



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:56 PM UTC

PDB ID : 4Q85 / pdb_00004q85
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 ⓘ 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:

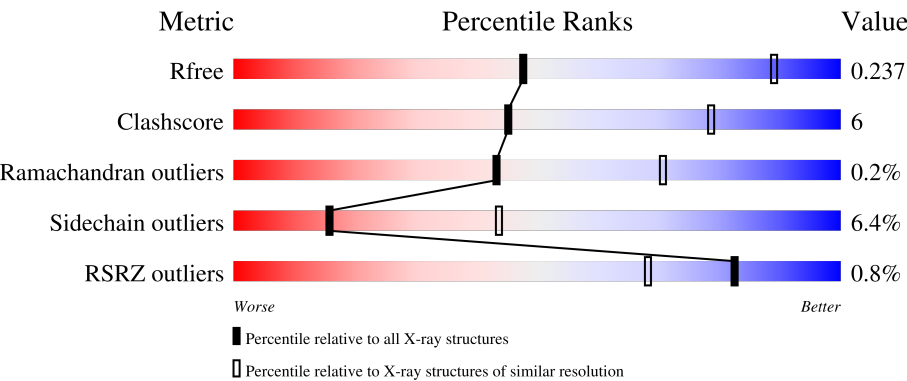
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	586	83%11%• 5%
1	B	586	84%12%• •
1	C	586	81%13%• •
1	D	586	83%13%• •
1	E	586	87%10%• •

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Mol	Chain	Length	Quality of chain
1	F	586	5% 72% 20% • • •
1	G	586	% 80% 11% • 7%
1	H	586	84% 13% • •

2 Entry composition

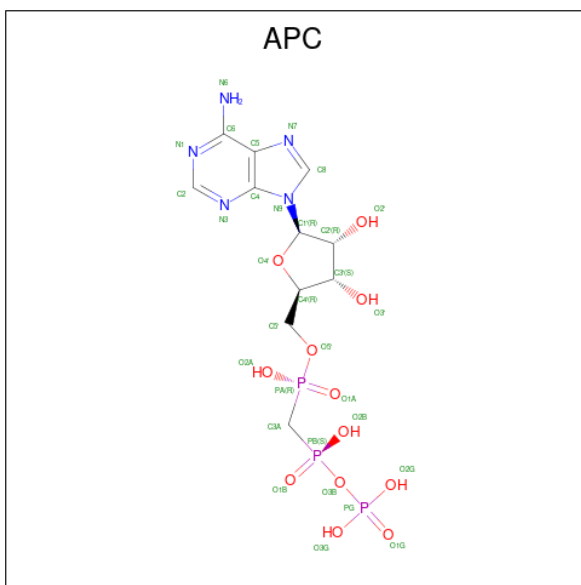
There are 4 unique types of molecules in this entry. The entry contains 36421 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

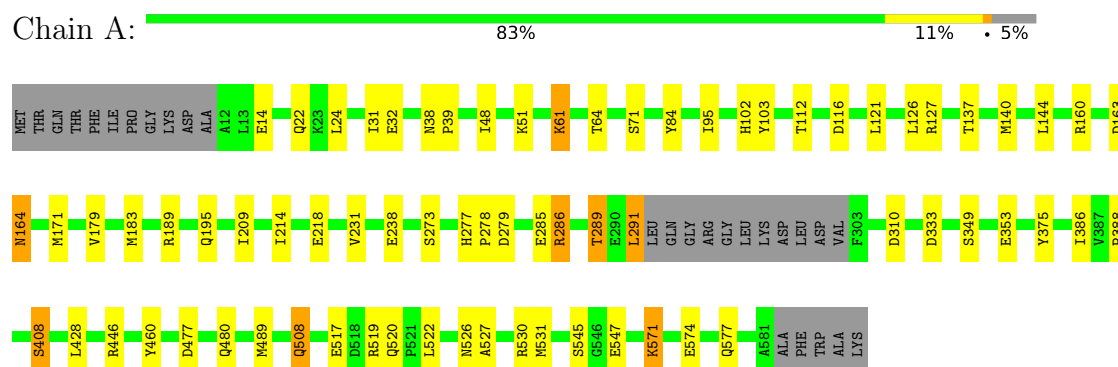
- Molecule 4 is water.

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

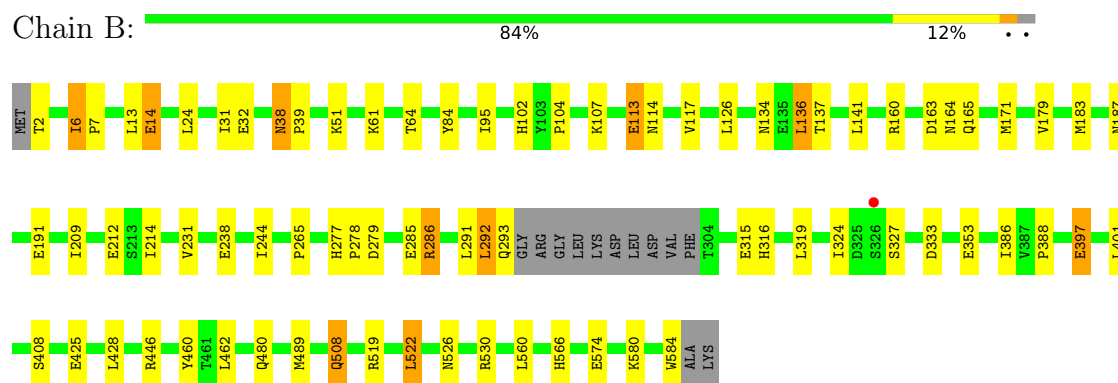
3 Residue-property plots

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.

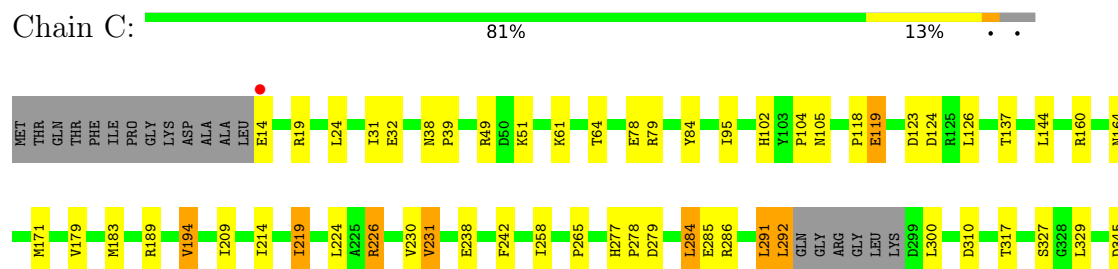
- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO



- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO



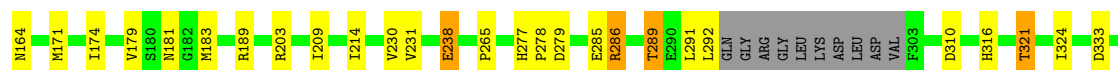
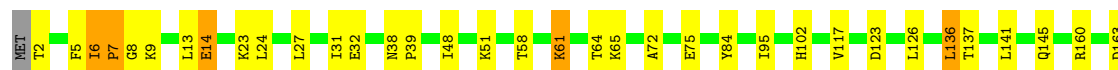
- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO





- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

Chain D: 83% 13% ..



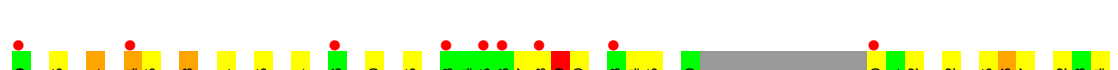
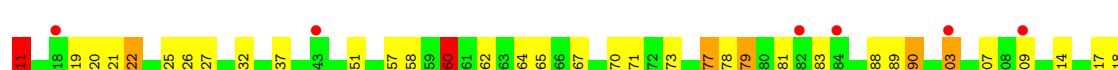
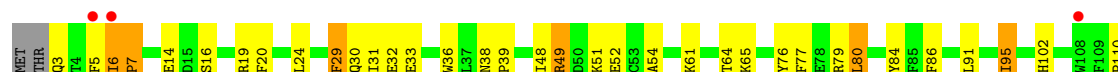
- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

Chain E: 87% 10% ..



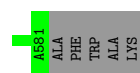
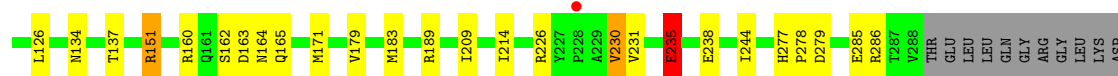
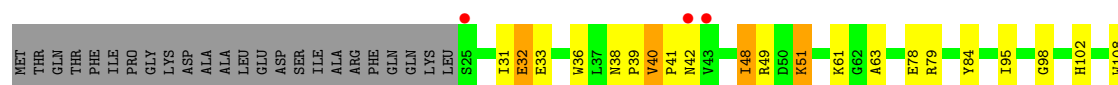
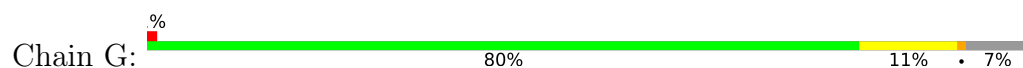
- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

Chain F: 5% 72% 20% ..

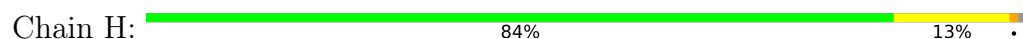




- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO



- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO



4 Data and refinement statistics

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 – 3.29 125.20 – 3.29	Depositor EDS
% Data completeness (in resolution range)	99.0 (125.20-3.29) 99.0 (125.20-3.29)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.97%)	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)	0.34 , 70.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.*

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: APC, MG

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	0.72	0/4534	0.92	5/6168 (0.1%)
1	B	0.76	0/4649	0.95	4/6326 (0.1%)
1	C	0.72	1/4560 (0.0%)	0.95	9/6204 (0.1%)
1	D	0.77	1/4636 (0.0%)	0.97	5/6307 (0.1%)
1	E	0.79	0/4642	0.95	6/6316 (0.1%)
1	F	0.81	2/4619 (0.0%)	1.06	19/6284 (0.3%)
1	G	0.72	1/4418 (0.0%)	0.98	8/6013 (0.1%)
1	H	0.82	1/4652 (0.0%)	0.97	10/6330 (0.2%)
All	All	0.77	6/36710 (0.0%)	0.97	66/49948 (0.1%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	119	GLU	CA-CB	6.76	1.64	1.53
1	D	321	THR	CA-CB	5.69	1.62	1.53
1	F	316	HIS	CA-CB	5.67	1.62	1.53
1	G	40	VAL	CA-C	5.35	1.57	1.52
1	H	432	GLU	CA-C	5.23	1.59	1.52
1	F	234	ILE	CA-CB	5.22	1.61	1.54

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	163	ASP	CB-CA-C	-13.18	88.08	110.09
1	G	40	VAL	N-CA-CB	-11.39	101.99	111.67
1	F	573	TYR	N-CA-CB	10.89	127.17	110.28
1	G	151	ARG	CG-CD-NE	9.72	133.39	112.00
1	F	7	PRO	N-CA-C	9.28	127.07	114.18
1	F	355	GLU	CA-CB-CG	-9.27	95.56	114.10
1	G	384	ARG	CG-CD-NE	9.20	132.25	112.00
1	H	163	ASP	N-CA-C	-8.32	97.96	109.95
1	H	163	ASP	CA-C-N	-7.96	106.33	121.54
1	H	163	ASP	C-N-CA	-7.96	106.33	121.54
1	G	40	VAL	CB-CA-C	7.70	121.90	110.97
1	F	426	ASP	CB-CA-C	7.48	123.21	110.79
1	C	19	ARG	CA-CB-CG	7.39	128.87	114.10
1	C	104	PRO	CA-C-N	7.18	132.19	120.63
1	C	104	PRO	C-N-CA	7.18	132.19	120.63
1	G	235	GLU	CA-CB-CG	6.93	127.95	114.10
1	C	231	VAL	N-CA-CB	6.87	119.06	110.47
1	H	420	SER	N-CA-C	6.56	124.77	110.80
1	A	571	LYS	CB-CG-CD	6.54	126.34	111.30
1	F	80	LEU	N-CA-CB	6.53	119.93	110.20
1	A	286	ARG	CB-CG-CD	-6.49	96.37	111.30
1	F	29	PHE	N-CA-C	6.39	118.78	109.07
1	F	279	ASP	N-CA-CB	6.17	120.54	110.17
1	B	38	ASN	CA-C-N	6.17	125.66	119.24
1	B	38	ASN	C-N-CA	6.17	125.66	119.24
1	E	578	ARG	CB-CG-CD	6.11	125.36	111.30
1	D	7	PRO	N-CA-C	6.01	124.86	112.47
1	D	163	ASP	N-CA-C	5.97	120.70	113.17
1	C	194	VAL	CB-CA-C	5.93	120.41	112.22
1	E	446	ARG	CG-CD-NE	-5.83	99.17	112.00
1	B	319	LEU	CA-CB-CG	5.81	136.63	116.30
1	F	477	ASP	CB-CA-C	5.67	121.15	111.68
1	B	292	LEU	N-CA-C	5.67	118.16	110.06
1	H	493	SER	CB-CA-C	5.61	121.33	110.46
1	F	477	ASP	N-CA-CB	5.56	119.76	110.53
1	C	355	GLU	CB-CG-CD	5.52	121.99	112.60
1	H	432	GLU	CB-CA-C	5.51	120.82	110.63
1	F	80	LEU	CA-CB-CG	5.43	135.31	116.30
1	F	234	ILE	N-CA-CB	5.43	119.63	110.56
1	F	6	ILE	CA-C-N	5.41	125.10	119.64
1	F	6	ILE	C-N-CA	5.41	125.10	119.64
1	G	32	GLU	CB-CA-C	-5.39	98.69	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	36	TRP	N-CA-CB	5.36	118.11	110.44
1	C	105	ASN	N-CA-C	5.32	119.25	112.34
1	A	164	ASN	N-CA-C	5.30	118.90	111.90
1	F	110	PRO	CA-C-N	5.27	129.78	121.56
1	F	110	PRO	C-N-CA	5.27	129.78	121.56
1	F	279	ASP	CB-CA-C	5.26	119.00	110.22
1	G	230	VAL	CB-CA-C	5.25	119.27	112.24
1	C	19	ARG	CB-CA-C	-5.25	102.58	110.92
1	H	520	GLN	CB-CA-C	-5.21	105.01	110.33
1	F	111	LEU	CA-C-O	-5.20	115.75	120.95
1	E	349	SER	N-CA-C	5.20	116.64	110.19
1	C	355	GLU	CG-CD-OE2	5.20	130.36	118.40
1	D	174	ILE	CB-CA-C	-5.20	105.23	111.88
1	D	8	GLY	N-CA-C	5.19	120.44	114.16
1	F	160	ARG	CG-CD-NE	-5.18	100.61	112.00
1	H	38	ASN	CA-C-N	5.17	126.30	119.84
1	H	38	ASN	C-N-CA	5.17	126.30	119.84
1	H	254	GLN	N-CA-C	5.16	116.71	111.14
1	E	38	ASN	CA-C-N	5.13	126.25	119.84
1	E	38	ASN	C-N-CA	5.13	126.25	119.84
1	E	174	ILE	CB-CA-C	-5.08	105.37	111.88
1	A	140	MET	CB-CA-C	5.08	120.53	110.17
1	A	349	SER	N-CA-C	5.05	116.46	110.19
1	F	95	ILE	CB-CA-C	-5.01	105.38	112.14

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

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	44	1
1	B	4535	0	4301	42	2
1	C	4450	0	4216	47	0
1	D	4523	0	4292	48	0
1	E	4530	0	4302	27	1
1	F	4507	0	4273	139	0
1	G	4309	0	4073	41	0
1	H	4537	0	4302	45	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
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	31	0
4	G	54	0	0	7	0
4	H	55	0	0	5	0
All	All	36421	0	34022	412	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 (412) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:467:LEU:HA	1:H:470:MET:HE2	1.55	0.89
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:F:400:TRP:O	1:F:406:MET:HE1	1.76	0.84
1:F:181:ASN:CB	1:F:393:ILE:HD11	2.09	0.83
1:C:400:TRP:O	1:C:406:MET:HE1	1.79	0.82
1:F:355:GLU:OE2	1:F:358:THR:OG1	1.98	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:MET:HE1	1:B:508:GLN:NE2	2.04	0.72
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:489:MET:HE1	1:F:508:GLN:NE2	2.04	0.72
1:F:29:PHE:CE1	1:F:575:LYS:HE3	2.23	0.72
1:A:489:MET:HE1	1:A:508:GLN:NE2	2.05	0.71
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:G:489:MET:HE1	1:G:508:GLN:NE2	2.08	0.68
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
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:H:489:MET:HE1	1:H:508:GLN:NE2	2.12	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:E:489:MET:HE1	1:E: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:489:MET:HE1	1:D:508:GLN:NE2	2.15	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:C:489:MET:HE1	1:C:508:GLN:NE2	2.18	0.59
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:G:32:GLU:CD	1:G:51:LYS:HG3	2.27	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
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: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:H:177:LEU:C	4:H:753:HOH:O	2.48	0.56
1:A:71:SER:OG	2:A:601:APC:O1A	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:439:PHE:HD1	4:F:653:HOH:O	1.89	0.56
1:F:400:TRP:O	1:F:406:MET:CE	2.51	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: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:F:355:GLU:N	1:F:355:GLU:CD	2.63	0.53
1:F:30:GLN:HB2	1:F:52:GLU:OE2	2.08	0.53
1:B:134:ASN:CG	1:H:133:GLU:OE1	2.51	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: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: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:C:400:TRP:O	1:C:406:MET:CE	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:195:GLN:NE2	1:A:286:ARG:NH2	2.59	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:279:ASP:C	1:C:279:ASP:OD1	2.56	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: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
1:F:16:SER:OG	1:F:20:PHE:CE2	2.61	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:HIS:CD2	1:A:278:PRO:HD2	2.49	0.47
1:B:279:ASP:OD1	1:B:279:ASP:C	2.57	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: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:E:242:PHE:CZ	1:E:300:LEU:HD12	2.50	0.47
1:G:279:ASP:OD1	1:G:279:ASP:C	2.57	0.47
1:F:102:HIS:CE1	1:F:171:MET:HG2	2.50	0.47
1:F:157:PRO:C	4:F:650:HOH:O	2.58	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:D:279:ASP:OD1	1:D:279:ASP:C	2.59	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
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:A:279:ASP:OD1	1:A:279:ASP:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:291:LEU:C	1:C:292:LEU:HG	2.41	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:F:374:ASP:OD1	1:F:381:TYR:OH	2.34	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
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:B:84:TYR:HB2	1:B:183:MET:HE1	2.00	0.44
1:G:519:ARG:NH1	1:H:333:ASP:CG	2.75	0.44
1:F:121:LEU:O	1:F:127:ARG:NH1	2.46	0.44
1:F:358:THR:HG21	4:F:666:HOH:O	2.17	0.44
1:H:279:ASP:C	1:H:279:ASP:OD1	2.59	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: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:E:279:ASP:C	1:E:279:ASP:OD1	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:277:HIS:CD2	1:F:278:PRO:HD2	2.53	0.44
1:E:112:THR:OG1	1:E:116:ASP:OD1	2.35	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:E:291:LEU:C	1:E:292:LEU:HG	2.42	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: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
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:112:THR:OG1	1:A:116:ASP:OD1	2.34	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:84:TYR:HB2	1:D:183:MET:HE1	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:84:TYR:HB2	1:C:183:MET:HE1	2.01	0.42
1:F:316:HIS:CD2	1:F:317:THR:HG23	2.54	0.42
1:H:470:MET:HE2	1:H:470:MET:HB2	1.87	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: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:F:84:TYR:HB2	1:F:183:MET:HE1	2.02	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:84:TYR:HB2	1:E:183:MET:HE1	2.01	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: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
1:G:84:TYR:HB2	1:G:183:MET:HE1	2.02	0.41
1:D:429:ASN:OD1	1:D:429:ASN:C	2.63	0.41
1:B:580:LYS:O	1:B:584:TRP:HE3	2.04	0.41
1:G:519:ARG:NH1	1:H:333:ASP:OD2	2.53	0.41
1:H:84:TYR:HB2	1:H:183:MET:HE1	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:477:ASP:OD1	1:A:477:ASP:C	2.64	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:G:108:TRP:NE1	1:G:151:ARG:NH1	2.69	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:A:84:TYR:HB2	1:A:183:MET:HE1	2.03	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
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
1:G:387:VAL:O	1:G:388:PRO:C	2.64	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%)	43	71
1	B	569/586 (97%)	541 (95%)	27 (5%)	1 (0%)	43	71
1	C	558/586 (95%)	532 (95%)	24 (4%)	2 (0%)	30	60
1	D	568/586 (97%)	539 (95%)	28 (5%)	1 (0%)	43	71
1	E	569/586 (97%)	540 (95%)	27 (5%)	2 (0%)	30	60
1	F	566/586 (97%)	535 (94%)	30 (5%)	1 (0%)	43	71
1	G	541/586 (92%)	514 (95%)	26 (5%)	1 (0%)	43	71
1	H	569/586 (97%)	544 (96%)	23 (4%)	2 (0%)	30	60
All	All	4495/4688 (96%)	4274 (95%)	210 (5%)	11 (0%)	43	71

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 ⓘ

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%)	446 (96%)	20 (4%)	26	54
1	B	477/487 (98%)	447 (94%)	30 (6%)	16	44
1	C	470/487 (96%)	441 (94%)	29 (6%)	16	45
1	D	476/487 (98%)	442 (93%)	34 (7%)	13	40
1	E	478/487 (98%)	451 (94%)	27 (6%)	19	47
1	F	475/487 (98%)	433 (91%)	42 (9%)	9	32
1	G	454/487 (93%)	423 (93%)	31 (7%)	14	42
1	H	477/487 (98%)	450 (94%)	27 (6%)	18	47
All	All	3773/3896 (97%)	3533 (94%)	240 (6%)	16	44

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	51	LYS
1	A	61	LYS
1	A	64	THR
1	A	95	ILE
1	A	137	THR
1	A	164	ASN
1	A	189	ARG
1	A	231	VAL
1	A	238	GLU
1	A	285	GLU
1	A	289	THR
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

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Mol	Chain	Res	Type
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	95	ILE
1	B	113	GLU
1	B	136	LEU
1	B	137	THR
1	B	164	ASN
1	B	165	GLN
1	B	231	VAL
1	B	238	GLU
1	B	285	GLU
1	B	286	ARG
1	B	291	LEU
1	B	292	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
1	B	522	LEU
1	B	530	ARG
1	B	574	GLU
1	C	14	GLU
1	C	32	GLU
1	C	51	LYS
1	C	61	LYS
1	C	64	THR
1	C	95	ILE
1	C	119	GLU
1	C	137	THR
1	C	164	ASN
1	C	189	ARG
1	C	219	ILE

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Mol	Chain	Res	Type
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	317	THR
1	C	406	MET
1	C	408	SER
1	C	428	LEU
1	C	480	GLN
1	C	492	ASN
1	C	522	LEU
1	C	547	GLU
1	C	574	GLU
1	C	578	ARG
1	D	6	ILE
1	D	7	PRO
1	D	14	GLU
1	D	32	GLU
1	D	51	LYS
1	D	61	LYS
1	D	64	THR
1	D	95	ILE
1	D	136	LEU
1	D	137	THR
1	D	145	GLN
1	D	164	ASN
1	D	189	ARG
1	D	231	VAL
1	D	238	GLU
1	D	285	GLU
1	D	286	ARG
1	D	289	THR
1	D	291	LEU
1	D	292	LEU
1	D	316	HIS
1	D	321	THR
1	D	405	SER
1	D	408	SER

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Mol	Chain	Res	Type
1	D	428	LEU
1	D	429	ASN
1	D	455	SER
1	D	480	GLN
1	D	495	VAL
1	D	517	GLU
1	D	522	LEU
1	D	547	GLU
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	95	ILE
1	E	137	THR
1	E	164	ASN
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	315	GLU
1	E	316	HIS
1	E	397	GLU
1	E	408	SER
1	E	428	LEU
1	E	480	GLN
1	E	492	ASN
1	E	520	GLN
1	E	522	LEU
1	E	530	ARG
1	E	574	GLU
1	F	6	ILE
1	F	32	GLU
1	F	49	ARG
1	F	51	LYS
1	F	61	LYS

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Mol	Chain	Res	Type
1	F	64	THR
1	F	95	ILE
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	177	LEU
1	F	189	ARG
1	F	190	ASN
1	F	203	ARG
1	F	231	VAL
1	F	234	ILE
1	F	238	GLU
1	F	279	ASP
1	F	285	GLU
1	F	300	LEU
1	F	302	VAL
1	F	312	GLU
1	F	315	GLU
1	F	355	GLU
1	F	397	GLU
1	F	406	MET
1	F	408	SER
1	F	413	THR
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	573	TYR
1	F	574	GLU
1	F	575	LYS
1	F	578	ARG
1	G	48	ILE
1	G	51	LYS
1	G	61	LYS
1	G	95	ILE
1	G	134	ASN

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Mol	Chain	Res	Type
1	G	137	THR
1	G	164	ASN
1	G	165	GLN
1	G	189	ARG
1	G	230	VAL
1	G	231	VAL
1	G	235	GLU
1	G	238	GLU
1	G	285	GLU
1	G	286	ARG
1	G	312	GLU
1	G	316	HIS
1	G	384	ARG
1	G	408	SER
1	G	415	LEU
1	G	421	GLU
1	G	425	GLU
1	G	428	LEU
1	G	446	ARG
1	G	455	SER
1	G	480	GLN
1	G	492	ASN
1	G	517	GLU
1	G	522	LEU
1	G	574	GLU
1	G	578	ARG
1	H	6	ILE
1	H	7	PRO
1	H	32	GLU
1	H	51	LYS
1	H	61	LYS
1	H	64	THR
1	H	80	LEU
1	H	95	ILE
1	H	137	THR
1	H	165	GLN
1	H	189	ARG
1	H	231	VAL
1	H	238	GLU
1	H	285	GLU
1	H	286	ARG
1	H	291	LEU

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Mol	Chain	Res	Type
1	H	292	LEU
1	H	304	THR
1	H	316	HIS
1	H	408	SER
1	H	428	LEU
1	H	432	GLU
1	H	455	SER
1	H	480	GLN
1	H	492	ASN
1	H	495	VAL
1	H	522	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	195	GLN
1	A	492	ASN
1	A	567	GLN
1	B	42	ASN
1	B	59	ASN
1	B	134	ASN
1	B	161	GLN
1	B	492	ASN
1	B	508	GLN
1	C	30	GLN
1	C	42	ASN
1	C	59	ASN
1	C	492	ASN
1	C	566	HIS
1	D	30	GLN
1	D	59	ASN
1	D	102	HIS
1	D	161	GLN
1	D	316	HIS
1	D	492	ASN
1	E	97	ASN
1	E	161	GLN
1	E	316	HIS
1	E	492	ASN
1	E	567	GLN
1	F	30	GLN

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Mol	Chain	Res	Type
1	F	59	ASN
1	F	102	HIS
1	F	190	ASN
1	F	195	GLN
1	F	316	HIS
1	F	492	ASN
1	F	508	GLN
1	F	567	GLN
1	G	30	GLN
1	G	102	HIS
1	G	161	GLN
1	G	190	ASN
1	G	492	ASN
1	G	567	GLN
1	H	22	GLN
1	H	30	GLN
1	H	97	ASN
1	H	161	GLN
1	H	165	GLN
1	H	195	GLN
1	H	316	HIS
1	H	492	ASN

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 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	29,33,33	1.89	6 (20%)	44,52,52	1.95	15 (34%)
2	APC	A	601	3	29,33,33	1.86	8 (27%)	44,52,52	1.80	12 (27%)
2	APC	D	601	3	29,33,33	2.05	10 (34%)	44,52,52	2.36	17 (38%)
2	APC	H	601	3	29,33,33	2.34	9 (31%)	44,52,52	2.54	21 (47%)
2	APC	E	601	3	29,33,33	2.09	7 (24%)	44,52,52	1.79	13 (29%)

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	-	4/19/38/38	0/3/3/3
2	APC	A	601	3	-	7/19/38/38	0/3/3/3
2	APC	D	601	3	-	6/19/38/38	0/3/3/3
2	APC	H	601	3	-	7/19/38/38	0/3/3/3
2	APC	E	601	3	-	4/19/38/38	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	APC	C5-C4	6.62	1.50	1.39
2	E	601	APC	C5-C4	6.15	1.50	1.39
2	D	601	APC	C5-C4	6.11	1.50	1.39
2	B	601	APC	C5-C4	5.78	1.49	1.39
2	A	601	APC	C5-C4	5.43	1.48	1.39
2	H	601	APC	C5-N7	-5.01	1.29	1.39
2	E	601	APC	PB-O3B	4.54	1.63	1.58
2	H	601	APC	C4-N9	-4.49	1.28	1.37
2	B	601	APC	C5-N7	-4.31	1.31	1.39
2	E	601	APC	C4-N9	-4.12	1.29	1.37
2	A	601	APC	PB-O3B	4.06	1.62	1.58
2	D	601	APC	C5-N7	-3.89	1.32	1.39
2	E	601	APC	C5-N7	-3.79	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	APC	PA-O2A	3.67	1.65	1.56
2	B	601	APC	C4-N9	-3.55	1.30	1.37
2	A	601	APC	C5-N7	-3.43	1.32	1.39
2	D	601	APC	C4-N9	-3.37	1.30	1.37
2	H	601	APC	C5'-C4'	3.24	1.61	1.51
2	B	601	APC	PB-O2B	3.04	1.63	1.56
2	H	601	APC	C8-N7	2.94	1.37	1.31
2	H	601	APC	C1'-N9	2.90	1.54	1.46
2	A	601	APC	C4-N9	-2.86	1.31	1.37
2	D	601	APC	C1'-N9	2.59	1.53	1.46
2	A	601	APC	PA-O2A	2.50	1.62	1.56
2	H	601	APC	C2-N1	2.49	1.38	1.33
2	D	601	APC	C2-N1	2.41	1.38	1.33
2	E	601	APC	PA-O2A	2.39	1.62	1.56
2	A	601	APC	PB-O2B	2.38	1.62	1.56
2	D	601	APC	C5-C6	2.36	1.47	1.41
2	H	601	APC	PB-O2B	2.30	1.62	1.56
2	B	601	APC	PB-O3B	2.29	1.61	1.58
2	D	601	APC	C2-N3	2.29	1.38	1.33
2	A	601	APC	C8-N7	2.25	1.36	1.31
2	D	601	APC	PB-O3B	2.25	1.60	1.58
2	E	601	APC	PB-O2B	2.20	1.61	1.56
2	A	601	APC	C1'-N9	2.11	1.52	1.46
2	B	601	APC	C8-N7	2.10	1.35	1.31
2	D	601	APC	PA-O2A	2.09	1.61	1.56
2	D	601	APC	PB-O1B	-2.07	1.46	1.51
2	E	601	APC	C8-N7	2.02	1.35	1.31

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	APC	C2'-C1'-N9	7.52	132.00	113.30
2	D	601	APC	O4'-C1'-N9	6.51	120.59	108.09
2	D	601	APC	PB-O3B-PG	-6.03	110.85	132.45
2	D	601	APC	C5-C4-N3	-4.42	120.63	126.72
2	H	601	APC	O2'-C2'-C3'	-4.34	97.90	111.82
2	B	601	APC	O4'-C1'-N9	4.32	116.39	108.09
2	H	601	APC	O4'-C4'-C3'	-4.30	96.62	105.15
2	D	601	APC	N3-C4-N9	4.06	134.07	127.17
2	B	601	APC	C5-C4-N3	-4.04	121.15	126.72
2	A	601	APC	N3-C2-N1	-3.79	122.84	128.58
2	E	601	APC	C5-C4-N3	-3.77	121.52	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	APC	N6-C6-N1	3.76	126.76	118.38
2	D	601	APC	N6-C6-N1	3.74	126.70	118.38
2	H	601	APC	N9-C8-N7	3.67	119.15	113.94
2	H	601	APC	PB-O3B-PG	-3.67	119.29	132.45
2	H	601	APC	O1A-PA-C3A	-3.64	99.48	109.05
2	B	601	APC	N3-C4-N9	3.61	133.30	127.17
2	H	601	APC	C4-N9-C8	-3.53	102.03	105.74
2	A	601	APC	N3-C4-N9	3.53	133.17	127.17
2	A	601	APC	C5-C4-N3	-3.52	121.88	126.72
2	E	601	APC	O4'-C1'-N9	3.48	114.77	108.09
2	B	601	APC	N3-C2-N1	-3.46	123.35	128.58
2	H	601	APC	N6-C6-N1	3.45	126.06	118.38
2	E	601	APC	C2-N1-C6	3.43	124.36	118.73
2	H	601	APC	O1B-PB-C3A	3.42	118.07	109.05
2	H	601	APC	C5-C4-N3	-3.40	122.03	126.72
2	E	601	APC	N6-C6-N1	3.32	125.78	118.38
2	A	601	APC	O4'-C1'-N9	3.29	114.41	108.09
2	D	601	APC	O4'-C4'-C5'	3.18	119.53	109.33
2	E	601	APC	N3-C4-N9	3.17	132.57	127.17
2	D	601	APC	O1A-PA-C3A	3.13	117.30	109.05
2	A	601	APC	O2A-PA-O1A	-3.06	100.00	109.95
2	A	601	APC	C2-N1-C6	3.05	123.75	118.73
2	B	601	APC	PB-O3B-PG	-3.02	121.63	132.45
2	B	601	APC	C4'-O4'-C1'	-3.01	102.82	109.47
2	A	601	APC	N6-C6-N1	2.99	125.03	118.38
2	D	601	APC	N3-C2-N1	-2.97	124.08	128.58
2	D	601	APC	C2-N3-C4	2.94	119.00	111.83
2	B	601	APC	C2-N1-C6	2.82	123.36	118.73
2	H	601	APC	O3G-PG-O2G	2.78	118.24	107.80
2	B	601	APC	C2'-C1'-N9	2.78	120.21	113.30
2	E	601	APC	C3'-C2'-C1'	-2.77	96.22	101.46
2	D	601	APC	C4-N9-C1'	2.70	132.94	126.63
2	A	601	APC	C2-N3-C4	2.69	118.40	111.83
2	H	601	APC	C5-N7-C8	-2.67	99.25	103.45
2	D	601	APC	C5'-C4'-C3'	-2.64	105.70	115.21
2	B	601	APC	C2-N3-C4	2.56	118.09	111.83
2	A	601	APC	O5'-C5'-C4'	2.51	117.53	108.99
2	H	601	APC	O3'-C3'-C4'	-2.49	103.92	111.08
2	H	601	APC	O4'-C4'-C5'	2.49	117.31	109.33
2	D	601	APC	O3G-PG-O2G	2.49	117.12	107.80
2	E	601	APC	O2'-C2'-C3'	2.48	119.78	111.82
2	H	601	APC	C2-N1-C6	2.48	122.80	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	APC	O4'-C1'-C2'	-2.45	101.37	106.62
2	D	601	APC	C5-C6-N6	-2.43	117.27	123.29
2	B	601	APC	C5'-C4'-C3'	-2.43	106.47	115.21
2	H	601	APC	C4'-O4'-C1'	2.42	114.80	109.47
2	D	601	APC	C1'-N9-C8	-2.40	121.77	127.09
2	B	601	APC	O3G-PG-O2G	2.36	116.66	107.80
2	E	601	APC	C1'-N9-C8	-2.36	121.86	127.09
2	E	601	APC	O3'-C3'-C2'	2.36	119.37	111.82
2	A	601	APC	O1B-PB-C3A	2.35	115.24	109.05
2	H	601	APC	N3-C2-N1	-2.29	125.11	128.58
2	H	601	APC	O5'-C5'-C4'	2.29	116.79	108.99
2	A	601	APC	O2A-PA-C3A	2.28	116.17	106.73
2	H	601	APC	O3B-PG-O1G	-2.27	99.09	111.04
2	B	601	APC	C5-C6-N6	-2.24	117.75	123.29
2	E	601	APC	C5'-C4'-C3'	-2.21	107.26	115.21
2	D	601	APC	O5'-C5'-C4'	2.14	116.28	108.99
2	B	601	APC	O2'-C2'-C1'	2.13	117.44	110.10
2	B	601	APC	O4'-C1'-C2'	-2.09	102.14	106.62
2	E	601	APC	C6-C5-C4	2.09	120.03	117.18
2	E	601	APC	N3-C2-N1	-2.08	125.44	128.58
2	H	601	APC	C2-N3-C4	2.07	116.89	111.83
2	D	601	APC	O4'-C1'-C2'	-2.03	102.26	106.62
2	A	601	APC	PB-O3B-PG	-2.02	125.20	132.45
2	E	601	APC	O3'-C3'-C4'	-2.02	105.29	111.08
2	D	601	APC	O3'-C3'-C4'	-2.00	105.33	111.08

There are no chirality outliers.

All (28) 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	C5'-O5'-PA-C3A
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

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Mol	Chain	Res	Type	Atoms
2	H	601	APC	PA-C3A-PB-O3B
2	H	601	APC	C4'-C5'-O5'-PA
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	H	601	APC	O4'-C4'-C5'-O5'
2	D	601	APC	C4'-C5'-O5'-PA
2	E	601	APC	PB-O3B-PG-O1G
2	A	601	APC	C3'-C4'-C5'-O5'
2	A	601	APC	PA-C3A-PB-O2B
2	A	601	APC	PB-C3A-PA-O5'
2	H	601	APC	O4'-C1'-N9-C4
2	B	601	APC	O4'-C1'-N9-C4
2	B	601	APC	PA-C3A-PB-O1B
2	A	601	APC	C4'-C5'-O5'-PA
2	B	601	APC	O4'-C1'-N9-C8

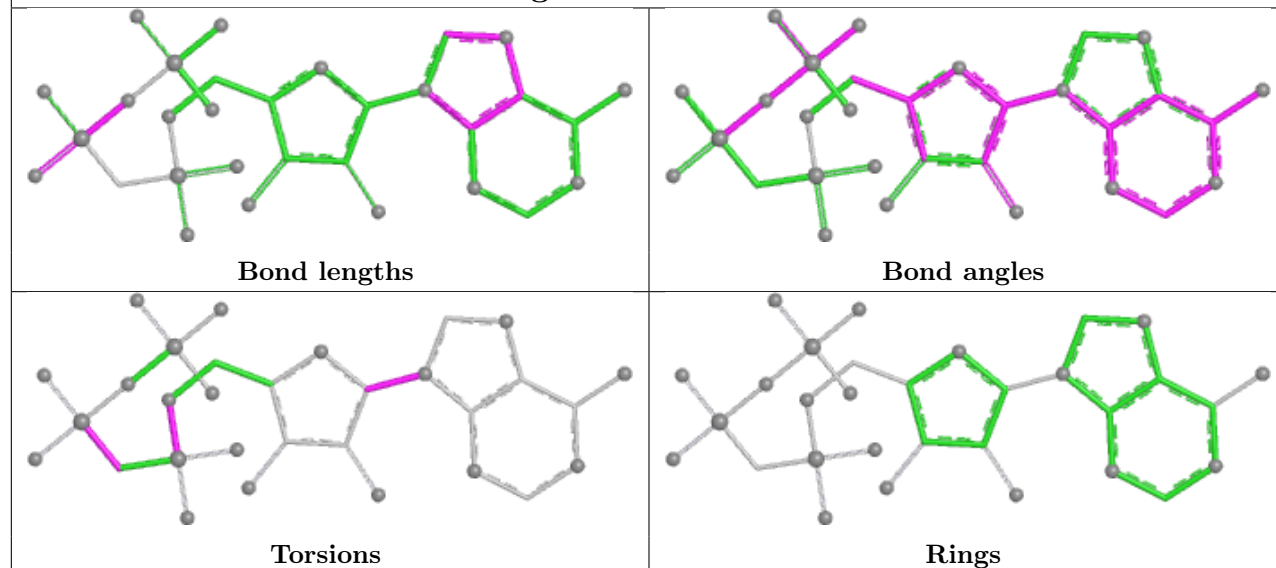
There are no ring outliers.

4 monomers are involved in 10 short contacts:

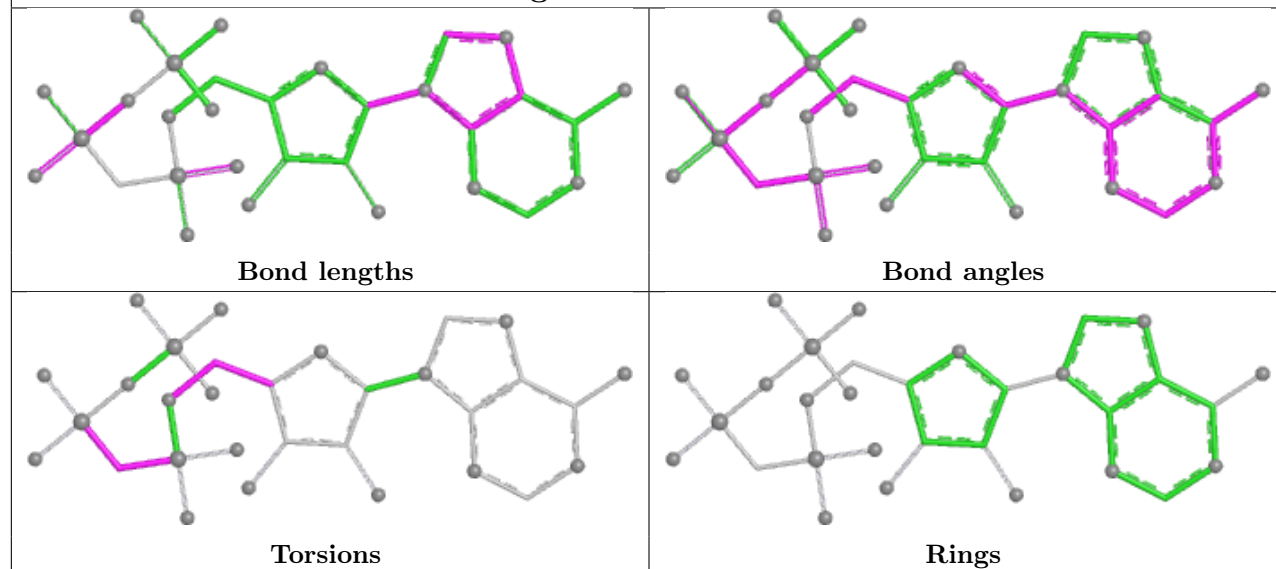
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	APC	2	0
2	A	601	APC	1	0
2	D	601	APC	3	0
2	H	601	APC	4	0

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 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.

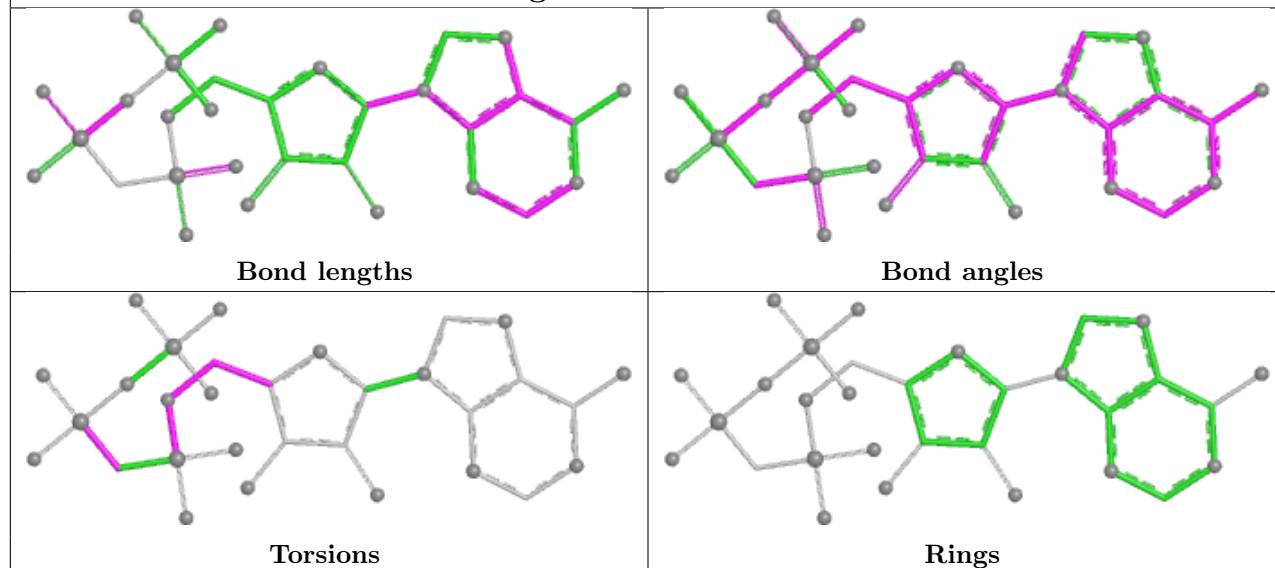
Ligand APC B 601



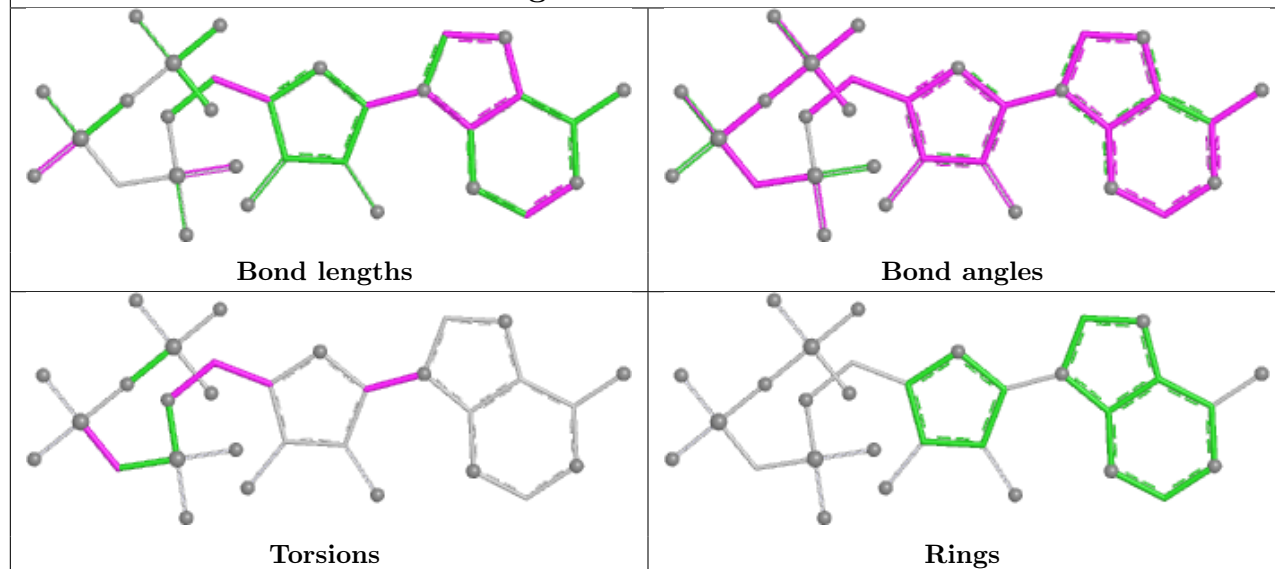
Ligand APC A 601

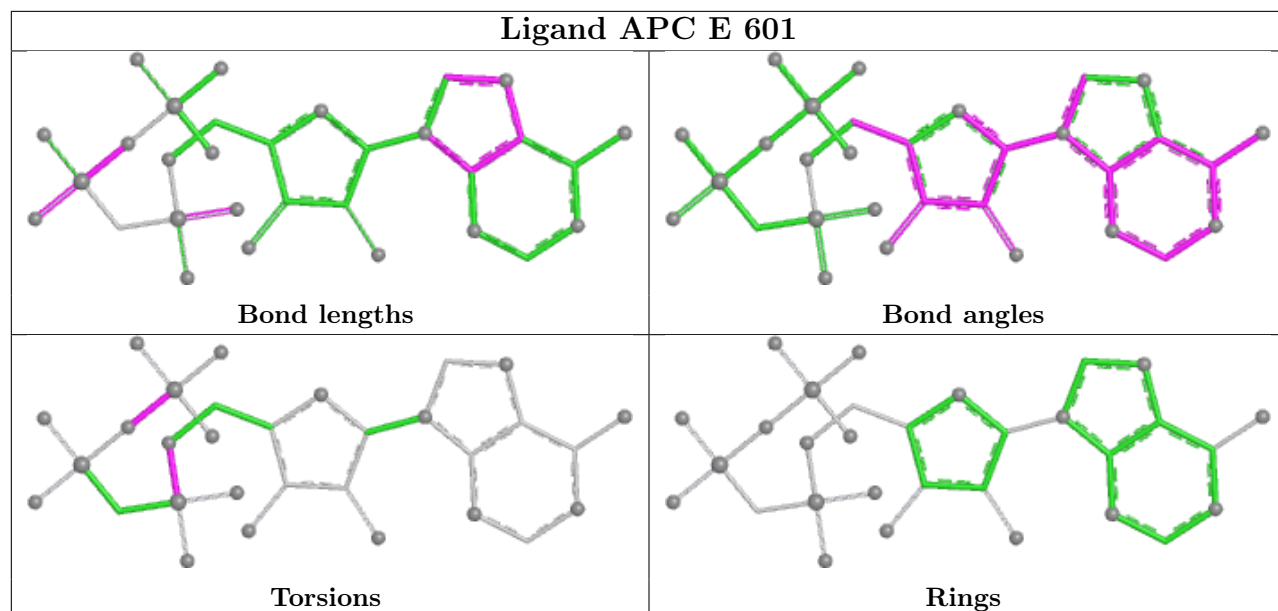


Ligand APC D 601



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 ⓘ

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	559/586 (95%)	-0.36	0 100 100	33, 59, 87, 111	0
1	B	573/586 (97%)	-0.31	1 (0%) 91 86	29, 54, 94, 130	0
1	C	562/586 (95%)	-0.19	1 (0%) 91 86	36, 63, 93, 112	0
1	D	572/586 (97%)	-0.28	0 100 100	29, 56, 89, 123	0
1	E	573/586 (97%)	-0.38	0 100 100	28, 50, 83, 112	0
1	F	570/586 (97%)	0.56	27 (4%) 36 24	54, 93, 124, 198	0
1	G	545/586 (93%)	-0.04	5 (0%) 81 65	36, 70, 107, 185	0
1	H	573/586 (97%)	-0.41	0 100 100	28, 49, 80, 125	0
All	All	4527/4688 (96%)	-0.18	34 (0%) 82 68	28, 60, 104, 198	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	573	TYR	5.6
1	F	182	GLY	4.1
1	F	300	LEU	3.8
1	B	326	SER	3.7
1	F	6	ILE	3.1
1	F	283	ALA	3.0
1	F	184	SER	3.0
1	F	108	TRP	2.8
1	F	275	GLY	2.8
1	F	348	PHE	2.6
1	F	363	PHE	2.6
1	F	219	ILE	2.5
1	C	14	GLU	2.5
1	F	203	ARG	2.5
1	F	391	SER	2.5
1	F	276	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	256	PRO	2.4
1	F	278	PRO	2.4
1	G	228	PRO	2.3
1	F	383	CYS	2.3
1	F	273	SER	2.3
1	G	43	VAL	2.2
1	G	42	ASN	2.2
1	F	209	ILE	2.2
1	F	143	ASP	2.2
1	F	234	ILE	2.2
1	G	379	GLY	2.2
1	G	25	SER	2.1
1	F	118	PRO	2.1
1	F	5	PHE	2.1
1	F	384	ARG	2.1
1	F	522	LEU	2.1
1	F	359	LEU	2.0
1	F	386	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(Å ²)	Q<0.9
3	MG	C	602	1/1	0.90	0.17	28,28,28,28	0
2	APC	D	601	31/31	0.95	0.09	33,45,59,60	0
2	APC	A	601	31/31	0.95	0.07	57,76,98,107	0
2	APC	E	601	31/31	0.96	0.07	32,42,54,60	0
2	APC	B	601	31/31	0.96	0.08	33,48,59,60	0

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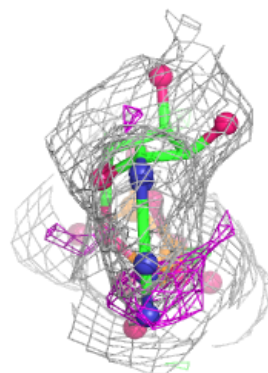
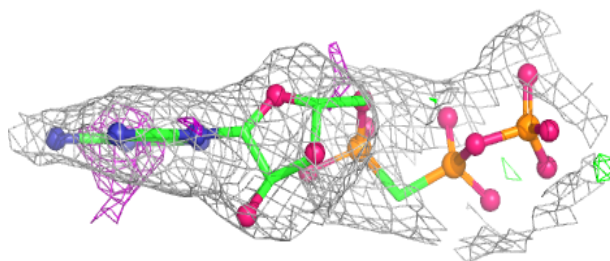
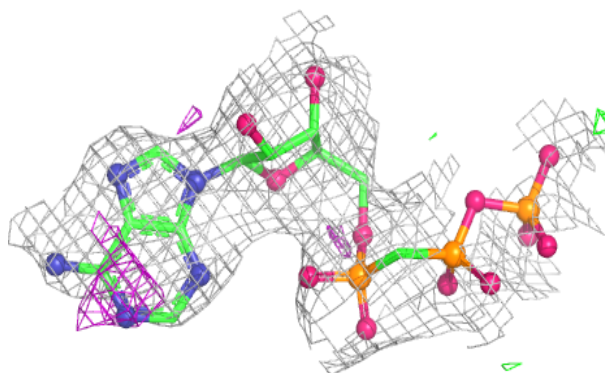
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	C	601	1/1	0.97	0.03	39,39,39,39	0
2	APC	H	601	31/31	0.97	0.08	24,38,49,54	0
3	MG	H	603	1/1	0.97	0.07	16,16,16,16	0
3	MG	H	605	1/1	0.97	0.11	62,62,62,62	0
3	MG	E	602	1/1	0.98	0.03	17,17,17,17	0
3	MG	E	603	1/1	0.98	0.03	22,22,22,22	0
3	MG	H	602	1/1	0.98	0.04	9,9,9,9	0
3	MG	A	604	1/1	0.98	0.02	31,31,31,31	0
3	MG	D	602	1/1	0.98	0.04	15,15,15,15	0
3	MG	D	604	1/1	0.99	0.03	19,19,19,19	0
3	MG	E	604	1/1	0.99	0.02	23,23,23,23	0
3	MG	B	603	1/1	0.99	0.05	9,9,9,9	0
3	MG	A	603	1/1	0.99	0.03	24,24,24,24	0
3	MG	G	601	1/1	0.99	0.02	22,22,22,22	0
3	MG	A	602	1/1	0.99	0.02	6,6,6,6	0
3	MG	B	602	1/1	0.99	0.03	24,24,24,24	0
3	MG	H	604	1/1	0.99	0.04	20,20,20,20	0
3	MG	D	603	1/1	0.99	0.06	24,24,24,24	0
3	MG	B	604	1/1	1.00	0.09	9,9,9,9	0

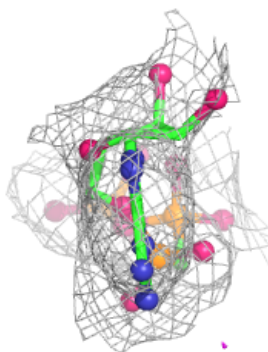
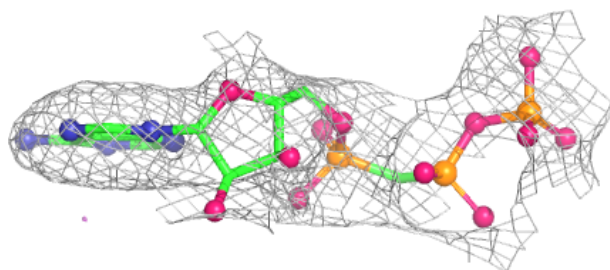
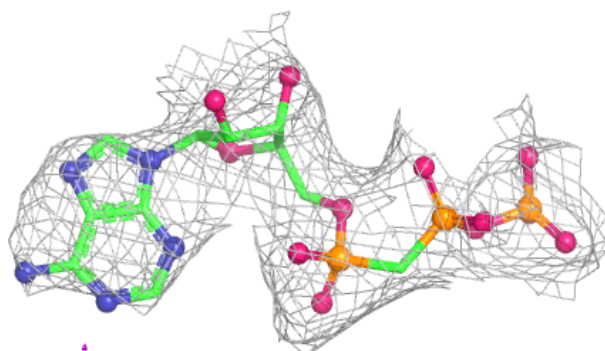
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around APC 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)

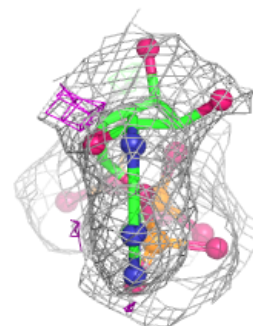
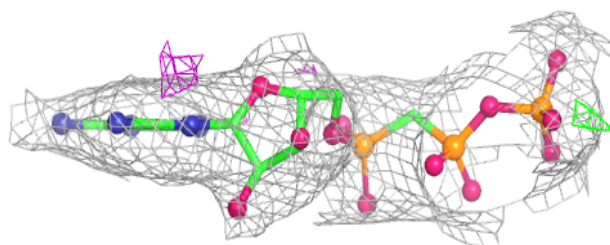
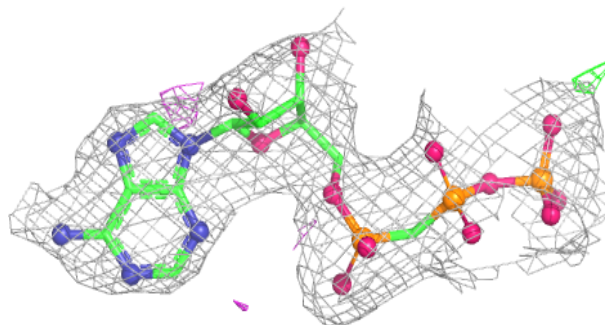
**Electron density around APC A 601:**

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

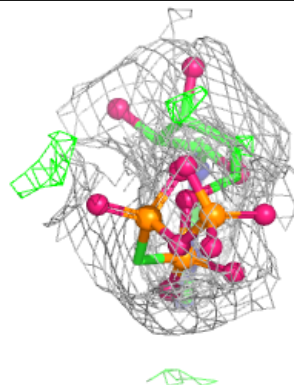
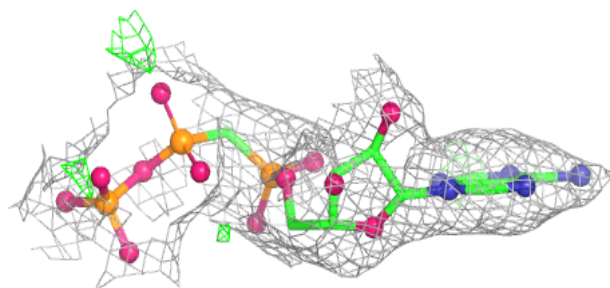
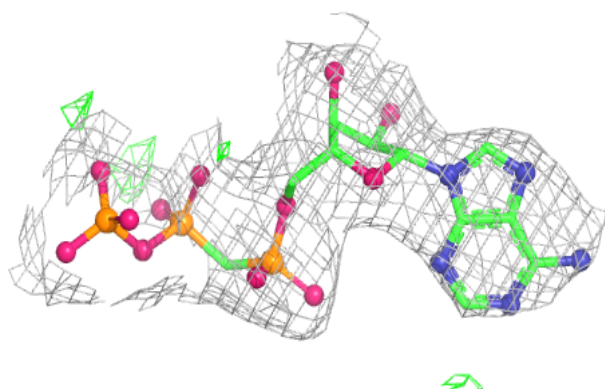


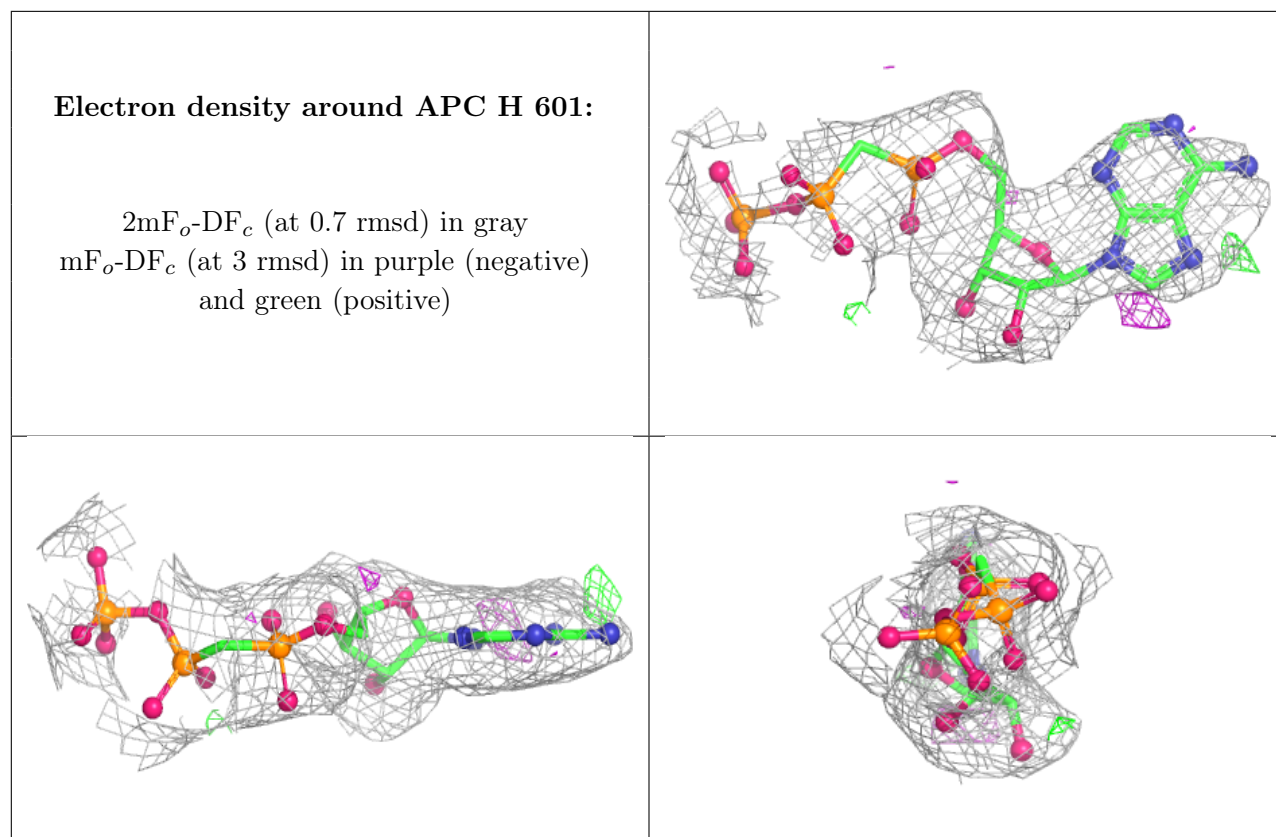
Electron density around APC E 601:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.