Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2024 – 02:54 AM EST

PDB ID	:	4Q85
Title	:	YcaO with Non-hydrolyzable ATP (AMPCPP) Bound
Authors	:	Chekan, J.R.; Nair, S.K.
Deposited on	:	2014-04-25
Resolution	:	3.29 Å(reported)

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

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

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

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

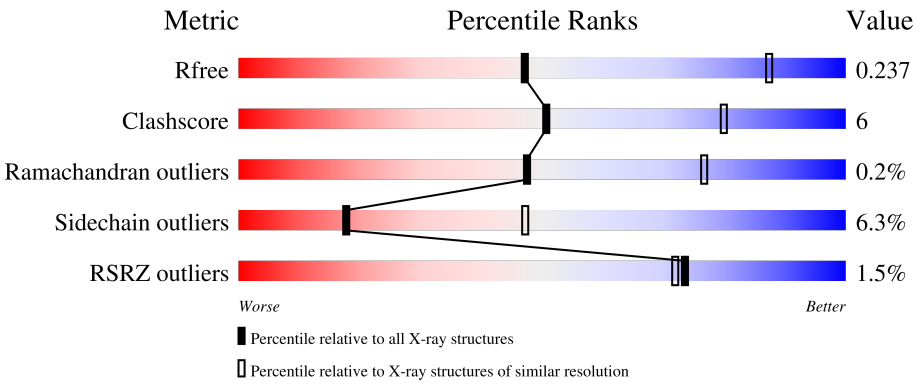
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	586	84% 10% • 5%
1	B	586	85% 11% • •
1	C	586	82% 13% • •
1	D	586	83% 13% • •
1	E	586	88% 9% • •

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Mol	Chain	Length	Quality of chain
1	F	586	8% 73% 20%
1	G	586	2% 80% 11% 7%
1	H	586	84% 12%

2 Entry composition (i)

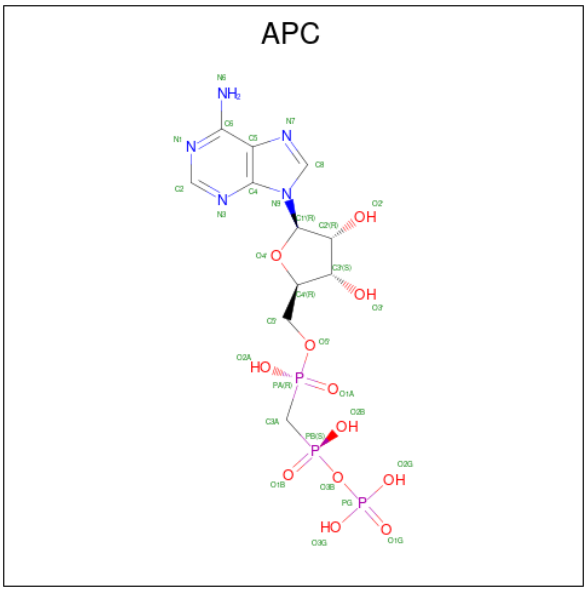
There are 4 unique types of molecules in this entry. The entry contains 36421 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribosomal protein S12 methylthiotransferase accessory factor YcaO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	559	4424	2823	718	866	17	0	0	0
1	B	573	4535	2896	736	886	17	0	0	0
1	C	562	4450	2839	721	873	17	0	0	0
1	D	572	4523	2889	733	884	17	0	0	0
1	E	573	4530	2892	734	887	17	0	0	0
1	F	570	4507	2876	731	883	17	0	0	0
1	G	545	4309	2750	698	844	17	0	0	0
1	H	573	4537	2900	735	885	17	0	0	0

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



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	3	3	3	0	0
3	B	3	3	3	0	0
3	C	2	2	2	0	0
3	D	3	3	3	0	0
3	E	3	3	3	0	0
3	G	1	1	1	0	0
3	H	4	4	4	0	0

- Molecule 4 is water.

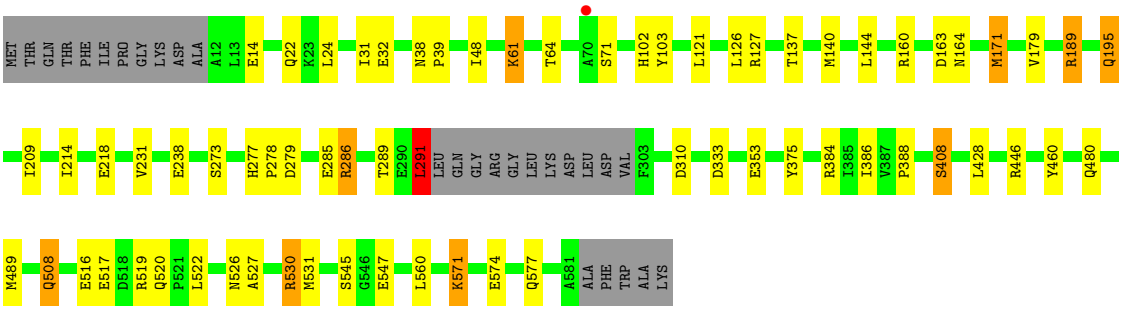
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	53	53	53	0	0
			Total	O		
4	B	42	42	42	0	0
			Total	O		
4	C	42	42	42	0	0
			Total	O		
4	D	60	60	60	0	0
			Total	O		
4	E	50	50	50	0	0
			Total	O		
4	F	76	76	76	0	0
			Total	O		
4	G	54	54	54	0	0
			Total	O		
4	H	55	55	55	0	0

3 Residue-property plots (i)

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

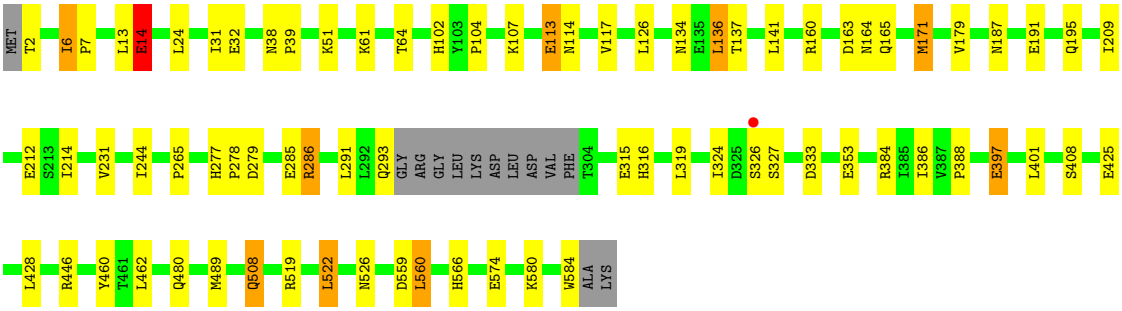
• Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

Chain A: 84% 10% • 5%



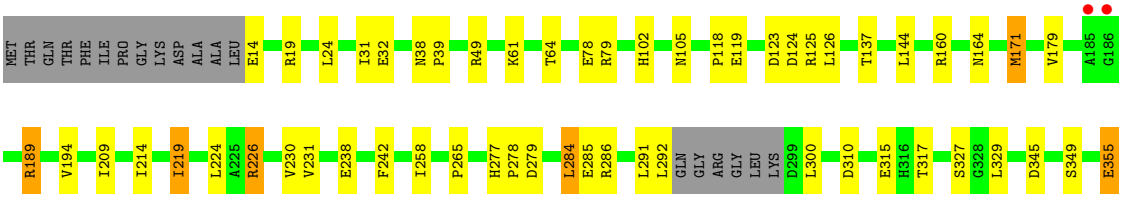
• Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

Chain B: 85% 11% • •



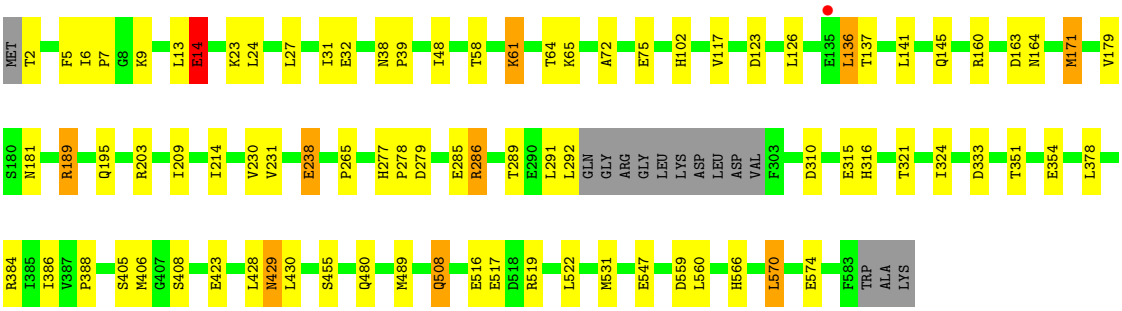
• Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

Chain C: 82% 13% • •



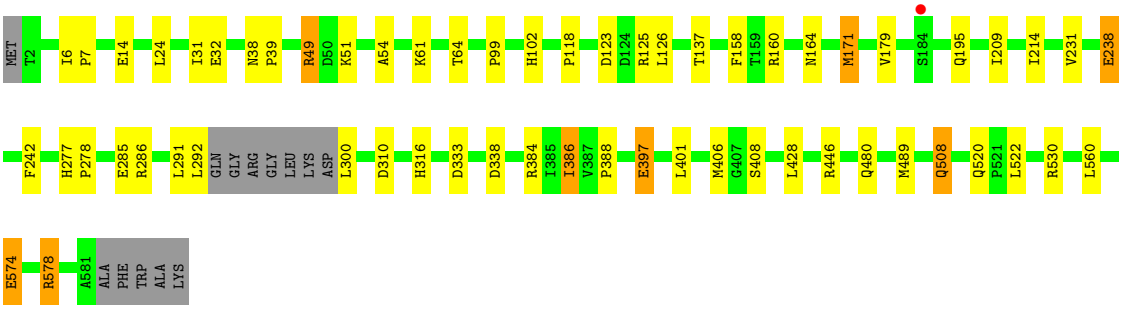
• Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

Chain D:



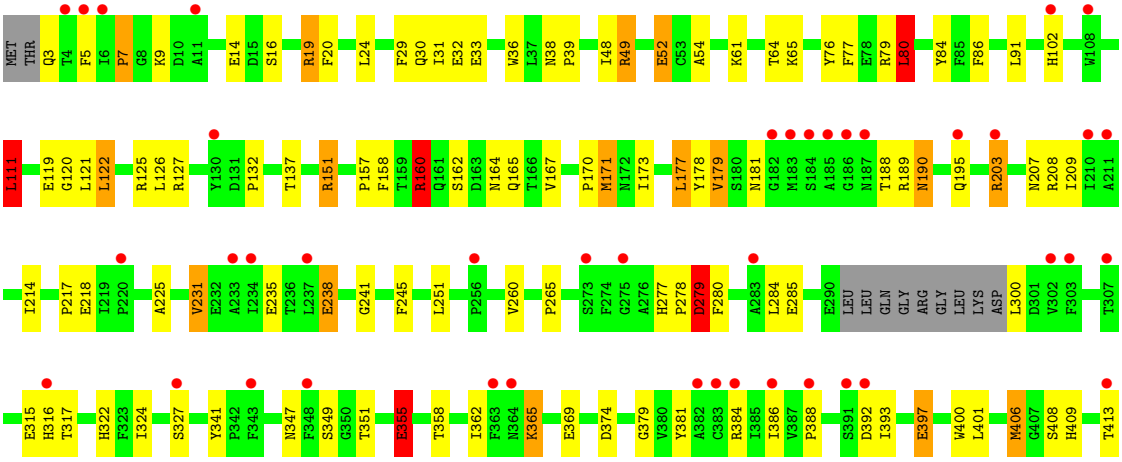
• Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

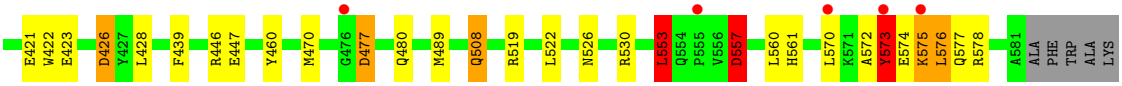
Chain E:



• Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

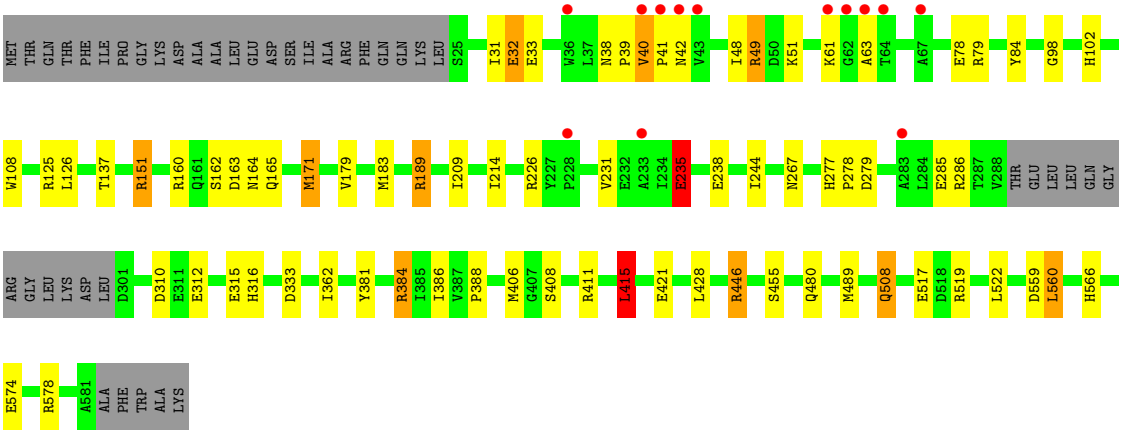
Chain F:





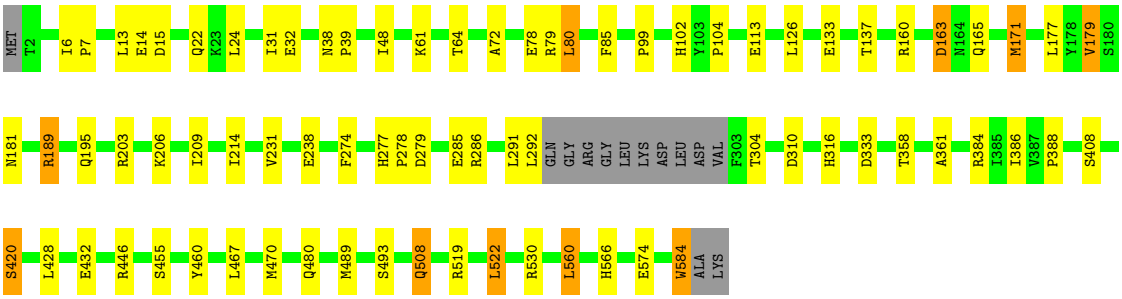
• Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

Chain G:



• Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	110.28Å 112.40Å 130.68Å 89.40° 73.63° 77.62°	Depositor
Resolution (Å)	125.20 – 3.29 125.21 – 3.29	Depositor EDS
% Data completeness (in resolution range)	99.0 (125.20-3.29) 99.0 (125.21-3.29)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 3.26Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.190 , 0.239 0.192 , 0.237	Depositor DCC
R_{free} test set	4442 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	63.4	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	36421	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.54	0/4534	0.73	13/6168 (0.2%)
1	B	0.58	0/4649	0.75	6/6326 (0.1%)
1	C	0.56	0/4560	0.75	8/6204 (0.1%)
1	D	0.58	0/4636	0.77	9/6307 (0.1%)
1	E	0.60	0/4642	0.75	6/6316 (0.1%)
1	F	0.61	1/4619 (0.0%)	0.90	23/6284 (0.4%)
1	G	0.55	0/4418	0.80	14/6013 (0.2%)
1	H	0.62	2/4652 (0.0%)	0.77	8/6330 (0.1%)
All	All	0.58	3/36710 (0.0%)	0.78	87/49948 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
1	F	0	3
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	584	TRP	CB-CG	6.58	1.62	1.50
1	F	573	TYR	CB-CG	-6.44	1.42	1.51
1	H	493	SER	CA-CB	5.66	1.61	1.52

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	208	ARG	NE-CZ-NH1	11.64	126.12	120.30
1	D	163	ASP	CB-CA-C	-11.16	88.08	110.40
1	G	384	ARG	NE-CZ-NH2	-11.06	114.77	120.30
1	F	208	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	G	151	ARG	CG-CD-NE	10.28	133.39	111.80
1	G	446	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	G	384	ARG	CG-CD-NE	9.74	132.25	111.80
1	B	319	LEU	CA-CB-CG	9.28	136.63	115.30
1	F	573	TYR	N-CA-CB	9.20	127.17	110.60
1	F	426	ASP	CB-CG-OD2	-9.20	110.02	118.30
1	F	557	ASP	CB-CG-OD2	9.20	126.58	118.30
1	F	80	LEU	CA-CB-CG	8.70	135.31	115.30
1	F	355	GLU	CA-CB-CG	-8.11	95.56	113.40
1	F	576	LEU	CB-CG-CD2	7.72	124.13	111.00
1	G	446	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	E	384	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	C	19	ARG	CA-CB-CG	7.03	128.87	113.40
1	F	384	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	H	560	LEU	CB-CG-CD2	6.91	122.74	111.00
1	A	560	LEU	CB-CG-CD1	6.88	122.70	111.00
1	F	576	LEU	CA-CB-CG	6.85	131.06	115.30
1	F	576	LEU	CB-CG-CD1	-6.84	99.38	111.00
1	A	291	LEU	CA-CB-CG	6.73	130.77	115.30
1	H	384	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	G	235	GLU	CA-CB-CG	6.61	127.95	113.40
1	E	560	LEU	CB-CG-CD1	6.59	122.21	111.00
1	E	386	ILE	CG1-CB-CG2	-6.58	96.93	111.40
1	C	560	LEU	CB-CG-CD2	6.57	122.17	111.00
1	A	530	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	F	426	ASP	CB-CA-C	6.41	123.21	110.40
1	A	384	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	319	LEU	CB-CG-CD2	6.37	121.82	111.00
1	F	553	LEU	CA-CB-CG	6.36	129.92	115.30
1	G	415	LEU	CA-CB-CG	6.36	129.92	115.30
1	D	560	LEU	CB-CG-CD1	6.33	121.76	111.00
1	F	560	LEU	CB-CG-CD1	6.32	121.74	111.00
1	G	560	LEU	CB-CG-CD2	6.30	121.71	111.00
1	B	560	LEU	CB-CG-CD2	6.15	121.46	111.00
1	H	163	ASP	C-N-CA	-6.15	106.33	121.70
1	B	384	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	C	384	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	C	355	GLU	CG-CD-OE2	6.03	130.36	118.30
1	E	446	ARG	CG-CD-NE	-6.01	99.17	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	125	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	H	493	SER	CB-CA-C	5.91	121.33	110.10
1	D	384	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	286	ARG	CB-CG-CD	-5.86	96.37	111.60
1	G	32	GLU	CB-CA-C	-5.86	98.69	110.40
1	D	189	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	D	163	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	H	189	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	F	7	PRO	N-CA-C	5.76	127.07	112.10
1	C	189	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	571	LYS	CB-CG-CD	5.67	126.34	111.60
1	F	151	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	C	355	GLU	CG-CD-OE1	-5.55	107.19	118.30
1	G	49	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	G	40	VAL	CB-CA-C	5.53	121.90	111.40
1	F	279	ASP	N-CA-CB	5.52	120.54	110.60
1	G	189	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	326	SER	N-CA-CB	5.47	118.71	110.50
1	F	560	LEU	CA-CB-CG	5.46	127.85	115.30
1	A	189	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	516	GLU	CG-CD-OE2	5.41	129.12	118.30
1	A	560	LEU	CA-CB-CG	5.40	127.71	115.30
1	F	477	ASP	CB-CA-C	5.37	121.15	110.40
1	D	560	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	140	MET	CA-CB-CG	5.37	122.42	113.30
1	F	160	ARG	CG-CD-NE	-5.33	100.61	111.80
1	A	560	LEU	CB-CG-CD2	-5.33	101.95	111.00
1	E	578	ARG	CB-CG-CD	5.29	125.36	111.60
1	D	516	GLU	CG-CD-OE1	-5.25	107.81	118.30
1	E	560	LEU	CA-CB-CG	5.25	127.36	115.30
1	F	151	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	H	432	GLU	CB-CA-C	5.21	120.82	110.40
1	C	125	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	F	111	LEU	CA-CB-CG	5.17	127.19	115.30
1	B	14	GLU	CG-CD-OE1	-5.15	108.00	118.30
1	G	446	ARG	CD-NE-CZ	5.15	130.81	123.60
1	H	420	SER	N-CA-C	5.10	124.77	111.00
1	D	14	GLU	CG-CD-OE1	-5.09	108.13	118.30
1	F	477	ASP	N-CA-CB	5.09	119.76	110.60
1	A	140	MET	CB-CA-C	5.07	120.53	110.40
1	D	516	GLU	CG-CD-OE2	5.05	128.41	118.30
1	C	105	ASN	N-CA-CB	-5.05	101.52	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	516	GLU	CG-CD-OE1	-5.04	108.21	118.30
1	H	163	ASP	CA-C-N	5.01	128.22	117.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	324	ILE	Peptide
1	D	324	ILE	Peptide
1	F	120	GLY	Peptide
1	F	324	ILE	Peptide
1	F	5	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4424	0	4193	42	1
1	B	4535	0	4301	42	2
1	C	4450	0	4216	46	0
1	D	4523	0	4292	46	0
1	E	4530	0	4302	24	1
1	F	4507	0	4273	140	0
1	G	4309	0	4073	39	0
1	H	4537	0	4302	42	0
2	A	31	0	14	1	0
2	B	31	0	14	2	0
2	D	31	0	14	3	0
2	E	31	0	14	0	0
2	H	31	0	14	4	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	G	1	0	0	0	0
3	H	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	53	0	0	9	0
4	B	42	0	0	6	0
4	C	42	0	0	6	0
4	D	60	0	0	7	0
4	E	50	0	0	4	0
4	F	76	0	0	30	0
4	G	54	0	0	7	0
4	H	55	0	0	5	0
All	All	36421	0	34022	401	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (401) 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:F:570:LEU:CD2	1:F:573:TYR:OH	1.82	1.27
1:F:16:SER:O	1:F:20:PHE:HD2	1.24	1.18
1:G:32:GLU:OE1	1:G:49:ARG:NH1	1.79	1.16
1:F:158:PHE:HA	4:F:650:HOH:O	1.52	1.09
1:F:181:ASN:HB2	1:F:393:ILE:HD11	1.27	1.05
1:F:355:GLU:OE2	1:F:355:GLU:HA	1.51	1.05
1:F:231:VAL:O	1:F:235:GLU:OE1	1.73	1.04
1:F:91:LEU:HD22	1:F:573:TYR:CZ	1.95	1.01
1:F:570:LEU:HD22	1:F:573:TYR:CZ	1.95	1.01
1:C:349:SER:HA	1:C:355:GLU:OE1	1.60	1.00
1:F:570:LEU:HD22	1:F:573:TYR:OH	1.57	1.00
1:F:16:SER:O	1:F:20:PHE:CD2	2.16	0.99
1:F:29:PHE:CD1	1:F:575:LYS:HE3	2.00	0.96
1:F:167:VAL:HB	4:F:619:HOH:O	1.64	0.94
1:F:347:ASN:ND2	4:F:613:HOH:O	1.95	0.94
1:F:570:LEU:CD2	1:F:573:TYR:CZ	2.52	0.92
1:B:2:THR:O	1:B:14:GLU:HG3	1.69	0.92
1:F:151:ARG:NH1	4:F:607:HOH:O	2.05	0.90
1:C:258:ILE:HG21	1:C:284:LEU:HD23	1.54	0.89
1:D:2:THR:O	1:D:14:GLU:HG3	1.71	0.89
1:D:9:LYS:HB3	4:D:706:HOH:O	1.74	0.88
1:B:293:GLN:N	4:B:740:HOH:O	2.07	0.86
1:H:467:LEU:HA	1:H:470:MET:HE2	1.58	0.85
1:F:181:ASN:CB	1:F:393:ILE:HD11	2.09	0.83
1:F:355:GLU:OE2	1:F:358:THR:OG1	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:ASN:OD1	1:G:63:ALA:HB1	1.81	0.80
1:F:24:LEU:HD22	1:F:29:PHE:CZ	2.17	0.80
1:F:557:ASP:OD2	1:F:561:HIS:HB2	1.82	0.79
1:B:134:ASN:ND2	1:H:133:GLU:OE1	2.15	0.79
1:F:570:LEU:HD21	1:F:573:TYR:OH	1.83	0.79
1:F:327:SER:HA	4:F:669:HOH:O	1.82	0.79
1:C:230:VAL:HG11	1:C:284:LEU:HD13	1.63	0.79
1:F:125:ARG:HD3	1:F:369:GLU:OE1	1.84	0.78
1:C:519:ARG:NH2	1:D:310:ASP:OD1	2.16	0.77
1:A:408:SER:OG	4:A:750:HOH:O	2.01	0.77
1:A:526:ASN:HB2	4:A:729:HOH:O	1.84	0.76
1:E:49:ARG:HG2	4:E:732:HOH:O	1.84	0.76
1:F:160:ARG:HH12	1:F:369:GLU:HB3	1.50	0.75
1:G:489:MET:HG2	4:G:753:HOH:O	1.85	0.75
2:D:601:APC:PG	4:D:708:HOH:O	2.44	0.75
1:F:362:ILE:HA	4:F:616:HOH:O	1.86	0.75
1:A:545:SER:HB3	1:C:525:LEU:HD21	1.69	0.74
1:F:260:VAL:HG21	4:F:606:HOH:O	1.87	0.73
1:F:33:GLU:OE1	1:F:36:TRP:CZ2	2.41	0.73
1:F:24:LEU:CD2	1:F:29:PHE:CZ	2.72	0.73
1:C:230:VAL:HG11	1:C:284:LEU:CD1	2.17	0.72
1:F:24:LEU:HD22	1:F:29:PHE:CE2	2.23	0.72
1:F:29:PHE:CE1	1:F:575:LYS:HE3	2.23	0.72
1:B:397:GLU:OE1	1:B:401:LEU:HD12	1.91	0.71
1:C:194:VAL:HG23	1:C:359:LEU:HD12	1.71	0.71
1:F:397:GLU:OE1	1:F:401:LEU:HD12	1.90	0.71
1:E:158:PHE:CE2	1:E:386:ILE:HD13	2.25	0.71
1:E:397:GLU:OE1	1:E:401:LEU:HD12	1.91	0.71
1:F:284:LEU:HD12	4:F:606:HOH:O	1.91	0.70
2:D:601:APC:O3G	4:D:708:HOH:O	2.08	0.70
1:F:3:GLN:O	1:F:7:PRO:HG3	1.89	0.70
1:F:225:ALA:O	4:F:652:HOH:O	2.10	0.69
1:F:157:PRO:O	4:F:650:HOH:O	2.11	0.69
1:C:560:LEU:HD13	1:C:566:HIS:CE1	2.28	0.69
2:D:601:APC:O2B	2:D:601:APC:O1G	2.11	0.69
1:E:310:ASP:OD1	1:F:519:ARG:NH2	2.28	0.67
1:H:48:ILE:HD12	1:H:72:ALA:HB1	1.77	0.67
1:F:570:LEU:HD23	1:F:573:TYR:OH	1.86	0.66
1:F:260:VAL:CG2	4:F:606:HOH:O	2.43	0.66
1:F:577:GLN:HB3	4:F:626:HOH:O	1.96	0.66
1:F:160:ARG:HH21	1:F:162:SER:HB3	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:LEU:O	4:B:729:HOH:O	2.13	0.65
1:F:203:ARG:NH2	1:F:392:ASP:O	2.29	0.65
1:F:160:ARG:NH1	1:F:369:GLU:HB3	2.11	0.65
1:F:570:LEU:CD2	1:F:573:TYR:HH	2.05	0.65
1:D:48:ILE:HG13	1:D:58:THR:HG22	1.80	0.64
1:G:560:LEU:HD13	1:G:566:HIS:CE1	2.32	0.64
1:F:19:ARG:NH2	1:F:379:GLY:O	2.30	0.64
1:F:355:GLU:OE2	1:F:355:GLU:CA	2.36	0.63
1:F:20:PHE:HD1	1:F:77:PHE:CD2	2.17	0.63
1:F:86:PHE:CE2	1:F:573:TYR:HD1	2.17	0.62
1:F:489:MET:HE1	1:F:508:GLN:NE2	2.14	0.62
1:F:241:GLY:HA2	4:F:622:HOH:O	1.99	0.62
1:G:235:GLU:OE1	1:G:235:GLU:HA	2.00	0.62
1:F:447:GLU:HG2	4:F:675:HOH:O	1.99	0.62
1:B:353:GLU:HB2	4:B:713:HOH:O	1.99	0.62
1:H:15:ASP:HB3	4:H:707:HOH:O	1.99	0.62
1:C:78:GLU:OE2	1:C:79:ARG:NH1	2.33	0.62
1:F:151:ARG:NE	4:F:667:HOH:O	2.31	0.62
1:A:273:SER:HB2	1:A:291:LEU:CD1	2.30	0.61
1:A:520:GLN:NE2	1:C:517:GLU:O	2.34	0.61
1:G:226:ARG:CG	4:G:731:HOH:O	2.47	0.61
1:A:22:GLN:HG3	4:A:726:HOH:O	2.01	0.61
1:F:24:LEU:CD2	1:F:29:PHE:HZ	2.13	0.60
1:F:86:PHE:CD2	1:F:573:TYR:CD1	2.89	0.60
1:C:226:ARG:NH2	1:C:345:ASP:OD2	2.34	0.60
1:D:58:THR:HG21	1:D:72:ALA:O	2.02	0.60
1:F:251:LEU:HA	1:F:341:TYR:CD2	2.37	0.59
1:C:310:ASP:OD1	1:D:519:ARG:NH2	2.35	0.59
1:G:519:ARG:NH1	1:H:333:ASP:OD1	2.36	0.59
1:C:219:ILE:HG12	1:C:224:LEU:HG	1.85	0.59
1:F:132:PRO:HB3	4:F:637:HOH:O	2.02	0.59
1:C:258:ILE:HG21	1:C:284:LEU:CD2	2.31	0.59
1:C:329:LEU:HA	4:C:739:HOH:O	2.02	0.59
1:F:400:TRP:O	1:F:406:MET:CE	2.51	0.58
1:H:78:GLU:OE2	1:H:79:ARG:NH1	2.35	0.58
1:G:78:GLU:OE2	1:G:79:ARG:NH1	2.35	0.58
1:F:91:LEU:HD22	1:F:573:TYR:OH	2.02	0.58
1:F:217:PRO:HA	4:F:605:HOH:O	2.03	0.58
1:F:577:GLN:CB	4:F:626:HOH:O	2.51	0.58
1:B:2:THR:O	1:B:14:GLU:CG	2.49	0.58
1:F:570:LEU:HD23	1:F:573:TYR:CZ	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:GLU:HA	4:B:704:HOH:O	2.04	0.57
1:B:560:LEU:HD13	1:B:566:HIS:CE1	2.39	0.57
1:D:423:GLU:HB3	4:D:710:HOH:O	2.03	0.57
1:H:467:LEU:HD12	1:H:470:MET:CE	2.35	0.57
1:A:333:ASP:OD1	1:B:519:ARG:NH1	2.38	0.57
1:C:400:TRP:O	1:C:406:MET:CE	2.53	0.57
1:F:16:SER:OG	1:F:20:PHE:HE2	1.87	0.57
1:D:48:ILE:CG1	1:D:58:THR:HG22	2.35	0.56
1:C:516:GLU:HB3	4:C:705:HOH:O	2.05	0.56
1:F:111:LEU:HD23	1:F:111:LEU:H	1.68	0.56
1:G:519:ARG:NH2	1:H:310:ASP:OD1	2.32	0.56
1:E:99:PRO:HA	1:H:99:PRO:HA	1.87	0.56
1:F:439:PHE:HD1	4:F:653:HOH:O	1.89	0.56
1:G:489:MET:HE1	1:G:508:GLN:NE2	2.21	0.56
1:D:2:THR:O	1:D:14:GLU:CG	2.50	0.55
1:D:48:ILE:HG12	1:D:58:THR:CG2	2.36	0.55
1:F:49:ARG:NH1	1:F:54:ALA:O	2.39	0.55
1:H:560:LEU:HD13	1:H:566:HIS:CE1	2.41	0.55
1:D:27:LEU:HD21	1:D:378:LEU:HD22	1.89	0.55
1:D:23:LYS:O	1:D:27:LEU:HD13	2.05	0.55
1:F:322:HIS:HE1	4:F:659:HOH:O	1.89	0.55
1:D:6:ILE:HG12	1:D:9:LYS:HG2	1.88	0.55
1:C:124:ASP:HB2	4:C:735:HOH:O	2.06	0.55
1:H:48:ILE:HD12	1:H:72:ALA:CB	2.37	0.54
1:D:48:ILE:CG1	1:D:58:THR:CG2	2.85	0.54
1:F:400:TRP:O	1:F:406:MET:HE3	2.05	0.54
1:F:280:PHE:N	4:F:613:HOH:O	2.36	0.54
1:F:358:THR:CG2	4:F:666:HOH:O	2.55	0.54
1:E:238:GLU:OE2	1:F:530:ARG:NH2	2.35	0.54
1:F:178:TYR:O	1:F:393:ILE:HD12	2.07	0.54
1:H:31:ILE:HG23	1:H:48:ILE:HG23	1.90	0.54
1:E:49:ARG:NH1	1:E:54:ALA:O	2.41	0.54
1:B:522:LEU:HB2	4:B:733:HOH:O	2.07	0.54
1:D:65:LYS:HB3	4:D:748:HOH:O	2.07	0.53
1:G:32:GLU:CD	1:G:51:LYS:HG3	2.27	0.53
1:F:30:GLN:HB2	1:F:52:GLU:OE2	2.08	0.53
1:C:489:MET:HE1	1:C:508:GLN:NE2	2.24	0.53
2:H:601:APC:N3	2:H:601:APC:H5'2	2.24	0.53
1:F:31:ILE:HG21	1:F:48:ILE:HD11	1.91	0.53
1:F:173:ILE:HG23	1:F:177:LEU:HD22	1.91	0.53
1:B:489:MET:HE1	1:B:508:GLN:NE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:409:HIS:HB2	4:F:631:HOH:O	2.08	0.53
1:H:522:LEU:HB2	4:H:745:HOH:O	2.09	0.52
1:C:49:ARG:HD3	4:C:703:HOH:O	2.08	0.52
1:A:526:ASN:OD1	1:A:527:ALA:N	2.42	0.52
1:G:162:SER:HA	4:G:742:HOH:O	2.10	0.52
1:H:177:LEU:C	4:H:753:HOH:O	2.48	0.52
1:H:489:MET:HE1	1:H:508:GLN:NE2	2.25	0.52
1:G:39:PRO:HA	4:G:719:HOH:O	2.09	0.52
1:E:333:ASP:OD1	1:F:519:ARG:NH1	2.42	0.51
4:E:717:HOH:O	1:F:265:PRO:CB	2.58	0.51
1:D:48:ILE:HG12	1:D:58:THR:HG23	1.93	0.51
2:H:601:APC:O2A	2:H:601:APC:C3'	2.59	0.51
1:F:29:PHE:CD1	1:F:575:LYS:CE	2.86	0.51
1:C:452:ALA:H	1:C:566:HIS:HD2	1.59	0.51
1:C:530:ARG:NH2	1:D:238:GLU:OE2	2.30	0.51
1:E:277:HIS:CD2	1:E:278:PRO:HD2	2.46	0.51
1:F:24:LEU:HD23	1:F:29:PHE:CZ	2.45	0.51
1:H:574:GLU:HG2	4:H:720:HOH:O	2.10	0.51
1:D:58:THR:OG1	1:D:75:GLU:HB3	2.11	0.50
1:A:530:ARG:NE	4:A:712:HOH:O	2.20	0.50
1:B:277:HIS:CG	1:B:278:PRO:HD2	2.46	0.50
1:B:277:HIS:CD2	1:B:278:PRO:HD2	2.47	0.50
1:C:278:PRO:HB2	1:C:355:GLU:OE1	2.12	0.50
1:G:31:ILE:HG23	1:G:48:ILE:HG23	1.92	0.50
1:G:108:TRP:CD1	1:G:151:ARG:NH1	2.80	0.50
1:D:489:MET:HE1	1:D:508:GLN:NE2	2.26	0.50
1:A:195:GLN:NE2	1:A:286:ARG:NH2	2.59	0.50
1:A:489:MET:HE2	1:A:508:GLN:HG3	1.94	0.50
1:G:277:HIS:CD2	1:G:278:PRO:HD2	2.46	0.50
1:A:277:HIS:CG	1:A:278:PRO:HD2	2.47	0.49
1:F:91:LEU:HB3	1:F:573:TYR:CE2	2.47	0.49
1:D:351:THR:HG22	1:D:354:GLU:HG3	1.94	0.49
1:G:33:GLU:HA	1:G:48:ILE:CD1	2.42	0.49
1:D:136:LEU:HD11	1:D:141:LEU:HD11	1.95	0.49
1:C:531:MET:O	1:D:265:PRO:HB3	2.12	0.49
1:F:91:LEU:HD22	1:F:573:TYR:CE1	2.43	0.49
1:G:411:ARG:HG2	1:G:415:LEU:HD22	1.95	0.49
1:F:355:GLU:N	1:F:355:GLU:CD	2.63	0.49
1:C:242:PHE:CZ	1:C:300:LEU:HD12	2.48	0.48
1:F:111:LEU:H	1:F:111:LEU:CD2	2.26	0.48
1:A:31:ILE:HG21	1:A:48:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:SER:OG	1:F:20:PHE:CE2	2.61	0.48
1:B:134:ASN:CG	1:H:133:GLU:OE1	2.51	0.48
1:G:333:ASP:OD1	1:H:519:ARG:NH1	2.46	0.48
1:F:33:GLU:OE1	1:F:36:TRP:CH2	2.66	0.48
1:E:277:HIS:CG	1:E:278:PRO:HD2	2.49	0.48
1:G:33:GLU:HA	1:G:48:ILE:HD13	1.96	0.48
1:B:136:LEU:HD11	1:B:141:LEU:HD11	1.96	0.48
1:E:489:MET:HE1	1:E:508:GLN:NE2	2.29	0.48
1:H:22:GLN:HA	1:H:22:GLN:NE2	2.29	0.48
1:G:244:ILE:O	1:H:530:ARG:NH2	2.47	0.48
1:D:61:LYS:HB2	1:D:289:THR:CG2	2.44	0.48
1:F:251:LEU:HD22	1:F:341:TYR:HE2	1.79	0.48
1:H:277:HIS:CG	1:H:278:PRO:HD2	2.49	0.48
1:C:405:SER:HB2	4:C:730:HOH:O	2.13	0.47
1:B:104:PRO:HG2	1:B:584:TRP:CE3	2.49	0.47
1:C:277:HIS:CD2	1:C:278:PRO:HD2	2.49	0.47
1:D:230:VAL:HG23	4:D:734:HOH:O	2.13	0.47
1:F:422:TRP:CB	1:F:426:ASP:OD1	2.62	0.47
1:F:423:GLU:O	1:F:426:ASP:OD1	2.32	0.47
1:A:277:HIS:CD2	1:A:278:PRO:HD2	2.49	0.47
1:D:5:PHE:HA	1:D:9:LYS:NZ	2.29	0.47
1:F:365:LYS:HE3	1:F:365:LYS:HB3	1.71	0.47
1:A:71:SER:OG	2:A:601:APC:O1A	2.21	0.47
1:A:489:MET:HE3	1:A:489:MET:HB2	1.53	0.47
1:B:160:ARG:NH1	1:B:163:ASP:OD2	2.48	0.47
1:F:111:LEU:HD23	1:F:111:LEU:N	2.28	0.47
1:F:126:LEU:CD2	1:F:388:PRO:HG3	2.45	0.47
1:C:400:TRP:O	1:C:406:MET:HE3	2.14	0.47
1:E:242:PHE:CZ	1:E:300:LEU:HD12	2.50	0.47
1:F:102:HIS:CE1	1:F:171:MET:HG2	2.50	0.47
1:F:422:TRP:HB3	1:F:426:ASP:OD1	2.15	0.47
1:D:126:LEU:CD2	1:D:388:PRO:HG3	2.45	0.46
1:G:102:HIS:CE1	1:G:171:MET:HG2	2.49	0.46
1:C:277:HIS:CG	1:C:278:PRO:HD2	2.50	0.46
1:D:429:ASN:OD1	1:D:430:LEU:N	2.48	0.46
1:F:572:ALA:O	1:F:575:LYS:HD3	2.16	0.46
1:F:351:THR:HB	4:F:628:HOH:O	2.16	0.46
2:H:601:APC:O2A	2:H:601:APC:C4'	2.63	0.46
1:A:171:MET:CE	4:A:748:HOH:O	2.63	0.46
1:A:519:ARG:NH1	1:B:333:ASP:OD1	2.48	0.46
1:B:286:ARG:NH1	2:B:601:APC:H3A1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:GLU:OE1	1:E:14:GLU:N	2.48	0.46
1:F:86:PHE:CD2	1:F:573:TYR:HD1	2.30	0.46
1:F:245:PHE:HA	4:F:630:HOH:O	2.15	0.46
1:C:194:VAL:HG23	1:C:359:LEU:CD1	2.43	0.46
1:F:31:ILE:CG2	1:F:48:ILE:HD11	2.46	0.46
1:H:160:ARG:NH1	1:H:163:ASP:OD2	2.49	0.46
1:A:126:LEU:CD2	1:A:388:PRO:HG3	2.46	0.46
1:D:6:ILE:HD13	1:D:13:LEU:HD21	1.98	0.46
1:D:38:ASN:N	1:D:39:PRO:CD	2.78	0.46
1:D:277:HIS:CD2	1:D:278:PRO:HD2	2.51	0.46
1:F:179:VAL:CG2	1:F:393:ILE:HD13	2.46	0.46
1:F:218:GLU:HG3	4:F:623:HOH:O	2.16	0.46
1:G:126:LEU:CD2	1:G:388:PRO:HG3	2.45	0.46
1:H:179:VAL:HG13	4:H:753:HOH:O	2.16	0.46
1:C:327:SER:O	1:C:327:SER:OG	2.32	0.46
1:B:126:LEU:CD2	1:B:388:PRO:HG3	2.47	0.45
1:F:203:ARG:NH2	1:F:207:ASN:ND2	2.65	0.45
1:F:470:MET:SD	1:F:553:LEU:HD21	2.57	0.45
1:G:277:HIS:CG	1:G:278:PRO:HD2	2.51	0.45
1:A:577:GLN:HG3	4:A:708:HOH:O	2.15	0.45
1:C:102:HIS:CE1	1:C:171:MET:HG2	2.52	0.45
4:E:717:HOH:O	1:F:265:PRO:HB3	2.16	0.45
1:F:76:TYR:O	1:F:80:LEU:HD23	2.16	0.45
1:F:557:ASP:OD2	1:F:561:HIS:CB	2.61	0.45
1:E:386:ILE:HG22	1:E:388:PRO:HD3	1.97	0.45
1:F:209:ILE:HA	1:F:214:ILE:HD12	1.98	0.45
1:F:238:GLU:HG3	4:F:624:HOH:O	2.15	0.45
1:G:98:GLY:O	1:G:151:ARG:NH2	2.46	0.45
1:F:470:MET:SD	1:F:553:LEU:CD2	3.05	0.45
1:H:102:HIS:CE1	1:H:171:MET:HG2	2.51	0.45
1:A:310:ASP:OD1	1:B:519:ARG:NH2	2.41	0.45
1:H:277:HIS:CD2	1:H:278:PRO:HD2	2.51	0.45
1:C:519:ARG:NH1	1:D:333:ASP:OD1	2.49	0.45
1:D:277:HIS:CG	1:D:278:PRO:HD2	2.52	0.45
1:B:446:ARG:HD3	1:B:460:TYR:HA	1.99	0.45
1:C:126:LEU:CD2	1:C:388:PRO:HG3	2.47	0.45
1:D:566:HIS:HD2	1:D:570:LEU:HD22	1.82	0.45
1:A:102:HIS:CE1	1:A:171:MET:HG2	2.51	0.45
1:B:24:LEU:HD13	1:B:31:ILE:HG13	1.99	0.45
1:H:126:LEU:CD2	1:H:388:PRO:HG3	2.46	0.45
1:B:102:HIS:CE1	1:B:171:MET:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:TRP:O	1:C:406:MET:HE1	2.17	0.45
1:E:126:LEU:CD2	1:E:388:PRO:HG3	2.47	0.45
1:F:14:GLU:OE1	1:F:14:GLU:N	2.48	0.44
1:F:79:ARG:HD3	1:F:84:TYR:HB3	1.99	0.44
1:F:121:LEU:O	1:F:127:ARG:NH1	2.46	0.44
1:C:279:ASP:C	1:C:279:ASP:OD1	2.56	0.44
1:F:358:THR:HG21	4:F:666:HOH:O	2.17	0.44
1:C:209:ILE:HA	1:C:214:ILE:HD12	1.99	0.44
1:F:132:PRO:HG3	4:F:637:HOH:O	2.17	0.44
1:G:84:TYR:HB2	1:G:183:MET:HE1	1.99	0.44
1:B:14:GLU:OE1	1:B:14:GLU:N	2.49	0.44
1:F:421:GLU:N	4:F:651:HOH:O	2.51	0.44
1:A:24:LEU:HD13	1:A:31:ILE:HG13	2.00	0.44
1:B:327:SER:O	1:B:327:SER:OG	2.33	0.44
1:F:277:HIS:CD2	1:F:278:PRO:HD2	2.53	0.44
1:F:277:HIS:CG	1:F:278:PRO:HD2	2.52	0.44
1:C:38:ASN:N	1:C:39:PRO:CD	2.81	0.43
1:F:446:ARG:HD3	1:F:460:TYR:HA	2.00	0.43
1:F:570:LEU:HA	1:F:573:TYR:CE1	2.53	0.43
1:B:6:ILE:HD13	1:B:13:LEU:HD21	1.99	0.43
1:F:570:LEU:HD23	1:F:573:TYR:CE1	2.53	0.43
1:G:209:ILE:HA	1:G:214:ILE:HD12	2.00	0.43
1:F:122:LEU:HD13	1:F:170:PRO:HD3	2.00	0.43
1:G:38:ASN:N	1:G:39:PRO:CD	2.82	0.43
1:G:160:ARG:NH1	1:G:163:ASP:OD2	2.52	0.43
1:A:144:LEU:HA	4:A:750:HOH:O	2.17	0.43
1:B:113:GLU:HG3	1:B:114:ASN:N	2.33	0.43
1:B:209:ILE:HA	1:B:214:ILE:HD12	2.01	0.43
1:C:386:ILE:HG22	1:C:388:PRO:HD3	2.01	0.43
1:E:102:HIS:CE1	1:E:171:MET:HG2	2.54	0.43
1:A:446:ARG:HD3	1:A:460:TYR:HA	1.99	0.43
1:B:117:VAL:CG2	1:B:136:LEU:HD13	2.49	0.43
1:B:279:ASP:OD1	1:B:279:ASP:C	2.57	0.43
1:H:38:ASN:N	1:H:39:PRO:CD	2.81	0.43
1:B:117:VAL:HG21	1:B:136:LEU:HD13	2.01	0.43
1:B:286:ARG:NH1	2:B:601:APC:C3A	2.82	0.43
1:G:386:ILE:HG22	1:G:388:PRO:HD3	2.00	0.43
1:A:103:TYR:CZ	1:A:375:TYR:CE1	3.07	0.43
1:D:117:VAL:HG21	1:D:136:LEU:HD13	2.01	0.43
1:G:381:TYR:HB3	4:G:709:HOH:O	2.19	0.43
1:H:386:ILE:HG22	1:H:388:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:HB2	1:A:289:THR:CG2	2.49	0.43
1:A:386:ILE:HG22	1:A:388:PRO:HD3	2.00	0.43
1:C:144:LEU:HA	4:C:730:HOH:O	2.19	0.43
1:A:31:ILE:CG2	1:A:48:ILE:HD11	2.49	0.42
1:F:24:LEU:HD13	1:F:31:ILE:HG13	2.00	0.42
1:A:531:MET:O	1:B:265:PRO:HB3	2.19	0.42
1:A:547:GLU:OE2	1:C:529:VAL:HG11	2.19	0.42
1:D:27:LEU:CD2	1:D:378:LEU:HD22	2.50	0.42
1:D:117:VAL:CG2	1:D:136:LEU:HD13	2.48	0.42
1:E:574:GLU:HB3	1:E:578:ARG:NH1	2.34	0.42
1:F:160:ARG:NE	1:F:162:SER:OG	2.52	0.42
1:A:14:GLU:OE1	1:A:14:GLU:N	2.49	0.42
1:D:209:ILE:HA	1:D:214:ILE:HD12	2.01	0.42
1:D:386:ILE:HG22	1:D:388:PRO:HD3	2.00	0.42
1:A:160:ARG:NH1	1:A:163:ASP:OD2	2.52	0.42
1:B:38:ASN:N	1:B:39:PRO:CD	2.80	0.42
1:F:316:HIS:CD2	1:F:317:THR:HG23	2.54	0.42
1:A:209:ILE:HA	1:A:214:ILE:HD12	2.00	0.42
1:B:386:ILE:HG22	1:B:388:PRO:HD3	2.01	0.42
1:G:279:ASP:OD1	1:G:279:ASP:C	2.57	0.42
1:G:560:LEU:HD13	1:G:566:HIS:NE2	2.34	0.42
1:H:6:ILE:HD13	1:H:13:LEU:HD21	2.00	0.42
1:H:181:ASN:OD1	1:H:203:ARG:HD2	2.18	0.42
1:G:40:VAL:HG13	1:G:41:PRO:HD2	2.02	0.42
1:B:212:GLU:HG2	4:B:704:HOH:O	2.18	0.42
1:D:102:HIS:CE1	1:D:171:MET:HG2	2.54	0.42
1:F:36:TRP:CD1	1:F:65:LYS:HE3	2.54	0.42
1:H:24:LEU:HD13	1:H:31:ILE:HG13	2.00	0.42
1:H:104:PRO:HG2	1:H:584:TRP:CE3	2.54	0.42
1:H:446:ARG:HD3	1:H:460:TYR:HA	2.01	0.42
1:D:181:ASN:OD1	1:D:203:ARG:HD2	2.20	0.42
1:D:286:ARG:NH2	4:D:744:HOH:O	2.53	0.42
1:E:38:ASN:N	1:E:39:PRO:CD	2.83	0.42
1:E:209:ILE:HA	1:E:214:ILE:HD12	2.01	0.42
1:H:14:GLU:OE1	1:H:14:GLU:N	2.48	0.42
1:E:24:LEU:HD13	1:E:31:ILE:HG13	2.02	0.42
1:E:489:MET:HB2	1:E:489:MET:HE3	1.75	0.42
1:F:177:LEU:N	1:F:177:LEU:CD1	2.83	0.42
1:D:123:ASP:OD2	1:D:160:ARG:NH1	2.53	0.41
1:F:179:VAL:HG23	1:F:393:ILE:HD13	2.02	0.41
1:F:386:ILE:HG22	1:F:388:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:MET:HB2	1:B:489:MET:HE3	1.62	0.41
1:B:580:LYS:O	1:B:584:TRP:HE3	2.04	0.41
1:D:279:ASP:OD1	1:D:279:ASP:C	2.59	0.41
1:F:327:SER:O	1:F:327:SER:OG	2.32	0.41
1:G:519:ARG:NH1	1:H:333:ASP:OD2	2.53	0.41
1:H:209:ILE:HA	1:H:214:ILE:HD12	2.01	0.41
1:D:24:LEU:HD13	1:D:31:ILE:HG13	2.02	0.41
1:A:121:LEU:O	1:A:127:ARG:NH1	2.48	0.41
1:C:24:LEU:HD13	1:C:31:ILE:HG13	2.02	0.41
1:C:265:PRO:HB3	1:D:531:MET:O	2.19	0.41
1:F:188:THR:OG1	1:F:190:ASN:ND2	2.53	0.41
1:F:38:ASN:N	1:F:39:PRO:CD	2.83	0.41
1:A:279:ASP:OD1	1:A:279:ASP:C	2.58	0.41
1:H:80:LEU:CD1	1:H:85:PHE:CE2	3.03	0.41
1:A:22:GLN:CG	4:A:726:HOH:O	2.64	0.41
1:A:517:GLU:O	1:C:520:GLN:NE2	2.54	0.41
1:E:125:ARG:HD3	4:E:726:HOH:O	2.21	0.41
1:F:400:TRP:O	1:F:406:MET:HE1	2.21	0.41
1:F:573:TYR:HA	1:F:576:LEU:HD13	2.01	0.41
1:D:14:GLU:OE1	1:D:14:GLU:N	2.48	0.41
1:E:520:GLN:HA	1:E:520:GLN:OE1	2.21	0.41
1:G:310:ASP:OD1	1:H:519:ARG:NH2	2.49	0.41
1:G:362:ILE:HG23	4:G:717:HOH:O	2.20	0.41
1:H:206:LYS:HG3	1:H:274:PHE:CD1	2.56	0.41
1:A:530:ARG:NH2	1:B:244:ILE:O	2.54	0.41
1:F:29:PHE:CE2	1:F:31:ILE:HD11	2.56	0.41
1:F:29:PHE:HE2	1:F:31:ILE:HD11	1.85	0.41
1:F:160:ARG:NH2	1:F:162:SER:HB3	2.32	0.41
1:F:374:ASP:OD1	1:F:381:TYR:OH	2.34	0.41
1:F:489:MET:HB2	1:F:489:MET:HE3	1.76	0.41
1:G:108:TRP:NE1	1:G:151:ARG:NH1	2.69	0.41
1:H:279:ASP:C	1:H:279:ASP:OD1	2.59	0.41
1:A:38:ASN:N	1:A:39:PRO:CD	2.84	0.40
1:H:358:THR:O	1:H:361:ALA:HB3	2.21	0.40
1:B:187:ASN:HB2	1:B:191:GLU:OE1	2.22	0.40
1:C:123:ASP:OD2	1:C:160:ARG:NH1	2.55	0.40
1:F:203:ARG:CZ	1:F:392:ASP:O	2.68	0.40
1:F:279:ASP:HB3	1:F:349:SER:HB3	2.03	0.40
1:F:422:TRP:HB2	1:F:426:ASP:OD1	2.22	0.40
1:F:526:ASN:O	1:F:530:ARG:HG3	2.22	0.40
1:C:560:LEU:CD1	1:C:566:HIS:CE1	3.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:LEU:CD2	1:F:573:TYR:OH	2.69	0.40
1:G:226:ARG:HD3	4:G:731:HOH:O	2.22	0.40
1:H:80:LEU:HD13	1:H:85:PHE:CE2	2.57	0.40
1:A:218:GLU:HB3	4:A:730:HOH:O	2.21	0.40
1:A:273:SER:CB	1:A:291:LEU:CD1	2.99	0.40
1:E:123:ASP:OD2	1:E:160:ARG:NH1	2.54	0.40
2:H:601:APC:O2A	2:H:601:APC:H4'	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:GLU:OE1	1:B:107:LYS:NZ[1_455]	1.85	0.35
1:B:526:ASN:OD1	1:E:338:ASP:OD2[1_456]	1.89	0.31

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	555/586 (95%)	529 (95%)	25 (4%)	1 (0%)	47	77
1	B	569/586 (97%)	541 (95%)	27 (5%)	1 (0%)	47	77
1	C	558/586 (95%)	532 (95%)	24 (4%)	2 (0%)	34	66
1	D	568/586 (97%)	539 (95%)	28 (5%)	1 (0%)	47	77
1	E	569/586 (97%)	540 (95%)	27 (5%)	2 (0%)	34	66
1	F	566/586 (97%)	535 (94%)	30 (5%)	1 (0%)	47	77
1	G	541/586 (92%)	514 (95%)	26 (5%)	1 (0%)	47	77
1	H	569/586 (97%)	544 (96%)	23 (4%)	2 (0%)	34	66
All	All	4495/4688 (96%)	4274 (95%)	210 (5%)	11 (0%)	47	77

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	VAL
1	B	179	VAL
1	C	179	VAL
1	D	179	VAL
1	E	179	VAL
1	F	179	VAL
1	G	179	VAL
1	H	179	VAL
1	H	420	SER
1	E	118	PRO
1	C	118	PRO

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	466/487 (96%)	447 (96%)	19 (4%)	30	61
1	B	477/487 (98%)	448 (94%)	29 (6%)	18	48
1	C	470/487 (96%)	442 (94%)	28 (6%)	19	49
1	D	476/487 (98%)	441 (93%)	35 (7%)	13	40
1	E	478/487 (98%)	451 (94%)	27 (6%)	21	52
1	F	475/487 (98%)	431 (91%)	44 (9%)	9	30
1	G	454/487 (93%)	424 (93%)	30 (7%)	16	46
1	H	477/487 (98%)	452 (95%)	25 (5%)	23	54
All	All	3773/3896 (97%)	3536 (94%)	237 (6%)	18	47

All (237) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	61	LYS
1	A	64	THR

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Mol	Chain	Res	Type
1	A	137	THR
1	A	164	ASN
1	A	171	MET
1	A	189	ARG
1	A	195	GLN
1	A	231	VAL
1	A	238	GLU
1	A	285	GLU
1	A	291	LEU
1	A	408	SER
1	A	428	LEU
1	A	480	GLN
1	A	508	GLN
1	A	522	LEU
1	A	571	LYS
1	A	574	GLU
1	B	6	ILE
1	B	7	PRO
1	B	14	GLU
1	B	32	GLU
1	B	51	LYS
1	B	61	LYS
1	B	64	THR
1	B	113	GLU
1	B	136	LEU
1	B	137	THR
1	B	164	ASN
1	B	165	GLN
1	B	171	MET
1	B	195	GLN
1	B	231	VAL
1	B	285	GLU
1	B	286	ARG
1	B	291	LEU
1	B	315	GLU
1	B	316	HIS
1	B	397	GLU
1	B	408	SER
1	B	425	GLU
1	B	428	LEU
1	B	480	GLN
1	B	508	GLN

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Mol	Chain	Res	Type
1	B	522	LEU
1	B	559	ASP
1	B	574	GLU
1	C	14	GLU
1	C	32	GLU
1	C	61	LYS
1	C	64	THR
1	C	119	GLU
1	C	137	THR
1	C	164	ASN
1	C	171	MET
1	C	189	ARG
1	C	219	ILE
1	C	226	ARG
1	C	231	VAL
1	C	238	GLU
1	C	284	LEU
1	C	285	GLU
1	C	286	ARG
1	C	291	LEU
1	C	292	LEU
1	C	315	GLU
1	C	317	THR
1	C	406	MET
1	C	408	SER
1	C	428	LEU
1	C	480	GLN
1	C	522	LEU
1	C	547	GLU
1	C	574	GLU
1	C	578	ARG
1	D	7	PRO
1	D	14	GLU
1	D	32	GLU
1	D	61	LYS
1	D	64	THR
1	D	136	LEU
1	D	137	THR
1	D	145	GLN
1	D	164	ASN
1	D	171	MET
1	D	189	ARG

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Mol	Chain	Res	Type
1	D	195	GLN
1	D	231	VAL
1	D	238	GLU
1	D	285	GLU
1	D	286	ARG
1	D	291	LEU
1	D	292	LEU
1	D	315	GLU
1	D	316	HIS
1	D	321	THR
1	D	405	SER
1	D	406	MET
1	D	408	SER
1	D	428	LEU
1	D	429	ASN
1	D	455	SER
1	D	480	GLN
1	D	508	GLN
1	D	517	GLU
1	D	522	LEU
1	D	547	GLU
1	D	559	ASP
1	D	570	LEU
1	D	574	GLU
1	E	6	ILE
1	E	7	PRO
1	E	32	GLU
1	E	49	ARG
1	E	51	LYS
1	E	61	LYS
1	E	64	THR
1	E	137	THR
1	E	164	ASN
1	E	171	MET
1	E	195	GLN
1	E	231	VAL
1	E	238	GLU
1	E	285	GLU
1	E	286	ARG
1	E	291	LEU
1	E	292	LEU
1	E	316	HIS

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Mol	Chain	Res	Type
1	E	397	GLU
1	E	406	MET
1	E	408	SER
1	E	428	LEU
1	E	480	GLN
1	E	508	GLN
1	E	522	LEU
1	E	530	ARG
1	E	574	GLU
1	F	9	LYS
1	F	19	ARG
1	F	32	GLU
1	F	49	ARG
1	F	52	GLU
1	F	61	LYS
1	F	64	THR
1	F	80	LEU
1	F	111	LEU
1	F	119	GLU
1	F	122	LEU
1	F	137	THR
1	F	160	ARG
1	F	164	ASN
1	F	165	GLN
1	F	171	MET
1	F	177	LEU
1	F	189	ARG
1	F	190	ASN
1	F	195	GLN
1	F	203	ARG
1	F	231	VAL
1	F	238	GLU
1	F	279	ASP
1	F	285	GLU
1	F	300	LEU
1	F	315	GLU
1	F	355	GLU
1	F	365	LYS
1	F	397	GLU
1	F	406	MET
1	F	408	SER
1	F	413	THR

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Mol	Chain	Res	Type
1	F	428	LEU
1	F	477	ASP
1	F	480	GLN
1	F	508	GLN
1	F	522	LEU
1	F	553	LEU
1	F	557	ASP
1	F	573	TYR
1	F	574	GLU
1	F	575	LYS
1	F	578	ARG
1	G	61	LYS
1	G	137	THR
1	G	164	ASN
1	G	165	GLN
1	G	171	MET
1	G	189	ARG
1	G	231	VAL
1	G	235	GLU
1	G	238	GLU
1	G	267	ASN
1	G	285	GLU
1	G	286	ARG
1	G	312	GLU
1	G	315	GLU
1	G	316	HIS
1	G	384	ARG
1	G	406	MET
1	G	408	SER
1	G	415	LEU
1	G	421	GLU
1	G	428	LEU
1	G	446	ARG
1	G	455	SER
1	G	480	GLN
1	G	508	GLN
1	G	517	GLU
1	G	522	LEU
1	G	559	ASP
1	G	574	GLU
1	G	578	ARG
1	H	7	PRO

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Mol	Chain	Res	Type
1	H	32	GLU
1	H	61	LYS
1	H	64	THR
1	H	80	LEU
1	H	113	GLU
1	H	137	THR
1	H	165	GLN
1	H	171	MET
1	H	189	ARG
1	H	195	GLN
1	H	231	VAL
1	H	238	GLU
1	H	285	GLU
1	H	286	ARG
1	H	291	LEU
1	H	292	LEU
1	H	304	THR
1	H	316	HIS
1	H	408	SER
1	H	428	LEU
1	H	455	SER
1	H	480	GLN
1	H	508	GLN
1	H	522	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	195	GLN
1	A	492	ASN
1	A	508	GLN
1	A	567	GLN
1	B	134	ASN
1	B	293	GLN
1	B	492	ASN
1	B	508	GLN
1	C	38	ASN
1	C	134	ASN
1	C	492	ASN
1	C	508	GLN
1	C	566	HIS

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Mol	Chain	Res	Type
1	D	38	ASN
1	D	102	HIS
1	D	134	ASN
1	D	187	ASN
1	D	492	ASN
1	D	508	GLN
1	E	134	ASN
1	E	322	HIS
1	E	492	ASN
1	E	508	GLN
1	E	567	GLN
1	F	102	HIS
1	F	134	ASN
1	F	316	HIS
1	F	492	ASN
1	F	508	GLN
1	F	567	GLN
1	G	102	HIS
1	G	190	ASN
1	G	492	ASN
1	G	508	GLN
1	G	567	GLN
1	H	22	GLN
1	H	38	ASN
1	H	134	ASN
1	H	165	GLN
1	H	187	ASN
1	H	492	ASN
1	H	508	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 19 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	APC	B	601	3	27,33,33	1.49	6 (22%)	31,52,52	1.81	9 (29%)
2	APC	A	601	3	27,33,33	1.69	6 (22%)	31,52,52	1.76	8 (25%)
2	APC	E	601	3	27,33,33	1.85	9 (33%)	31,52,52	1.76	9 (29%)
2	APC	D	601	3	27,33,33	1.89	10 (37%)	31,52,52	2.24	11 (35%)
2	APC	H	601	3	27,33,33	1.89	10 (37%)	31,52,52	2.40	18 (58%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	APC	B	601	3	-	2/15/38/38	0/3/3/3
2	APC	A	601	3	-	6/15/38/38	0/3/3/3
2	APC	E	601	3	-	4/15/38/38	0/3/3/3
2	APC	D	601	3	-	6/15/38/38	0/3/3/3
2	APC	H	601	3	-	6/15/38/38	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	APC	PB-O3B	4.56	1.63	1.58
2	D	601	APC	PA-O5'	4.50	1.64	1.57
2	A	601	APC	PA-O5'	4.14	1.63	1.57
2	A	601	APC	PB-O3B	4.08	1.62	1.58
2	H	601	APC	PA-O2A	3.82	1.65	1.56
2	H	601	APC	C5-C4	3.77	1.50	1.40
2	D	601	APC	C2-N3	3.67	1.38	1.32
2	E	601	APC	C5-C4	3.45	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	APC	C5-C4	3.42	1.50	1.40
2	H	601	APC	C4-N3	-3.37	1.31	1.35
2	B	601	APC	C5-C4	3.20	1.49	1.40
2	B	601	APC	PB-O2B	3.17	1.63	1.56
2	E	601	APC	PA-O5'	3.13	1.62	1.57
2	H	601	APC	C5'-C4'	3.11	1.61	1.51
2	B	601	APC	C2-N3	3.10	1.37	1.32
2	A	601	APC	C5-C4	2.96	1.48	1.40
2	E	601	APC	C2'-C1'	-2.93	1.49	1.53
2	D	601	APC	C2'-C1'	-2.88	1.49	1.53
2	H	601	APC	C2-N3	2.77	1.36	1.32
2	H	601	APC	C5-N7	-2.70	1.29	1.39
2	A	601	APC	PA-O2A	2.61	1.62	1.56
2	E	601	APC	C4-N3	-2.54	1.32	1.35
2	E	601	APC	PA-O2A	2.49	1.62	1.56
2	A	601	APC	PB-O2B	2.48	1.62	1.56
2	E	601	APC	C2-N3	2.46	1.36	1.32
2	H	601	APC	PA-O5'	2.45	1.61	1.57
2	A	601	APC	O4'-C1'	2.42	1.44	1.41
2	H	601	APC	PB-O2B	2.40	1.62	1.56
2	H	601	APC	C2-N1	2.39	1.38	1.33
2	B	601	APC	C5-N7	-2.34	1.31	1.39
2	B	601	APC	PB-O3B	2.32	1.61	1.58
2	D	601	APC	C2-N1	2.31	1.38	1.33
2	E	601	APC	PB-O2B	2.30	1.61	1.56
2	D	601	APC	PB-O3B	2.27	1.60	1.58
2	B	601	APC	PA-O5'	2.25	1.60	1.57
2	H	601	APC	O4'-C1'	2.22	1.44	1.41
2	D	601	APC	PA-O2A	2.18	1.61	1.56
2	D	601	APC	C5-N7	-2.14	1.32	1.39
2	E	601	APC	C5-N7	-2.08	1.32	1.39
2	D	601	APC	PB-O1B	-2.05	1.46	1.51
2	D	601	APC	PB-O2B	2.02	1.61	1.56

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	APC	PB-O3B-PG	-6.18	110.85	132.62
2	H	601	APC	O2'-C2'-C3'	-4.31	97.90	111.82
2	H	601	APC	O4'-C4'-C3'	-4.29	96.62	105.11
2	B	601	APC	N6-C6-N1	3.94	126.76	118.57
2	D	601	APC	N6-C6-N1	3.92	126.70	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	601	APC	O4'-C1'-C2'	-3.80	101.37	106.93
2	H	601	APC	PB-O3B-PG	-3.78	119.29	132.62
2	A	601	APC	N3-C2-N1	-3.73	122.84	128.68
2	H	601	APC	O1A-PA-C3A	-3.63	99.48	109.07
2	H	601	APC	N6-C6-N1	3.61	126.06	118.57
2	D	601	APC	C1'-N9-C4	3.59	132.94	126.64
2	E	601	APC	N6-C6-N1	3.47	125.78	118.57
2	E	601	APC	C5-C6-N1	-3.41	112.62	120.35
2	B	601	APC	N3-C2-N1	-3.41	123.35	128.68
2	H	601	APC	O1B-PB-C3A	3.40	118.07	109.07
2	E	601	APC	C2-N1-C6	3.28	124.36	118.75
2	B	601	APC	O4'-C1'-C2'	-3.27	102.14	106.93
2	D	601	APC	O4'-C1'-C2'	-3.19	102.26	106.93
2	E	601	APC	C3'-C2'-C1'	-3.16	96.22	100.98
2	B	601	APC	PB-O3B-PG	-3.12	121.63	132.62
2	D	601	APC	O1A-PA-C3A	3.11	117.30	109.07
2	A	601	APC	N6-C6-N1	3.11	125.03	118.57
2	D	601	APC	O4'-C4'-C5'	3.09	119.53	109.37
2	A	601	APC	O2A-PA-O1A	-3.02	100.00	110.07
2	D	601	APC	N3-C2-N1	-2.94	124.08	128.68
2	A	601	APC	C2-N1-C6	2.92	123.75	118.75
2	H	601	APC	O3G-PG-O2G	2.77	118.24	107.64
2	H	601	APC	C5-C6-N1	-2.76	114.08	120.35
2	B	601	APC	C2-N1-C6	2.69	123.36	118.75
2	D	601	APC	C5'-C4'-C3'	-2.53	105.70	115.18
2	E	601	APC	C1'-N9-C4	2.53	131.08	126.64
2	H	601	APC	C1'-N9-C4	2.48	131.00	126.64
2	D	601	APC	O3G-PG-O2G	2.48	117.12	107.64
2	A	601	APC	O5'-C5'-C4'	2.48	117.53	108.99
2	H	601	APC	O3'-C3'-C4'	-2.46	103.92	111.05
2	E	601	APC	O2'-C2'-C3'	2.46	119.78	111.82
2	H	601	APC	O4'-C4'-C5'	2.41	117.31	109.37
2	B	601	APC	C1'-N9-C4	2.40	130.85	126.64
2	H	601	APC	C2-N1-C6	2.37	122.80	118.75
2	B	601	APC	O3G-PG-O2G	2.36	116.66	107.64
2	A	601	APC	O2A-PA-C3A	2.35	116.17	106.58
2	E	601	APC	O3'-C3'-C2'	2.33	119.37	111.82
2	A	601	APC	O1B-PB-C3A	2.33	115.24	109.07
2	B	601	APC	C5'-C4'-C3'	-2.32	106.47	115.18
2	H	601	APC	N3-C2-N1	-2.28	125.11	128.68
2	H	601	APC	O5'-C5'-C4'	2.27	116.79	108.99
2	H	601	APC	O3B-PG-O1G	-2.18	99.09	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	601	APC	C4-C5-N7	2.16	111.65	109.40
2	B	601	APC	C5-C6-N1	-2.14	115.49	120.35
2	D	601	APC	O5'-C5'-C4'	2.12	116.28	108.99
2	E	601	APC	C5'-C4'-C3'	-2.11	107.26	115.18
2	A	601	APC	PB-O3B-PG	-2.11	125.20	132.62
2	E	601	APC	N3-C2-N1	-2.07	125.44	128.68
2	H	601	APC	C3'-C2'-C1'	2.07	104.09	100.98
2	D	601	APC	C5-C6-N6	-2.03	117.27	120.35

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	APC	PB-C3A-PA-O1A
2	A	601	APC	PB-C3A-PA-O2A
2	B	601	APC	C5'-O5'-PA-O2A
2	D	601	APC	PA-C3A-PB-O1B
2	D	601	APC	PA-C3A-PB-O2B
2	D	601	APC	O4'-C4'-C5'-O5'
2	E	601	APC	C5'-O5'-PA-O1A
2	E	601	APC	C5'-O5'-PA-O2A
2	E	601	APC	C5'-O5'-PA-C3A
2	H	601	APC	PA-C3A-PB-O1B
2	H	601	APC	PA-C3A-PB-O2B
2	H	601	APC	PA-C3A-PB-O3B
2	H	601	APC	C4'-C5'-O5'-PA
2	H	601	APC	O4'-C4'-C5'-O5'
2	A	601	APC	O4'-C4'-C5'-O5'
2	D	601	APC	C3'-C4'-C5'-O5'
2	H	601	APC	C3'-C4'-C5'-O5'
2	D	601	APC	C5'-O5'-PA-C3A
2	E	601	APC	PB-O3B-PG-O1G
2	D	601	APC	C4'-C5'-O5'-PA
2	A	601	APC	C3'-C4'-C5'-O5'
2	A	601	APC	PB-C3A-PA-O5'
2	B	601	APC	PA-C3A-PB-O1B
2	A	601	APC	C4'-C5'-O5'-PA

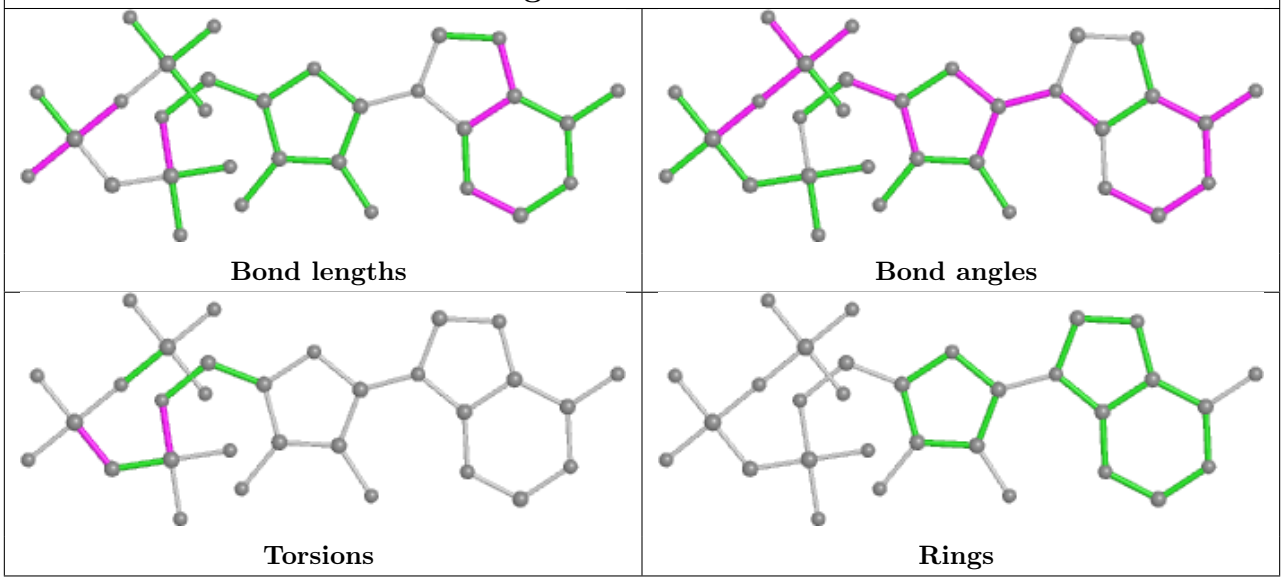
There are no ring outliers.

4 monomers are involved in 10 short contacts:

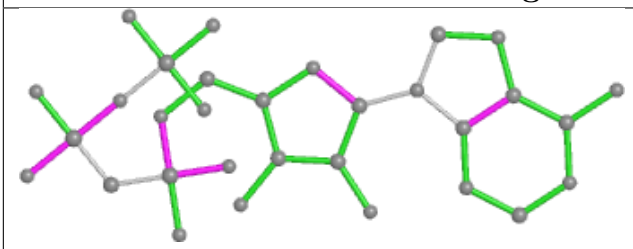
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	APC	2	0
2	A	601	APC	1	0
2	D	601	APC	3	0
2	H	601	APC	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

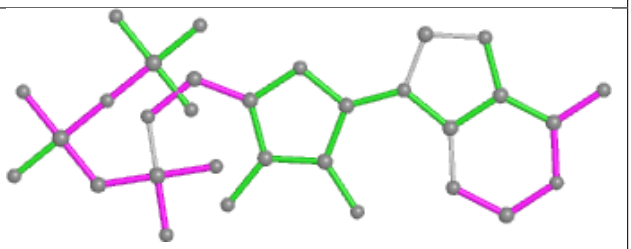
Ligand APC B 601



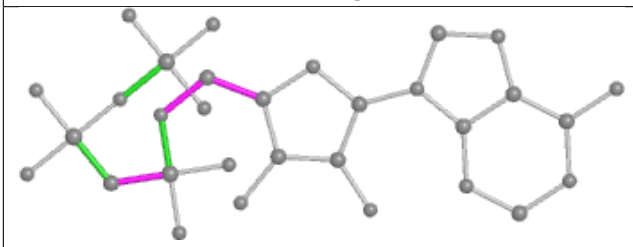
Ligand APC A 601



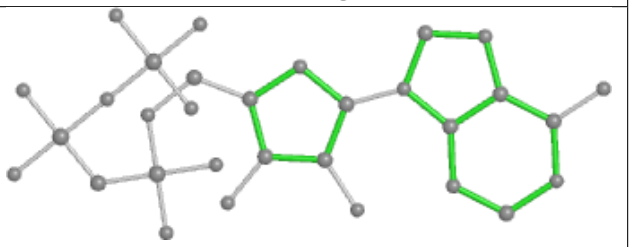
Bond lengths



Bond angles

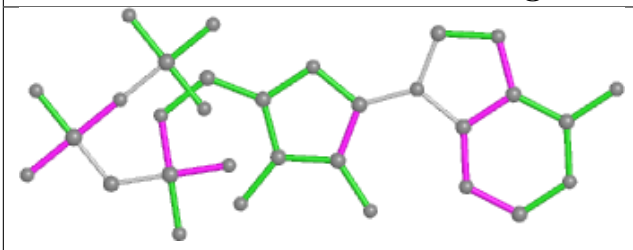


Torsions

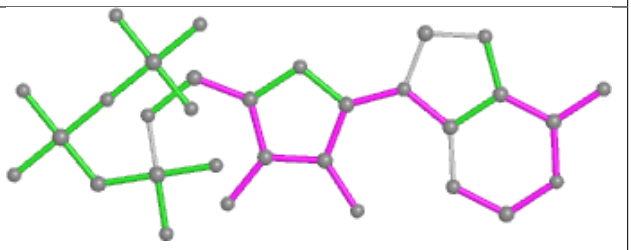


Rings

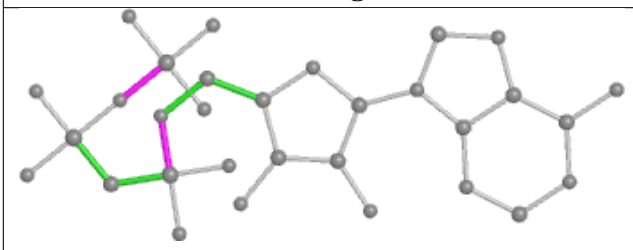
Ligand APC E 601



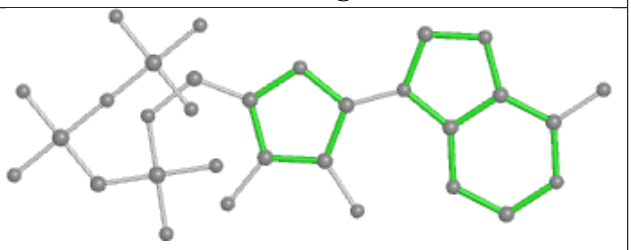
Bond lengths



Bond angles

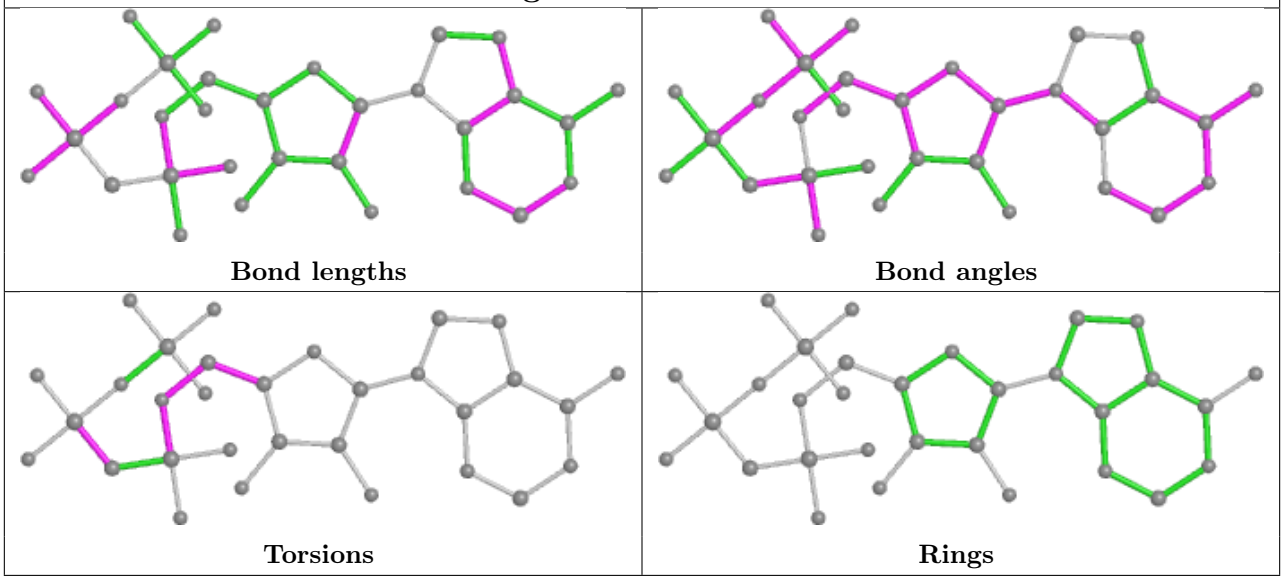


Torsions

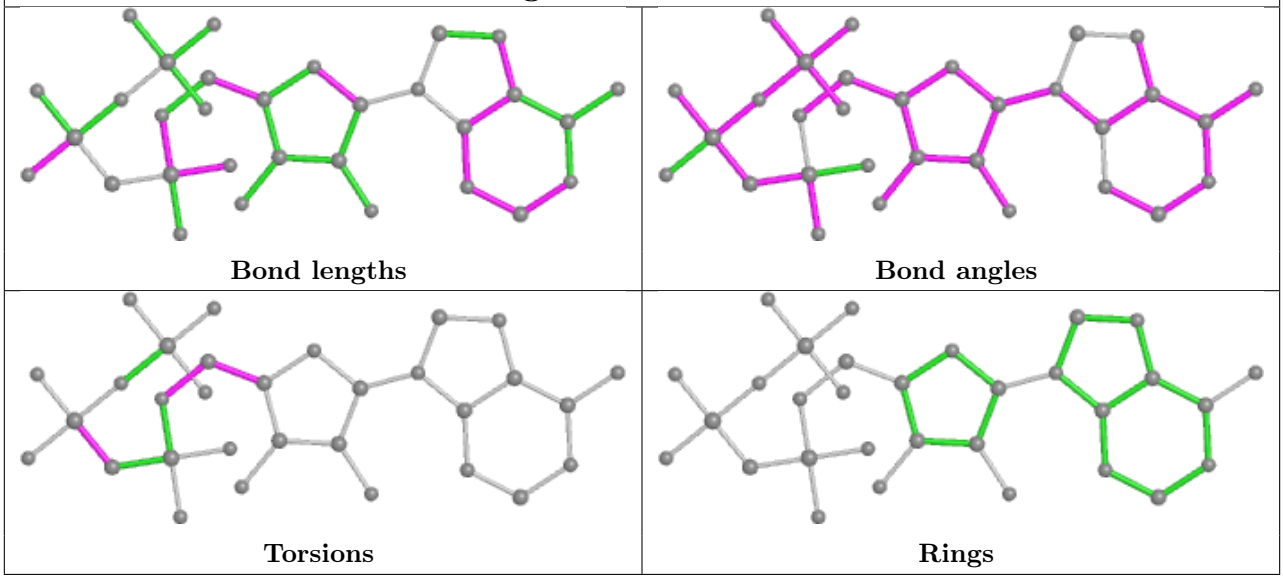


Rings

Ligand APC D 601



Ligand APC H 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	559/586 (95%)	-0.11	1 (0%)	95	96	33, 59, 87, 111	0
1	B	573/586 (97%)	-0.10	1 (0%)	95	96	29, 54, 94, 130	0
1	C	562/586 (95%)	-0.04	2 (0%)	92	93	36, 63, 93, 112	0
1	D	572/586 (97%)	-0.11	1 (0%)	95	96	29, 56, 89, 123	0
1	E	573/586 (97%)	-0.12	1 (0%)	95	96	28, 50, 83, 112	0
1	F	570/586 (97%)	0.51	47 (8%)	11	11	54, 93, 124, 198	0
1	G	545/586 (93%)	0.06	13 (2%)	59	56	36, 70, 107, 185	0
1	H	573/586 (97%)	-0.16	0	100	100	28, 49, 80, 125	0
All	All	4527/4688 (96%)	-0.01	66 (1%)	73	72	28, 60, 104, 198	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	184	SER	6.2
1	G	36	TRP	6.0
1	F	573	TYR	5.9
1	F	4	THR	4.7
1	F	283	ALA	4.4
1	G	42	ASN	4.3
1	F	182	GLY	4.3
1	F	203	ARG	4.2
1	F	185	ALA	3.9
1	F	327	SER	3.9
1	F	186	GLY	3.8
1	G	43	VAL	3.7
1	F	391	SER	3.7
1	G	63	ALA	3.7
1	F	413	THR	3.6
1	F	570	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	348	PHE	3.3
1	F	183	MET	3.3
1	G	41	PRO	3.2
1	C	186	GLY	3.2
1	G	62	GLY	3.1
1	F	187	ASN	3.0
1	D	135	GLU	2.9
1	F	210	ILE	2.9
1	G	64	THR	2.9
1	F	108	TRP	2.8
1	B	326	SER	2.8
1	G	67	ALA	2.7
1	F	364	ASN	2.7
1	F	233	ALA	2.7
1	F	195	GLN	2.6
1	F	303	PHE	2.6
1	F	307	THR	2.5
1	F	11	ALA	2.5
1	F	302	VAL	2.5
1	F	275	GLY	2.5
1	G	233	ALA	2.5
1	F	383	CYS	2.5
1	F	384	ARG	2.4
1	F	343	PHE	2.4
1	F	382	ALA	2.3
1	F	234	ILE	2.3
1	F	237	LEU	2.3
1	F	6	ILE	2.3
1	F	555	PRO	2.3
1	C	185	ALA	2.2
1	F	211	ALA	2.2
1	F	388	PRO	2.2
1	G	228	PRO	2.2
1	F	386	ILE	2.2
1	F	256	PRO	2.2
1	F	316	HIS	2.2
1	F	5	PHE	2.2
1	F	220	PRO	2.2
1	F	392	ASP	2.1
1	A	70	ALA	2.1
1	E	184	SER	2.1
1	G	283	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	363	PHE	2.1
1	F	476	GLY	2.0
1	F	102	HIS	2.0
1	F	575	LYS	2.0
1	G	61	LYS	2.0
1	F	273	SER	2.0
1	F	130	TYR	2.0
1	G	40	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	E	603	1/1	0.82	0.09	22,22,22,22	0
3	MG	C	602	1/1	0.94	0.20	28,28,28,28	0
2	APC	A	601	31/31	0.94	0.23	57,76,98,107	0
3	MG	G	601	1/1	0.94	0.05	22,22,22,22	0
3	MG	C	601	1/1	0.95	0.06	39,39,39,39	0
3	MG	B	602	1/1	0.95	0.08	24,24,24,24	0
2	APC	E	601	31/31	0.96	0.21	32,42,54,60	0
3	MG	D	603	1/1	0.96	0.13	24,24,24,24	0
3	MG	E	604	1/1	0.96	0.09	23,23,23,23	0
2	APC	B	601	31/31	0.96	0.22	33,48,59,60	0
2	APC	D	601	31/31	0.96	0.22	33,45,59,60	0
3	MG	H	602	1/1	0.96	0.13	9,9,9,9	0
3	MG	B	604	1/1	0.97	0.13	9,9,9,9	0
3	MG	A	602	1/1	0.97	0.10	6,6,6,6	0
3	MG	A	604	1/1	0.97	0.04	31,31,31,31	0

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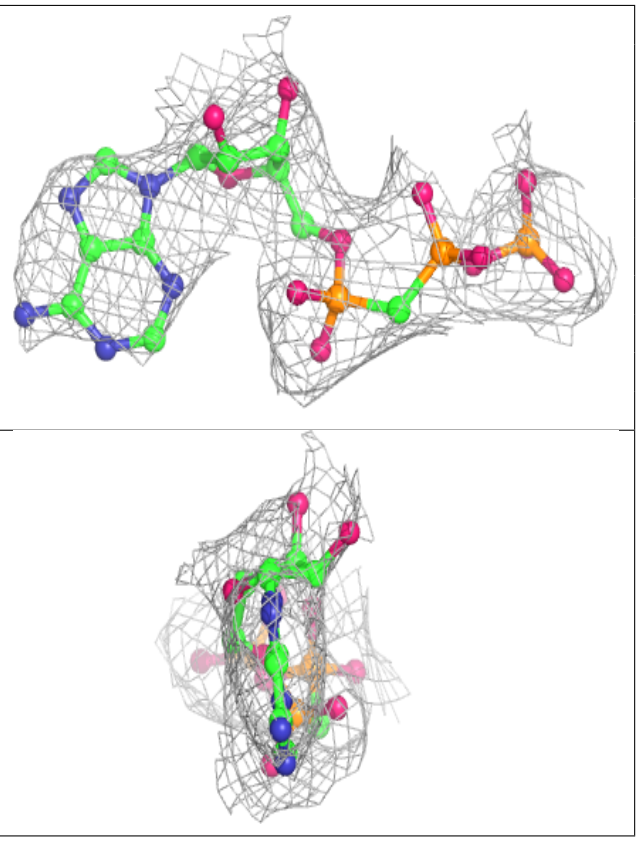
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	APC	H	601	31/31	0.97	0.19	24,38,49,54	0
3	MG	A	603	1/1	0.98	0.10	24,24,24,24	0
3	MG	E	602	1/1	0.98	0.11	17,17,17,17	0
3	MG	D	602	1/1	0.98	0.10	15,15,15,15	0
3	MG	B	603	1/1	0.98	0.14	9,9,9,9	0
3	MG	D	604	1/1	0.98	0.11	19,19,19,19	0
3	MG	H	603	1/1	0.98	0.12	16,16,16,16	0
3	MG	H	605	1/1	0.98	0.54	62,62,62,62	0
3	MG	H	604	1/1	0.99	0.12	20,20,20,20	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.

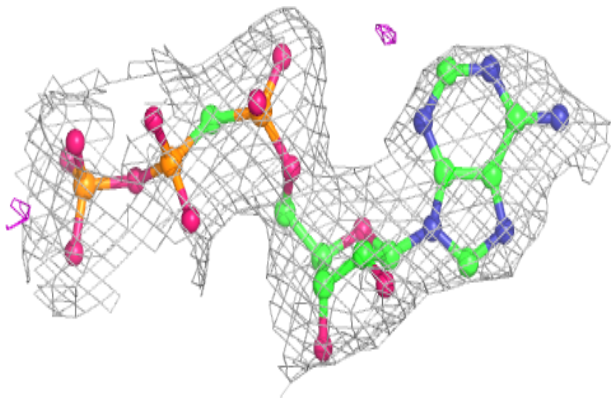
Electron density around APC A 601:

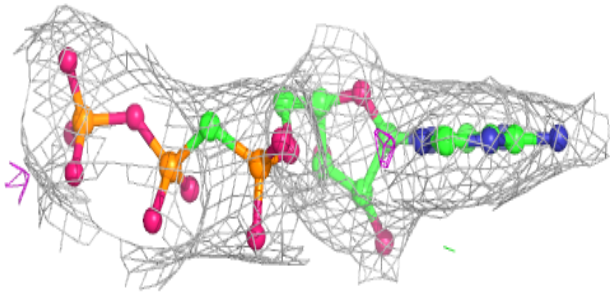
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

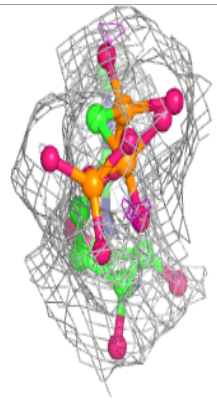


Electron density around APC E 601:

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

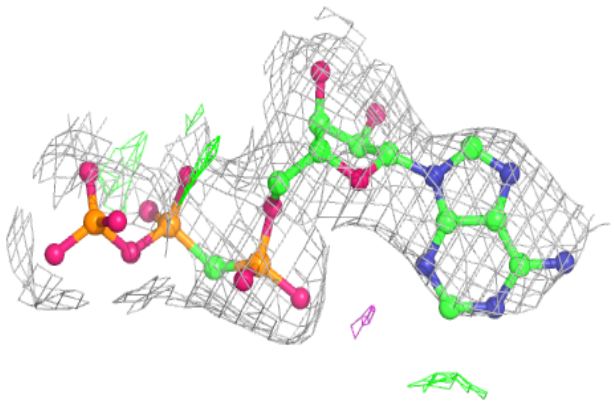


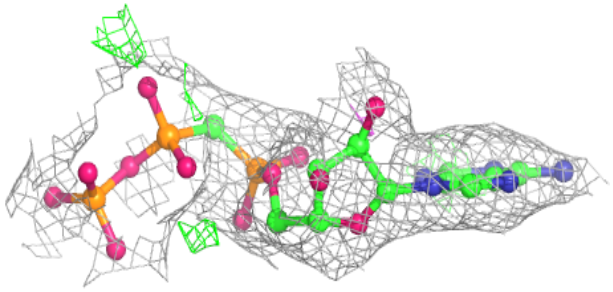


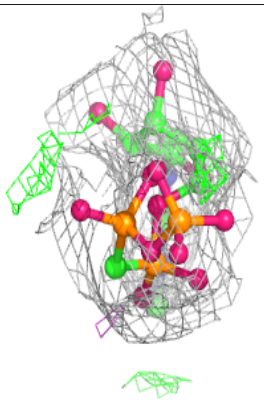


Electron density around APC B 601:

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

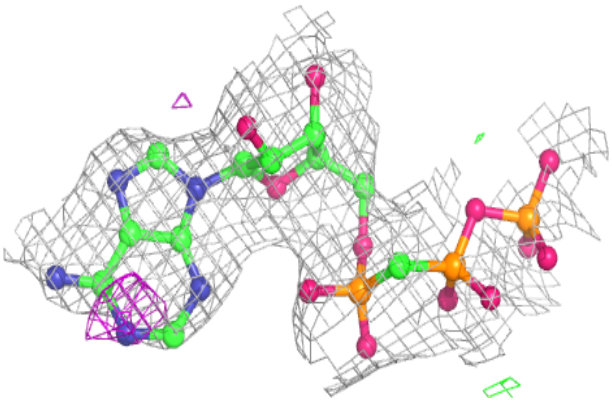


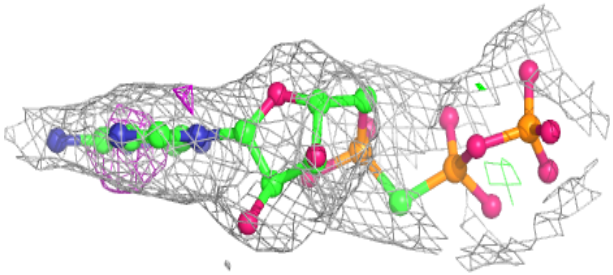


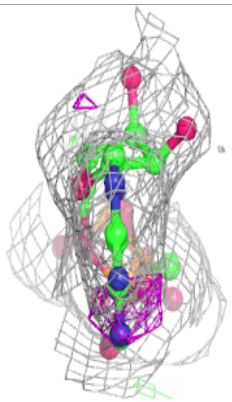


Electron density around APC D 601:

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

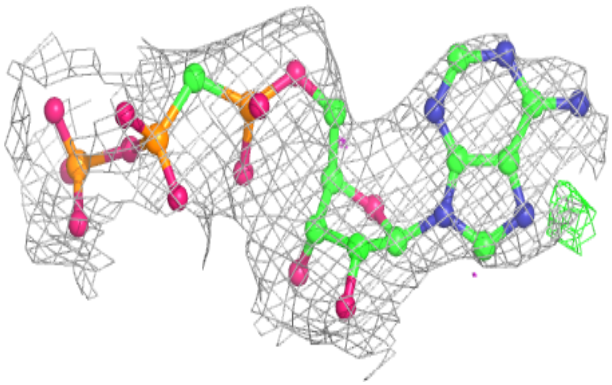


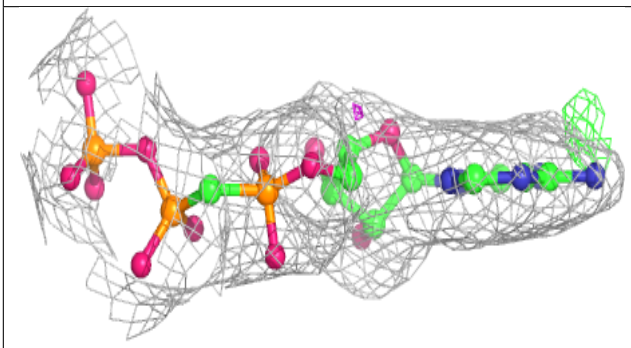


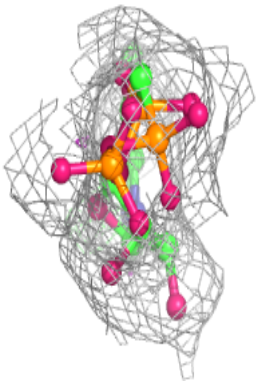


Electron density around APC H 601:

$2mF_o$-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.