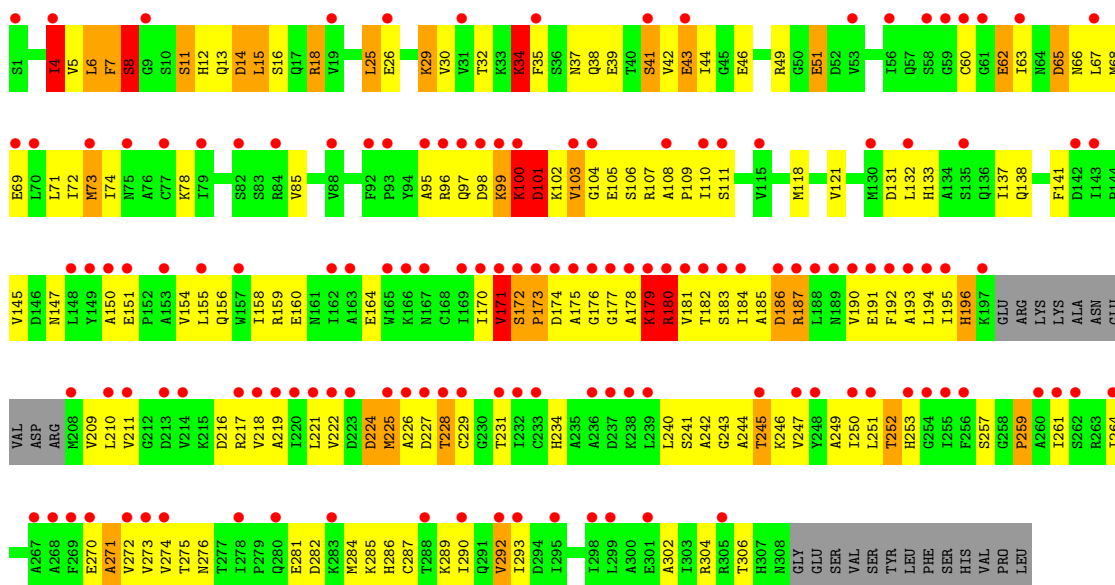




- Molecule 1: Isoform 2 of Ribose-phosphate pyrophosphokinase 2

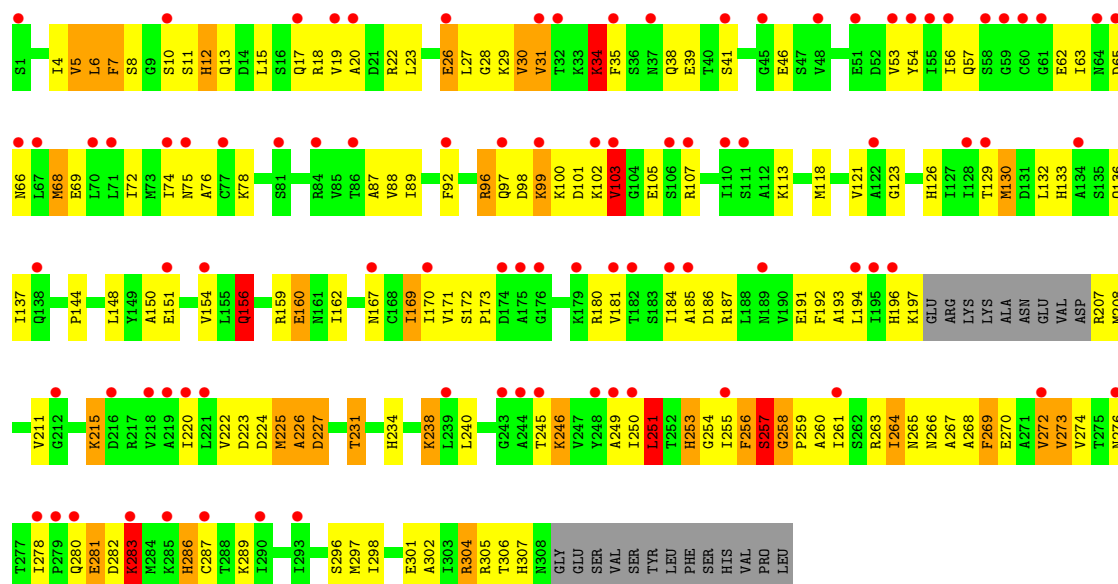


- Molecule 1: Isoform 2 of Ribose-phosphate pyrophosphokinase 2

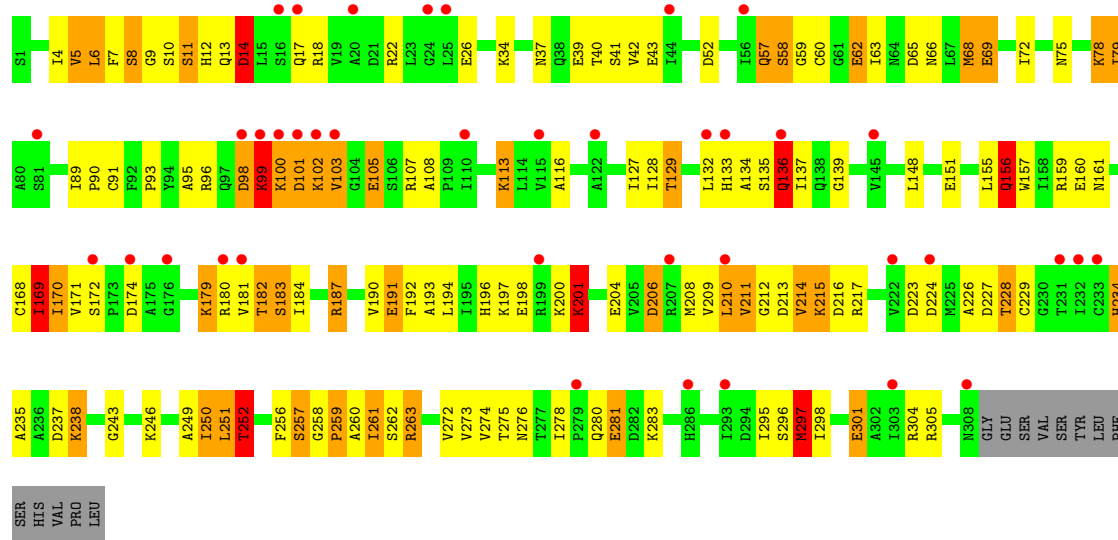


- Molecule 1: Isoform 2 of Ribose-phosphate pyrophosphokinase 2





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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	2789 reflections (4.50%)	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	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.80	84/2387 (3.5%)	1.33	27/3229 (0.8%)
1	B	1.62	41/2281 (1.8%)	1.19	19/3087 (0.6%)
1	C	1.38	20/2261 (0.9%)	1.33	33/3059 (1.1%)
1	D	1.40	33/2296 (1.4%)	1.20	20/3108 (0.6%)
1	E	1.61	51/2307 (2.2%)	1.20	20/3122 (0.6%)
1	F	1.94	100/2383 (4.2%)	1.28	32/3224 (1.0%)
All	All	1.64	329/13915 (2.4%)	1.26	151/18829 (0.8%)

All (329) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	PRO	C-O	-12.36	1.08	1.24
1	A	253	HIS	CE1-NE2	-12.09	1.20	1.32
1	B	110	ILE	C-O	-11.21	1.12	1.24
1	A	272	VAL	C-O	-11.10	1.12	1.24
1	A	195	ILE	C-O	-10.84	1.12	1.24
1	F	42	VAL	C-O	-10.59	1.12	1.24
1	F	237	ASP	C-O	-10.41	1.11	1.24
1	F	250	ILE	C-O	-10.29	1.12	1.24
1	A	6	LEU	C-O	-10.09	1.11	1.24
1	A	179	LYS	C-O	-10.01	1.12	1.24
1	F	252	THR	C-O	-9.91	1.12	1.24
1	D	5	VAL	C-O	-9.89	1.12	1.24
1	F	62	GLU	C-O	-9.75	1.11	1.23
1	F	201	LYS	N-CA	-9.64	1.34	1.45
1	F	256	PHE	C-O	-9.54	1.11	1.23
1	A	8	SER	C-O	-9.24	1.12	1.24
1	A	184	ILE	C-O	-9.23	1.13	1.24
1	C	43	GLU	C-O	-9.15	1.13	1.24
1	A	169	ILE	C-O	-9.06	1.15	1.24
1	A	70	LEU	C-O	-9.05	1.13	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	HIS	C-O	-8.97	1.13	1.24
1	D	4	ILE	C-O	-8.79	1.14	1.24
1	F	37	ASN	C-O	-8.71	1.12	1.24
1	A	151	GLU	C-O	-8.63	1.16	1.24
1	A	187	ARG	C-O	-8.59	1.13	1.24
1	F	63	ILE	C-O	-8.53	1.14	1.24
1	F	297	MET	C-O	-8.52	1.13	1.24
1	F	259	PRO	C-O	-8.50	1.15	1.23
1	F	34	LYS	C-O	-8.46	1.13	1.23
1	F	6	LEU	C-O	-8.46	1.13	1.24
1	E	223	ASP	C-O	-8.34	1.14	1.23
1	B	151	GLU	C-O	-8.32	1.16	1.24
1	F	151	GLU	C-O	-8.29	1.16	1.24
1	B	69	GLU	C-O	-8.25	1.14	1.24
1	A	196	HIS	C-O	-8.25	1.14	1.24
1	A	5	VAL	C-O	-8.24	1.15	1.24
1	D	29	LYS	C-O	-8.23	1.14	1.24
1	F	156	GLN	C-O	-8.22	1.14	1.24
1	F	228	THR	C-O	-8.21	1.13	1.24
1	A	7	PHE	C-O	-8.20	1.13	1.24
1	B	2	PRO	C-O	-8.18	1.14	1.23
1	F	68	MET	C-O	-8.15	1.14	1.24
1	E	180	ARG	N-CA	-8.14	1.36	1.46
1	E	105	GLU	C-O	-8.12	1.16	1.24
1	E	270	GLU	C-O	-8.07	1.14	1.24
1	B	128	ILE	C-O	-8.05	1.15	1.24
1	F	7	PHE	C-O	-8.04	1.13	1.24
1	F	213	ASP	C-O	-8.02	1.14	1.24
1	E	238	LYS	C-O	-8.01	1.14	1.24
1	A	12	HIS	C-O	-7.99	1.14	1.23
1	E	227	ASP	C-O	-7.98	1.14	1.24
1	A	43	GLU	C-O	-7.97	1.15	1.24
1	A	237	ASP	C-O	-7.95	1.14	1.24
1	A	211	VAL	C-O	-7.92	1.15	1.24
1	F	116	ALA	C-N	7.86	1.44	1.34
1	B	243	GLY	C-N	-7.79	1.22	1.33
1	F	190	VAL	C-O	-7.78	1.14	1.23
1	B	166	LYS	C-O	-7.74	1.14	1.24
1	F	13	GLN	CA-C	-7.74	1.42	1.52
1	F	211	VAL	C-O	-7.72	1.15	1.24
1	F	4	ILE	C-O	-7.72	1.15	1.24
1	F	57	GLN	C-O	-7.71	1.15	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	41	SER	C-O	-7.68	1.15	1.24
1	A	263	ARG	C-O	-7.67	1.15	1.24
1	D	43	GLU	C-O	-7.67	1.14	1.24
1	A	147	ASN	C-O	-7.63	1.15	1.23
1	A	305	ARG	C-O	-7.63	1.15	1.24
1	E	269	PHE	C-O	-7.63	1.14	1.24
1	B	238	LYS	C-O	-7.61	1.15	1.24
1	E	105	GLU	CA-CB	-7.61	1.43	1.53
1	A	9	GLY	C-O	-7.60	1.16	1.23
1	F	281	GLU	C-O	-7.58	1.15	1.24
1	E	8	SER	C-O	-7.55	1.14	1.24
1	F	283	LYS	C-O	-7.53	1.15	1.24
1	A	283	LYS	C-O	-7.50	1.14	1.24
1	A	8	SER	CA-C	-7.49	1.43	1.52
1	E	5	VAL	C-O	-7.46	1.16	1.24
1	C	63	ILE	CA-C	-7.43	1.43	1.52
1	F	14	ASP	C-O	-7.42	1.15	1.24
1	A	297	MET	C-O	-7.42	1.15	1.24
1	A	145	VAL	C-O	-7.41	1.16	1.24
1	F	59	GLY	C-O	-7.39	1.14	1.23
1	E	4	ILE	C-O	-7.37	1.15	1.24
1	F	234	HIS	C-O	-7.33	1.15	1.24
1	C	167	ASN	CA-C	-7.27	1.49	1.53
1	F	135	SER	C-O	-7.25	1.15	1.24
1	E	68	MET	C-O	-7.25	1.15	1.24
1	A	217	ARG	C-O	-7.25	1.14	1.23
1	F	210	LEU	C-O	-7.24	1.15	1.24
1	B	113	LYS	C-O	-7.16	1.15	1.24
1	B	57	GLN	C-O	-7.15	1.15	1.23
1	E	246	LYS	C-O	-7.11	1.15	1.23
1	F	238	LYS	C-O	-7.07	1.15	1.24
1	A	271	ALA	C-O	-7.06	1.15	1.23
1	A	212	GLY	C-O	-7.06	1.16	1.23
1	D	6	LEU	C-O	-7.03	1.15	1.24
1	E	156	GLN	C-O	-7.01	1.15	1.24
1	A	259	PRO	C-O	-6.99	1.14	1.24
1	B	18	ARG	C-O	-6.98	1.16	1.24
1	B	173	PRO	C-O	-6.96	1.14	1.24
1	F	281	GLU	N-CA	-6.96	1.38	1.46
1	C	68	MET	C-O	-6.96	1.16	1.24
1	F	301	GLU	C-O	-6.93	1.15	1.24
1	B	307	HIS	C-O	-6.93	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	7	PHE	C-O	-6.93	1.15	1.23
1	F	58	SER	CA-CB	-6.88	1.42	1.53
1	D	78	LYS	C-O	-6.86	1.16	1.24
1	F	127	ILE	C-O	-6.85	1.17	1.24
1	F	136	GLN	C-N	-6.81	1.26	1.34
1	C	159	ARG	N-CA	-6.81	1.38	1.46
1	F	68	MET	C-N	-6.80	1.24	1.33
1	A	207	ARG	C-O	-6.78	1.15	1.23
1	A	12	HIS	CA-C	-6.78	1.45	1.53
1	A	210	LEU	C-O	-6.78	1.15	1.24
1	A	253	HIS	CG-ND1	-6.77	1.30	1.38
1	F	113	LYS	C-O	-6.77	1.16	1.24
1	F	179	LYS	C-O	-6.77	1.16	1.24
1	F	214	VAL	CA-C	-6.77	1.44	1.53
1	F	261	ILE	C-O	-6.77	1.16	1.24
1	F	305	ARG	C-O	-6.75	1.16	1.24
1	B	197	LYS	C-O	-6.74	1.16	1.24
1	E	226	ALA	C-O	-6.74	1.16	1.24
1	E	253	HIS	CE1-NE2	-6.73	1.25	1.32
1	E	6	LEU	C-O	-6.71	1.16	1.24
1	F	5	VAL	C-O	-6.71	1.17	1.24
1	A	142	ASP	C-O	-6.68	1.14	1.24
1	B	246	LYS	C-O	-6.66	1.15	1.23
1	C	117	ASN	C-O	-6.66	1.16	1.24
1	E	29	LYS	C-O	-6.63	1.16	1.24
1	D	253	HIS	C-N	-6.63	1.23	1.33
1	F	258	GLY	C-O	-6.58	1.15	1.24
1	F	260	ALA	C-O	-6.58	1.16	1.24
1	F	171	VAL	C-O	-6.58	1.17	1.24
1	B	11	SER	CA-C	-6.58	1.44	1.52
1	A	4	ILE	C-O	-6.57	1.17	1.24
1	B	180	ARG	C-O	-6.57	1.16	1.24
1	A	208	MET	C-O	-6.57	1.16	1.24
1	E	304	ARG	C-O	-6.56	1.16	1.24
1	F	251	LEU	C-O	-6.53	1.15	1.24
1	D	65	ASP	C-O	-6.53	1.16	1.24
1	F	135	SER	N-CA	-6.51	1.38	1.46
1	F	169	ILE	C-O	-6.47	1.17	1.24
1	F	22	ARG	C-O	-6.45	1.16	1.24
1	C	159	ARG	C-O	-6.44	1.16	1.24
1	E	180	ARG	C-O	-6.43	1.16	1.24
1	F	246	LYS	C-O	-6.42	1.16	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	257	SER	C-O	-6.41	1.15	1.23
1	E	162	ILE	C-O	-6.40	1.17	1.24
1	F	58	SER	C-O	-6.35	1.15	1.23
1	F	234	HIS	N-CA	-6.33	1.38	1.46
1	E	31	VAL	C-O	-6.31	1.17	1.24
1	C	231	THR	N-CA	-6.30	1.39	1.46
1	F	215	LYS	C-O	-6.30	1.16	1.23
1	E	254	GLY	C-O	-6.30	1.15	1.23
1	A	202	ALA	C-N	-6.29	1.25	1.33
1	E	160	GLU	C-O	-6.29	1.15	1.24
1	B	29	LYS	N-CA	-6.28	1.38	1.46
1	A	3	ASN	C-O	-6.27	1.15	1.23
1	A	281	GLU	C-O	-6.26	1.16	1.24
1	D	15	LEU	C-O	-6.26	1.16	1.24
1	F	40	THR	C-O	-6.25	1.16	1.23
1	C	40	THR	C-O	-6.21	1.16	1.23
1	E	305	ARG	C-O	-6.18	1.16	1.24
1	A	149	TYR	C-O	-6.18	1.16	1.23
1	D	49	ARG	C-O	-6.17	1.16	1.23
1	F	13	GLN	N-CA	-6.17	1.38	1.46
1	E	231	THR	C-O	-6.15	1.17	1.24
1	A	184	ILE	N-CA	-6.13	1.39	1.46
1	A	154	VAL	C-O	-6.11	1.16	1.24
1	E	251	LEU	C-O	-6.11	1.16	1.23
1	E	215	LYS	C-O	-6.10	1.16	1.24
1	E	253	HIS	C-O	-6.09	1.16	1.24
1	D	131	ASP	C-O	-6.09	1.14	1.23
1	E	7	PHE	C-O	-6.08	1.16	1.23
1	F	187	ARG	C-O	-6.07	1.16	1.24
1	E	187	ARG	N-CA	-6.07	1.38	1.46
1	A	286	HIS	CA-CB	-6.02	1.44	1.53
1	B	263	ARG	C-O	-6.02	1.17	1.24
1	E	169	ILE	C-O	-6.02	1.17	1.23
1	F	156	GLN	CA-C	-6.01	1.45	1.52
1	F	197	LYS	C-O	-5.99	1.16	1.24
1	F	13	GLN	C-O	-5.97	1.16	1.24
1	B	11	SER	C-O	-5.96	1.17	1.24
1	B	193	ALA	CA-C	-5.96	1.45	1.52
1	C	15	LEU	C-O	-5.94	1.17	1.24
1	A	11	SER	N-CA	-5.91	1.39	1.46
1	B	187	ARG	CA-CB	-5.87	1.43	1.53
1	B	289	LYS	C-O	-5.87	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	10	SER	C-O	-5.87	1.17	1.24
1	A	187	ARG	N-CA	-5.86	1.39	1.46
1	B	196	HIS	C-O	-5.85	1.16	1.23
1	F	129	THR	C-O	-5.84	1.17	1.24
1	F	206	ASP	C-O	-5.83	1.17	1.24
1	F	41	SER	CA-C	-5.83	1.45	1.52
1	E	13	GLN	CA-C	-5.82	1.45	1.52
1	B	29	LYS	C-O	-5.82	1.17	1.24
1	E	34	LYS	N-CA	-5.81	1.39	1.46
1	A	13	GLN	CA-C	-5.80	1.45	1.52
1	D	304	ARG	C-O	-5.80	1.17	1.24
1	A	294	ASP	C-O	-5.79	1.17	1.24
1	A	102	LYS	C-O	-5.79	1.16	1.24
1	A	271	ALA	CA-C	-5.79	1.45	1.52
1	E	224	ASP	C-O	-5.78	1.17	1.24
1	F	136	GLN	C-O	-5.76	1.16	1.24
1	A	150	ALA	C-O	-5.76	1.16	1.24
1	A	69	GLU	C-O	-5.76	1.17	1.24
1	F	78	LYS	C-O	-5.75	1.17	1.24
1	F	11	SER	C-O	-5.74	1.17	1.24
1	A	10	SER	C-O	-5.74	1.16	1.24
1	D	25	LEU	C-O	-5.73	1.16	1.23
1	D	62	GLU	C-O	-5.73	1.17	1.24
1	B	189	ASN	C-O	-5.72	1.16	1.23
1	B	174	ASP	CA-CB	5.72	1.61	1.53
1	A	203	ASN	C-N	-5.71	1.25	1.33
1	F	52	ASP	C-O	-5.71	1.17	1.23
1	A	142	ASP	CA-C	-5.71	1.45	1.52
1	D	29	LYS	CA-C	-5.69	1.45	1.52
1	A	270	GLU	C-O	-5.68	1.17	1.24
1	C	238	LYS	C-O	-5.68	1.17	1.24
1	F	297	MET	N-CA	-5.67	1.39	1.46
1	A	283	LYS	CA-C	-5.67	1.44	1.52
1	F	159	ARG	C-O	-5.67	1.17	1.24
1	C	156	GLN	C-O	-5.66	1.17	1.24
1	A	286	HIS	C-O	-5.66	1.16	1.24
1	F	43	GLU	C-O	-5.65	1.17	1.24
1	A	215	LYS	C-O	-5.64	1.17	1.24
1	A	11	SER	CA-C	-5.63	1.45	1.52
1	F	63	ILE	CA-C	-5.63	1.46	1.52
1	D	51	GLU	C-O	-5.62	1.16	1.23
1	E	69	GLU	CA-C	-5.62	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	LEU	C-O	-5.60	1.16	1.23
1	A	197	LYS	C-O	-5.57	1.17	1.23
1	B	15	LEU	C-O	-5.57	1.17	1.24
1	F	105	GLU	C-O	-5.57	1.17	1.23
1	D	51	GLU	CA-C	-5.57	1.46	1.52
1	F	128	ILE	C-O	-5.56	1.18	1.24
1	A	226	ALA	N-CA	-5.54	1.39	1.46
1	D	281	GLU	C-O	-5.54	1.17	1.24
1	F	216	ASP	CA-C	-5.54	1.45	1.53
1	F	11	SER	CA-C	-5.54	1.45	1.52
1	B	41	SER	C-O	-5.53	1.17	1.23
1	E	68	MET	N-CA	-5.53	1.39	1.46
1	A	269	PHE	C-O	-5.52	1.17	1.23
1	A	268	ALA	C-O	-5.52	1.16	1.24
1	F	170	ILE	C-O	-5.52	1.17	1.24
1	E	5	VAL	CA-CB	-5.50	1.47	1.54
1	E	105	GLU	CA-C	-5.50	1.46	1.53
1	F	7	PHE	CA-C	-5.49	1.46	1.52
1	A	64	ASN	C-O	-5.49	1.17	1.24
1	B	110	ILE	N-CA	-5.49	1.39	1.46
1	F	223	ASP	C-O	-5.48	1.17	1.23
1	A	184	ILE	CA-CB	-5.47	1.47	1.54
1	D	34	LYS	C-O	-5.47	1.17	1.24
1	D	5	VAL	CA-CB	-5.46	1.47	1.54
1	F	281	GLU	CA-C	-5.46	1.45	1.52
1	E	266	ASN	C-O	-5.45	1.17	1.24
1	D	259	PRO	C-O	-5.44	1.16	1.24
1	F	212	GLY	C-O	-5.43	1.18	1.23
1	D	224	ASP	C-O	-5.43	1.17	1.24
1	A	179	LYS	C-N	-5.41	1.27	1.33
1	B	84	ARG	C-O	-5.41	1.17	1.23
1	A	255	ILE	C-O	-5.40	1.18	1.24
1	F	8	SER	C-O	-5.40	1.17	1.24
1	E	159	ARG	N-CA	-5.38	1.39	1.46
1	F	4	ILE	N-CA	-5.37	1.39	1.46
1	F	9	GLY	C-O	-5.37	1.17	1.23
1	A	292	VAL	C-O	-5.37	1.18	1.24
1	B	13	GLN	C-O	-5.37	1.17	1.24
1	D	171	VAL	N-CA	5.37	1.52	1.46
1	B	238	LYS	CA-C	-5.35	1.46	1.52
1	A	266	ASN	C-O	-5.32	1.16	1.24
1	B	69	GLU	CA-C	-5.30	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	62	GLU	CD-OE1	-5.29	1.15	1.25
1	F	12	HIS	C-O	-5.27	1.16	1.23
1	C	10	SER	N-CA	-5.26	1.39	1.46
1	F	237	ASP	N-CA	-5.24	1.40	1.46
1	E	27	LEU	N-CA	-5.24	1.38	1.45
1	F	8	SER	CA-CB	-5.24	1.45	1.53
1	C	118	MET	C-O	-5.24	1.17	1.24
1	F	39	GLU	C-O	-5.24	1.17	1.23
1	D	65	ASP	N-CA	-5.23	1.40	1.46
1	C	29	LYS	C-O	-5.22	1.17	1.24
1	A	11	SER	C-O	-5.21	1.18	1.24
1	A	13	GLN	CA-CB	-5.21	1.45	1.53
1	F	95	ALA	C-N	-5.21	1.26	1.33
1	A	62	GLU	C-O	-5.21	1.17	1.24
1	F	26	GLU	C-O	-5.21	1.17	1.23
1	E	234	HIS	C-O	-5.20	1.18	1.24
1	B	294	ASP	C-O	-5.19	1.17	1.24
1	D	46	GLU	C-O	-5.19	1.17	1.23
1	C	16	SER	CA-C	-5.19	1.46	1.52
1	F	69	GLU	C-O	-5.17	1.18	1.24
1	A	179	LYS	CA-C	-5.17	1.46	1.52
1	E	160	GLU	N-CA	-5.17	1.39	1.46
1	A	13	GLN	C-O	-5.16	1.18	1.24
1	A	281	GLU	N-CA	-5.16	1.40	1.46
1	F	262	SER	CA-C	-5.16	1.46	1.52
1	E	29	LYS	N-CA	-5.15	1.39	1.46
1	B	223	ASP	C-O	-5.15	1.19	1.24
1	B	110	ILE	CA-C	-5.14	1.46	1.53
1	C	22	ARG	C-O	-5.14	1.17	1.24
1	D	4	ILE	CA-C	-5.14	1.46	1.52
1	F	174	ASP	C-O	-5.14	1.17	1.23
1	F	192	PHE	CA-C	-5.13	1.46	1.52
1	C	14	ASP	C-O	-5.13	1.18	1.24
1	E	304	ARG	CA-C	-5.12	1.46	1.52
1	B	110	ILE	CA-CB	-5.11	1.48	1.54
1	D	95	ALA	C-O	-5.10	1.18	1.24
1	B	242	ALA	C-N	5.10	1.41	1.33
1	E	173	PRO	C-N	-5.10	1.27	1.33
1	F	262	SER	C-O	-5.09	1.18	1.24
1	B	78	LYS	C-O	-5.09	1.18	1.24
1	C	108	ALA	C-N	-5.08	1.22	1.33
1	E	12	HIS	CA-C	-5.08	1.47	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	193	ALA	C-O	-5.08	1.17	1.23
1	D	196	HIS	C-O	-5.08	1.17	1.23
1	D	8	SER	C-O	-5.07	1.17	1.23
1	A	245	THR	C-N	-5.07	1.27	1.33
1	C	56	ILE	C-O	-5.07	1.18	1.24
1	A	253	HIS	CD2-NE2	-5.05	1.32	1.37
1	A	257	SER	C-O	-5.05	1.17	1.23
1	D	43	GLU	N-CA	-5.05	1.40	1.46
1	E	301	GLU	C-O	-5.04	1.18	1.24
1	D	29	LYS	N-CA	-5.04	1.40	1.46
1	E	26	GLU	C-N	-5.04	1.26	1.33
1	D	172	SER	N-CA	5.03	1.49	1.46
1	A	184	ILE	CA-C	-5.03	1.46	1.52
1	A	253	HIS	ND1-CE1	-5.02	1.27	1.32
1	E	103	VAL	C-O	-5.01	1.18	1.24

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	SER	N-CA-C	12.04	124.48	111.36
1	E	11	SER	N-CA-C	11.79	124.13	111.28
1	A	199	ARG	CA-C-N	-11.65	104.47	120.90
1	A	199	ARG	C-N-CA	-11.65	104.47	120.90
1	C	258	GLY	CA-C-N	11.33	131.00	119.56
1	C	258	GLY	C-N-CA	11.33	131.00	119.56
1	D	224	ASP	N-CA-C	10.95	122.97	111.14
1	F	11	SER	N-CA-C	10.50	122.31	111.07
1	A	101	ASP	CA-C-N	-10.49	101.50	121.54
1	A	101	ASP	C-N-CA	-10.49	101.50	121.54
1	B	63	ILE	N-CA-C	10.40	121.28	110.36
1	F	102	LYS	CA-C-N	-9.72	105.75	120.82
1	F	102	LYS	C-N-CA	-9.72	105.75	120.82
1	A	13	GLN	N-CA-C	9.43	121.63	111.36
1	C	300	ALA	CA-C-N	9.06	133.15	120.29
1	C	300	ALA	C-N-CA	9.06	133.15	120.29
1	A	200	LYS	N-CA-C	9.00	122.93	110.24
1	C	270	GLU	N-CA-C	-8.13	102.36	111.14
1	A	197	LYS	CB-CA-C	-8.10	95.84	109.53
1	A	102	LYS	CA-C-N	8.07	131.31	120.50
1	A	102	LYS	C-N-CA	8.07	131.31	120.50
1	A	101	ASP	CA-CB-CG	7.88	120.48	112.60
1	A	229	CYS	N-CA-C	7.85	122.44	112.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	ALA	N-CA-C	7.66	119.41	111.14
1	F	99	LYS	CA-C-N	7.62	132.94	122.19
1	F	99	LYS	C-N-CA	7.62	132.94	122.19
1	D	292	VAL	N-CA-C	7.52	118.64	108.11
1	A	153	ALA	CA-C-N	7.50	131.07	120.42
1	A	153	ALA	C-N-CA	7.50	131.07	120.42
1	D	11	SER	N-CA-C	7.49	119.08	111.07
1	D	100	LYS	N-CA-C	7.44	120.66	108.08
1	B	116	ALA	O-C-N	7.40	129.97	122.12
1	B	11	SER	N-CA-C	7.32	119.05	111.14
1	C	167	ASN	N-CA-C	-7.23	102.85	108.78
1	F	192	PHE	N-CA-C	7.00	119.13	109.18
1	C	224	ASP	N-CA-C	6.92	118.61	111.14
1	D	171	VAL	N-CA-C	6.92	119.16	108.44
1	C	14	ASP	N-CA-C	6.91	118.81	111.28
1	A	305	ARG	CB-CA-C	-6.91	99.32	110.79
1	C	98	ASP	CB-CA-C	6.87	120.36	111.50
1	F	101	ASP	CA-C-N	6.86	133.82	121.89
1	F	101	ASP	C-N-CA	6.86	133.82	121.89
1	F	100	LYS	CA-C-N	6.83	134.59	121.54
1	F	100	LYS	C-N-CA	6.83	134.59	121.54
1	A	305	ARG	CG-CD-NE	6.78	126.92	112.00
1	A	62	GLU	N-CA-C	-6.76	97.53	108.41
1	B	173	PRO	CB-CA-C	-6.75	101.76	111.62
1	D	102	LYS	CA-C-N	-6.74	113.94	122.37
1	D	102	LYS	C-N-CA	-6.74	113.94	122.37
1	C	63	ILE	CA-C-N	-6.74	110.55	120.38
1	C	63	ILE	C-N-CA	-6.74	110.55	120.38
1	A	254	GLY	CA-C-N	6.71	129.14	120.56
1	A	254	GLY	C-N-CA	6.71	129.14	120.56
1	C	218	VAL	CB-CA-C	-6.67	104.03	111.23
1	B	270	GLU	N-CA-C	-6.66	103.95	111.14
1	C	292	VAL	N-CA-C	6.64	117.41	108.11
1	B	173	PRO	N-CA-CB	-6.57	97.28	103.52
1	B	104	GLY	N-CA-C	6.51	122.83	115.08
1	C	192	PHE	N-CA-C	6.50	119.29	109.41
1	F	260	ALA	N-CA-C	6.50	118.37	111.28
1	C	179	LYS	N-CA-C	-6.47	104.23	111.28
1	A	146	ASP	CB-CA-C	-6.42	99.66	110.19
1	F	68	MET	CA-C-O	6.38	127.18	120.42
1	C	151	GLU	CA-C-N	-6.36	111.99	119.05
1	C	151	GLU	C-N-CA	-6.36	111.99	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	103	VAL	N-CA-C	6.35	117.86	110.62
1	D	102	LYS	N-CA-C	-6.35	101.02	110.23
1	E	100	LYS	N-CA-C	-6.33	95.98	107.75
1	F	252	THR	CB-CA-C	6.25	121.48	110.85
1	F	191	GLU	N-CA-C	6.18	119.56	110.59
1	F	62	GLU	CA-C-N	6.17	128.34	120.56
1	F	62	GLU	C-N-CA	6.17	128.34	120.56
1	E	273	VAL	N-CA-C	6.16	116.80	108.17
1	B	258	GLY	N-CA-C	6.13	124.85	112.34
1	F	211	VAL	N-CA-CB	-6.12	103.75	111.46
1	F	63	ILE	N-CA-C	6.08	116.26	110.42
1	E	269	PHE	CA-C-N	6.06	130.94	120.58
1	E	269	PHE	C-N-CA	6.06	130.94	120.58
1	B	131	ASP	N-CA-C	6.05	119.59	111.24
1	F	10	SER	N-CA-C	6.05	117.88	111.28
1	E	260	ALA	N-CA-C	6.01	117.50	111.07
1	E	256	PHE	CA-C-O	-6.00	114.69	122.14
1	C	98	ASP	CA-CB-CG	5.99	118.59	112.60
1	C	289	LYS	N-CA-C	5.97	117.87	111.36
1	C	158	ILE	CB-CA-C	-5.94	104.37	111.97
1	C	130	MET	N-CA-C	5.92	118.77	108.76
1	D	187	ARG	N-CA-C	-5.85	106.11	113.18
1	F	100	LYS	O-C-N	5.82	130.21	122.41
1	F	103	VAL	CA-C-O	-5.82	113.81	119.92
1	F	6	LEU	N-CA-CB	-5.81	100.92	110.68
1	A	252	THR	CB-CA-C	-5.78	98.59	110.38
1	D	101	ASP	N-CA-C	5.72	120.05	111.81
1	A	207	ARG	N-CA-C	5.71	118.77	109.06
1	C	164	GLU	CA-C-N	-5.71	112.63	120.28
1	C	164	GLU	C-N-CA	-5.71	112.63	120.28
1	C	286	HIS	CB-CA-C	-5.70	100.55	110.17
1	E	246	LYS	N-CA-C	5.68	118.04	109.23
1	D	234	HIS	N-CA-C	-5.66	105.11	111.28
1	C	40	THR	N-CA-CB	-5.63	101.07	109.69
1	E	101	ASP	N-CA-C	5.62	117.89	108.73
1	F	168	CYS	CA-C-N	-5.62	115.19	122.99
1	F	168	CYS	C-N-CA	-5.62	115.19	122.99
1	B	267	ALA	N-CA-C	5.55	118.70	110.48
1	A	292	VAL	N-CA-C	5.54	116.45	108.48
1	E	265	ASN	N-CA-C	-5.53	105.25	111.28
1	E	227	ASP	CA-C-O	-5.52	116.62	119.77
1	F	261	ILE	CA-C-N	5.46	127.59	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	261	ILE	C-N-CA	5.46	127.59	120.28
1	E	105	GLU	N-CA-C	5.46	115.44	108.24
1	C	60	CYS	N-CA-C	5.42	122.36	110.80
1	C	158	ILE	CA-C-N	-5.42	113.39	120.44
1	C	158	ILE	C-N-CA	-5.42	113.39	120.44
1	D	179	LYS	N-CA-C	-5.42	99.25	110.80
1	E	207	ARG	CA-C-N	-5.38	115.29	122.72
1	E	207	ARG	C-N-CA	-5.38	115.29	122.72
1	E	283	LYS	CA-C-O	5.37	125.27	119.15
1	B	109	PRO	N-CA-C	-5.35	101.45	112.47
1	C	173	PRO	N-CA-CB	-5.35	97.84	103.19
1	E	226	ALA	N-CA-CB	-5.32	102.42	110.77
1	B	116	ALA	CA-C-N	-5.29	112.26	120.31
1	B	116	ALA	C-N-CA	-5.29	112.26	120.31
1	E	156	GLN	CB-CA-C	5.29	119.84	110.85
1	C	25	LEU	N-CA-C	5.22	117.12	109.24
1	D	180	ARG	CA-C-N	5.19	127.10	120.56
1	D	180	ARG	C-N-CA	5.19	127.10	120.56
1	B	243	GLY	O-C-N	-5.17	115.98	122.70
1	A	154	VAL	CA-CB-CG1	5.17	119.19	110.40
1	F	100	LYS	CA-C-O	-5.16	115.14	121.28
1	E	10	SER	N-CA-C	5.13	116.87	111.28
1	A	280	GLN	CA-C-N	-5.13	113.41	120.28
1	A	280	GLN	C-N-CA	-5.13	113.41	120.28
1	A	297	MET	N-CA-CB	5.11	117.72	110.16
1	A	199	ARG	CB-CA-C	-5.10	101.92	110.29
1	F	4	ILE	CB-CA-C	-5.09	103.52	110.96
1	D	62	GLU	N-CA-C	-5.08	99.50	108.20
1	F	301	GLU	N-CA-C	5.08	116.90	111.36
1	F	98	ASP	O-C-N	-5.07	116.42	122.46
1	D	111	SER	N-CA-C	5.06	116.88	111.36
1	D	245	THR	CB-CA-C	-5.06	102.94	110.88
1	B	242	ALA	O-C-N	5.06	129.35	122.37
1	B	63	ILE	CB-CA-C	-5.05	105.41	111.88
1	C	273	VAL	N-CA-C	5.05	115.58	108.36
1	F	98	ASP	CA-C-N	-5.05	110.90	121.80
1	F	98	ASP	C-N-CA	-5.05	110.90	121.80
1	D	100	LYS	CB-CA-C	-5.04	110.78	116.63
1	D	131	ASP	CA-CB-CG	-5.03	107.57	112.60
1	E	257	SER	CB-CA-C	-5.03	101.97	113.33
1	B	193	ALA	CA-C-N	-5.02	114.60	122.73
1	B	193	ALA	C-N-CA	-5.02	114.60	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	14	ASP	N-CA-C	5.01	116.43	111.07
1	C	118	MET	CA-C-O	-5.00	115.12	120.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2355	0	2403	89	0
1	B	2251	0	2293	119	0
1	C	2232	0	2270	176	0
1	D	2265	0	2309	187	0
1	E	2276	0	2325	149	0
1	F	2351	0	2401	97	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	15	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	14085	780	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 28.

All (780) 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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:96:ARG:NE	1:C:225:MET:HE1	1.75	1.00
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:A:101:ASP:O	1:A:102:LYS:C	1.96	0.97
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: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:D:96:ARG:NE	1:D:225:MET:SD	2.42	0.91
1:D:171:VAL:HG13	1:D:193:ALA:C	1.95	0.91
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:PHE:HB3	1:C:143:ILE:HG22	1.54	0.89
1:B:34:LYS:HE2	1:B:38:GLN:C	1.98	0.88
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:B:96:ARG:HD3	1:B:225:MET:HE1	1.57	0.87
1:E:99:LYS:H	2:E:1001:APC:H3'	1.40	0.87
1:C:102:LYS:HG2	1:C:103:VAL:N	1.84	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:F:208:MET:HE1	1:F:235:ALA:HA	1.58	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: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: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:C:96:ARG:CD	1:C:225:MET:HE1	2.09	0.83
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: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:A:169:ILE:HD11	1:A:217:ARG:HD3	1.61	0.81
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:B:294:ASP:CG	1:B:296:SER:HG	1.89	0.80
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:171:VAL:CG1	1:D:193:ALA:C	2.55	0.80
1:E:297:MET:HE1	1:E:304:ARG:HH22	1.46	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: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: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:E:281:GLU:N	1:E:281:GLU:CD	2.43	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
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:C:96:ARG:CZ	1:C:225:MET:HE3	2.16	0.74
1:D:42:VAL:O	1:D:43:GLU:HG2	1.87	0.74
1:E:130:MET:HE1	1:E:150:ALA:HB2	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:178:ALA:C	1:D:180:ARG:H	1.96	0.72
1:D:63:ILE:CD1	1:E:39:GLU:HG3	2.19	0.72
1:A:115:VAL:HA	1:A:118:MET:HE2	1.71	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: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:F:208:MET:HE1	1:F:235:ALA:CA	2.21	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:E:68:MET:HE3	1:E:72:ILE:HD11	1.74	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
1:C:22:ARG:NE	1:C:296:SER:HB2	2.06	0.69
1:B:208:MET:HE1	1:B:235:ALA:HA	1.74	0.69
1:C:196:HIS:HE1	1:D:186:ASP:OD2	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:68:MET:HE3	1:F:72:ILE:HG13	1.75	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: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:125:ASP:C	1:C:143:ILE:HD11	2.20	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: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
1:D:178:ALA:C	1:D:180:ARG:N	2.47	0.65
1:A:77:CYS:O	1:A:82:SER:OG	2.13	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:68:MET:HE3	1:F:72:ILE:CG1	2.28	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:B:159:ARG:NH2	6:B:2103:HOH:O	2.31	0.62
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:PHE:CD2	2:C:1002:APC:C6	2.83	0.62
1:B:118:MET:HE1	1:C:68:MET:HE1	1.82	0.62
1:D:173:PRO:CB	1:D:231:THR:HG22	2.23	0.62
1:B:256:PHE:HB3	1:B:283:LYS:HE2	1.80	0.61
1:C:63:ILE:O	1:C:64:ASN:C	2.38	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
1:E:34:LYS:HZ3	1:E:38:GLN:HE21	1.50	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
1:E:297:MET:HE1	1:E:304:ARG:NH2	2.16	0.59

Continued on next page...

Continued from previous page...

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: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:F:297:MET:HE2	1:F:298:ILE:HG13	1.84	0.59
1:B:274:VAL:O	1:B:292:VAL:HA	2.02	0.59
1:C:32:THR:HG21	1:C:69:GLU:CD	2.26	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:42:VAL:C	1:D:43:GLU:HG2	2.26	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:A:208:MET:HE1	1:A:235:ALA:HA	1.85	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:F:208:MET:HE1	1:F:235:ALA:N	2.20	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:GLN:O	1:E:281:GLU:C	2.48	0.57
1:C:171:VAL:O	1:C:221:LEU:HA	2.05	0.57
1:C:157:TRP:CH2	1:C:273:VAL:HG21	2.40	0.56
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:B:151:GLU:O	1:B:152:PRO:C	2.44	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:257:SER:O	1:E:258:GLY:C	2.48	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:210:LEU:HB2	1:F:238:LYS:HE3	1.89	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:D:62:GLU:O	1:D:62:GLU:HG3	2.05	0.53
1:E:68:MET:CE	1:E:72:ILE:HD11	2.37	0.53
1:E:98:ASP:HA	2:E:1001:APC:HO2'	1.73	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:D:240:LEU:O	1:D:241:SER:C	2.50	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:C:107:ARG:O	1:C:108:ALA:C	2.52	0.53
1:C:158:ILE:O	1:C:159:ARG:C	2.45	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:E:68:MET:HE3	1:E:72:ILE:CD1	2.38	0.52
1:D:217:ARG:O	1:D:244:ALA:CA	2.58	0.52
1:A:199:ARG:O	1:A:200:LYS:C	2.48	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:151:GLU:O	1:C:152:PRO:C	2.49	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: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:96:ARG:HH22	1:F:227:ASP:CG	2.06	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:B:115:VAL:HA	1:B:118:MET:HE2	1.94	0.50
1:C:62:GLU:CG	1:C:65:ASP:CG	2.84	0.50
1:E:286:HIS:ND1	1:E:286:HIS:N	2.59	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HD23	1:A:70:LEU:C	2.36	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: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: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:A:70:LEU:C	1:A:70:LEU:CD2	2.85	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: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:A:195:ILE:CG2	1:A:208:MET:HE3	2.43	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:30:VAL:HG11	1:D:73:MET:HE3	1.93	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:C:169:ILE:CD1	1:C:191:GLU:C	2.86	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:F:11:SER:OG	1:F:57:GLN:OE1	2.25	0.48
1:C:157:TRP:CZ2	1:C:273:VAL:HG21	2.49	0.48
1:C:96:ARG:CG	1:C:225:MET:HE1	2.44	0.47
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:192:PHE:CD1	1:D:192:PHE:C	2.92	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:C:197:LYS:HD3	1:C:197:LYS:C	2.40	0.47
1:D:99:LYS:HB2	1:D:107:ARG:HD2	1.97	0.47
1:D:240:LEU:C	1:D:242:ALA:N	2.69	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:A:75:ASN:HD22	1:A:75:ASN:C	2.22	0.46
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:159:ARG:HA	1:C:165:TRP:CD1	2.51	0.46
1:D:97:GLN:CG	1:D:98:ASP:N	2.79	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
1:C:62:GLU:HG3	1:C:65:ASP:CG	2.40	0.46
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:A:195:ILE:HG23	1:A:208:MET:HE3	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: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:181:VAL:HG23	1:C:182:THR:H	1.81	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:208:MET:HE3	1:E:208:MET:HB2	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:118:MET:HE3	1:E:118:MET:SD	2.57	0.45
1:E:54:TYR:OH	1:E:307:HIS:HB2	2.16	0.45
1:E:238:LYS:O	1:E:238:LYS:HG3	2.15	0.45
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:E:130:MET:HB3	1:E:130:MET:HE2	1.49	0.44
1:E:136:GLN:CD	1:E:136:GLN:H	2.24	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
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:C:178:ALA:O	1:C:179:LYS:C	2.59	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:E:249:ALA:HB3	1:E:272:VAL:HG22	1.99	0.44
1:D:39:GLU:CD	2:E:1001:APC:HN62	2.19	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:C:136:GLN:H	1:C:136:GLN:CD	2.25	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:E:281:GLU:CD	1:E:281:GLU:H	2.14	0.43
1:F:208:MET:HE1	1:F:234:HIS:C	2.43	0.43
1:B:225:MET:HB3	1:B:253:HIS:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:37:ASN:HD21	1:A:39:GLU:CD	2.26	0.43
1:A:130:MET:HE1	1:A:295:ILE:HB	2.01	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
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:C:164:GLU:O	1:C:165:TRP:C	2.60	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:171:VAL:C	1:E:181:VAL:HG21	2.44	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:F:297:MET:HE2	1:F:298:ILE:CG1	2.49	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: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
1:F:68:MET:HE3	1:F:72:ILE:CD1	2.49	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:D:158:ILE:O	1:D:159:ARG:C	2.61	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: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:C:280:GLN:O	1:C:281:GLU:C	2.62	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:F:134:ALA:HB1	1:F:136:GLN:NE2	2.35	0.41
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:F:68:MET:CE	1:F:72:ILE:HD11	2.51	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: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:74:ILE:C	1:E:76:ALA:H	2.28	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:E:225:MET:HE3	1:E:225:MET:HB3	1.51	0.40
1:F:68:MET:HE3	1:F:72:ILE:HD11	2.02	0.40
1:B:275:THR:HG22	1:B:295:ILE:CG1	2.50	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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%)	12	22
1	B	290/321 (90%)	279 (96%)	11 (4%)	0	100	100
1	C	286/321 (89%)	264 (92%)	21 (7%)	1 (0%)	36	54
1	D	294/321 (92%)	275 (94%)	14 (5%)	5 (2%)	7	12
1	E	295/321 (92%)	274 (93%)	20 (7%)	1 (0%)	36	54
1	F	306/321 (95%)	287 (94%)	18 (6%)	1 (0%)	36	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1778/1926 (92%)	1666 (94%)	101 (6%)	11 (1%)	21	36

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%)	233 (90%)	26 (10%)	7	14
1	B	248/271 (92%)	230 (93%)	18 (7%)	13	24
1	C	246/271 (91%)	222 (90%)	24 (10%)	7	14
1	D	250/271 (92%)	227 (91%)	23 (9%)	8	16
1	E	251/271 (93%)	225 (90%)	26 (10%)	7	13
1	F	259/271 (96%)	237 (92%)	22 (8%)	10	18
All	All	1513/1626 (93%)	1374 (91%)	139 (9%)	8	16

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	25	LEU
1	A	26	GLU
1	A	34	LYS
1	A	43	GLU
1	A	62	GLU
1	A	70	LEU
1	A	75	ASN
1	A	82	SER
1	A	99	LYS
1	A	100	LYS
1	A	101	ASP
1	A	102	LYS
1	A	151	GLU
1	A	184	ILE
1	A	207	ARG
1	A	209	VAL
1	A	211	VAL
1	A	228	THR
1	A	251	LEU
1	A	275	THR
1	A	281	GLU
1	A	283	LYS
1	A	293	ILE
1	A	297	MET
1	A	305	ARG
1	B	4	ILE
1	B	18	ARG
1	B	57	GLN
1	B	62	GLU
1	B	78	LYS
1	B	83	SER
1	B	107	ARG
1	B	110	ILE
1	B	114	LEU
1	B	130	MET
1	B	136	GLN
1	B	181	VAL
1	B	190	VAL
1	B	225	MET
1	B	228	THR
1	B	252	THR
1	B	263	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	295	ILE
1	C	11	SER
1	C	13	GLN
1	C	25	LEU
1	C	43	GLU
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	136	GLN
1	C	155	LEU
1	C	168	CYS
1	C	170	ILE
1	C	179	LYS
1	C	184	ILE
1	C	191	GLU
1	C	216	ASP
1	C	218	VAL
1	C	228	THR
1	C	238	LYS
1	C	272	VAL
1	C	292	VAL
1	D	4	ILE
1	D	8	SER
1	D	18	ARG
1	D	25	LEU
1	D	26	GLU
1	D	29	LYS
1	D	34	LYS
1	D	41	SER
1	D	51	GLU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	186	ASP
1	D	225	MET
1	D	228	THR
1	D	252	THR
1	D	259	PRO
1	D	292	VAL
1	E	26	GLU
1	E	30	VAL
1	E	31	VAL
1	E	34	LYS
1	E	96	ARG
1	E	97	GLN
1	E	99	LYS
1	E	102	LYS
1	E	103	VAL
1	E	107	ARG
1	E	130	MET
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	272	VAL
1	E	278	ILE
1	E	281	GLU
1	E	283	LYS
1	E	286	HIS
1	F	5	VAL
1	F	6	LEU
1	F	8	SER
1	F	14	ASP
1	F	79	ILE
1	F	99	LYS
1	F	100	LYS
1	F	103	VAL
1	F	136	GLN
1	F	156	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	169	ILE
1	F	182	THR
1	F	183	SER
1	F	191	GLU
1	F	201	LYS
1	F	252	THR
1	F	257	SER
1	F	261	ILE
1	F	263	ARG
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 (30) 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	161	ASN
1	B	189	ASN
1	C	13	GLN
1	C	38	GLN
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	138	GLN
1	D	286	HIS
1	E	38	GLN
1	E	66	ASN
1	E	138	GLN
1	E	156	GLN
1	E	189	ASN
1	E	280	GLN
1	F	38	GLN
1	F	64	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	75	ASN
1	F	136	GLN
1	F	161	ASN
1	F	234	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	D	1004	-	4,4,4	1.78	1 (25%)	6,6,6	1.39	1 (16%)
3	HSX	B	2001	-	14,14,14	1.37	2 (14%)	19,21,21	1.05	1 (5%)
3	HSX	E	1002	-	14,14,14	1.41	2 (14%)	19,21,21	1.91	9 (47%)
3	HSX	A	1002	-	14,14,14	2.05	8 (57%)	19,21,21	3.07	12 (63%)
2	APC	E	1001	-	29,33,33	1.06	3 (10%)	44,52,52	0.90	1 (2%)
5	PO4	F	2003	-	4,4,4	3.38	3 (75%)	6,6,6	3.51	5 (83%)
5	PO4	A	1006	-	4,4,4	2.09	2 (50%)	6,6,6	1.87	2 (33%)
2	APC	A	1004	-	29,33,33	2.03	10 (34%)	44,52,52	2.53	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	APC	D	1001	-	29,33,33	2.00	10 (34%)	44,52,52	2.54	19 (43%)
5	PO4	A	1007	-	4,4,4	2.83	3 (75%)	6,6,6	2.22	3 (50%)
3	HSX	F	2001	-	14,14,14	2.37	9 (64%)	19,21,21	3.25	12 (63%)
2	APC	C	1001	-	29,33,33	2.03	10 (34%)	44,52,52	2.56	20 (45%)
2	APC	C	1002	-	29,33,33	1.90	9 (31%)	44,52,52	2.55	21 (47%)
3	HSX	C	1003	-	14,14,14	1.27	1 (7%)	19,21,21	1.02	1 (5%)
5	PO4	A	1005	-	4,4,4	2.55	3 (75%)	6,6,6	1.44	2 (33%)
3	HSX	D	1002	-	14,14,14	1.20	1 (7%)	19,21,21	1.14	2 (10%)
2	APC	A	1001	-	29,33,33	1.07	3 (10%)	44,52,52	1.16	3 (6%)

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	E	1002	-	-	1/6/22/22	0/1/1/1
3	HSX	A	1002	-	-	3/6/22/22	0/1/1/1
2	APC	E	1001	-	-	4/19/38/38	0/3/3/3
2	APC	A	1004	-	-	9/19/38/38	0/3/3/3
2	APC	D	1001	-	-	11/19/38/38	0/3/3/3
3	HSX	F	2001	-	-	6/6/22/22	0/1/1/1
2	APC	C	1001	-	-	2/19/38/38	0/3/3/3
2	APC	C	1002	-	-	6/19/38/38	0/3/3/3
3	HSX	C	1003	-	-	3/6/22/22	0/1/1/1
3	HSX	D	1002	-	-	1/6/22/22	0/1/1/1
2	APC	A	1001	-	-	4/19/38/38	0/3/3/3

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	2003	PO4	P-O1	-4.66	1.39	1.50
2	A	1004	APC	PB-O3B	3.93	1.62	1.58
3	F	2001	HSX	P'-O5	-3.85	1.48	1.60
2	C	1001	APC	PB-O3B	3.82	1.62	1.58
5	A	1007	PO4	P-O3	-3.68	1.43	1.54
2	C	1002	APC	C2-N3	3.53	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	APC	C2-N3	3.50	1.40	1.33
5	F	2003	PO4	P-O2	-3.50	1.44	1.54
2	C	1002	APC	PB-O2B	-3.48	1.47	1.56
2	C	1001	APC	C2-N3	3.48	1.40	1.33
2	A	1004	APC	PB-O2B	-3.47	1.47	1.56
2	D	1001	APC	PB-O3B	3.47	1.62	1.58
2	A	1001	APC	PB-O2B	-3.38	1.48	1.56
2	C	1001	APC	PA-O2A	-3.38	1.48	1.56
3	F	2001	HSX	P'-O3X	-3.38	1.42	1.54
2	A	1004	APC	C2-N3	3.35	1.39	1.33
2	A	1004	APC	C5-N7	-3.31	1.33	1.39
2	D	1001	APC	PB-O2B	-3.30	1.48	1.56
2	C	1001	APC	PB-O2B	-3.30	1.48	1.56
3	C	1003	HSX	C1-C2	-3.27	1.49	1.52
5	F	2003	PO4	P-O4	-3.27	1.45	1.54
2	C	1002	APC	PA-O2A	-3.26	1.48	1.56
2	D	1001	APC	C2-N1	3.26	1.39	1.33
2	C	1001	APC	C5-N7	-3.24	1.33	1.39
5	A	1007	PO4	P-O2	-3.24	1.45	1.54
2	D	1001	APC	C5-N7	-3.23	1.33	1.39
2	A	1004	APC	PA-O2A	-3.21	1.48	1.56
2	D	1001	APC	PA-O2A	-3.20	1.48	1.56
5	A	1005	PO4	P-O2	-3.20	1.45	1.54
2	C	1002	APC	C2-N1	3.18	1.39	1.33
2	C	1001	APC	C2-N1	3.16	1.39	1.33
2	A	1004	APC	C2-N1	3.15	1.39	1.33
3	F	2001	HSX	P'-O2X	-3.15	1.43	1.54
2	C	1002	APC	C5-N7	-3.11	1.33	1.39
5	A	1005	PO4	P-O3	-2.98	1.45	1.54
2	C	1001	APC	C5-C4	-2.98	1.33	1.39
2	A	1004	APC	C5-C4	-2.95	1.33	1.39
2	C	1002	APC	C5-C4	-2.89	1.33	1.39
3	A	1002	HSX	P'-O2X	-2.83	1.44	1.54
2	E	1001	APC	PA-O2A	-2.82	1.49	1.56
2	D	1001	APC	C5-C4	-2.82	1.34	1.39
3	A	1002	HSX	O4-C1	-2.75	1.39	1.43
3	F	2001	HSX	C3-C4	-2.74	1.46	1.53
3	F	2001	HSX	O4-C4	-2.72	1.38	1.45
2	A	1004	APC	C5-C6	-2.70	1.33	1.41
2	C	1002	APC	C5-C6	-2.67	1.33	1.41
2	D	1001	APC	C5-C6	-2.66	1.33	1.41
2	E	1001	APC	PB-O2B	-2.66	1.49	1.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	APC	C5-C6	-2.65	1.33	1.41
3	F	2001	HSX	O3-C3	-2.57	1.36	1.43
2	C	1002	APC	C8-N9	-2.53	1.33	1.37
3	A	1002	HSX	P'-O5	-2.48	1.52	1.60
5	D	1004	PO4	P-O4	-2.46	1.47	1.54
2	D	1001	APC	C8-N9	-2.46	1.33	1.37
2	E	1001	APC	PG-O2G	-2.42	1.45	1.54
3	A	1002	HSX	C1-C2	2.40	1.55	1.52
2	A	1004	APC	C8-N9	-2.38	1.33	1.37
2	C	1001	APC	C8-N9	-2.36	1.33	1.37
5	A	1006	PO4	P-O3	-2.35	1.47	1.54
5	A	1006	PO4	P-O4	-2.32	1.47	1.54
2	A	1004	APC	O4'-C1'	2.28	1.47	1.42
3	A	1002	HSX	C3-C4	-2.27	1.47	1.53
2	C	1001	APC	O4'-C1'	2.26	1.47	1.42
3	F	2001	HSX	O5-C5	-2.25	1.36	1.44
5	A	1005	PO4	P-O4	-2.22	1.48	1.54
3	A	1002	HSX	O4-C4	-2.22	1.40	1.45
3	E	1002	HSX	O4-C4	-2.21	1.40	1.45
2	C	1002	APC	O4'-C1'	2.20	1.47	1.42
2	D	1001	APC	O4'-C1'	2.19	1.47	1.42
3	E	1002	HSX	C3-C4	-2.19	1.47	1.53
3	F	2001	HSX	C1-C2	2.19	1.55	1.52
2	A	1001	APC	PA-O2A	-2.18	1.51	1.56
3	D	1002	HSX	C1-C2	-2.17	1.50	1.52
2	A	1001	APC	PB-O3B	2.16	1.60	1.58
3	A	1002	HSX	P'-O1X	-2.11	1.43	1.50
3	A	1002	HSX	P'-O3X	-2.11	1.47	1.54
3	B	2001	HSX	O4-C1	-2.10	1.40	1.43
3	F	2001	HSX	C5-C4	-2.09	1.45	1.51
5	A	1007	PO4	P-O1	-2.09	1.45	1.50
3	B	2001	HSX	O4-C4	-2.04	1.40	1.45

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2001	HSX	O3-C3-C4	-8.05	87.96	111.08
3	A	1002	HSX	O1-C1-O4	-7.48	101.59	111.12
2	D	1001	APC	N3-C2-N1	-7.01	117.97	128.58
2	A	1004	APC	N3-C2-N1	-6.99	118.00	128.58
2	C	1001	APC	N3-C2-N1	-6.95	118.06	128.58
2	C	1002	APC	N3-C2-N1	-6.71	118.42	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	2003	PO4	O4-P-O3	5.77	125.86	107.91
2	C	1001	APC	C5-C4-N3	-5.51	119.14	126.72
2	A	1004	APC	C5-C4-N3	-5.28	119.45	126.72
2	D	1001	APC	C5-C4-N3	-5.26	119.48	126.72
2	C	1001	APC	C1'-N9-C8	-5.24	115.46	127.09
2	D	1001	APC	C1'-N9-C8	-5.23	115.49	127.09
2	C	1002	APC	C5-C4-N3	-5.20	119.55	126.72
2	A	1004	APC	C1'-N9-C8	-5.16	115.64	127.09
3	F	2001	HSX	O3X-P'-O5	-4.92	93.84	106.67
2	C	1002	APC	C1'-N9-C8	-4.59	116.91	127.09
2	A	1004	APC	C4-N9-C1'	4.52	137.21	126.63
2	C	1001	APC	C4-N9-C1'	4.51	137.19	126.63
3	F	2001	HSX	O5-C5-C4	-4.50	93.66	108.99
2	D	1001	APC	C4-N9-C1'	4.44	137.01	126.63
3	A	1002	HSX	O3-C3-C4	-4.22	98.97	111.08
2	A	1001	APC	PB-O3B-PG	4.15	147.32	132.45
2	C	1002	APC	PB-O3B-PG	-4.14	117.63	132.45
5	F	2003	PO4	O3-P-O2	-3.99	95.49	107.91
3	A	1002	HSX	O2X-P'-O5	-3.98	96.30	106.67
2	C	1002	APC	N9-C8-N7	-3.82	108.52	113.94
2	C	1002	APC	C4-N9-C1'	3.74	135.38	126.63
2	D	1001	APC	N9-C8-N7	-3.74	108.63	113.94
2	C	1001	APC	N9-C8-N7	-3.73	108.65	113.94
3	F	2001	HSX	O2-C2-C1	3.72	122.19	111.85
2	C	1001	APC	C2-N3-C4	3.72	120.91	111.83
3	A	1002	HSX	O3X-P'-O2X	3.67	121.58	107.80
3	A	1002	HSX	C5-C4-C3	-3.66	102.02	115.21
2	A	1004	APC	C2-N3-C4	3.64	120.72	111.83
2	D	1001	APC	C2-N3-C4	3.61	120.66	111.83
5	A	1007	PO4	O3-P-O1	-3.61	98.17	110.95
3	A	1002	HSX	O4-C1-C2	3.60	109.67	104.67
2	A	1004	APC	N9-C8-N7	-3.57	108.88	113.94
3	F	2001	HSX	C5-C4-C3	-3.51	102.58	115.21
3	F	2001	HSX	O2X-P'-O5	3.48	115.74	106.67
2	C	1002	APC	C2-N3-C4	3.44	120.24	111.83
3	F	2001	HSX	O3X-P'-O1X	3.42	124.18	110.83
3	A	1002	HSX	O2-C2-C1	3.38	121.26	111.85
2	C	1001	APC	N3-C4-N9	3.37	132.90	127.17
2	D	1001	APC	N3-C4-N9	3.29	132.76	127.17
3	F	2001	HSX	O5-P'-O1X	-3.26	97.64	106.44
2	C	1002	APC	N3-C4-N9	3.25	132.70	127.17
5	F	2003	PO4	O3-P-O1	-3.25	99.45	110.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1006	PO4	O3-P-O2	3.23	117.95	107.91
2	A	1004	APC	N3-C4-N9	3.20	132.62	127.17
2	E	1001	APC	PB-O3B-PG	3.19	143.88	132.45
3	E	1002	HSX	C1-C2-C3	3.12	106.12	102.29
2	C	1002	APC	C6-C5-C4	3.10	121.41	117.18
2	C	1001	APC	O2A-PA-O1A	3.03	119.81	109.95
2	C	1002	APC	O2A-PA-O1A	3.03	119.80	109.95
2	C	1002	APC	O3B-PG-O1G	-3.02	95.15	111.04
2	C	1001	APC	C5-C6-N6	-3.01	115.83	123.29
2	A	1004	APC	C2'-C3'-C4'	-2.98	96.85	102.61
2	D	1001	APC	O2A-PA-O1A	2.98	119.64	109.95
2	C	1001	APC	C6-C5-C4	2.97	121.24	117.18
3	F	2001	HSX	O4-C4-C3	2.97	111.04	105.15
5	A	1007	PO4	O4-P-O1	2.96	121.43	110.95
2	C	1001	APC	O2B-PB-O1B	2.95	119.55	109.95
2	D	1001	APC	C6-C5-C4	2.94	121.20	117.18
2	D	1001	APC	C5-N7-C8	2.92	108.03	103.45
2	A	1004	APC	C6-C5-C4	2.91	121.15	117.18
2	C	1002	APC	C5-N7-C8	2.89	108.00	103.45
2	D	1001	APC	C5-C6-N6	-2.89	116.13	123.29
2	C	1001	APC	C5-N7-C8	2.88	107.97	103.45
3	A	1002	HSX	C2-C3-C4	2.87	108.15	102.61
2	A	1004	APC	C5-C6-N6	-2.85	116.23	123.29
2	C	1001	APC	O3G-PG-O2G	2.85	118.48	107.80
2	A	1004	APC	O2B-PB-O1B	2.85	119.21	109.95
2	C	1002	APC	O2B-PB-O1B	2.84	119.21	109.95
2	C	1002	APC	O3G-PG-O2G	2.83	118.42	107.80
2	C	1002	APC	C5-C6-N6	-2.82	116.31	123.29
2	D	1001	APC	O2B-PB-O1B	2.81	119.09	109.95
2	A	1004	APC	C5-N7-C8	2.80	107.85	103.45
3	A	1002	HSX	O5-C5-C4	-2.79	99.51	108.99
2	A	1004	APC	O2A-PA-O1A	2.78	119.01	109.95
2	A	1004	APC	O3G-PG-O2G	2.76	118.14	107.80
2	D	1001	APC	O3G-PG-O2G	2.76	118.14	107.80
3	E	1002	HSX	O1-C1-O4	-2.72	107.66	111.12
3	D	1002	HSX	O3X-P'-O2X	2.68	117.84	107.80
2	C	1001	APC	O3G-PG-O3B	-2.65	95.73	104.64
3	E	1002	HSX	O3X-P'-O2X	2.64	117.72	107.80
3	A	1002	HSX	O3X-P'-O5	-2.64	99.80	106.67
2	D	1001	APC	O3B-PG-O1G	-2.62	97.27	111.04
2	A	1004	APC	O2G-PG-O3B	-2.60	95.90	104.64
2	C	1002	APC	C2'-C3'-C4'	-2.59	97.60	102.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1002	HSX	C5-C4-C3	-2.59	105.88	115.21
5	D	1004	PO4	O4-P-O1	-2.58	101.83	110.95
2	D	1001	APC	O2G-PG-O3B	-2.56	96.05	104.64
2	A	1004	APC	O3B-PG-O1G	-2.53	97.74	111.04
2	C	1001	APC	PB-O3B-PG	-2.52	123.41	132.45
2	A	1001	APC	O2A-PA-O1A	2.52	118.16	109.95
2	C	1002	APC	O4'-C4'-C3'	-2.38	100.43	105.15
3	E	1002	HSX	O5-P'-O1X	-2.37	100.03	106.44
5	F	2003	PO4	O2-P-O1	2.36	119.29	110.95
3	C	1003	HSX	O2-C2-C1	-2.36	105.29	111.85
3	A	1002	HSX	O5-P'-O1X	2.36	112.81	106.44
2	C	1001	APC	O3B-PG-O1G	-2.33	98.76	111.04
2	D	1001	APC	PB-O3B-PG	-2.32	124.14	132.45
3	E	1002	HSX	O3-C3-C4	-2.30	104.47	111.08
2	C	1002	APC	O2G-PG-O3B	-2.30	96.93	104.64
5	A	1006	PO4	O2-P-O1	-2.28	102.89	110.95
2	D	1001	APC	C2'-C3'-C4'	-2.28	98.21	102.61
3	F	2001	HSX	O4-C1-C2	2.27	107.82	104.67
3	A	1002	HSX	O4-C4-C3	2.27	109.65	105.15
5	A	1007	PO4	O4-P-O3	2.25	114.92	107.91
3	D	1002	HSX	O2X-P'-O5	-2.25	100.81	106.67
2	C	1002	APC	C4-C5-N7	-2.22	108.04	110.58
3	E	1002	HSX	O2X-P'-O1X	2.22	119.47	110.83
2	D	1001	APC	C4-C5-N7	-2.18	108.09	110.58
3	E	1002	HSX	O5-C5-C4	-2.17	101.60	108.99
3	B	2001	HSX	C5-C4-C3	-2.17	107.40	115.21
5	F	2003	PO4	O4-P-O1	-2.17	103.29	110.95
3	F	2001	HSX	O1-C1-O4	-2.16	108.36	111.12
2	C	1001	APC	C4-C5-N7	-2.16	108.12	110.58
3	E	1002	HSX	C2-C3-C4	-2.13	98.49	102.61
2	A	1001	APC	C4-N9-C1'	2.12	131.59	126.63
2	A	1004	APC	C4-C5-N7	-2.08	108.21	110.58
5	A	1005	PO4	O2-P-O1	2.08	118.30	110.95
2	A	1004	APC	PB-O3B-PG	-2.07	125.02	132.45
3	F	2001	HSX	C2-C3-C4	2.07	106.61	102.61
2	C	1001	APC	C2'-C1'-N9	2.07	118.44	113.30
5	A	1005	PO4	O4-P-O2	-2.04	101.56	107.91
2	C	1001	APC	O2G-PG-O3B	-2.04	97.81	104.64
2	C	1002	APC	O3G-PG-O1G	2.03	118.74	110.83
2	C	1001	APC	C5'-C4'-C3'	-2.01	107.97	115.21
2	D	1001	APC	O4'-C4'-C3'	-2.01	101.17	105.15
2	C	1002	APC	O2G-PG-O1G	2.00	118.64	110.83

There are no chirality outliers.

All (50) 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
2	D	1001	APC	C5'-O5'-PA-O1A
2	E	1001	APC	C5'-O5'-PA-C3A
3	C	1003	HSX	C4-C5-O5-P'
3	D	1002	HSX	C4-C5-O5-P'
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	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	O4-C4-C5-O5
3	F	2001	HSX	C3-C4-C5-O5
2	A	1001	APC	O4'-C4'-C5'-O5'
3	C	1003	HSX	O4-C4-C5-O5
3	C	1003	HSX	C3-C4-C5-O5
2	A	1001	APC	C2'-C1'-N9-C4
2	A	1004	APC	C2'-C1'-N9-C4
2	C	1002	APC	C2'-C1'-N9-C4
2	D	1001	APC	C2'-C1'-N9-C4
2	E	1001	APC	C3'-C4'-C5'-O5'
2	A	1001	APC	C2'-C1'-N9-C8
2	A	1004	APC	C2'-C1'-N9-C8
2	C	1002	APC	C2'-C1'-N9-C8
2	D	1001	APC	C2'-C1'-N9-C8
2	E	1001	APC	C2'-C1'-N9-C8
2	A	1001	APC	PA-C3A-PB-O2B
2	C	1002	APC	PB-C3A-PA-O2A
2	D	1001	APC	PA-C3A-PB-O3B
3	F	2001	HSX	C4-C5-O5-P'
2	E	1001	APC	C2'-C1'-N9-C4
3	A	1002	HSX	O4-C4-C5-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1002	HSX	C4-C5-O5-P'
2	A	1004	APC	C5'-O5'-PA-O2A
2	C	1002	APC	C5'-O5'-PA-O2A
2	D	1001	APC	PB-C3A-PA-O1A
2	D	1001	APC	C5'-O5'-PA-O2A
2	D	1001	APC	O4'-C1'-N9-C8
2	A	1004	APC	C5'-O5'-PA-C3A
2	C	1001	APC	C5'-O5'-PA-C3A
3	A	1002	HSX	C3-C4-C5-O5
3	E	1002	HSX	C4-C5-O5-P'

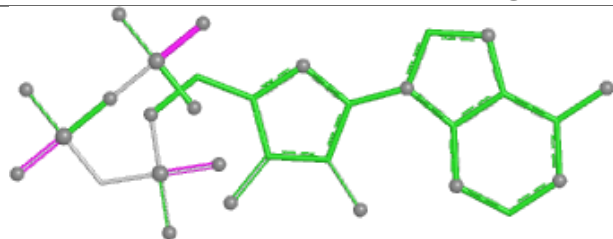
There are no ring outliers.

14 monomers are involved in 61 short contacts:

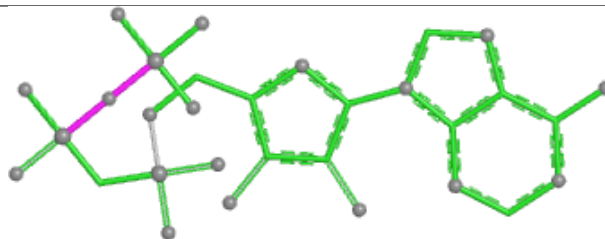
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1004	PO4	1	0
3	B	2001	HSX	1	0
3	E	1002	HSX	2	0
3	A	1002	HSX	1	0
2	E	1001	APC	15	0
5	F	2003	PO4	2	0
2	A	1004	APC	3	0
2	D	1001	APC	12	0
3	F	2001	HSX	5	0
2	C	1001	APC	2	0
2	C	1002	APC	6	0
5	A	1005	PO4	2	0
3	D	1002	HSX	6	0
2	A	1001	APC	3	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

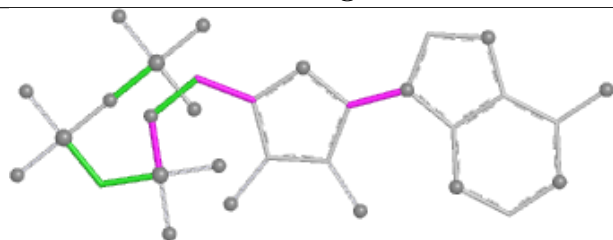
Ligand APC E 1001



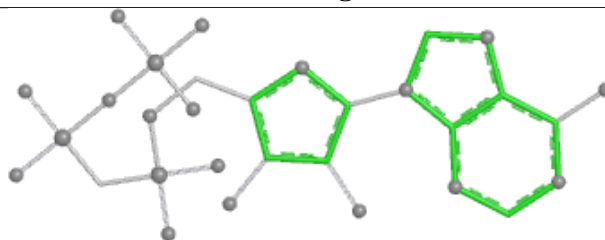
Bond lengths



Bond angles

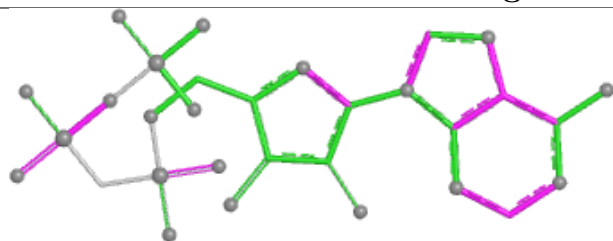


Torsions

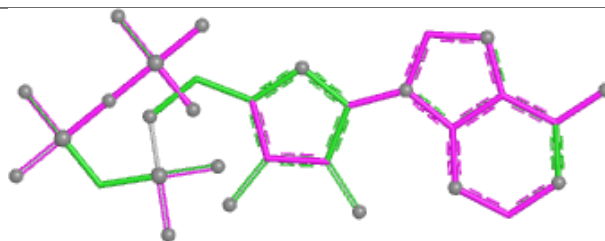


Rings

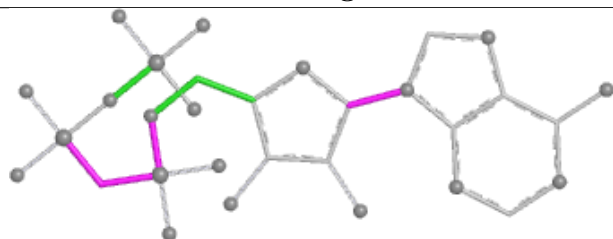
Ligand APC A 1004



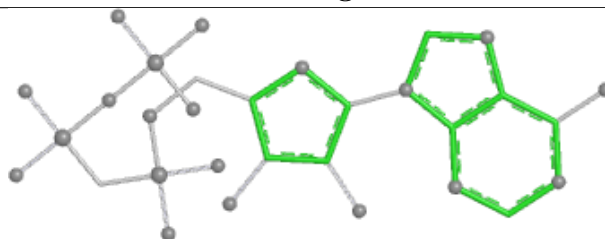
Bond lengths



Bond angles

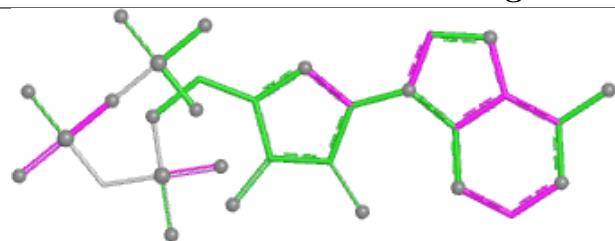


Torsions

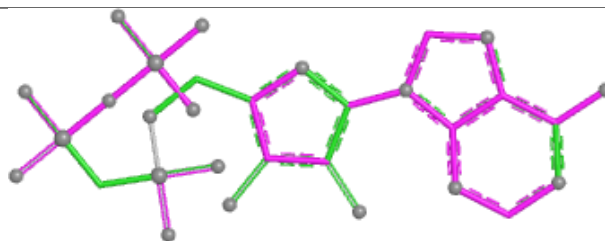


Rings

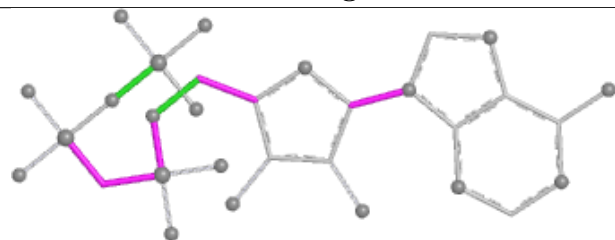
Ligand APC D 1001



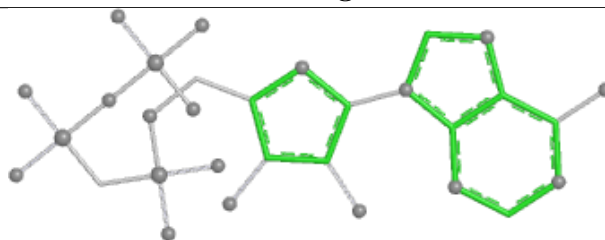
Bond lengths



Bond angles

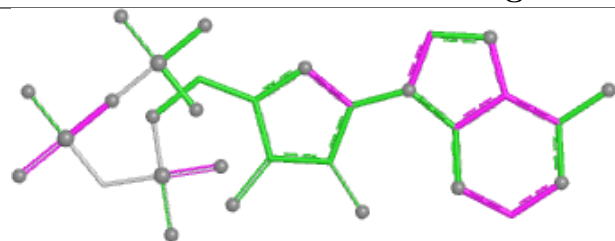


Torsions

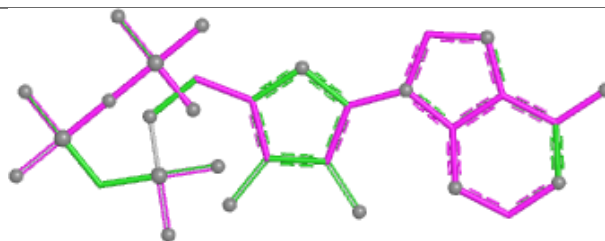


Rings

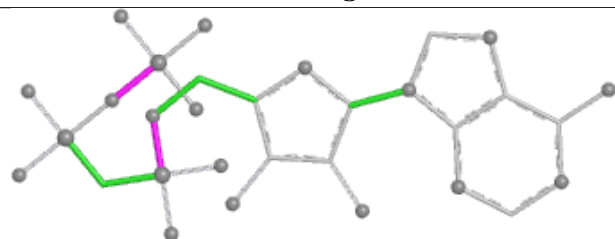
Ligand APC C 1001



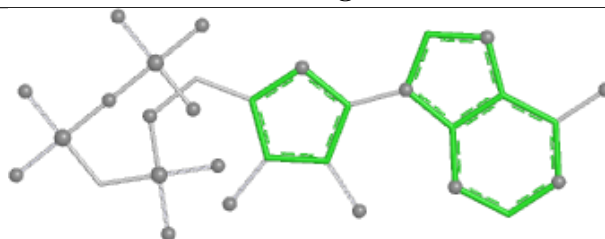
Bond lengths



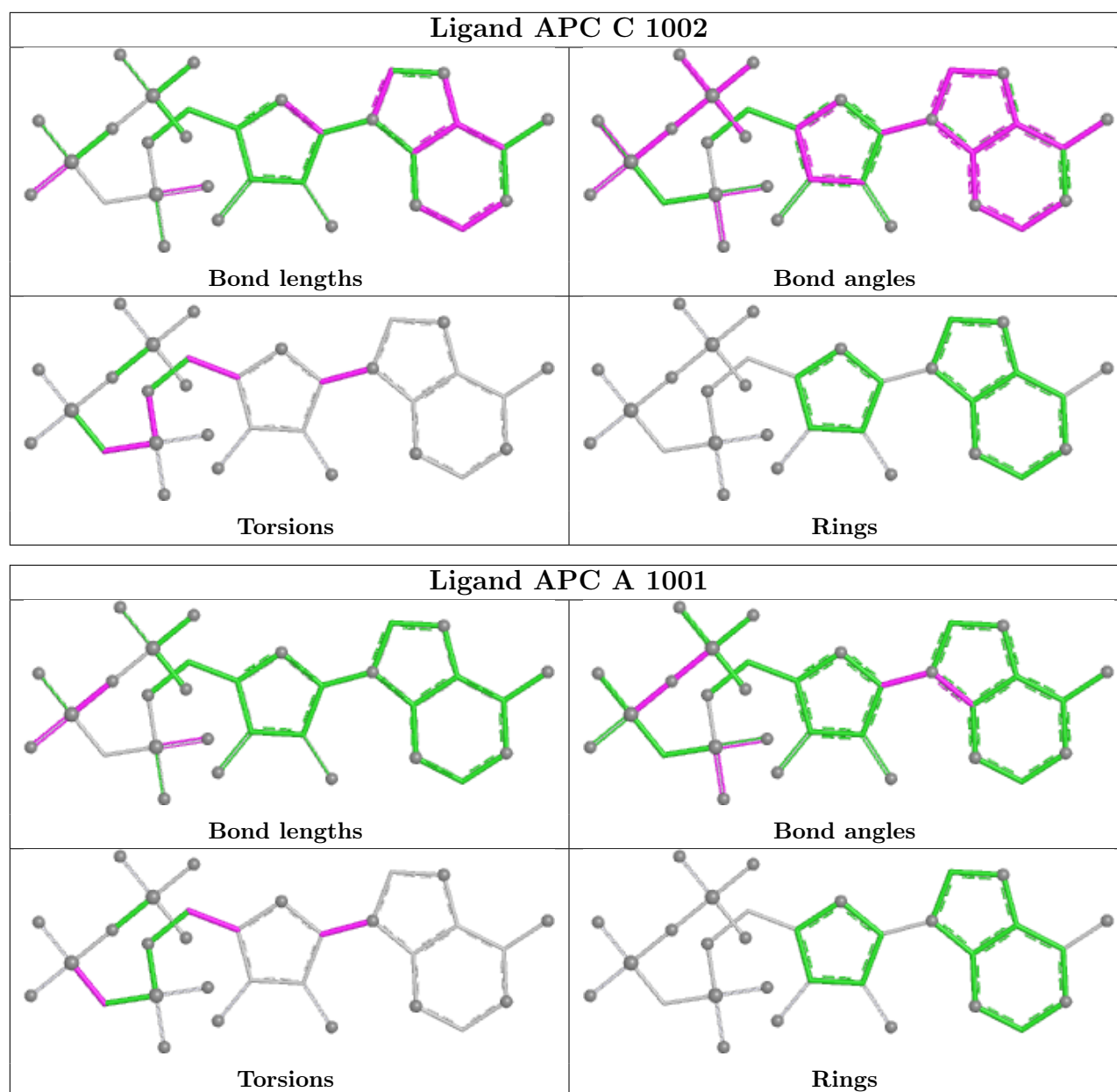
Bond angles



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, 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	309/321 (96%)	1.17	43 (13%) 6 6	16, 31, 52, 99	0
1	B	296/321 (92%)	1.52	82 (27%) 1 1	27, 47, 65, 78	0
1	C	294/321 (91%)	1.82	104 (35%) 1 1	35, 64, 88, 99	0
1	D	298/321 (92%)	2.05	140 (46%) 0 0	33, 66, 96, 113	0
1	E	299/321 (93%)	1.62	89 (29%) 1 1	30, 47, 69, 94	0
1	F	308/321 (95%)	1.02	39 (12%) 8 8	16, 30, 49, 98	0
All	All	1804/1926 (93%)	1.53	497 (27%) 1 1	16, 45, 85, 113	0

All (497) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	98	ASP	7.1
1	C	221	LEU	7.1
1	B	4	ILE	6.9
1	C	250	ILE	6.8
1	D	268	ALA	6.3
1	D	172	SER	6.2
1	C	249	ALA	5.9
1	C	154	VAL	5.6
1	E	181	VAL	5.5
1	A	175	ALA	5.4
1	B	97	GLN	5.4
1	D	179	LYS	5.3
1	E	174	ASP	5.1
1	D	251	LEU	5.1
1	D	173	PRO	5.1
1	C	248	TYR	5.0
1	D	236	ALA	4.9
1	D	184	ILE	4.9
1	C	254	GLY	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	103	VAL	4.9
1	D	150	ALA	4.8
1	D	95	ALA	4.7
1	B	154	VAL	4.7
1	C	268	ALA	4.6
1	D	267	ALA	4.6
1	C	192	PHE	4.6
1	E	290	ILE	4.6
1	D	295	ILE	4.6
1	D	225	MET	4.5
1	E	66	ASN	4.5
1	D	197	LYS	4.5
1	D	59	GLY	4.5
1	D	178	ALA	4.5
1	C	280	GLN	4.5
1	C	220	ILE	4.4
1	C	173	PRO	4.4
1	C	103	VAL	4.3
1	A	136	GLN	4.3
1	B	175	ALA	4.3
1	D	1	SER	4.3
1	C	175	ALA	4.3
1	B	19	VAL	4.2
1	C	300	ALA	4.2
1	D	9	GLY	4.2
1	D	171	VAL	4.2
1	C	226	ALA	4.2
1	D	174	ASP	4.2
1	A	176	GLY	4.1
1	D	193	ALA	4.1
1	E	220	ILE	4.1
1	C	188	LEU	4.0
1	E	61	GLY	4.0
1	B	304	ARG	3.9
1	A	150	ALA	3.9
1	D	61	GLY	3.9
1	D	58	SER	3.9
1	C	21	ASP	3.9
1	C	88	VAL	3.9
1	E	32	THR	3.8
1	F	99	LYS	3.8
1	D	250	ILE	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	175	ALA	3.8
1	E	293	ILE	3.8
1	B	103	VAL	3.8
1	E	99	LYS	3.8
1	B	5	VAL	3.8
1	D	222	VAL	3.8
1	D	60	CYS	3.8
1	D	142	ASP	3.8
1	D	208	MET	3.8
1	C	8	SER	3.8
1	D	269	PHE	3.8
1	F	100	LYS	3.8
1	C	279	PRO	3.8
1	E	97	GLN	3.7
1	E	60	CYS	3.7
1	A	1	SER	3.7
1	D	169	ILE	3.7
1	C	134	ALA	3.7
1	D	245	THR	3.7
1	C	208	MET	3.7
1	D	155	LEU	3.6
1	E	179	LYS	3.6
1	C	224	ASP	3.6
1	D	194	LEU	3.6
1	C	255	ILE	3.6
1	E	20	ALA	3.6
1	F	172	SER	3.6
1	C	278	ILE	3.5
1	D	175	ALA	3.5
1	E	176	GLY	3.5
1	C	42	VAL	3.5
1	C	190	VAL	3.5
1	A	15	LEU	3.5
1	E	81	SER	3.5
1	C	165	TRP	3.5
1	B	25	LEU	3.5
1	A	206	ASP	3.5
1	C	102	LYS	3.5
1	E	194	LEU	3.5
1	C	56	ILE	3.5
1	D	100	LYS	3.5
1	F	24	GLY	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	174	ASP	3.5
1	C	194	LEU	3.5
1	B	250	ILE	3.4
1	E	110	ILE	3.4
1	E	184	ILE	3.4
1	B	165	TRP	3.4
1	E	55	ILE	3.4
1	F	81	SER	3.4
1	B	32	THR	3.4
1	A	167	ASN	3.4
1	B	280	GLN	3.4
1	F	101	ASP	3.4
1	B	158	ILE	3.4
1	D	226	ALA	3.4
1	E	75	ASN	3.4
1	B	224	ASP	3.3
1	C	179	LYS	3.3
1	B	67	LEU	3.3
1	C	263	ARG	3.3
1	C	163	ALA	3.3
1	B	223	ASP	3.3
1	B	1	SER	3.3
1	D	221	LEU	3.3
1	A	95	ALA	3.3
1	C	108	ALA	3.3
1	D	237	ASP	3.3
1	D	223	ASP	3.3
1	F	199	ARG	3.2
1	E	17	GLN	3.2
1	D	248	TYR	3.2
1	C	7	PHE	3.2
1	C	143	ILE	3.2
1	A	174	ASP	3.2
1	B	188	LEU	3.2
1	B	61	GLY	3.2
1	E	248	TYR	3.2
1	D	211	VAL	3.2
1	A	245	THR	3.2
1	C	275	THR	3.2
1	F	16	SER	3.2
1	C	297	MET	3.2
1	B	71	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	26	GLU	3.2
1	D	151	GLU	3.2
1	A	236	ALA	3.2
1	F	181	VAL	3.2
1	D	130	MET	3.1
1	F	286	HIS	3.1
1	D	176	GLY	3.1
1	E	45	GLY	3.1
1	B	122	ALA	3.1
1	C	260	ALA	3.1
1	C	195	ILE	3.1
1	D	191	GLU	3.1
1	B	293	ILE	3.1
1	E	276	ASN	3.1
1	B	26	GLU	3.1
1	E	280	GLN	3.1
1	C	244	ALA	3.1
1	E	219	ALA	3.1
1	F	210	LEU	3.1
1	A	100	LYS	3.1
1	A	220	ILE	3.1
1	D	214	VAL	3.1
1	D	239	LEU	3.0
1	E	261	ILE	3.0
1	D	149	TYR	3.0
1	A	99	LYS	3.0
1	D	210	LEU	3.0
1	C	228	THR	3.0
1	F	103	VAL	3.0
1	C	26	GLU	3.0
1	D	170	ILE	3.0
1	E	278	ILE	3.0
1	C	150	ALA	3.0
1	D	165	TRP	2.9
1	D	135	SER	2.9
1	D	213	ASP	2.9
1	B	47	SER	2.9
1	C	229	CYS	2.9
1	D	167	ASN	2.9
1	D	261	ILE	2.9
1	D	92	PHE	2.9
1	D	247	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	19	VAL	2.9
1	D	4	ILE	2.9
1	D	293	ILE	2.9
1	A	103	VAL	2.9
1	A	181	VAL	2.9
1	A	194	LEU	2.9
1	E	107	ARG	2.9
1	D	227	ASP	2.9
1	B	212	GLY	2.9
1	D	79	ILE	2.8
1	D	254	GLY	2.8
1	B	77	CYS	2.8
1	D	153	ALA	2.8
1	B	264	ILE	2.8
1	D	262	SER	2.8
1	D	264	ILE	2.8
1	D	177	GLY	2.8
1	C	269	PHE	2.8
1	D	218	VAL	2.8
1	E	35	PHE	2.8
1	C	55	ILE	2.8
1	D	278	ILE	2.8
1	E	196	HIS	2.8
1	F	102	LYS	2.8
1	E	58	SER	2.8
1	C	272	VAL	2.8
1	C	162	ILE	2.7
1	E	167	ASN	2.7
1	A	252	THR	2.7
1	B	281	GLU	2.7
1	C	19	VAL	2.7
1	C	216	ASP	2.7
1	E	244	ALA	2.7
1	C	149	TYR	2.7
1	F	279	PRO	2.7
1	D	238	LYS	2.7
1	D	132	LEU	2.7
1	D	104	GLY	2.7
1	E	1	SER	2.7
1	B	121	VAL	2.7
1	B	226	ALA	2.7
1	B	119	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	70	LEU	2.7
1	E	10	SER	2.7
1	F	207	ARG	2.7
1	B	76	ALA	2.7
1	B	271	ALA	2.7
1	D	108	ALA	2.7
1	B	255	ILE	2.7
1	C	110	ILE	2.7
1	E	77	CYS	2.7
1	B	45	GLY	2.7
1	C	243	GLY	2.7
1	B	106	SER	2.7
1	A	76	ALA	2.7
1	B	20	ALA	2.7
1	D	53	VAL	2.7
1	C	245	THR	2.7
1	C	142	ASP	2.7
1	B	295	ILE	2.6
1	D	219	ALA	2.6
1	D	186	ASP	2.6
1	B	248	TYR	2.6
1	D	195	ILE	2.6
1	F	293	ILE	2.6
1	B	62	GLU	2.6
1	B	215	LYS	2.6
1	D	272	VAL	2.6
1	A	279	PRO	2.6
1	B	86	THR	2.6
1	F	136	GLN	2.6
1	C	227	ASP	2.6
1	B	284	MET	2.6
1	F	303	ILE	2.6
1	A	164	GLU	2.6
1	D	260	ALA	2.6
1	C	44	ILE	2.6
1	D	110	ILE	2.6
1	F	180	ARG	2.6
1	D	43	GLU	2.6
1	E	185	ALA	2.6
1	F	17	GLN	2.6
1	F	308	ASN	2.6
1	D	82	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	56	ILE	2.5
1	C	158	ILE	2.5
1	C	210	LEU	2.5
1	C	197	LYS	2.5
1	D	96	ARG	2.5
1	A	204	GLU	2.5
1	E	243	GLY	2.5
1	D	93	PRO	2.5
1	D	190	VAL	2.5
1	D	231	THR	2.5
1	D	157	TRP	2.5
1	C	125	ASP	2.5
1	A	143	ILE	2.5
1	C	252	THR	2.5
1	E	129	THR	2.5
1	E	245	THR	2.5
1	E	56	ILE	2.5
1	D	253	HIS	2.5
1	A	190	VAL	2.5
1	C	181	VAL	2.5
1	E	103	VAL	2.5
1	D	182	THR	2.5
1	B	179	LYS	2.5
1	D	229	CYS	2.5
1	F	110	ILE	2.5
1	F	232	ILE	2.5
1	E	26	GLU	2.5
1	E	31	VAL	2.5
1	C	236	ALA	2.5
1	C	132	LEU	2.4
1	C	295	ILE	2.4
1	D	220	ILE	2.4
1	E	70	LEU	2.4
1	D	77	CYS	2.4
1	C	258	GLY	2.4
1	B	219	ALA	2.4
1	B	242	ALA	2.4
1	E	84	ARG	2.4
1	E	67	LEU	2.4
1	C	233	CYS	2.4
1	C	287	CYS	2.4
1	F	224	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	280	GLN	2.4
1	B	54	TYR	2.4
1	E	249	ALA	2.4
1	D	63	ILE	2.4
1	E	170	ILE	2.4
1	A	26	GLU	2.4
1	B	160	GLU	2.4
1	D	233	CYS	2.4
1	E	279	PRO	2.4
1	D	19	VAL	2.4
1	E	154	VAL	2.4
1	B	236	ALA	2.4
1	C	180	ARG	2.4
1	D	180	ARG	2.4
1	E	122	ALA	2.4
1	B	6	LEU	2.4
1	D	67	LEU	2.4
1	D	148	LEU	2.4
1	D	232	ILE	2.4
1	D	189	ASN	2.4
1	E	65	ASP	2.4
1	B	68	MET	2.4
1	C	104	GLY	2.4
1	B	38	GLN	2.4
1	B	85	VAL	2.4
1	D	181	VAL	2.4
1	D	256	PHE	2.4
1	E	239	LEU	2.3
1	E	128	ILE	2.3
1	E	51	GLU	2.3
1	C	183	SER	2.3
1	E	216	ASP	2.3
1	E	287	CYS	2.3
1	C	291	GLN	2.3
1	C	251	LEU	2.3
1	E	221	LEU	2.3
1	F	132	LEU	2.3
1	C	54	TYR	2.3
1	E	37	ASN	2.3
1	C	106	SER	2.3
1	D	217	ARG	2.3
1	B	181	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	30	VAL	2.3
1	D	115	VAL	2.3
1	D	292	VAL	2.3
1	D	35	PHE	2.3
1	D	299	LEU	2.3
1	B	55	ILE	2.3
1	B	63	ILE	2.3
1	B	220	ILE	2.3
1	E	195	ILE	2.3
1	F	133	HIS	2.3
1	C	166	LYS	2.3
1	D	166	LYS	2.3
1	A	115	VAL	2.3
1	E	53	VAL	2.3
1	C	256	PHE	2.3
1	E	92	PHE	2.3
1	C	232	ILE	2.3
1	A	101	ASP	2.3
1	B	262	SER	2.3
1	C	93	PRO	2.3
1	D	183	SER	2.3
1	E	71	LEU	2.3
1	D	143	ILE	2.2
1	D	283	LYS	2.2
1	E	102	LYS	2.2
1	E	86	THR	2.2
1	A	180	ARG	2.2
1	B	273	VAL	2.2
1	F	145	VAL	2.2
1	A	264	ILE	2.2
1	D	163	ALA	2.2
1	E	134	ALA	2.2
1	E	285	LYS	2.2
1	F	122	ALA	2.2
1	C	288	THR	2.2
1	D	84	ARG	2.2
1	D	187	ARG	2.2
1	A	93	PRO	2.2
1	C	139	GLY	2.2
1	D	41	SER	2.2
1	C	209	VAL	2.2
1	E	48	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	56	ILE	2.2
1	C	60	CYS	2.2
1	B	207	ARG	2.2
1	D	305	ARG	2.2
1	E	64	ASN	2.2
1	D	99	LYS	2.2
1	F	176	GLY	2.2
1	C	247	VAL	2.2
1	F	115	VAL	2.2
1	F	222	VAL	2.2
1	B	7	PHE	2.2
1	C	290	ILE	2.2
1	E	250	ILE	2.2
1	B	75	ASN	2.2
1	A	53	VAL	2.2
1	B	42	VAL	2.2
1	B	257	SER	2.2
1	C	218	VAL	2.2
1	E	74	ILE	2.2
1	B	256	PHE	2.2
1	D	192	PHE	2.2
1	A	163	ALA	2.1
1	A	178	ALA	2.1
1	C	164	GLU	2.1
1	D	69	GLU	2.1
1	B	91	CYS	2.1
1	E	138	GLN	2.1
1	A	188	LEU	2.1
1	C	25	LEU	2.1
1	A	28	GLY	2.1
1	A	14	ASP	2.1
1	A	133	HIS	2.1
1	B	82	SER	2.1
1	C	241	SER	2.1
1	D	162	ILE	2.1
1	D	255	ILE	2.1
1	E	41	SER	2.1
1	F	44	ILE	2.1
1	E	283	LYS	2.1
1	D	73	MET	2.1
1	E	54	TYR	2.1
1	B	104	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	44	ILE	2.1
1	C	292	VAL	2.1
1	D	273	VAL	2.1
1	E	272	VAL	2.1
1	E	106	SER	2.1
1	E	111	SER	2.1
1	F	20	ALA	2.1
1	B	180	ARG	2.1
1	B	275	THR	2.1
1	D	97	GLN	2.1
1	A	59	GLY	2.1
1	E	212	GLY	2.1
1	B	162	ILE	2.1
1	C	185	ALA	2.1
1	D	270	GLU	2.1
1	D	228	THR	2.1
1	D	288	THR	2.1
1	B	276	ASN	2.1
1	B	168	CYS	2.1
1	C	133	HIS	2.1
1	C	212	GLY	2.1
1	F	233	CYS	2.1
1	A	232	ILE	2.1
1	D	290	ILE	2.1
1	B	292	VAL	2.1
1	D	31	VAL	2.1
1	D	88	VAL	2.1
1	D	274	VAL	2.1
1	C	131	ASP	2.0
1	D	301	GLU	2.0
1	E	151	GLU	2.0
1	D	111	SER	2.0
1	B	33	LYS	2.0
1	B	102	LYS	2.0
1	F	231	THR	2.0
1	B	208	MET	2.0
1	A	239	LEU	2.0
1	C	67	LEU	2.0
1	F	25	LEU	2.0
1	B	230	GLY	2.0
1	C	4	ILE	2.0
1	D	298	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	59	GLY	2.0
1	F	56	ILE	2.0
1	C	121	VAL	2.0
1	C	273	VAL	2.0
1	E	218	VAL	2.0
1	B	269	PHE	2.0
1	F	98	ASP	2.0
1	A	2	PRO	2.0
1	E	182	THR	2.0
1	C	240	LEU	2.0
1	D	188	LEU	2.0
1	A	177	GLY	2.0
1	C	63	ILE	2.0
1	D	75	ASN	2.0
1	E	189	ASN	2.0
1	E	255	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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

Continued on next page...

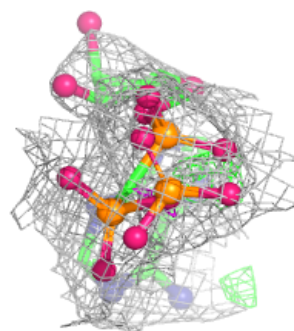
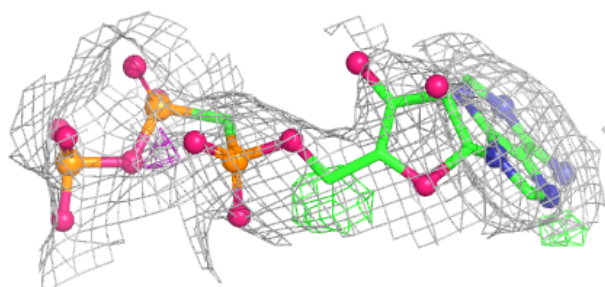
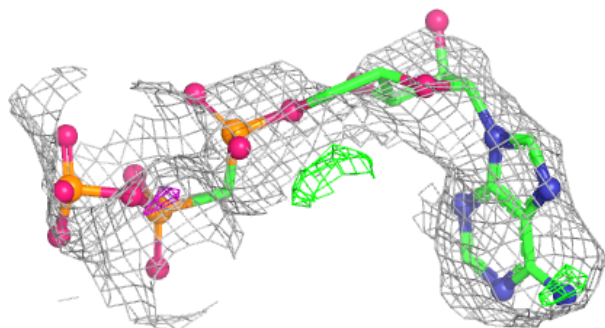
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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.

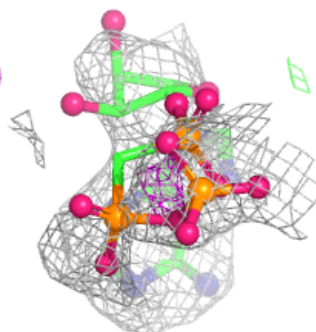
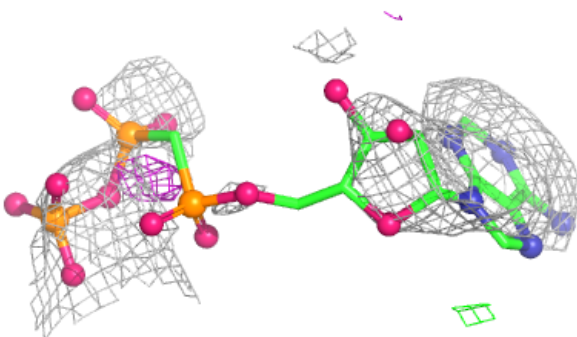
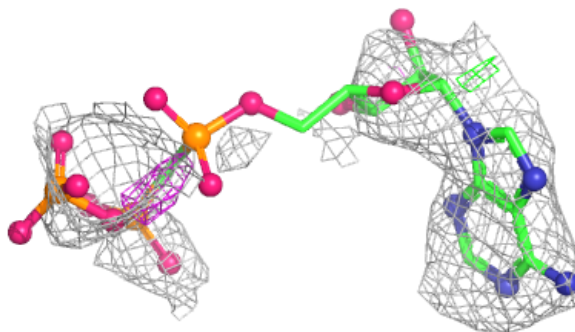
Electron density around APC C 1002:

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

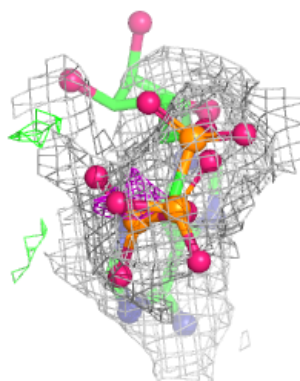
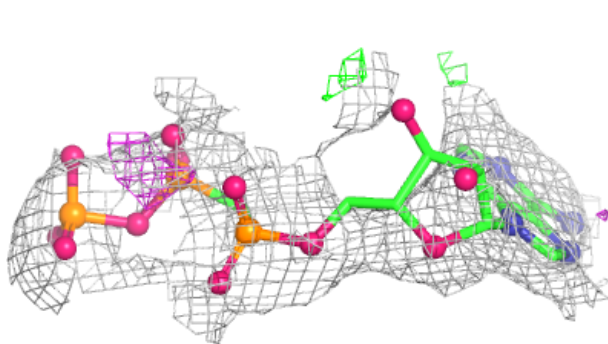
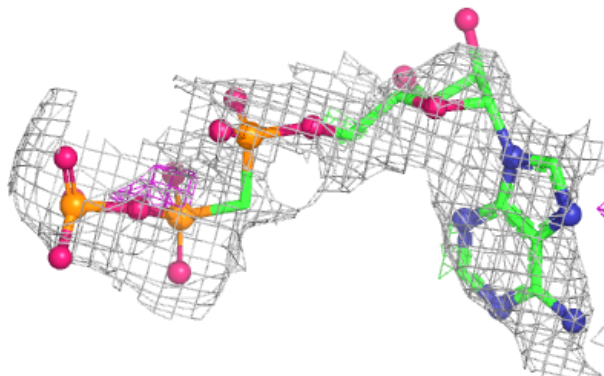


Electron density around APC D 1001:

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

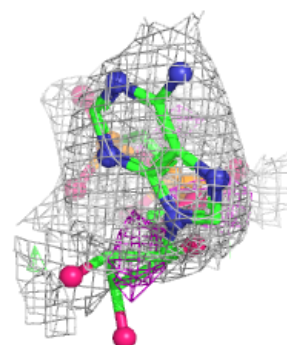
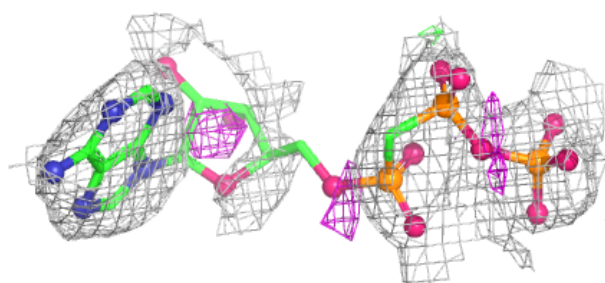
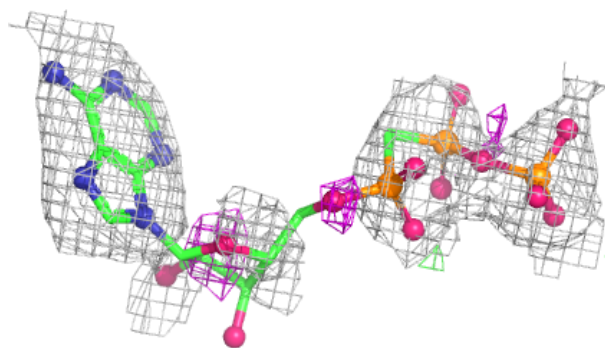
**Electron density around APC C 1001:**

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

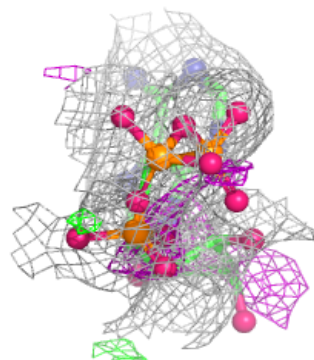
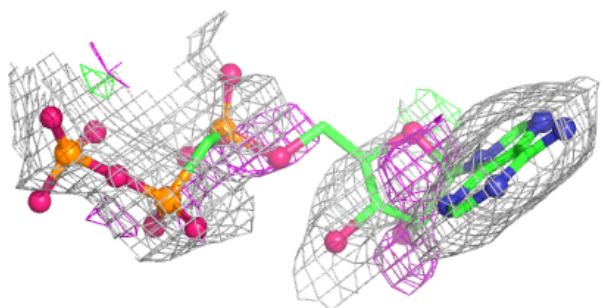
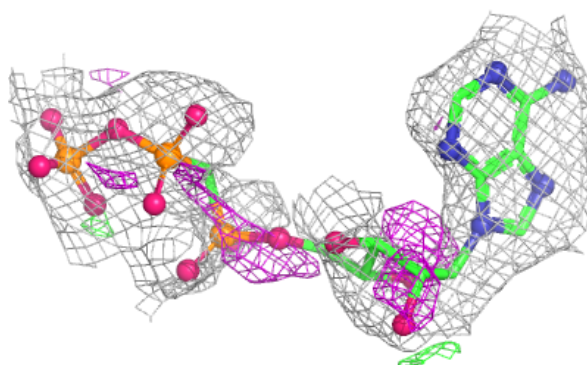


Electron density around APC E 1001:

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

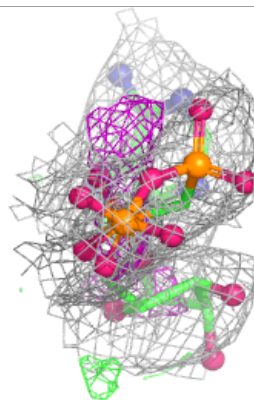
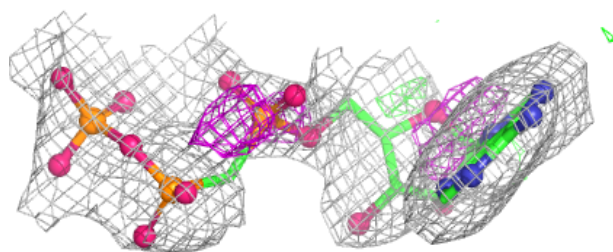
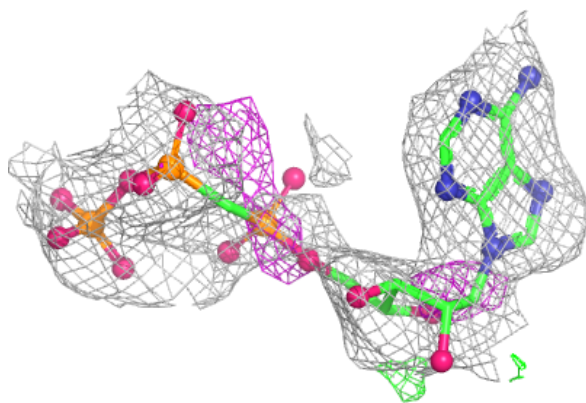
**Electron density around APC A 1004:**

$2mF_o-DF_c$ (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.