Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:55 am BST

PDB ID	:	6S84
Title	:	TsaBDE complex from Thermotoga maritima
Authors	:	Missoury, S.; Li-de-La-Sierra-Gallay, I.; van Tilbeurgh, H.
Deposited on	:	2019-07-08
Resolution	:	2.89 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 following versions of software and data (see references ⓘ) were used in the production of this report:

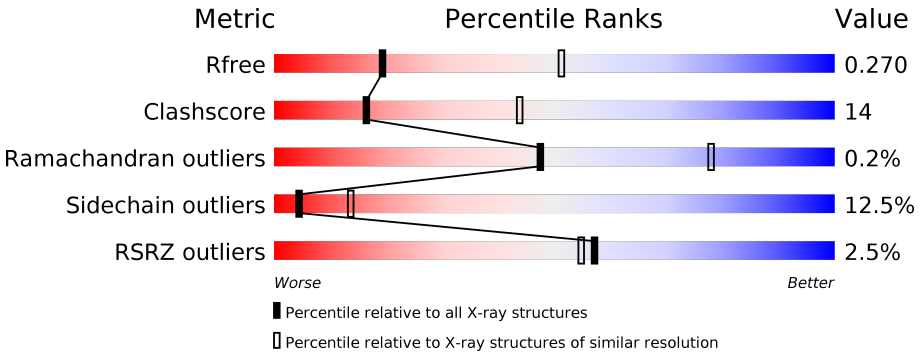
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	327	2% 65% 25% • 6%
1	D	327	2% 61% 28% 6% 6%
2	B	184	5% 60% 20% 7% 14%
2	E	184	5% 58% 26% • 12%
3	C	206	2% 76% 20% •
3	F	206	% 61% 32% 5% •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10687 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 tRNA N6-adenosine threonylcarbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2351	1510	399	433	9			
1	D	308	Total	C	N	O	S	0	0	0
			2368	1521	402	436	9			

- Molecule 2 is a protein called ATPase YjeE, predicted to have essential role in cell wall biosynthesis.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	162	Total	C	N	O	S	0	0	0
			1321	846	218	252	5			
2	B	159	Total	C	N	O	S	0	0	0
			1296	831	213	247	5			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-22	MET	-	initiating methionine	UNP R4NRX5
E	-21	GLY	-	expression tag	UNP R4NRX5
E	-20	HIS	-	expression tag	UNP R4NRX5
E	-19	HIS	-	expression tag	UNP R4NRX5
E	-18	HIS	-	expression tag	UNP R4NRX5
E	-17	HIS	-	expression tag	UNP R4NRX5
E	-16	HIS	-	expression tag	UNP R4NRX5
E	-15	HIS	-	expression tag	UNP R4NRX5
E	-14	GLU	-	expression tag	UNP R4NRX5
E	-13	ASN	-	expression tag	UNP R4NRX5
E	-12	LEU	-	expression tag	UNP R4NRX5
E	-11	TYR	-	expression tag	UNP R4NRX5
E	-10	PHE	-	expression tag	UNP R4NRX5
E	-9	GLN	-	expression tag	UNP R4NRX5
E	-8	GLY	-	expression tag	UNP R4NRX5

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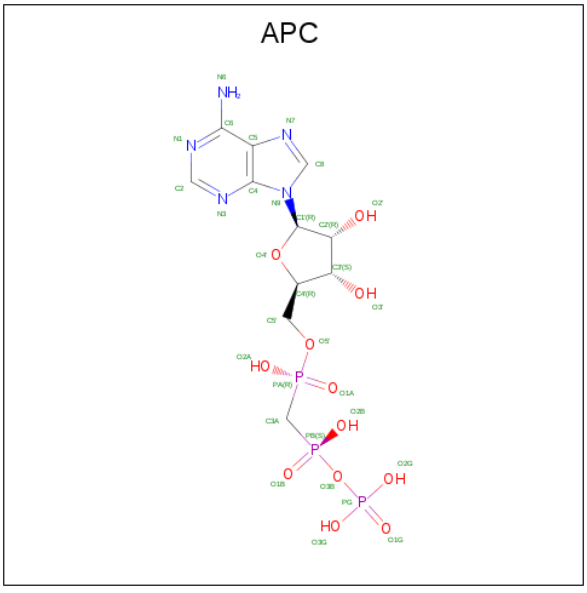
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	MET	-	initiating methionine	UNP R4NRX5
B	-21	GLY	-	expression tag	UNP R4NRX5
B	-20	HIS	-	expression tag	UNP R4NRX5
B	-19	HIS	-	expression tag	UNP R4NRX5
B	-18	HIS	-	expression tag	UNP R4NRX5
B	-17	HIS	-	expression tag	UNP R4NRX5
B	-16	HIS	-	expression tag	UNP R4NRX5
B	-15	HIS	-	expression tag	UNP R4NRX5
B	-14	GLU	-	expression tag	UNP R4NRX5
B	-13	ASN	-	expression tag	UNP R4NRX5
B	-12	LEU	-	expression tag	UNP R4NRX5
B	-11	TYR	-	expression tag	UNP R4NRX5
B	-10	PHE	-	expression tag	UNP R4NRX5
B	-9	GLN	-	expression tag	UNP R4NRX5
B	-8	GLY	-	expression tag	UNP R4NRX5

- Molecule 3 is a protein called tRNA threonylcarbamoyladenosine biosynthesis protein TsaB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	205	Total	C	N	O	S	0	0	0
			1614	1040	269	301	4			
3	F	201	Total	C	N	O	S	0	1	0
			1585	1024	259	298	4			

- Molecule 4 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).

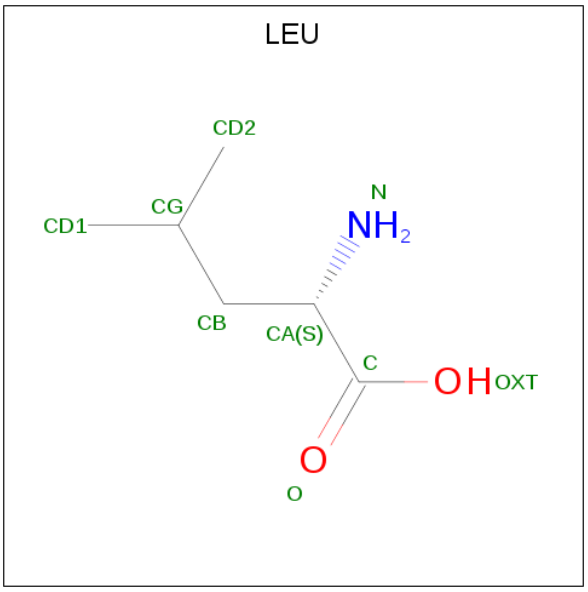


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
4	E	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
4	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		

- Molecule 6 is LEUCINE (three-letter code: LEU) (formula: $C_6H_{13}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			8	6	1	1		

- Molecule 7 is water.

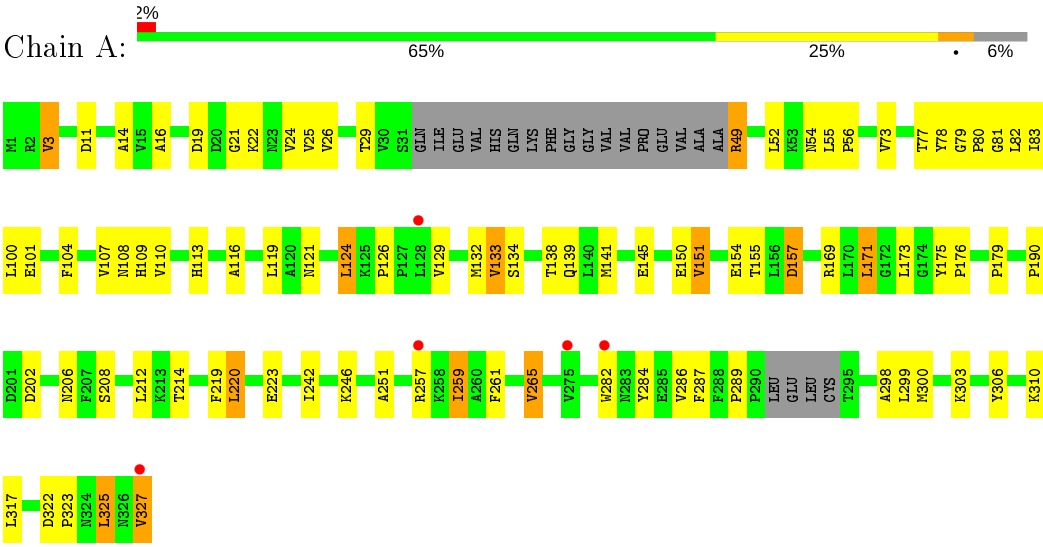
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	6	Total O 6 6	0	0
7	D	2	Total O 2 2	0	0
7	C	5	Total O 5 5	0	0
7	F	3	Total O 3 3	0	0
7	B	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

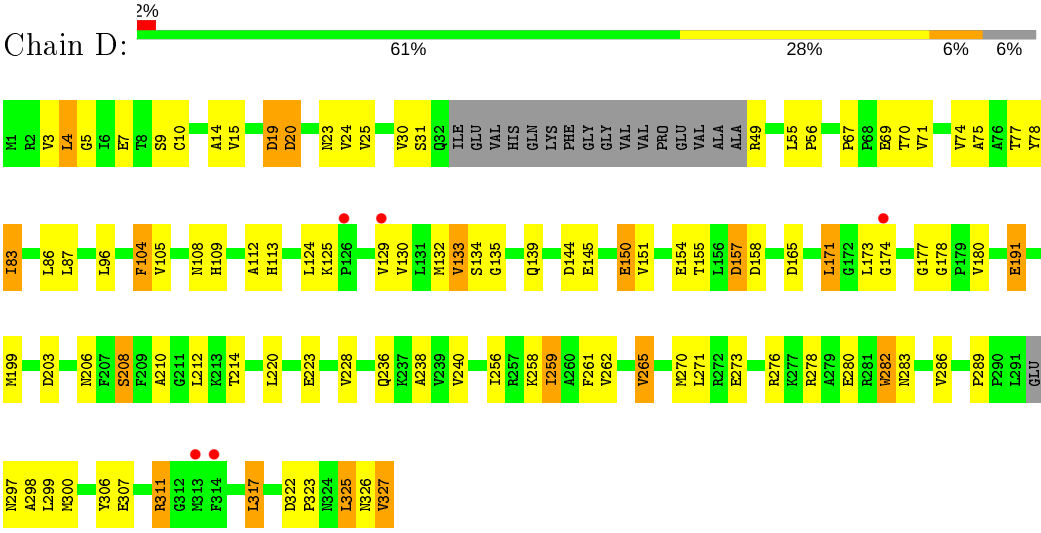
• Molecule 1: tRNA N6-adenosine threonylcarbamoyltransferase

Chain A:



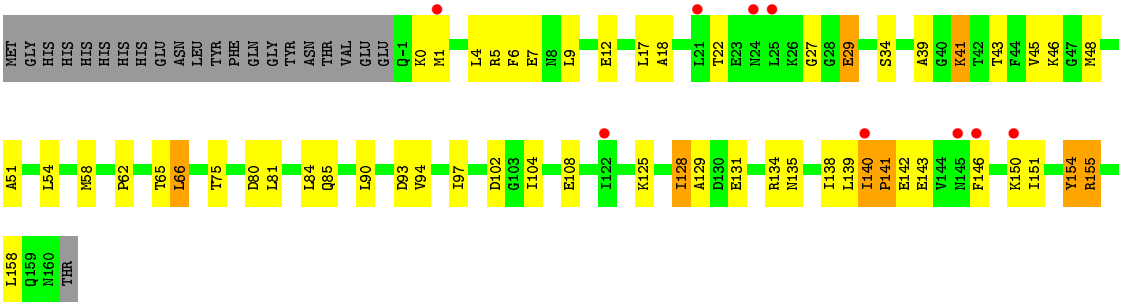
• Molecule 1: tRNA N6-adenosine threonylcarbamoyltransferase

Chain D:



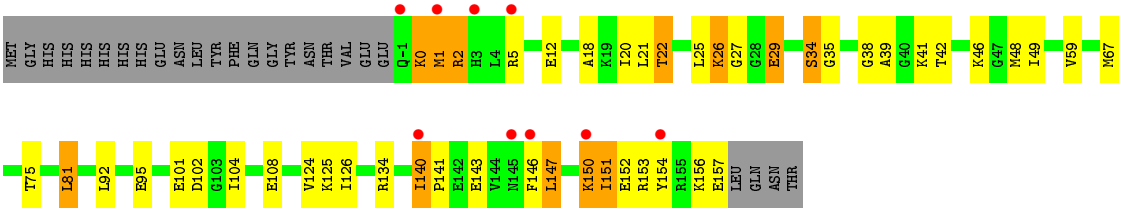
• Molecule 2: ATPase YjeE, predicted to have essential role in cell wall biosynthesis

Chain E:



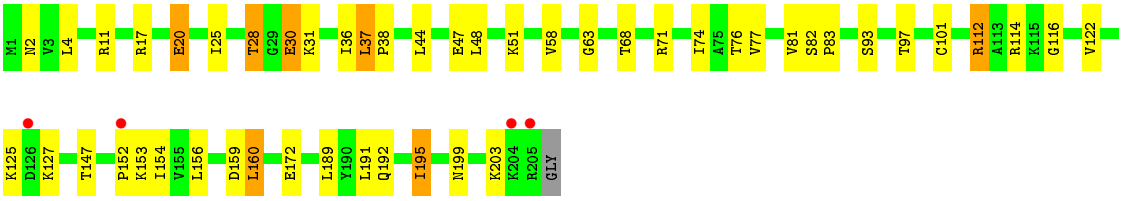
• Molecule 2: ATPase YjeE, predicted to have essential role in cell wall biosynthesis

Chain B:



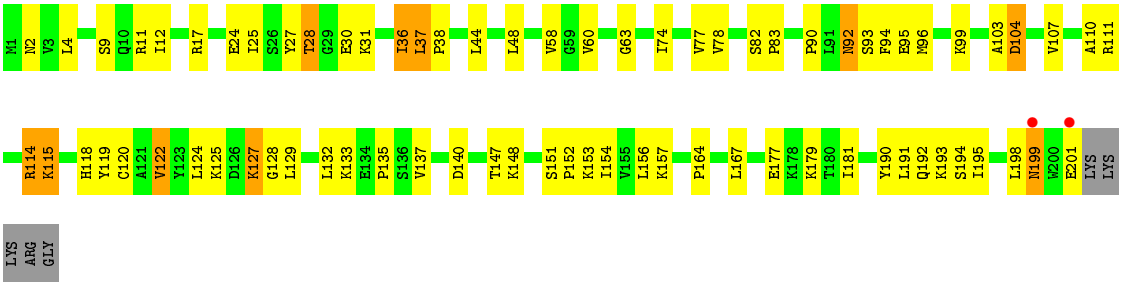
• Molecule 3: tRNA threonylcarbamoyladenosine biosynthesis protein TsaB

Chain C:



• Molecule 3: tRNA threonylcarbamoyladenosine biosynthesis protein TsaB

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.16Å 108.21Å 176.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.43 – 2.89 48.43 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.43-2.89) 80.5 (48.43-2.90)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.209 , 0.282 0.199 , 0.270	Depositor DCC
R_{free} test set	1494 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	65.6	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10687	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: APC, 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	0.27	0/2396	0.62	0/3242
1	D	0.27	0/2413	0.62	0/3265
2	B	0.27	0/1317	0.58	0/1773
2	E	0.28	0/1342	0.60	0/1807
3	C	0.27	0/1641	0.61	1/2217 (0.0%)
3	F	0.28	0/1616	0.60	0/2188
All	All	0.27	0/10725	0.61	1/14492 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	71	ARG	CG-CD-NE	-5.53	100.19	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2351	0	2400	63	9
1	D	2368	0	2419	67	0
2	B	1296	0	1314	38	0
2	E	1321	0	1339	57	9

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1614	0	1696	35	0
3	F	1585	0	1653	56	0
4	A	31	0	14	1	0
4	B	31	0	14	6	0
4	D	31	0	14	7	0
4	E	31	0	14	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
6	B	8	0	10	2	0
7	A	6	0	0	0	0
7	B	2	0	0	0	0
7	C	5	0	0	0	0
7	D	2	0	0	1	0
7	F	3	0	0	0	0
All	All	10687	0	10887	308	9

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 14.

All (308) 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)
2:E:140:ILE:HD13	2:E:146:PHE:CE2	1.31	1.62
2:E:140:ILE:HB	2:E:146:PHE:CZ	1.59	1.36
2:E:140:ILE:CB	2:E:146:PHE:HZ	1.38	1.35
2:E:140:ILE:CG1	2:E:146:PHE:CZ	2.09	1.34
2:E:140:ILE:CD1	2:E:146:PHE:CE2	2.18	1.25
2:E:140:ILE:HD13	2:E:146:PHE:CZ	1.72	1.24
2:E:140:ILE:CB	2:E:146:PHE:CZ	2.15	1.23
2:E:140:ILE:CD1	2:E:146:PHE:CZ	2.26	1.18
2:E:140:ILE:HG12	2:E:146:PHE:CZ	1.94	0.98
2:B:18:ALA:O	2:B:22:THR:HG22	1.65	0.96
2:E:140:ILE:HB	2:E:146:PHE:HZ	0.79	0.93
2:B:35:GLY:O	2:B:41:LYS:HE2	1.69	0.92
3:F:114:ARG:HD2	3:F:195:ILE:HG21	1.51	0.90
2:E:39:ALA:O	2:E:134:ARG:HD3	1.74	0.88
1:D:173:LEU:HB3	1:D:180:VAL:HG11	1.58	0.83
1:A:83:ILE:HG13	1:A:323:PRO:HG3	1.59	0.82
1:A:3:VAL:HB	1:A:73:VAL:HG13	1.61	0.81
2:B:18:ALA:O	2:B:22:THR:CG2	2.28	0.81
1:A:134:SER:HB2	4:A:400:APC:O2B	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:140:ILE:HD13	2:E:146:PHE:HE2	0.98	0.81
1:A:14:ALA:HB1	1:A:298:ALA:HB2	1.64	0.80
3:C:20:GLU:HG2	3:F:30:GLU:HG2	1.61	0.80
3:F:119:TYR:OH	3:F:192:GLN:CG	2.31	0.79
3:C:11:ARG:NH1	3:C:159:ASP:OD1	2.17	0.78
3:F:37:LEU:HB3	3:F:38:PRO:HD3	1.66	0.78
1:D:14:ALA:HB1	1:D:298:ALA:HB2	1.66	0.77
1:D:83:ILE:HD12	1:D:83:ILE:H	1.50	0.76
1:D:83:ILE:HG13	1:D:323:PRO:HG3	1.66	0.75
3:C:63:GLY:HA3	3:C:93:SER:H	1.52	0.75
3:C:114:ARG:NE	3:C:195:ILE:HD11	2.01	0.74
1:A:81:GLY:O	1:A:323:PRO:HB3	1.87	0.74
2:E:1:MET:HG3	2:E:141:PRO:HB3	1.71	0.73
1:D:134:SER:HB2	4:D:400:APC:O2B	1.90	0.72
2:B:34:SER:HB2	2:B:125:LYS:HD2	1.72	0.72
3:F:114:ARG:HD2	3:F:195:ILE:CG2	2.20	0.71
3:F:119:TYR:OH	3:F:192:GLN:HG2	1.91	0.71
1:A:83:ILE:HG13	1:A:323:PRO:CG	2.20	0.70
1:A:190:PRO:O	1:A:191:GLU:HG2	1.92	0.70
3:F:119:TYR:OH	3:F:192:GLN:HG3	1.91	0.70
2:E:140:ILE:CB	2:E:146:PHE:CE1	2.74	0.70
2:B:150:LYS:NZ	2:B:150:LYS:HB3	2.06	0.70
2:E:140:ILE:HG12	2:E:146:PHE:CE1	2.27	0.69
2:E:17:LEU:HD21	2:E:138:ILE:HD11	1.74	0.69
1:A:3:VAL:HG11	1:A:306:TYR:HB2	1.75	0.68
1:A:49:ARG:HD3	1:A:54:ASN:HD21	1.59	0.68
1:D:133:VAL:HB	1:D:265:VAL:HG22	1.77	0.67
1:D:24:VAL:HG12	1:D:299:LEU:HD22	1.76	0.67
1:D:135:GLY:H	4:D:400:APC:H4'	1.58	0.67
2:B:42:THR:OG1	4:B:203:APC:O1B	2.12	0.66
3:C:101:CYS:O	3:C:125:LYS:NZ	2.25	0.66
3:C:37:LEU:HB3	3:C:38:PRO:HD3	1.77	0.66
1:A:113:HIS:HD2	1:A:300:MET:CE	2.09	0.66
2:E:140:ILE:HB	2:E:146:PHE:CE1	2.27	0.65
1:A:11:ASP:O	1:A:49:ARG:N	2.30	0.65
1:D:78:TYR:CZ	1:D:325:LEU:HD11	2.32	0.64
1:D:133:VAL:CG2	1:D:265:VAL:HG22	2.28	0.64
2:E:151:ILE:O	2:E:154:TYR:HB2	1.97	0.64
1:A:49:ARG:HD3	1:A:54:ASN:ND2	2.13	0.63
3:C:97:THR:HG21	3:C:160:LEU:HG	1.80	0.62
1:A:154:GLU:H	1:A:206:ASN:HD22	1.45	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:ILE:HD12	2:B:59:VAL:HG23	1.82	0.62
3:C:195:ILE:HD13	3:C:195:ILE:C	2.20	0.62
3:F:92:ASN:HD22	3:F:95:GLU:H	1.46	0.62
1:A:132:MET:O	1:A:138:THR:HA	2.00	0.62
1:A:121:ASN:ND2	1:A:287:PHE:CD1	2.68	0.62
1:A:3:VAL:HB	1:A:73:VAL:CG1	2.29	0.62
1:D:19:ASP:HB2	1:D:23:ASN:HB3	1.80	0.62
3:F:127:LYS:H	3:F:127:LYS:HD3	1.65	0.61
3:F:63:GLY:HA3	3:F:93:SER:H	1.64	0.61
1:A:108:ASN:ND2	1:A:325:LEU:HD22	2.16	0.61
2:E:18:ALA:O	2:E:22:THR:HG22	2.00	0.61
1:D:151:VAL:HG12	1:D:327:VAL:HG23	1.82	0.61
1:D:297:ASN:ND2	7:D:501:HOH:O	2.33	0.60
2:E:140:ILE:HG21	2:E:146:PHE:HE1	1.65	0.60
2:E:4:LEU:HD22	2:E:150:LYS:NZ	2.15	0.60
1:D:296:ASP:HB3	1:D:299:LEU:HD12	1.83	0.60
2:E:140:ILE:HG21	2:E:146:PHE:CE1	2.36	0.60
1:D:282:TRP:CD1	1:D:282:TRP:N	2.71	0.59
3:F:92:ASN:O	3:F:96:MET:HG2	2.03	0.59
3:F:12:ILE:HD12	3:F:27:TYR:HD2	1.68	0.58
1:A:121:ASN:HB2	1:A:124:LEU:HD12	1.85	0.57
3:C:31:LYS:HD3	3:C:36:ILE:HD11	1.86	0.57
1:D:240:VAL:HG13	1:D:271:LEU:HD12	1.86	0.57
1:A:261:PHE:O	1:A:289:PRO:HD3	2.05	0.57
3:F:25:ILE:HD11	3:F:44:LEU:HD13	1.87	0.57
1:A:199:MET:O	1:A:202:ASP:HB2	2.06	0.56
3:F:127:LYS:N	3:F:127:LYS:HD3	2.20	0.56
3:C:154:ILE:HG23	3:F:103:ALA:HB2	1.88	0.56
1:A:311:ARG:HD3	1:A:311:ARG:N	2.21	0.56
2:E:22:THR:HG23	2:E:51:ALA:CB	2.35	0.56
3:F:12:ILE:HD13	3:F:36:ILE:HG23	1.87	0.56
1:A:171:LEU:HD12	1:A:220:LEU:HD21	1.87	0.56
3:F:82:SER:OG	3:F:83:PRO:HD3	2.05	0.56
1:A:157:ASP:OD2	1:A:208:SER:HA	2.06	0.56
2:B:143:GLU:HB2	2:B:146:PHE:HB3	1.88	0.56
2:B:41:LYS:NZ	4:B:203:APC:O3G	2.39	0.56
3:C:77:VAL:O	3:C:81:VAL:HG22	2.06	0.56
1:D:55:LEU:HB3	1:D:56:PRO:HD3	1.87	0.56
3:C:25:ILE:HD11	3:C:44:LEU:HD13	1.87	0.55
2:B:1:MET:HG3	2:B:141:PRO:HB3	1.88	0.55
3:F:124:LEU:O	3:F:129:LEU:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:PRO:HB2	1:A:145:GLU:HA	1.88	0.55
1:D:154:GLU:H	1:D:206:ASN:HD22	1.55	0.55
1:D:24:VAL:HG12	1:D:299:LEU:CD2	2.37	0.55
2:B:143:GLU:HB2	2:B:146:PHE:CB	2.37	0.55
3:F:104:ASP:HA	3:F:125:LYS:HE3	1.88	0.55
3:C:20:GLU:HG2	3:F:30:GLU:CG	2.36	0.55
2:E:142:GLU:HA	2:E:142:GLU:OE1	2.07	0.55
2:B:157:GLU:HG3	6:B:201:LEU:N	2.22	0.55
3:C:114:ARG:NE	3:C:195:ILE:CD1	2.70	0.54
3:C:97:THR:HG22	3:C:156:LEU:HD13	1.88	0.54
1:A:49:ARG:HG2	1:A:49:ARG:HH11	1.72	0.54
2:B:150:LYS:HZ2	2:B:150:LYS:HB3	1.73	0.54
2:E:4:LEU:HD22	2:E:150:LYS:HZ1	1.73	0.54
1:A:119:LEU:HD12	1:A:303:LYS:HE3	1.90	0.54
1:D:77:THR:HG22	1:D:79:GLY:H	1.72	0.54
2:B:39:ALA:O	4:B:203:APC:H3A1	2.06	0.54
3:C:114:ARG:CD	3:C:195:ILE:HD11	2.37	0.54
1:D:191:GLU:HG2	1:D:191:GLU:O	2.07	0.54
1:A:78:TYR:CZ	1:A:325:LEU:HD11	2.43	0.54
1:A:77:THR:HG22	1:A:79:GLY:H	1.71	0.54
1:A:133:VAL:HB	1:A:265:VAL:HG22	1.88	0.54
2:E:43:THR:O	2:E:46:LYS:HB2	2.08	0.53
1:D:171:LEU:CD1	1:D:220:LEU:HD11	2.38	0.53
2:B:39:ALA:O	4:B:203:APC:O2B	2.26	0.53
3:C:11:ARG:HD3	3:C:28:THR:HG23	1.91	0.53
3:F:12:ILE:HD13	3:F:36:ILE:CG2	2.39	0.52
1:A:83:ILE:HD12	1:A:83:ILE:H	1.74	0.52
1:D:134:SER:CB	4:D:400:APC:O2B	2.58	0.52
1:D:133:VAL:CB	1:D:265:VAL:HG22	2.40	0.52
3:F:90:PRO:HD3	3:F:181:ILE:HG12	1.92	0.52
1:A:311:ARG:CG	1:A:311:ARG:HH11	2.23	0.52
3:C:199:ASN:O	3:C:203:LYS:HB2	2.10	0.52
1:A:151:VAL:HG12	1:A:327:VAL:HG23	1.93	0.51
1:D:273:GLU:OE2	1:D:276:ARG:NH2	2.43	0.51
1:A:80:PRO:HD2	1:A:109:HIS:HB3	1.93	0.51
1:D:5:GLY:HA2	1:D:75:ALA:O	2.11	0.51
1:D:81:GLY:O	1:D:323:PRO:HB3	2.11	0.51
2:E:139:LEU:HD12	2:E:139:LEU:N	2.25	0.51
2:B:140:ILE:HD13	2:B:146:PHE:HB3	1.93	0.51
1:D:133:VAL:HB	1:D:265:VAL:CG2	2.40	0.50
1:D:210:ALA:O	1:D:214:THR:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:201:APC:H4'	1:D:214:THR:HG21	1.94	0.50
2:E:62:PRO:HG2	2:E:80:ASP:HB2	1.92	0.50
1:D:134:SER:HB2	4:D:400:APC:PB	2.52	0.50
3:F:11:ARG:HD3	3:F:28:THR:CG2	2.42	0.50
1:A:219:PHE:CE2	1:A:223:GLU:HG3	2.47	0.50
1:A:55:LEU:HB3	1:A:56:PRO:HD3	1.91	0.50
2:B:143:GLU:O	2:B:147:LEU:HG	2.12	0.50
2:B:134:ARG:HD3	4:B:203:APC:C6	2.42	0.50
2:E:140:ILE:CG2	2:E:146:PHE:CE1	2.94	0.49
1:D:165:ASP:HA	1:D:177:GLY:HA3	1.94	0.49
2:B:27:GLY:HA3	2:B:102:ASP:HA	1.94	0.49
3:F:103:ALA:O	3:F:125:LYS:HE2	2.12	0.49
3:F:107:VAL:HG22	3:F:154:ILE:HD13	1.94	0.49
3:F:11:ARG:HD3	3:F:28:THR:HG23	1.94	0.49
2:B:153:ARG:HA	2:B:156:LYS:HB2	1.95	0.49
2:B:22:THR:HG21	2:B:48:MET:HA	1.95	0.49
3:F:127:LYS:HG2	3:F:128:GLY:H	1.78	0.49
2:B:41:LYS:HB3	2:B:108:GLU:HG2	1.95	0.48
2:B:157:GLU:C	6:B:201:LEU:N	2.66	0.48
1:A:129:VAL:HG13	1:A:259:ILE:HD13	1.95	0.48
3:C:114:ARG:HD2	3:C:195:ILE:HD11	1.94	0.48
1:D:171:LEU:HG	1:D:228:VAL:HG13	1.95	0.48
1:D:3:VAL:HG11	1:D:306:TYR:HB2	1.95	0.48
3:F:2:ASN:HA	3:F:17:ARG:O	2.13	0.48
2:E:1:MET:HE3	2:E:1:MET:HA	1.94	0.48
3:F:9:SER:O	3:F:111:ARG:NH2	2.42	0.48
3:F:110:ALA:O	3:F:157:LYS:HA	2.14	0.48
2:B:124:VAL:HG12	2:B:126:ILE:HD11	1.95	0.48
2:E:140:ILE:HD11	2:E:143:GLU:H	1.78	0.48
1:A:129:VAL:HG11	1:A:251:ALA:HB2	1.95	0.47
1:D:256:ILE:HG22	1:D:258:LYS:H	1.79	0.47
1:D:108:ASN:CG	1:D:325:LEU:HD22	2.34	0.47
2:E:22:THR:HG23	2:E:51:ALA:HB3	1.96	0.47
1:A:108:ASN:ND2	1:A:325:LEU:CD2	2.77	0.47
1:D:259:ILE:O	1:D:286:VAL:HA	2.14	0.47
1:D:9:SER:HA	1:D:86:LEU:HD23	1.96	0.47
3:C:37:LEU:HD13	3:C:76:THR:HG21	1.95	0.47
1:D:80:PRO:CB	1:D:323:PRO:O	2.63	0.47
2:E:155:ARG:NH2	2:E:158:LEU:HD22	2.30	0.47
3:F:122:VAL:HG13	3:F:133:LYS:HB3	1.97	0.47
1:A:176:PRO:HG2	1:A:179:PRO:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:HIS:HD2	1:A:300:MET:HE1	1.80	0.47
1:A:259:ILE:HG23	1:A:286:VAL:HG12	1.97	0.47
3:F:122:VAL:HG22	3:F:132:LEU:HB2	1.96	0.46
2:B:41:LYS:HB2	4:B:203:APC:O2B	2.15	0.46
3:C:4:LEU:O	3:C:58:VAL:HA	2.15	0.46
2:E:41:LYS:HE3	2:E:108:GLU:HG2	1.96	0.46
1:A:306:TYR:CZ	1:A:310:LYS:HD3	2.51	0.46
2:E:93:ASP:O	2:E:97:ILE:HG13	2.16	0.46
2:E:155:ARG:HH11	2:E:155:ARG:HB2	1.80	0.46
1:A:200:LEU:HD13	1:A:242:ILE:HA	1.96	0.46
1:A:79:GLY:HA2	1:A:86:LEU:HD11	1.98	0.46
1:D:150:GLU:HA	1:D:327:VAL:HG22	1.98	0.45
1:D:236:GLN:HG2	1:D:270:MET:HG2	1.98	0.45
2:E:143:GLU:HA	2:E:143:GLU:OE1	2.17	0.45
3:F:74:ILE:O	3:F:78:VAL:HG23	2.15	0.45
1:D:133:VAL:HG23	1:D:265:VAL:HG22	1.97	0.45
3:F:177:GLU:HB2	3:F:179:LYS:HD2	1.99	0.45
1:A:157:ASP:OD2	1:A:208:SER:CA	2.65	0.45
2:E:140:ILE:CD1	2:E:146:PHE:HE2	1.89	0.45
3:C:82:SER:N	3:C:83:PRO:CD	2.79	0.45
3:F:60:VAL:HB	3:F:77:VAL:HG21	1.98	0.45
2:B:25:LEU:HD13	2:B:29:GLU:HG3	1.98	0.45
1:D:197:ARG:CZ	1:D:238:ALA:HA	2.47	0.45
2:E:34:SER:HB2	2:E:125:LYS:HD2	1.98	0.45
3:F:4:LEU:O	3:F:58:VAL:HA	2.17	0.45
1:D:80:PRO:HD2	1:D:109:HIS:HB3	1.98	0.44
2:E:90:LEU:HD23	2:E:94:VAL:HG21	2.00	0.44
1:A:171:LEU:HB3	1:A:173:LEU:HD12	2.00	0.44
2:E:1:MET:CE	2:E:1:MET:HA	2.47	0.44
2:E:6:PHE:HB3	2:E:9:LEU:HD11	1.99	0.44
3:F:147:THR:O	3:F:152:PRO:HD3	2.17	0.44
2:E:143:GLU:HB2	2:E:146:PHE:CE2	2.53	0.44
1:D:307:GLU:O	1:D:311:ARG:HD2	2.18	0.44
1:D:7:GLU:OE2	1:D:9:SER:HB3	2.17	0.44
3:F:118:HIS:HE1	3:F:140:ASP:OD1	2.00	0.44
3:F:119:TYR:CD1	3:F:191:LEU:HD23	2.52	0.44
3:F:118:HIS:O	3:F:137:VAL:HA	2.18	0.44
3:C:2:ASN:HA	3:C:17:ARG:O	2.17	0.44
3:F:154:ILE:CG2	3:F:156:LEU:HD21	2.48	0.44
1:A:133:VAL:CG2	1:A:265:VAL:HG22	2.47	0.44
2:B:25:LEU:HD11	2:B:104:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:PHE:O	1:D:289:PRO:HD3	2.18	0.44
3:F:37:LEU:HB3	3:F:38:PRO:CD	2.42	0.44
1:D:80:PRO:HB2	1:D:323:PRO:O	2.18	0.43
1:D:4:LEU:HB2	1:D:71:VAL:HG11	2.00	0.43
1:A:121:ASN:ND2	1:A:287:PHE:HD1	2.12	0.43
3:F:118:HIS:CE1	3:F:140:ASP:OD1	2.71	0.43
1:A:282:TRP:CD1	1:A:282:TRP:N	2.86	0.43
2:E:54:LEU:HD23	2:E:58:MET:SD	2.58	0.43
3:F:199:ASN:HD22	3:F:199:ASN:HA	1.61	0.43
1:A:24:VAL:O	1:A:24:VAL:HG23	2.17	0.43
1:A:116:ALA:HA	1:A:119:LEU:HB3	2.01	0.43
1:D:132:MET:HA	1:D:262:VAL:O	2.18	0.43
1:A:52:LEU:HD11	3:C:74:ILE:HG22	2.00	0.43
3:F:127:LYS:HG2	3:F:128:GLY:N	2.34	0.43
1:D:259:ILE:HG23	1:D:286:VAL:HG12	2.00	0.43
1:D:174:GLY:O	1:D:180:VAL:HG21	2.19	0.43
2:B:2:ARG:HH21	2:B:151:ILE:HD12	1.83	0.42
1:A:171:LEU:CD1	1:A:220:LEU:HD21	2.49	0.42
3:F:164:PRO:HA	3:F:167:LEU:HD12	2.01	0.42
3:C:30:GLU:H	3:C:30:GLU:HG3	1.68	0.42
1:D:129:VAL:HG13	1:D:259:ILE:HB	2.01	0.42
1:D:80:PRO:HB3	1:D:325:LEU:H	1.84	0.42
1:A:206:ASN:O	1:A:246:LYS:HE3	2.19	0.42
3:C:195:ILE:HD13	3:C:195:ILE:O	2.18	0.42
1:A:157:ASP:OD2	1:A:208:SER:CB	2.68	0.42
2:E:129:ALA:H	2:E:134:ARG:HA	1.85	0.42
3:F:99:LYS:HG3	3:F:129:LEU:HD23	2.01	0.42
2:B:42:THR:OG1	2:B:108:GLU:OE2	2.38	0.42
1:A:21:GLY:O	1:A:303:LYS:HE2	2.20	0.42
1:D:157:ASP:HB2	1:D:158:ASP:H	1.40	0.42
1:D:199:MET:HG2	1:D:208:SER:HB3	2.01	0.42
2:E:140:ILE:HA	2:E:141:PRO:HD3	1.92	0.42
2:B:26:LYS:HE3	2:B:26:LYS:HA	2.01	0.42
2:B:81:LEU:HD12	2:B:81:LEU:HA	1.91	0.42
3:C:37:LEU:CD1	3:C:76:THR:HG21	2.50	0.42
1:D:135:GLY:N	4:D:400:APC:H4'	2.31	0.42
3:F:120:CYS:O	3:F:135:PRO:HA	2.19	0.41
1:A:16:ALA:HB1	1:A:299:LEU:HD23	2.02	0.41
2:B:46:LYS:O	2:B:49:ILE:HG22	2.20	0.41
3:C:112:ARG:NH1	3:C:116:GLY:H	2.18	0.41
1:D:75:ALA:HA	1:D:105:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ALA:HB1	1:D:300:MET:HG2	2.02	0.41
2:E:39:ALA:O	2:E:134:ARG:CD	2.56	0.41
1:D:67:PRO:HB2	1:D:70:THR:HG23	2.01	0.41
1:A:121:ASN:HD21	1:A:287:PHE:HD1	1.69	0.41
3:C:195:ILE:HD12	2:B:95:GLU:OE2	2.20	0.41
3:C:25:ILE:HA	3:F:24:GLU:O	2.21	0.41
1:D:265:VAL:HG12	4:D:400:APC:H1'	2.02	0.41
3:F:82:SER:N	3:F:83:PRO:CD	2.83	0.41
1:A:214:THR:HG22	2:B:38:GLY:HA2	2.02	0.41
3:C:47:GLU:OE2	3:C:47:GLU:HA	2.21	0.41
1:D:317:LEU:HA	1:D:317:LEU:HD12	1.89	0.41
2:E:128:ILE:HA	2:E:134:ARG:HG2	2.03	0.41
1:A:87:LEU:HD12	1:A:87:LEU:HA	1.84	0.41
2:B:0:LYS:HG3	2:B:0:LYS:O	2.21	0.41
1:D:139:GLN:OE1	1:D:326:ASN:ND2	2.49	0.41
2:E:29:GLU:HG2	2:E:29:GLU:H	1.79	0.41
2:B:156:LYS:O	2:B:157:GLU:C	2.59	0.41
1:D:74:VAL:O	1:D:104:PHE:HA	2.21	0.41
2:E:22:THR:HG21	2:E:48:MET:HA	2.03	0.41
2:E:45:VAL:HA	2:E:48:MET:HB2	2.02	0.41
3:F:194:SER:O	3:F:198:LEU:HD23	2.20	0.41
2:B:35:GLY:O	2:B:41:LYS:CE	2.57	0.41
3:C:153:LYS:O	3:F:153:LYS:HE3	2.21	0.41
1:D:178:GLY:HA3	4:D:400:APC:C4	2.51	0.41
2:E:140:ILE:HD11	2:E:143:GLU:N	2.36	0.41
2:E:81:LEU:HG	2:E:84:LEU:HD22	2.03	0.41
3:F:92:ASN:HD21	3:F:94:PHE:HB2	1.86	0.41
1:A:257:ARG:HA	1:A:284:TYR:CD2	2.57	0.40
1:D:19:ASP:O	1:D:20:ASP:C	2.60	0.40
3:F:103:ALA:O	3:F:125:LYS:CE	2.69	0.40
2:E:7:GLU:HA	2:E:135:ASN:OD1	2.22	0.40
1:A:151:VAL:HG12	1:A:327:VAL:CG2	2.51	0.40
3:C:17:ARG:HD2	3:C:172:GLU:OE2	2.22	0.40
2:E:27:GLY:N	2:E:29:GLU:OE2	2.44	0.40
3:F:114:ARG:H	3:F:114:ARG:HG3	1.66	0.40
1:A:100:LEU:O	1:A:101:GLU:HB2	2.22	0.40
3:C:147:THR:O	3:C:152:PRO:HD3	2.20	0.40
1:D:282:TRP:HD1	1:D:282:TRP:H	1.70	0.40
2:E:66:LEU:HA	2:E:66:LEU:HD13	1.84	0.40
2:E:81:LEU:HD21	2:E:90:LEU:HD21	2.04	0.40
2:B:49:ILE:HD12	2:B:59:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:191:LEU:HD23	3:C:191:LEU:HA	1.94	0.40

All (9) 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:257:ARG:CZ	2:E:142:GLU:OE2[1_565]	0.73	1.47
1:A:257:ARG:NH1	2:E:142:GLU:OE2[1_565]	1.03	1.17
1:A:257:ARG:NE	2:E:142:GLU:OE2[1_565]	1.41	0.79
1:A:257:ARG:CZ	2:E:142:GLU:CD[1_565]	1.54	0.66
1:A:257:ARG:NH1	2:E:142:GLU:CD[1_565]	1.92	0.28
1:A:257:ARG:NH2	2:E:142:GLU:OE2[1_565]	1.97	0.23
1:A:257:ARG:NE	2:E:142:GLU:CD[1_565]	2.02	0.18
1:A:257:ARG:NH2	2:E:142:GLU:CD[1_565]	2.15	0.05
1:A:257:ARG:CD	2:E:142:GLU:OE2[1_565]	2.19	0.01

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	300/327 (92%)	290 (97%)	10 (3%)	0	100	100
1	D	302/327 (92%)	286 (95%)	16 (5%)	0	100	100
2	B	157/184 (85%)	145 (92%)	12 (8%)	0	100	100
2	E	160/184 (87%)	149 (93%)	10 (6%)	1 (1%)	25	58
3	C	203/206 (98%)	194 (96%)	9 (4%)	0	100	100
3	F	200/206 (97%)	188 (94%)	11 (6%)	1 (0%)	29	61
All	All	1322/1434 (92%)	1252 (95%)	68 (5%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	141	PRO
3	F	115	LYS

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	252/269 (94%)	219 (87%)	33 (13%)	4 12
1	D	254/269 (94%)	212 (84%)	42 (16%)	2 7
2	B	144/167 (86%)	122 (85%)	22 (15%)	2 8
2	E	147/167 (88%)	131 (89%)	16 (11%)	6 19
3	C	180/180 (100%)	166 (92%)	14 (8%)	12 34
3	F	177/180 (98%)	160 (90%)	17 (10%)	8 25
All	All	1154/1232 (94%)	1010 (88%)	144 (12%)	4 14

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	19	ASP
1	A	22	LYS
1	A	25	VAL
1	A	26	VAL
1	A	29	THR
1	A	49	ARG
1	A	82	LEU
1	A	87	LEU
1	A	104	PHE
1	A	107	VAL
1	A	110	VAL
1	A	124	LEU
1	A	133	VAL
1	A	139	GLN
1	A	141	MET
1	A	150	GLU

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Mol	Chain	Res	Type
1	A	151	VAL
1	A	155	THR
1	A	157	ASP
1	A	169	ARG
1	A	171	LEU
1	A	175	TYR
1	A	212	LEU
1	A	220	LEU
1	A	259	ILE
1	A	265	VAL
1	A	311	ARG
1	A	315	SER
1	A	317	LEU
1	A	322	ASP
1	A	325	LEU
1	A	327	VAL
2	E	0	LYS
2	E	5	ARG
2	E	12	GLU
2	E	29	GLU
2	E	41	LYS
2	E	65	THR
2	E	66	LEU
2	E	75	THR
2	E	85	GLN
2	E	102	ASP
2	E	104	ILE
2	E	128	ILE
2	E	131	GLU
2	E	140	ILE
2	E	154	TYR
2	E	155	ARG
1	D	4	LEU
1	D	10	CYS
1	D	15	VAL
1	D	19	ASP
1	D	20	ASP
1	D	25	VAL
1	D	30	VAL
1	D	31	SER
1	D	49	ARG
1	D	69	GLU

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Mol	Chain	Res	Type
1	D	83	ILE
1	D	87	LEU
1	D	96	LEU
1	D	104	PHE
1	D	113	HIS
1	D	124	LEU
1	D	125	LYS
1	D	130	VAL
1	D	133	VAL
1	D	144	ASP
1	D	145	GLU
1	D	150	GLU
1	D	155	THR
1	D	157	ASP
1	D	171	LEU
1	D	191	GLU
1	D	194	SER
1	D	203	ASP
1	D	208	SER
1	D	212	LEU
1	D	223	GLU
1	D	259	ILE
1	D	265	VAL
1	D	278	ARG
1	D	280	GLU
1	D	282	TRP
1	D	283	ASN
1	D	311	ARG
1	D	317	LEU
1	D	322	ASP
1	D	325	LEU
1	D	327	VAL
3	C	20	GLU
3	C	28	THR
3	C	30	GLU
3	C	37	LEU
3	C	48	LEU
3	C	51	LYS
3	C	68	THR
3	C	112	ARG
3	C	122	VAL
3	C	127	LYS

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Mol	Chain	Res	Type
3	C	160	LEU
3	C	189	LEU
3	C	192	GLN
3	C	195	ILE
3	F	28	THR
3	F	31	LYS
3	F	36	ILE
3	F	37	LEU
3	F	48	LEU
3	F	92	ASN
3	F	104	ASP
3	F	114	ARG
3	F	115	LYS
3	F	122	VAL
3	F	127	LYS
3	F	148	LYS
3	F	151	SER
3	F	190[A]	TYR
3	F	190[B]	TYR
3	F	199	ASN
3	F	201	GLU
2	B	0	LYS
2	B	1	MET
2	B	2	ARG
2	B	5	ARG
2	B	12	GLU
2	B	20	ILE
2	B	21	LEU
2	B	22	THR
2	B	26	LYS
2	B	29	GLU
2	B	34	SER
2	B	67	MET
2	B	75	THR
2	B	81	LEU
2	B	92	LEU
2	B	101	GLU
2	B	140	ILE
2	B	147	LEU
2	B	150	LYS
2	B	151	ILE
2	B	152	GLU

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Mol	Chain	Res	Type
2	B	154	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	109	HIS
1	A	113	HIS
1	A	206	ASN
1	A	268	ASN
2	E	24	ASN
1	D	32	GLN
1	D	109	HIS
1	D	113	HIS
1	D	206	ASN
1	D	268	ASN
1	D	283	ASN
3	C	10	GLN
3	F	33	HIS
3	F	92	ASN
3	F	118	HIS
3	F	199	ASN
2	B	145	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
4	APC	A	400	-	27,33,33	0.98	2 (7%)	31,52,52	0.86	1 (3%)
4	APC	D	400	-	27,33,33	1.00	3 (11%)	31,52,52	0.92	1 (3%)
4	APC	B	203	5	27,33,33	0.89	2 (7%)	31,52,52	0.89	2 (6%)
4	APC	E	201	5	27,33,33	0.92	2 (7%)	31,52,52	0.86	1 (3%)

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
4	APC	A	400	-	-	3/15/38/38	0/3/3/3
4	APC	D	400	-	-	2/15/38/38	0/3/3/3
4	APC	B	203	5	-	2/15/38/38	0/3/3/3
4	APC	E	201	5	-	5/15/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	203	APC	PB-O2B	-2.58	1.50	1.56
4	A	400	APC	PB-O2B	-2.44	1.50	1.56
4	E	201	APC	PB-O2B	-2.33	1.50	1.56
4	B	203	APC	PA-O2A	-2.32	1.50	1.56
4	D	400	APC	PB-O2B	-2.31	1.51	1.56
4	A	400	APC	PA-O2A	-2.31	1.51	1.56
4	E	201	APC	PA-O2A	-2.27	1.51	1.56
4	D	400	APC	PA-O2A	-2.26	1.51	1.56
4	D	400	APC	PB-O3B	2.25	1.60	1.58

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	201	APC	C5-C6-N6	2.44	124.07	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	400	APC	C5-C6-N6	2.43	124.04	120.35
4	B	203	APC	O2A-PA-O1A	2.34	117.88	110.07
4	D	400	APC	C5-C6-N6	2.31	123.86	120.35
4	B	203	APC	C5-C6-N6	2.28	123.82	120.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	201	APC	PB-C3A-PA-O1A
4	E	201	APC	PB-C3A-PA-O2A
4	E	201	APC	O4'-C4'-C5'-O5'
4	E	201	APC	C3'-C4'-C5'-O5'
4	B	203	APC	O4'-C4'-C5'-O5'
4	A	400	APC	C5'-O5'-PA-C3A
4	D	400	APC	C5'-O5'-PA-O1A
4	A	400	APC	PA-C3A-PB-O2B
4	B	203	APC	C3'-C4'-C5'-O5'
4	A	400	APC	PA-C3A-PB-O1B
4	D	400	APC	C5'-O5'-PA-O2A
4	E	201	APC	C5'-O5'-PA-O2A

There are no ring outliers.

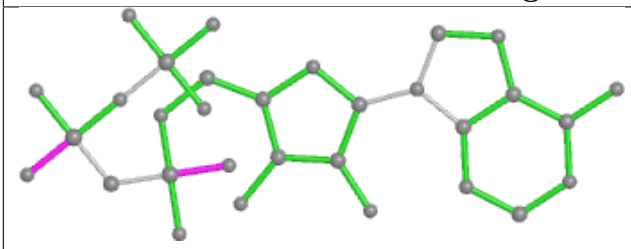
4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	400	APC	1	0
4	D	400	APC	7	0
4	B	203	APC	6	0
4	E	201	APC	1	0

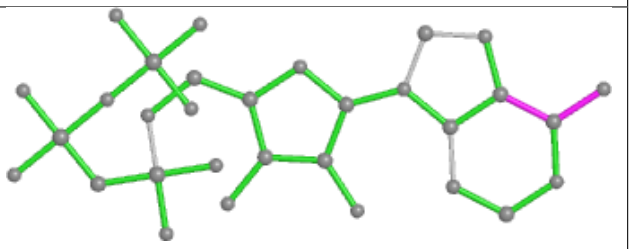
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

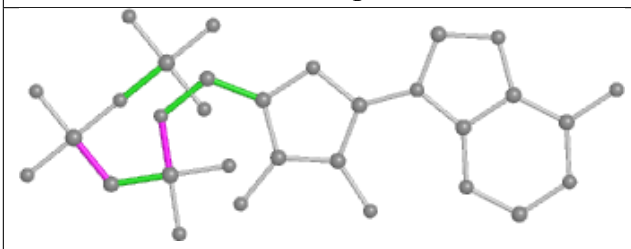
Ligand APC A 400



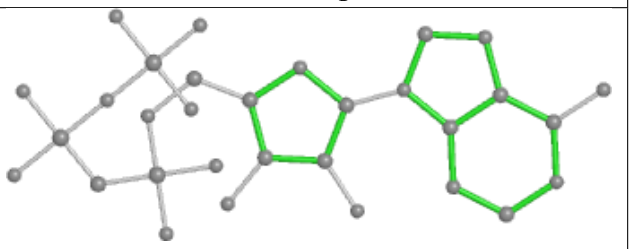
Bond lengths



Bond angles

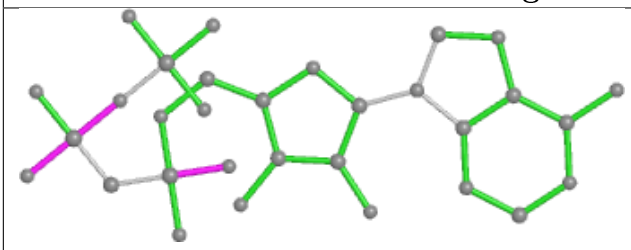


Torsions

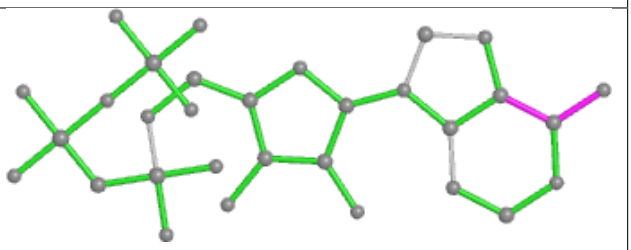


Rings

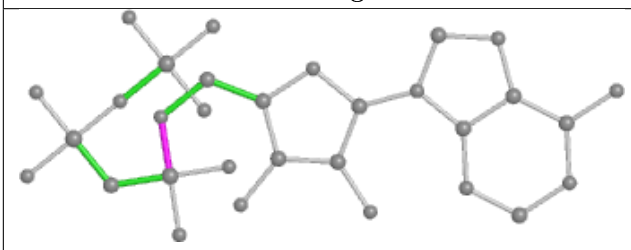
Ligand APC D 400



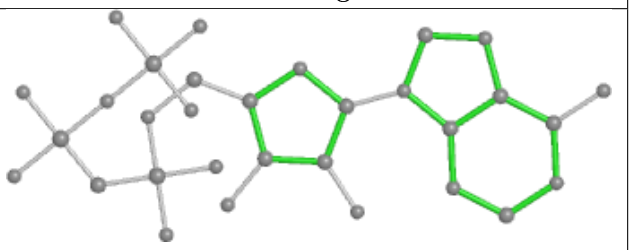
Bond lengths



Bond angles

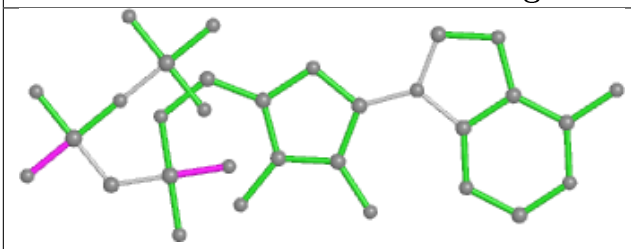


Torsions

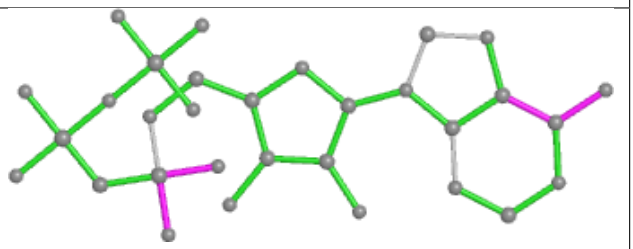


Rings

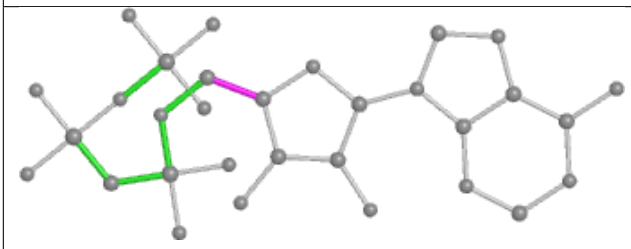
Ligand APC B 203



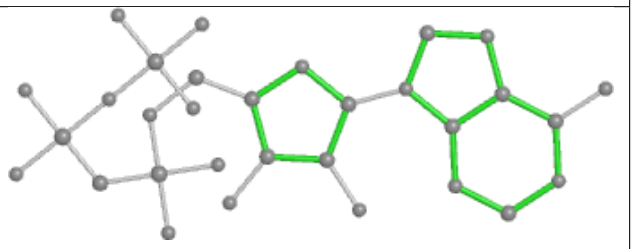
Bond lengths



Bond angles

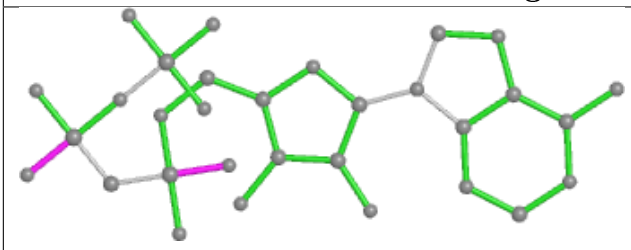


Torsions

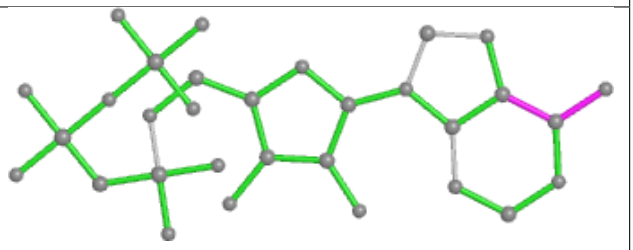


Rings

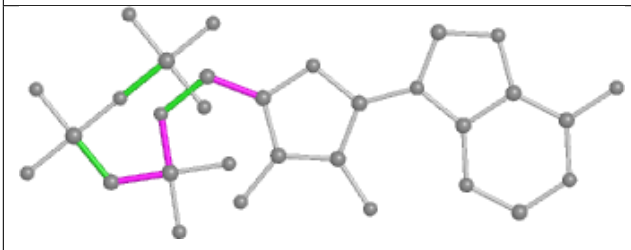
Ligand APC E 201



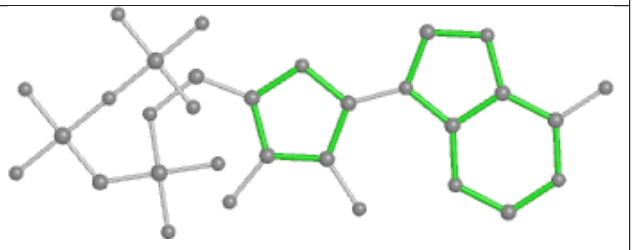
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	306/327 (93%)	0.14	5 (1%)	72	71	55, 82, 122, 148	0
1	D	308/327 (94%)	0.06	5 (1%)	72	71	58, 89, 126, 144	0
2	B	159/184 (86%)	0.15	9 (5%)	23	19	61, 82, 121, 150	0
2	E	162/184 (88%)	0.43	9 (5%)	24	20	79, 106, 142, 199	0
3	C	205/206 (99%)	-0.09	4 (1%)	65	63	51, 74, 109, 143	0
3	F	201/206 (97%)	-0.14	2 (0%)	82	82	53, 79, 115, 154	0
All	All	1341/1434 (93%)	0.08	34 (2%)	57	55	51, 84, 128, 199	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	24	ASN	5.9
2	E	146	PHE	5.6
1	A	257	ARG	3.4
2	B	-1	GLN	3.4
2	E	150	LYS	3.3
2	B	146	PHE	3.3
2	E	21	LEU	3.3
2	E	122	ILE	3.1
2	B	1	MET	3.0
2	B	154	TYR	2.9
2	E	140	ILE	2.9
2	B	150	LYS	2.8
2	E	25	LEU	2.7
3	F	201	GLU	2.7
3	C	152	PRO	2.6
1	D	174	GLY	2.6
2	B	5	ARG	2.6
2	E	145	ASN	2.6
3	C	126	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	205	ARG	2.5
1	A	128	LEU	2.5
1	A	282	TRP	2.5
1	D	313	MET	2.5
1	D	314	PHE	2.5
1	D	129	VAL	2.3
3	C	204	LYS	2.3
2	B	140	ILE	2.3
1	A	275	VAL	2.2
2	B	145	ASN	2.2
2	B	3	HIS	2.2
1	D	126	PRO	2.1
2	E	1	MET	2.1
3	F	199	ASN	2.0
1	A	327	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 carbohydrates in this entry.

6.4 Ligands (i)

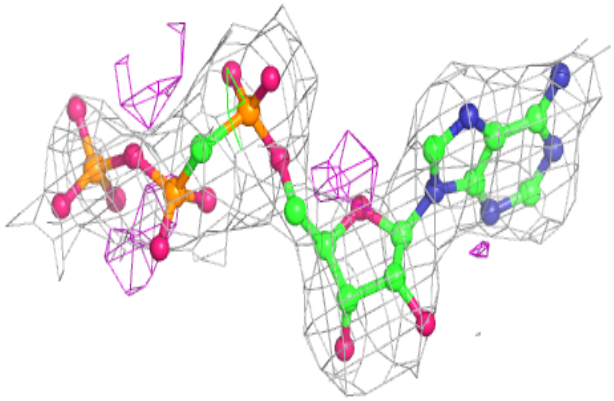
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

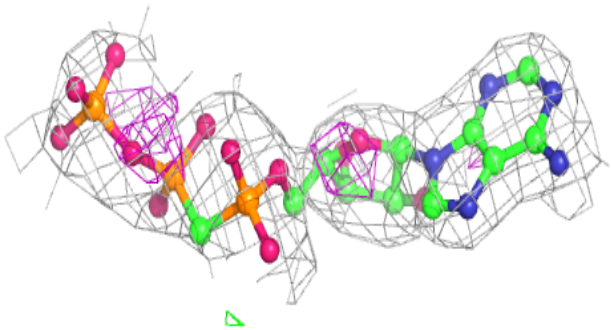
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	APC	A	400	31/31	0.89	0.21	86,94,174,176	0
6	LEU	B	201	8/9	0.89	0.12	95,98,103,103	0
4	APC	D	400	31/31	0.92	0.17	80,90,150,155	0
4	APC	E	201	31/31	0.95	0.18	80,93,102,106	0
4	APC	B	203	31/31	0.96	0.20	69,83,98,100	0
5	MG	E	200	1/1	0.97	0.14	67,67,67,67	0
5	MG	B	202	1/1	0.99	0.15	52,52,52,52	0

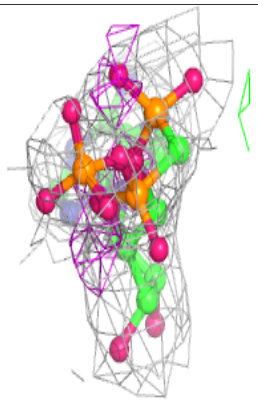
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around APC A 400:

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

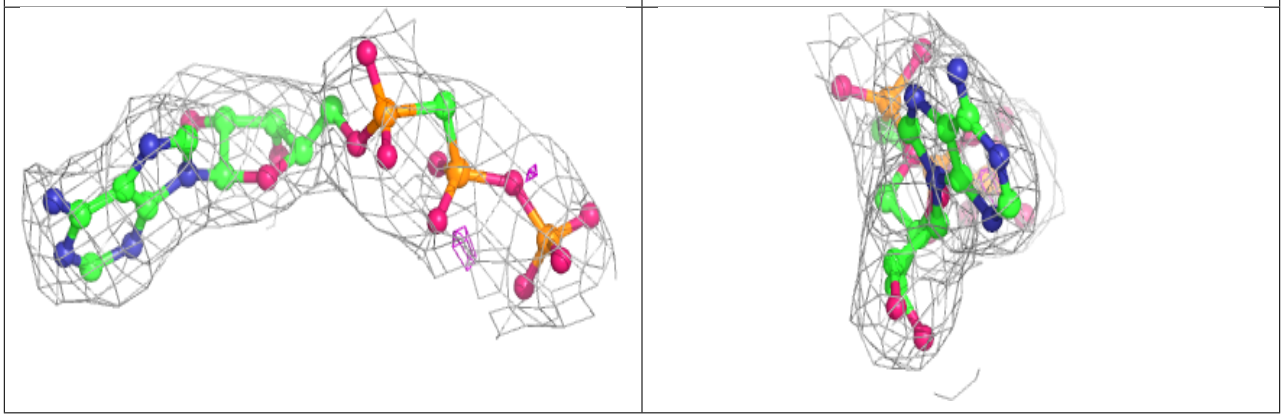






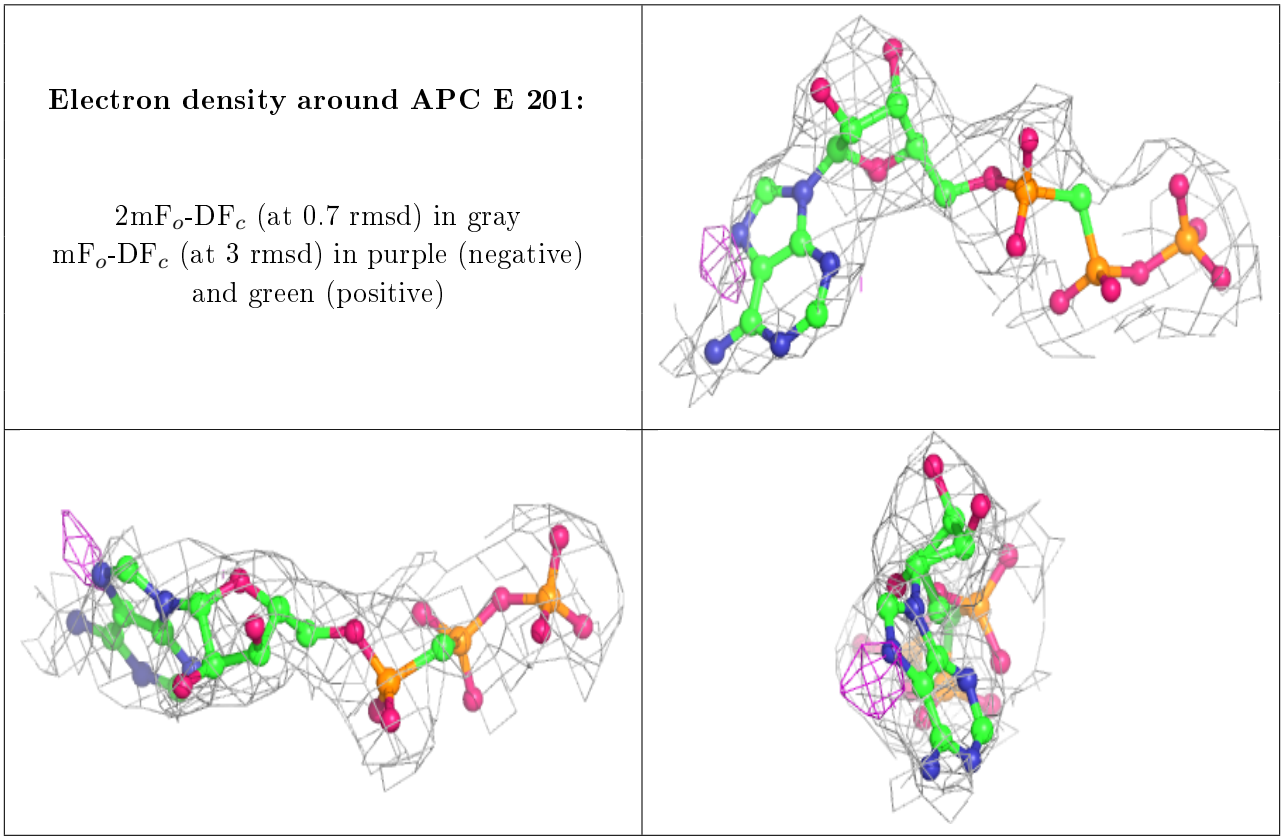
Electron density around APC D 400:

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



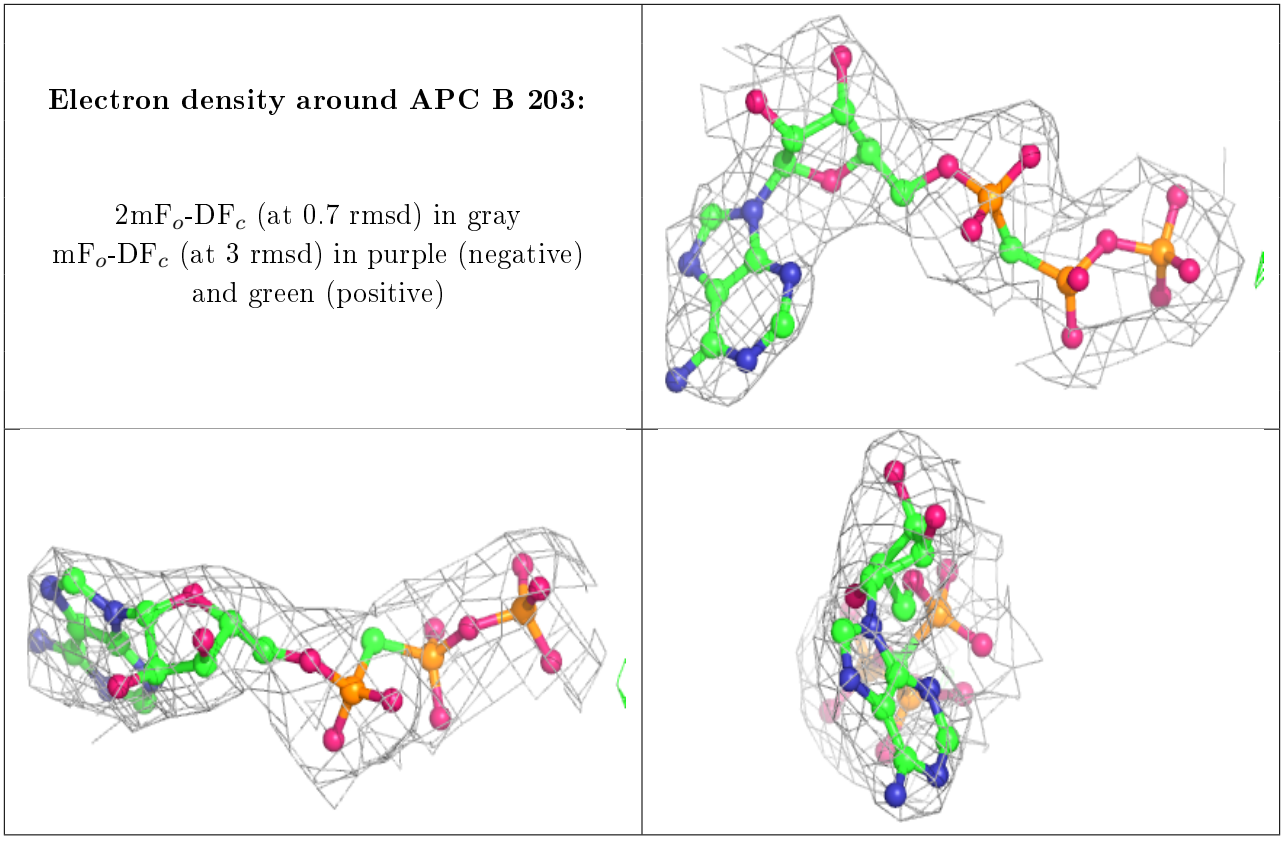
Electron density around APC E 201:

$2mF_o$-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 203:

$2mF_o$-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

There are no such residues in this entry.