



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:24 AM UTC

PDB ID : 6NAK / pdb_00006nak
Title : BACTERIAL PROTEIN COMPLEX TM BDE complex
Authors : Stec, B.
Deposited on : 2018-12-05
Resolution : 3.14 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

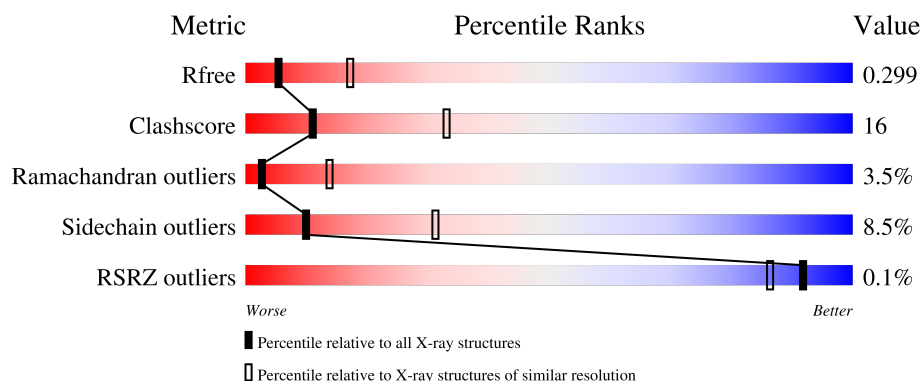
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	206	59% 35% 5%
1	C	206	60% 38%
2	B	327	58% 34% 6%
2	G	327	61% 30% 7%
3	D	184	54% 33% 10%

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Mol	Chain	Length	Quality of chain
3	E	184	53% 31% • • 12%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10983 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 threonylcarbamoyladenine biosynthesis protein TsaB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1594	1028	263	299	4			
1	C	206	Total	C	N	O	S	0	0	0
			1619	1042	270	303	4			

- Molecule 2 is a protein called tRNA N6-adenosine threonylcarbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	327	Total	C	N	O	S	0	0	0
			2510	1612	425	463	10			
2	G	321	Total	C	N	O	S	0	0	0
			2466	1581	418	457	10			

- Molecule 3 is a protein called TsaE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	165	Total	C	N	O	S	0	0	0
			1346	860	221	260	5			
3	E	161	Total	C	N	O	S	0	0	0
			1312	841	216	250	5			

There are 30 discrepancies between the modelled and reference sequences:

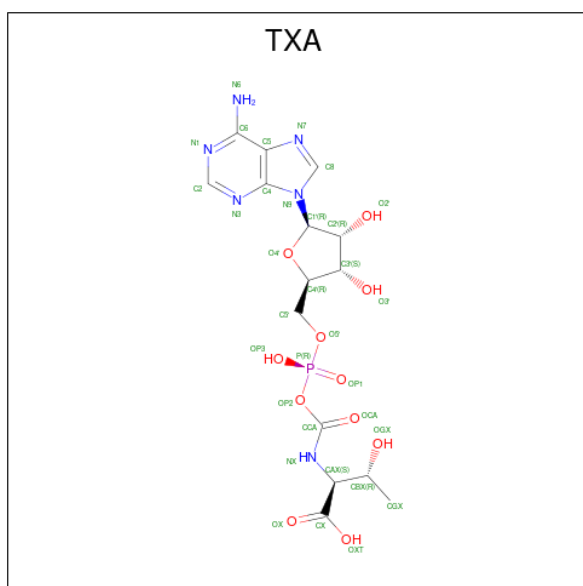
Chain	Residue	Modelled	Actual	Comment	Reference
D	-22	MET	-	expression tag	UNP R4NRX5
D	-21	GLY	-	expression tag	UNP R4NRX5
D	-20	HIS	-	expression tag	UNP R4NRX5
D	-19	HIS	-	expression tag	UNP R4NRX5
D	-18	HIS	-	expression tag	UNP R4NRX5
D	-17	HIS	-	expression tag	UNP R4NRX5
D	-16	HIS	-	expression tag	UNP R4NRX5
D	-15	HIS	-	expression tag	UNP R4NRX5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	GLU	-	expression tag	UNP R4NRX5
D	-13	ASN	-	expression tag	UNP R4NRX5
D	-12	LEU	-	expression tag	UNP R4NRX5
D	-11	TYR	-	expression tag	UNP R4NRX5
D	-10	PHE	-	expression tag	UNP R4NRX5
D	-9	GLN	-	expression tag	UNP R4NRX5
D	-8	GLY	-	expression tag	UNP R4NRX5
E	-22	MET	-	expression tag	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

- Molecule 4 is threonylcarbamoyladenylate (CCD ID: TXA) (formula: $C_{15}H_{21}N_6O_{11}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			33	15	6	11	1		
4	G	1	Total	C	N	O	P	0	0
			33	15	6	11	1		

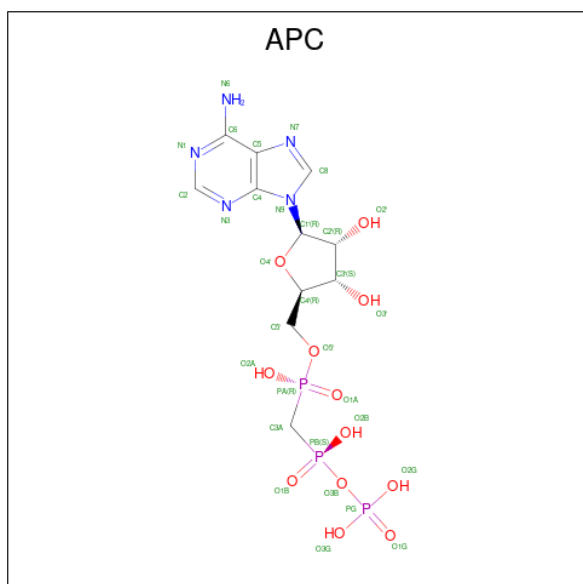
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	G	1	Total	Zn	0	0
			1	1		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		
6	E	1	Total	Mg	0	0
			1	1		

- Molecule 7 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

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

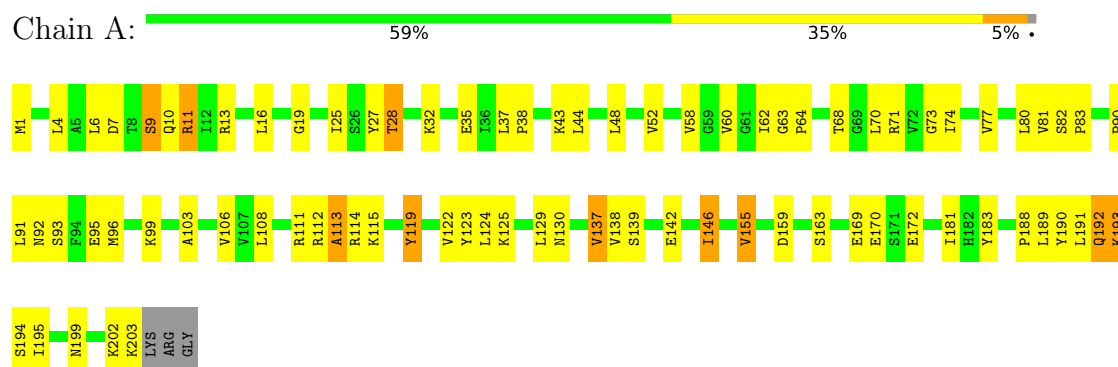
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	O	0	0
			2	2		
8	G	1	Total	O	0	0
			1	1		
8	E	1	Total	O	0	0
			1	1		

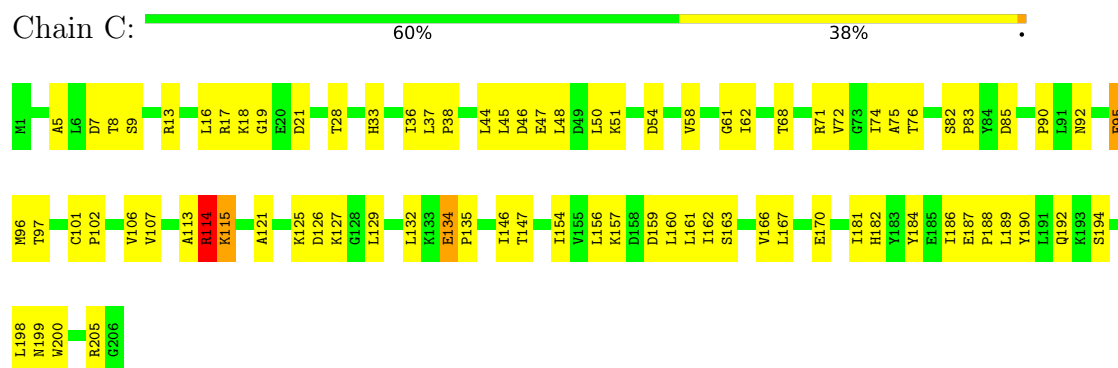
3 Residue-property plots [i](#)

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

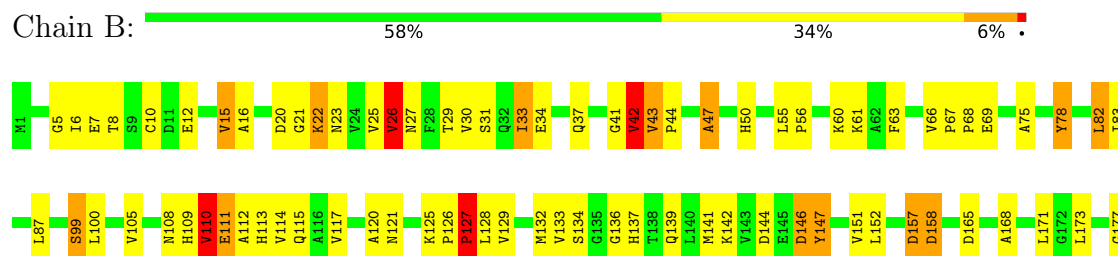
• Molecule 1: tRNA threonylcarbamoyladenosine biosynthesis protein TsaB



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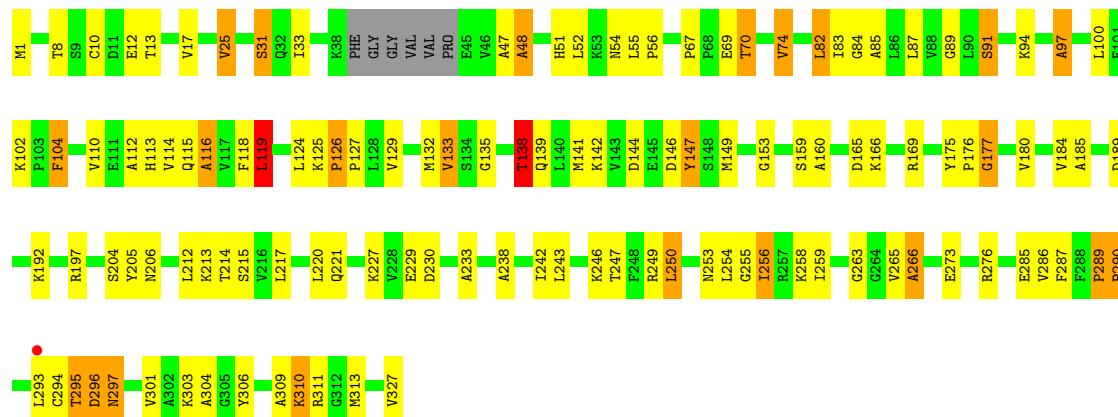
• Molecule 2: tRNA N6-adenosine threonylcarbamoyltransferase





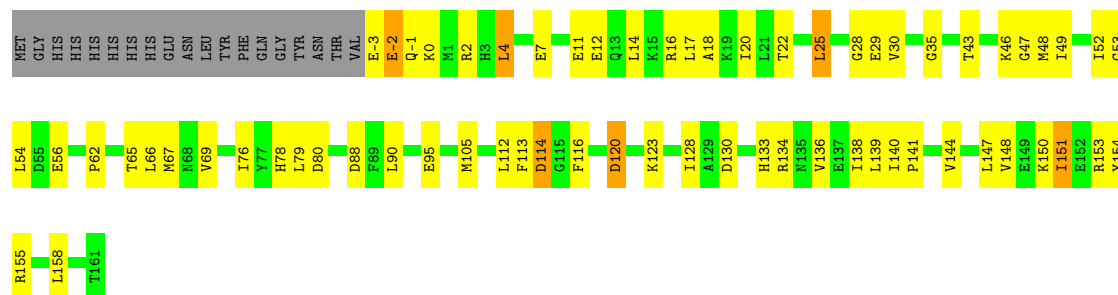
• Molecule 2: tRNA N6-adenosine threonylcarbamoyltransferase

Chain G: 61% 30% 7% ..



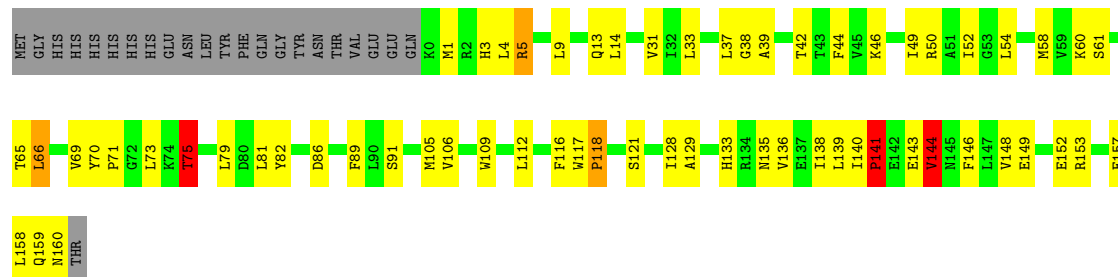
• Molecule 3: TsaE

Chain D: 54% 33% 10%



• Molecule 3: TsaE

Chain E: 53% 31% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.31Å 113.99Å 177.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.40 – 3.14 48.40 – 3.14	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.40-3.14) 99.0 (48.40-3.14)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.192 , 0.302 0.198 , 0.299	Depositor DCC
R_{free} test set	1550 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	93.4	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10983	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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, TXA, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.06	0/1621	1.55	4/2192 (0.2%)
1	C	1.07	0/1646	1.57	9/2222 (0.4%)
2	B	1.08	0/2560	1.54	4/3467 (0.1%)
2	G	1.09	0/2513	1.58	6/3402 (0.2%)
3	D	1.10	0/1367	1.53	2/1841 (0.1%)
3	E	1.04	0/1333	1.56	8/1795 (0.4%)
All	All	1.08	0/11040	1.56	33/14919 (0.2%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	126	PRO	N-CA-C	8.14	120.63	110.70
1	C	28	THR	CB-CA-C	7.36	121.74	110.62
2	B	78	TYR	CB-CA-C	6.35	120.35	109.24
3	E	75	THR	CB-CA-C	6.01	119.92	110.19
1	A	68	THR	CB-CA-C	5.94	122.08	110.67
2	G	290	PRO	CA-C-N	5.93	128.55	120.54
2	G	290	PRO	C-N-CA	5.93	128.55	120.54
1	A	68	THR	N-CA-C	-5.82	105.07	111.82
1	A	119	TYR	CA-C-O	-5.74	115.46	121.55
1	C	8	THR	CA-CB-OG1	-5.62	101.17	109.60
3	D	120	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	75	ALA	CA-C-O	-5.56	114.95	120.90
2	G	138	THR	CB-CA-C	5.52	119.31	109.65
3	E	86	ASP	CA-CB-CG	5.52	118.12	112.60
1	C	187	GLU	CB-CA-C	-5.49	104.50	110.98
3	E	50	ARG	CA-C-N	5.30	128.12	120.38
3	E	50	ARG	C-N-CA	5.30	128.12	120.38
3	D	35	GLY	CA-C-O	-5.26	117.25	121.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	TYR	N-CA-C	-5.21	103.27	110.35
2	B	127	PRO	N-CA-CB	-5.19	97.80	103.25
3	E	149	GLU	CA-C-N	5.17	127.21	120.28
3	E	149	GLU	C-N-CA	5.17	127.21	120.28
2	B	232	ALA	CA-C-N	5.14	127.13	120.44
2	B	232	ALA	C-N-CA	5.14	127.13	120.44
1	C	114	ARG	CA-C-N	5.12	131.32	121.54
1	C	114	ARG	C-N-CA	5.12	131.32	121.54
1	C	76	THR	N-CA-CB	5.11	117.72	110.16
2	G	69	GLU	CA-C-N	5.10	127.83	120.38
2	G	69	GLU	C-N-CA	5.10	127.83	120.38
1	C	58	VAL	CA-C-N	5.08	125.17	120.34
1	C	58	VAL	C-N-CA	5.08	125.17	120.34
3	E	118	PRO	N-CA-C	5.03	119.37	111.38
3	E	44	PHE	N-CA-C	-5.01	105.71	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1594	0	1670	67	0
1	C	1619	0	1699	47	0
2	B	2510	0	2562	90	0
2	G	2466	0	2510	90	0
3	D	1346	0	1358	43	0
3	E	1312	0	1331	42	0
4	B	33	0	20	1	0
4	G	33	0	20	0	0
5	B	1	0	0	0	0
5	G	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
7	D	31	0	14	1	0
7	E	31	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	2	0	0	0	0
8	E	1	0	0	0	0
8	G	1	0	0	0	0
All	All	10983	0	11198	364	0

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 16.

All (364) 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)
3:E:13:GLN:NE2	3:E:158:LEU:HD22	1.77	0.98
1:A:139:SER:OG	1:A:142:GLU:HB2	1.71	0.89
3:D:154:TYR:OH	3:D:158:LEU:HD12	1.79	0.81
1:C:101:CYS:O	1:C:125:LYS:NZ	2.13	0.81
2:B:247:THR:HG22	2:B:259:ILE:HD11	1.61	0.80
1:A:103:ALA:HB2	1:C:154:ILE:HD13	1.63	0.78
2:G:87:LEU:O	2:G:91:SER:HB2	1.84	0.77
3:E:13:GLN:HE21	3:E:158:LEU:HD22	1.45	0.77
1:C:97:THR:HG21	1:C:160:LEU:HD23	1.65	0.77
1:A:16:LEU:HD23	1:A:48:LEU:HD12	1.66	0.76
2:B:12:GLU:OE2	2:B:31:SER:OG	2.03	0.76
2:G:254:LEU:HD11	2:G:256:ILE:HG13	1.66	0.76
2:G:254:LEU:HD11	2:G:256:ILE:CG1	2.16	0.75
2:G:250:LEU:HD12	2:G:250:LEU:O	1.86	0.75
2:G:254:LEU:HD12	2:G:255:GLY:N	2.02	0.73
1:A:139:SER:HG	1:A:142:GLU:HB2	1.51	0.73
2:B:108:ASN:OD1	2:B:325:LEU:HD21	1.88	0.73
2:G:205:TYR:CD2	2:G:250:LEU:HD22	2.23	0.73
2:G:289:PRO:HB2	2:G:290:PRO:HD2	1.70	0.73
3:E:13:GLN:HE21	3:E:158:LEU:CD2	2.02	0.72
1:A:25:ILE:HD12	1:A:44:LEU:HD22	1.73	0.71
2:B:5:GLY:HA2	2:B:75:ALA:O	1.90	0.71
2:G:175:TYR:CG	2:G:176:PRO:HA	2.26	0.70
1:C:13:ARG:HD2	1:C:162:ILE:O	1.92	0.69
2:B:75:ALA:HA	2:B:105:VAL:O	1.93	0.69
1:C:96:MET:HE1	1:C:170:GLU:HG3	1.75	0.69
3:E:42:THR:OG1	7:E:201:APC:O2B	2.10	0.69
2:B:12:GLU:OE1	2:B:30:VAL:HG12	1.93	0.68
1:C:16:LEU:HD23	1:C:44:LEU:HG	1.74	0.68
2:G:247:THR:HG22	2:G:259:ILE:HD11	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:GLY:O	2:B:42:VAL:HG23	1.94	0.68
2:B:254:LEU:HD23	2:B:256:ILE:HD12	1.77	0.67
2:G:289:PRO:HB2	2:G:290:PRO:CD	2.23	0.67
1:C:126:ASP:OD1	1:C:127:LYS:N	2.27	0.67
1:C:92:ASN:HB3	1:C:95:GLU:HB2	1.76	0.66
2:B:25:VAL:O	2:B:26:VAL:HG23	1.94	0.66
2:G:139:GLN:NE2	2:G:141:MET:HE3	2.10	0.66
1:C:163:SER:HB3	1:C:166:VAL:HG23	1.77	0.66
2:G:13:THR:HG21	2:G:54:ASN:HB2	1.78	0.66
1:C:199:ASN:ND2	3:E:117:TRP:O	2.29	0.65
1:A:37:LEU:HB3	1:A:38:PRO:HD3	1.76	0.65
3:E:141:PRO:O	3:E:144:VAL:HG12	1.97	0.65
1:C:7:ASP:OD1	1:C:9:SER:HB3	1.95	0.65
2:G:144:ASP:HB3	2:G:146:ASP:OD1	1.97	0.65
2:B:125:LYS:C	2:B:127:PRO:HD3	2.22	0.65
2:B:257:ARG:NH2	2:B:283:ASN:O	2.30	0.65
3:E:13:GLN:NE2	3:E:158:LEU:CD2	2.57	0.64
2:B:281:ARG:O	2:B:282:TRP:HD1	1.80	0.64
3:E:31:VAL:HG12	3:E:33:LEU:CD1	2.27	0.64
2:B:16:ALA:HB2	2:B:27:ASN:HD22	1.63	0.64
1:A:11:ARG:HG2	1:A:28:THR:HA	1.80	0.64
1:A:114:ARG:HD2	3:D:95:GLU:OE2	1.98	0.64
2:B:294:CYS:SG	2:B:294:CYS:O	2.55	0.63
2:G:204:SER:O	2:G:249:ARG:NH1	2.32	0.63
2:G:13:THR:OG1	2:G:51:HIS:ND1	2.32	0.63
3:D:154:TYR:HH	3:D:158:LEU:HD12	1.62	0.63
2:G:91:SER:HA	2:G:94:LYS:HZ1	1.64	0.63
3:D:25:LEU:HB2	3:D:29:GLU:OE2	1.99	0.62
1:C:5:ALA:HB1	1:C:167:LEU:HB3	1.81	0.62
2:G:250:LEU:HD11	2:G:254:LEU:HD23	1.82	0.62
3:D:14:LEU:HD11	3:D:136:VAL:HG11	1.82	0.62
2:G:254:LEU:HD12	2:G:254:LEU:C	2.24	0.62
2:B:311:ARG:HB3	2:B:313:MET:HE2	1.82	0.61
3:D:46:LYS:O	3:D:49:ILE:HG22	2.01	0.61
2:G:294:CYS:O	2:G:294:CYS:SG	2.58	0.61
2:B:157:ASP:OD2	2:B:208:SER:HA	2.01	0.60
2:B:173:LEU:HB3	2:B:180:VAL:HG11	1.82	0.60
3:E:1:MET:HB3	3:E:141:PRO:HA	1.84	0.60
3:D:-1:GLN:HE22	3:D:123:LYS:CD	2.14	0.60
3:D:140:ILE:HG23	3:D:144:VAL:HB	1.84	0.60
2:G:114:VAL:HG11	2:G:149:MET:SD	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:VAL:HA	1:C:154:ILE:HG23	1.83	0.60
2:B:139:GLN:NE2	2:B:141:MET:HE2	2.16	0.59
1:A:193:LYS:HE3	3:D:88:ASP:OD1	2.02	0.59
1:C:18:LYS:HG3	1:C:50:LEU:HD13	1.84	0.59
3:E:153:ARG:O	3:E:157:GLU:HB2	2.02	0.59
1:A:190:TYR:O	1:A:191:LEU:C	2.46	0.58
2:B:254:LEU:O	2:B:254:LEU:HG	2.03	0.58
2:G:139:GLN:HA	2:G:153:GLY:O	2.03	0.58
2:G:206:ASN:O	2:G:246:LYS:NZ	2.24	0.58
3:E:138:ILE:HG22	3:E:140:ILE:HD11	1.84	0.58
3:D:53:GLY:C	3:D:54:LEU:HD12	2.29	0.58
1:C:97:THR:HG22	1:C:156:LEU:HD22	1.86	0.58
2:B:7:GLU:O	2:B:8:THR:HG23	2.04	0.58
2:G:294:CYS:O	2:G:296:ASP:N	2.36	0.58
1:A:74:ILE:O	1:A:77:VAL:HB	2.04	0.58
3:D:66:LEU:O	3:D:79:LEU:HA	2.04	0.58
2:B:146:ASP:O	2:B:147:TYR:HB2	2.03	0.58
2:B:245:GLU:O	2:B:249:ARG:HB2	2.04	0.57
1:A:114:ARG:NH2	3:D:116:PHE:O	2.37	0.57
2:B:199:MET:O	2:B:202:ASP:HB3	2.04	0.57
1:C:182:HIS:HD1	1:C:184:TYR:HH	1.52	0.57
2:G:180:VAL:O	2:G:184:VAL:HG13	2.04	0.57
2:G:250:LEU:HD12	2:G:250:LEU:C	2.29	0.57
2:G:74:VAL:O	2:G:104:PHE:HA	2.05	0.57
2:G:12:GLU:CG	2:G:31:SER:OG	2.52	0.56
1:A:62:ILE:HD12	1:A:189:LEU:HG	1.86	0.56
1:A:92:ASN:HB3	1:A:95:GLU:HB2	1.86	0.56
1:A:95:GLU:O	1:A:99:LYS:HG3	2.05	0.56
2:B:21:GLY:O	2:B:23:ASN:N	2.39	0.56
2:G:141:MET:HE2	2:G:327:VAL:HG21	1.86	0.56
1:A:77:VAL:HA	1:A:80:LEU:HD12	1.86	0.56
1:A:96:MET:SD	1:A:170:GLU:HG3	2.45	0.56
1:C:121:ALA:HB2	1:C:135:PRO:HA	1.86	0.56
2:G:146:ASP:O	2:G:147:TYR:HB2	2.06	0.56
1:C:126:ASP:CG	1:C:127:LYS:N	2.63	0.55
1:A:139:SER:OG	1:A:142:GLU:CB	2.50	0.55
2:B:248:PHE:C	2:B:250:LEU:H	2.14	0.55
3:D:150:LYS:O	3:D:153:ARG:HB3	2.07	0.55
3:D:18:ALA:HB3	3:D:47:GLY:HA3	1.87	0.55
2:B:239:VAL:O	2:B:240:VAL:C	2.50	0.55
2:G:33:ILE:HG22	2:G:33:ILE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:90:LEU:HD22	3:D:116:PHE:CE2	2.42	0.54
1:C:7:ASP:OD2	1:C:61:GLY:HA3	2.07	0.54
3:E:66:LEU:HD23	3:E:89:PHE:CZ	2.43	0.54
1:A:6:LEU:HD12	1:A:6:LEU:O	2.07	0.54
1:A:92:ASN:O	1:A:96:MET:HG2	2.08	0.54
1:C:114:ARG:HG2	1:C:115:LYS:N	2.22	0.54
2:G:17:VAL:O	2:G:25:VAL:HG12	2.08	0.54
1:A:37:LEU:O	1:A:38:PRO:C	2.51	0.54
2:B:311:ARG:CB	2:B:313:MET:HE2	2.36	0.54
1:C:82:SER:OG	1:C:83:PRO:HD3	2.08	0.54
2:G:141:MET:HE2	2:G:327:VAL:CG2	2.38	0.54
2:G:303:LYS:O	2:G:304:ALA:C	2.50	0.54
1:A:62:ILE:CD1	1:A:189:LEU:HG	2.38	0.54
2:B:132:MET:HA	2:B:262:VAL:HG13	1.90	0.54
2:G:192:LYS:HG2	2:G:230:ASP:HB3	1.89	0.54
1:A:82:SER:OG	1:A:83:PRO:HD3	2.07	0.53
3:E:129:ALA:HB2	3:E:135:ASN:ND2	2.23	0.53
2:G:259:ILE:CG2	2:G:286:VAL:HG12	2.38	0.53
2:G:254:LEU:HD11	2:G:256:ILE:HG12	1.89	0.53
2:B:110:VAL:O	2:B:112:ALA:N	2.40	0.53
3:D:128:ILE:HA	3:D:134:ARG:HD3	1.90	0.53
2:G:129:VAL:HG13	2:G:259:ILE:HG13	1.91	0.53
2:G:94:LYS:O	2:G:97:ALA:HB3	2.08	0.53
1:C:121:ALA:HB2	1:C:135:PRO:CA	2.38	0.53
2:B:126:PRO:HG2	2:B:147:TYR:CE1	2.44	0.53
3:D:29:GLU:OE1	3:D:29:GLU:N	2.41	0.53
2:G:142:LYS:O	2:G:149:MET:HA	2.08	0.53
2:B:110:VAL:C	2:B:112:ALA:N	2.67	0.52
2:G:204:SER:HB2	2:G:206:ASN:HD22	1.74	0.52
1:A:114:ARG:CD	3:D:95:GLU:OE2	2.58	0.52
3:E:69:VAL:O	3:E:71:PRO:HD3	2.08	0.52
3:D:67:MET:HA	3:D:78:HIS:O	2.09	0.52
2:B:111:GLU:O	2:B:115:GLN:HG2	2.09	0.52
2:G:263:GLY:O	2:G:266:ALA:HB3	2.10	0.52
2:B:133:VAL:O	2:B:265:VAL:HB	2.09	0.52
3:D:113:PHE:O	3:D:114:ASP:O	2.27	0.52
1:A:188:PRO:CG	1:A:190:TYR:CZ	2.93	0.51
1:A:90:PRO:HG3	1:A:181:ILE:HD13	1.91	0.51
1:C:71:ARG:NH1	2:G:84:GLY:HA3	2.25	0.51
3:E:144:VAL:HG23	3:E:146:PHE:CZ	2.46	0.51
3:E:60:LYS:O	3:E:61:SER:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:LEU:N	1:C:38:PRO:CD	2.74	0.51
2:B:171:LEU:HD22	2:B:228:VAL:HG13	1.92	0.51
2:G:116:ALA:O	2:G:119:LEU:HB3	2.11	0.51
2:B:55:LEU:N	2:B:56:PRO:CD	2.73	0.50
2:G:132:MET:O	2:G:138:THR:HA	2.11	0.50
3:E:52:ILE:HA	3:E:73:LEU:HB2	1.94	0.50
1:A:124:LEU:HB3	1:A:130:ASN:HB2	1.93	0.50
2:G:17:VAL:HB	2:G:25:VAL:HG13	1.91	0.50
3:E:138:ILE:CG2	3:E:140:ILE:HD11	2.41	0.50
2:G:295:THR:O	2:G:296:ASP:OD1	2.30	0.50
3:E:129:ALA:HB2	3:E:135:ASN:HD21	1.75	0.50
1:A:73:GLY:O	1:A:77:VAL:HG23	2.12	0.50
1:A:137:VAL:HG11	1:A:195:ILE:HG12	1.94	0.50
1:C:45:LEU:C	1:C:47:GLU:H	2.20	0.50
2:G:297:ASN:OD1	2:G:297:ASN:N	2.44	0.50
1:A:64:PRO:HB3	1:A:191:LEU:HG	1.94	0.49
2:B:63:PHE:CE1	2:B:68:PRO:HB3	2.47	0.49
3:D:-2:GLU:OE2	3:D:0:LYS:HE3	2.12	0.49
2:G:133:VAL:HB	2:G:265:VAL:HB	1.93	0.49
3:E:79:LEU:N	3:E:79:LEU:HD12	2.26	0.49
1:A:4:LEU:O	1:A:58:VAL:HA	2.12	0.49
3:E:109:TRP:HB3	3:E:112:LEU:HD12	1.95	0.49
2:B:129:VAL:HG11	2:B:251:ALA:HB2	1.93	0.49
3:E:54:LEU:HD22	3:E:58:MET:HE1	1.94	0.49
1:C:194:SER:O	1:C:198:LEU:HD13	2.13	0.49
1:C:134:GLU:HG3	1:C:135:PRO:CD	2.43	0.49
2:B:248:PHE:O	2:B:250:LEU:N	2.46	0.48
3:D:62:PRO:HG2	3:D:80:ASP:HB2	1.94	0.48
2:B:128:LEU:C	2:B:128:LEU:HD12	2.38	0.48
2:G:250:LEU:CD1	2:G:254:LEU:HD23	2.42	0.48
2:G:165:ASP:HA	2:G:177:GLY:HA3	1.95	0.48
3:E:31:VAL:O	3:E:106:VAL:HA	2.13	0.48
2:B:120:ALA:O	2:B:121:ASN:ND2	2.47	0.48
1:A:1:MET:CE	1:A:172:GLU:HG3	2.43	0.48
1:A:108:LEU:HD13	1:A:122:VAL:HG22	1.94	0.48
1:C:161:LEU:HD12	1:C:161:LEU:C	2.38	0.48
2:G:254:LEU:CD1	2:G:256:ILE:HG12	2.44	0.48
3:E:31:VAL:HG12	3:E:33:LEU:HD13	1.96	0.48
1:A:123:TYR:CD1	1:A:129:LEU:HD21	2.49	0.48
2:B:151:VAL:C	2:B:152:LEU:HD12	2.39	0.48
3:D:113:PHE:O	3:D:114:ASP:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ASP:O	2:B:168:ALA:HB3	2.13	0.48
2:B:248:PHE:C	2:B:250:LEU:N	2.71	0.48
3:E:14:LEU:HD23	7:E:201:APC:H2	1.96	0.48
2:B:263:GLY:O	2:B:266:ALA:HB3	2.14	0.48
3:D:14:LEU:CD1	3:D:136:VAL:HG11	2.43	0.48
1:A:81:VAL:C	1:A:83:PRO:HD2	2.39	0.47
2:G:1:MET:HE2	2:G:306:TYR:HD1	1.77	0.47
2:G:175:TYR:CD1	2:G:176:PRO:HA	2.48	0.47
3:E:148:VAL:O	3:E:152:GLU:HB2	2.14	0.47
2:G:12:GLU:HG2	2:G:31:SER:OG	2.14	0.47
1:A:6:LEU:HD12	1:A:6:LEU:C	2.39	0.47
2:G:67:PRO:O	2:G:70:THR:HG23	2.14	0.47
2:B:6:ILE:HG12	2:B:15:VAL:HG22	1.96	0.47
2:B:33:ILE:HG21	2:B:61:LYS:HE3	1.95	0.47
2:B:245:GLU:OE1	2:B:245:GLU:HA	2.15	0.47
2:G:12:GLU:HG3	2:G:31:SER:OG	2.15	0.47
2:G:119:LEU:HD12	2:G:119:LEU:O	2.15	0.47
2:B:47:ALA:HB3	2:B:50:HIS:HB2	1.96	0.47
2:B:110:VAL:C	2:B:112:ALA:H	2.23	0.47
3:D:22:THR:HG21	3:D:48:MET:HB3	1.97	0.47
2:G:133:VAL:HG12	2:G:160:ALA:HB3	1.95	0.47
2:G:205:TYR:CE2	2:G:250:LEU:HD22	2.50	0.47
1:A:115:LYS:HE3	3:D:28:GLY:O	2.14	0.47
3:D:11:GLU:HA	7:D:201:APC:C6	2.44	0.47
2:B:20:ASP:HA	2:B:306:TYR:CE1	2.50	0.46
2:B:83:ILE:HG22	2:B:87:LEU:HD11	1.96	0.46
2:G:115:GLN:O	2:G:118:PHE:N	2.44	0.46
1:A:63:GLY:HA3	1:A:93:SER:H	1.80	0.46
3:E:38:GLY:O	3:E:39:ALA:C	2.57	0.46
1:A:32:LYS:HD3	2:B:320:ASN:HD21	1.79	0.46
2:B:134:SER:HG	2:B:137:HIS:H	1.63	0.46
1:C:62:ILE:C	1:C:62:ILE:HD12	2.40	0.46
1:A:7:ASP:OD2	1:A:9:SER:HB3	2.16	0.46
1:A:82:SER:HA	1:A:183:TYR:CE2	2.50	0.46
3:D:139:LEU:O	3:D:140:ILE:HG13	2.15	0.46
1:A:74:ILE:O	1:A:77:VAL:N	2.49	0.46
2:B:263:GLY:O	2:B:266:ALA:N	2.43	0.46
1:C:134:GLU:HG3	1:C:135:PRO:HD3	1.97	0.46
2:B:33:ILE:HG22	2:B:37:GLN:HE21	1.80	0.46
2:B:165:ASP:HA	2:B:177:GLY:HA3	1.98	0.46
1:C:161:LEU:HD12	1:C:161:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:LYS:CD	2:B:254:LEU:HD21	2.46	0.46
2:B:214:THR:O	2:B:217:LEU:N	2.48	0.46
1:A:188:PRO:HG2	1:A:190:TYR:CZ	2.50	0.46
2:B:114:VAL:O	2:B:117:VAL:HG23	2.16	0.46
2:B:281:ARG:O	2:B:281:ARG:HG2	2.15	0.46
2:B:125:LYS:HG2	2:B:127:PRO:HD3	1.97	0.45
2:G:212:LEU:O	2:G:213:LYS:C	2.59	0.45
1:A:1:MET:HE3	1:A:172:GLU:HG3	1.97	0.45
3:E:138:ILE:HG22	3:E:140:ILE:CD1	2.47	0.45
1:A:91:LEU:HD22	1:A:96:MET:HE3	1.97	0.45
2:B:125:LYS:C	2:B:127:PRO:CD	2.90	0.45
1:C:33:HIS:HB3	1:C:72:VAL:HG11	1.98	0.45
2:B:189:ASP:HB3	2:B:192:LYS:HB2	1.99	0.45
3:D:43:THR:O	3:D:46:LYS:HB2	2.17	0.45
1:C:114:ARG:HG2	1:C:115:LYS:HB2	1.99	0.45
3:E:37:LEU:HD11	3:E:82:TYR:HE2	1.81	0.45
3:D:53:GLY:O	3:D:54:LEU:HD12	2.17	0.45
3:E:71:PRO:HA	3:E:75:THR:HB	1.97	0.45
1:A:188:PRO:HG2	1:A:190:TYR:CE2	2.52	0.45
2:B:171:LEU:HD21	2:B:231:VAL:HG11	1.99	0.45
2:B:83:ILE:HG22	2:B:87:LEU:CD1	2.47	0.45
1:A:111:ARG:O	1:A:113:ALA:N	2.51	0.44
2:B:195:PHE:HB3	2:B:196:PRO:HD2	1.99	0.44
1:C:74:ILE:HG22	2:G:52:LEU:HD11	1.99	0.44
3:E:13:GLN:HE22	3:E:158:LEU:HD22	1.75	0.44
1:A:32:LYS:O	1:A:35:GLU:HB2	2.17	0.44
2:B:66:VAL:O	2:B:67:PRO:C	2.60	0.44
3:E:118:PRO:HD2	3:E:121:SER:OG	2.18	0.44
2:G:133:VAL:CG1	2:G:160:ALA:HB3	2.48	0.44
2:G:311:ARG:HB2	2:G:313:MET:HG3	2.00	0.44
2:B:43:VAL:HB	2:B:44:PRO:CD	2.47	0.44
2:B:178:GLY:O	2:B:179:PRO:C	2.61	0.44
2:G:100:LEU:HB3	2:G:102:LYS:HG3	1.99	0.44
1:A:96:MET:HE1	1:A:170:GLU:HG3	2.00	0.44
1:A:142:GLU:O	1:A:146:ILE:HG12	2.18	0.44
2:B:109:HIS:O	2:B:112:ALA:HB3	2.17	0.44
2:G:8:THR:OG1	2:G:89:GLY:HA3	2.17	0.44
2:B:60:LYS:O	2:B:61:LYS:C	2.60	0.44
3:E:144:VAL:O	3:E:144:VAL:HG13	2.17	0.44
2:B:113:HIS:CE1	2:B:295:THR:HB	2.52	0.44
3:D:-1:GLN:HE22	3:D:123:LYS:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:125:LYS:C	2:G:127:PRO:HD2	2.43	0.43
3:E:46:LYS:O	3:E:49:ILE:HG22	2.17	0.43
3:D:16:ARG:NH1	3:D:158:LEU:HD13	2.32	0.43
3:D:30:VAL:HG22	3:D:105:MET:HB3	2.00	0.43
1:C:113:ALA:O	1:C:114:ARG:O	2.35	0.43
3:E:3:HIS:C	3:E:4:LEU:HD12	2.43	0.43
2:G:17:VAL:O	2:G:25:VAL:CG1	2.66	0.43
2:G:263:GLY:O	2:G:266:ALA:CB	2.66	0.43
1:A:188:PRO:HG3	1:A:190:TYR:OH	2.18	0.43
1:C:37:LEU:HB3	1:C:38:PRO:HD3	2.00	0.43
2:B:144:ASP:O	2:B:147:TYR:N	2.52	0.43
3:D:12:GLU:OE2	3:D:16:ARG:HG3	2.18	0.43
3:D:52:ILE:HG13	3:D:54:LEU:HD13	2.00	0.43
2:B:157:ASP:HB2	2:B:158:ASP:H	1.54	0.43
1:C:17:ARG:HA	1:C:21:ASP:O	2.19	0.43
2:G:1:MET:HE1	2:G:309:ALA:HB3	2.00	0.43
2:G:67:PRO:HD2	2:G:70:THR:HG21	2.00	0.43
3:D:130:ASP:HB3	3:D:133:HIS:H	1.84	0.43
2:B:134:SER:OG	2:B:136:GLY:N	2.52	0.43
3:D:17:LEU:HD21	3:D:138:ILE:HD11	2.01	0.43
3:E:70:TYR:O	3:E:75:THR:HA	2.19	0.43
1:A:103:ALA:O	1:A:125:LYS:HD3	2.18	0.43
2:B:21:GLY:O	2:B:22:LYS:C	2.61	0.43
1:A:60:VAL:HB	1:A:77:VAL:HG21	2.00	0.42
2:G:189:ASP:HB3	2:G:192:LYS:HB2	1.99	0.42
1:A:27:TYR:OH	1:C:21:ASP:OD1	2.37	0.42
2:G:10:CYS:SG	2:G:296:ASP:OD2	2.77	0.42
2:B:68:PRO:HB2	2:B:100:LEU:HD21	2.02	0.42
2:G:135:GLY:O	2:G:159:SER:CB	2.68	0.42
2:G:185:ALA:HB1	2:G:233:ALA:HA	2.02	0.42
2:G:197:ARG:HG3	2:G:197:ARG:HH11	1.83	0.42
1:C:16:LEU:HG	1:C:48:LEU:HD12	2.02	0.42
2:G:55:LEU:HB3	2:G:56:PRO:HD3	2.02	0.42
3:E:54:LEU:HB3	3:E:58:MET:HE3	2.01	0.42
2:B:303:LYS:C	2:B:305:GLY:N	2.77	0.42
2:B:139:GLN:HE22	2:B:141:MET:HE2	1.84	0.42
1:A:25:ILE:CD1	1:A:44:LEU:HD22	2.45	0.42
1:A:80:LEU:O	2:B:99:SER:HB3	2.20	0.42
1:A:111:ARG:HB3	1:A:119:TYR:HB2	2.02	0.42
2:B:247:THR:CG2	2:B:259:ILE:HD11	2.42	0.42
1:A:138:VAL:HB	1:A:142:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:GLY:O	2:B:266:ALA:CB	2.68	0.41
1:C:90:PRO:HD3	1:C:181:ILE:HG12	2.02	0.41
1:A:190:TYR:O	1:A:192:GLN:N	2.52	0.41
2:G:47:ALA:O	2:G:48:ALA:C	2.62	0.41
2:G:212:LEU:HD23	2:G:212:LEU:HA	1.91	0.41
2:B:252:ARG:O	2:B:255:GLY:N	2.50	0.41
1:C:114:ARG:NH2	3:E:116:PHE:O	2.53	0.41
2:G:258:LYS:HA	2:G:285:GLU:O	2.20	0.41
3:E:5:ARG:HE	3:E:5:ARG:HB2	1.65	0.41
1:A:155:VAL:O	1:A:155:VAL:CG2	2.68	0.41
2:G:82:LEU:O	2:G:83:ILE:C	2.63	0.41
2:B:82:LEU:CD1	2:B:82:LEU:N	2.83	0.41
2:B:108:ASN:ND2	2:B:110:VAL:HG23	2.35	0.41
1:A:43:LYS:CD	1:C:47:GLU:OE2	2.68	0.41
2:B:113:HIS:NE2	2:B:295:THR:HB	2.36	0.41
2:G:124:LEU:HD13	2:G:287:PHE:CZ	2.55	0.41
3:D:2:ARG:HD2	3:D:148:VAL:HG21	2.03	0.41
3:D:4:LEU:HD21	3:D:151:ILE:HB	2.02	0.41
3:D:151:ILE:O	3:D:153:ARG:N	2.54	0.41
1:C:82:SER:N	1:C:83:PRO:CD	2.84	0.41
2:G:8:THR:O	2:G:85:ALA:HB1	2.21	0.41
2:G:55:LEU:HB3	2:G:56:PRO:CD	2.49	0.41
2:G:126:PRO:HG2	2:G:147:TYR:CE1	2.56	0.41
2:G:238:ALA:O	2:G:242:ILE:HG22	2.21	0.41
3:E:144:VAL:CG2	3:E:146:PHE:CZ	3.04	0.41
1:A:6:LEU:HA	1:A:13:ARG:O	2.20	0.41
2:G:166:LYS:O	2:G:169:ARG:HB3	2.21	0.41
3:E:9:LEU:O	3:E:133:HIS:HA	2.21	0.41
1:A:193:LYS:HE2	1:A:193:LYS:HB3	1.77	0.40
2:B:293:LEU:HD11	4:B:401:TXA:OP3	2.21	0.40
1:C:106:VAL:O	1:C:154:ILE:HG22	2.21	0.40
2:G:176:PRO:O	2:G:180:VAL:HG23	2.21	0.40
3:E:1:MET:HE3	3:E:139:LEU:HB3	2.03	0.40
1:A:82:SER:N	1:A:83:PRO:CD	2.84	0.40
1:A:106:VAL:HG22	1:A:124:LEU:HD13	2.03	0.40
2:G:112:ALA:O	2:G:115:GLN:HB2	2.20	0.40
1:A:70:LEU:O	1:A:71:ARG:C	2.64	0.40
1:A:114:ARG:NE	3:D:95:GLU:OE2	2.55	0.40
2:B:33:ILE:HG22	2:B:37:GLN:NE2	2.37	0.40
1:C:181:ILE:HD11	1:C:186:ILE:HG12	2.03	0.40
1:C:188:PRO:HG2	1:C:190:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:LYS:O	1:C:54:ASP:HB2	2.21	0.40
2:G:273:GLU:OE1	2:G:276:ARG:NH1	2.54	0.40
2:B:158:ASP:OD1	2:B:158:ASP:N	2.55	0.40
2:B:193:TYR:CE2	2:B:230:ASP:HB3	2.57	0.40
3:D:147:LEU:O	3:D:150:LYS:N	2.54	0.40
3:D:154:TYR:O	3:D:155:ARG:C	2.64	0.40

There are no symmetry-related clashes.

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	201/206 (98%)	164 (82%)	32 (16%)	5 (2%)	4	19
1	C	204/206 (99%)	170 (83%)	27 (13%)	7 (3%)	3	14
2	B	325/327 (99%)	255 (78%)	52 (16%)	18 (6%)	1	7
2	G	317/327 (97%)	261 (82%)	43 (14%)	13 (4%)	2	11
3	D	163/184 (89%)	134 (82%)	26 (16%)	3 (2%)	6	25
3	E	159/184 (86%)	136 (86%)	21 (13%)	2 (1%)	9	32
All	All	1369/1434 (96%)	1120 (82%)	201 (15%)	48 (4%)	3	14

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	ARG
2	B	22	LYS
2	B	43	VAL
2	B	293	LEU
3	D	114	ASP
1	C	114	ARG

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Mol	Chain	Res	Type
1	C	115	LYS
2	G	119	LEU
2	G	293	LEU
2	G	295	THR
1	A	19	GLY
1	A	199	ASN
2	B	42	VAL
2	B	47	ALA
2	B	111	GLU
2	B	127	PRO
2	B	147	TYR
2	B	199	MET
2	B	225	GLY
1	C	19	GLY
2	G	48	ALA
2	G	147	TYR
2	G	266	ALA
2	G	296	ASP
3	E	144	VAL
1	A	113	ALA
1	A	202	LYS
2	B	249	ARG
1	C	205	ARG
2	G	97	ALA
2	B	69	GLU
3	D	151	ILE
1	C	46	ASP
1	C	85	ASP
2	G	116	ALA
3	E	141	PRO
2	B	259	ILE
2	B	290	PRO
2	G	243	LEU
2	G	310	LYS
2	B	226	TYR
2	B	234	SER
2	B	26	VAL
2	B	110	VAL
1	C	102	PRO
2	G	177	GLY
2	G	289	PRO
3	D	141	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	178/180 (99%)	163 (92%)	15 (8%)	10	32
1	C	180/180 (100%)	167 (93%)	13 (7%)	13	37
2	B	269/269 (100%)	247 (92%)	22 (8%)	10	32
2	G	264/269 (98%)	239 (90%)	25 (10%)	8	27
3	D	150/167 (90%)	138 (92%)	12 (8%)	11	33
3	E	146/167 (87%)	132 (90%)	14 (10%)	8	27
All	All	1187/1232 (96%)	1086 (92%)	101 (8%)	10	31

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	10	GLN
1	A	11	ARG
1	A	28	THR
1	A	52	VAL
1	A	137	VAL
1	A	146	ILE
1	A	155	VAL
1	A	159	ASP
1	A	163	SER
1	A	169	GLU
1	A	192	GLN
1	A	193	LYS
1	A	194	SER
1	A	203	LYS
2	B	10	CYS
2	B	15	VAL
2	B	26	VAL
2	B	29	THR
2	B	33	ILE
2	B	34	GLU
2	B	42	VAL

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Mol	Chain	Res	Type
2	B	78	TYR
2	B	82	LEU
2	B	99	SER
2	B	110	VAL
2	B	127	PRO
2	B	146	ASP
2	B	157	ASP
2	B	158	ASP
2	B	181	ILE
2	B	204	SER
2	B	231	VAL
2	B	245	GLU
2	B	311	ARG
2	B	315	SER
2	B	327	VAL
3	D	-3	GLU
3	D	-2	GLU
3	D	4	LEU
3	D	7	GLU
3	D	20	ILE
3	D	25	LEU
3	D	56	GLU
3	D	65	THR
3	D	69	VAL
3	D	76	ILE
3	D	112	LEU
3	D	120	ASP
1	C	36	ILE
1	C	68	THR
1	C	95	GLU
1	C	129	LEU
1	C	132	LEU
1	C	134	GLU
1	C	146	ILE
1	C	147	THR
1	C	157	LYS
1	C	159	ASP
1	C	189	LEU
1	C	192	GLN
1	C	200	TRP
2	G	25	VAL
2	G	31	SER

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Mol	Chain	Res	Type
2	G	70	THR
2	G	74	VAL
2	G	82	LEU
2	G	91	SER
2	G	104	PHE
2	G	110	VAL
2	G	113	HIS
2	G	119	LEU
2	G	133	VAL
2	G	138	THR
2	G	214	THR
2	G	215	SER
2	G	217	LEU
2	G	220	LEU
2	G	221	GLN
2	G	227	LYS
2	G	229	GLU
2	G	250	LEU
2	G	253	ASN
2	G	256	ILE
2	G	297	ASN
2	G	301	VAL
2	G	310	LYS
3	E	5	ARG
3	E	65	THR
3	E	66	LEU
3	E	75	THR
3	E	81	LEU
3	E	91	SER
3	E	105	MET
3	E	128	ILE
3	E	136	VAL
3	E	141	PRO
3	E	143	GLU
3	E	144	VAL
3	E	159	GLN
3	E	160	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	27	ASN

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Mol	Chain	Res	Type
2	B	37	GLN
2	B	121	ASN
2	B	139	GLN
2	B	297	ASN
2	B	324	ASN
3	D	-1	GLN
3	D	135	ASN
1	C	118	HIS
2	G	32	GLN
2	G	108	ASN
2	G	121	ASN
2	G	139	GLN
2	G	206	ASN
2	G	320	ASN
3	E	159	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	TXA	G	401	-	34,35,35	2.16	5 (14%)	50,52,52	3.24	13 (26%)
7	APC	D	201	6	29,33,33	0.76	2 (6%)	44,52,52	0.80	2 (4%)
7	APC	E	201	6	29,33,33	0.72	2 (6%)	44,52,52	0.90	1 (2%)
4	TXA	B	401	5	34,35,35	2.24	6 (17%)	50,52,52	2.66	12 (24%)

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	TXA	G	401	-	-	0/25/43/43	0/3/3/3
7	APC	D	201	6	-	3/19/38/38	0/3/3/3
7	APC	E	201	6	-	10/19/38/38	0/3/3/3
4	TXA	B	401	5	-	2/25/43/43	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	TXA	C2-N1	7.56	1.47	1.33
4	B	401	TXA	C2-N3	7.50	1.47	1.33
4	G	401	TXA	C2-N3	7.34	1.47	1.33
4	G	401	TXA	C2-N1	7.29	1.46	1.33
4	B	401	TXA	C5-C4	4.51	1.47	1.39
4	G	401	TXA	C5-C4	4.35	1.46	1.39
4	G	401	TXA	C5-C6	2.97	1.49	1.41
4	B	401	TXA	C5-C6	2.69	1.48	1.41
7	D	201	APC	PB-O2B	-2.53	1.50	1.56
4	B	401	TXA	C5-N7	-2.40	1.34	1.39
4	G	401	TXA	C8-N7	2.37	1.36	1.31
4	B	401	TXA	C8-N7	2.35	1.36	1.31
7	E	201	APC	PB-O2B	-2.22	1.51	1.56
7	D	201	APC	PA-O2A	-2.04	1.51	1.56
7	E	201	APC	PA-O2A	-2.02	1.51	1.56

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	401	TXA	OP2-CCA-NX	15.81	119.27	109.91
4	B	401	TXA	OP2-CCA-NX	10.72	116.26	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	401	TXA	N3-C2-N1	-9.67	113.95	128.58
4	B	401	TXA	N3-C2-N1	-8.83	115.22	128.58
4	G	401	TXA	C2-N3-C4	5.17	124.47	111.83
4	B	401	TXA	C5-C4-N3	-4.88	120.00	126.72
4	G	401	TXA	C5-C4-N3	-4.80	120.10	126.72
4	B	401	TXA	C2-N3-C4	4.69	123.29	111.83
4	B	401	TXA	CBX-CAX-CX	4.13	117.23	110.03
4	G	401	TXA	N3-C4-N9	3.91	133.81	127.17
4	B	401	TXA	N3-C4-N9	3.88	133.76	127.17
4	G	401	TXA	C4-C5-N7	-3.83	106.20	110.58
4	G	401	TXA	C4-N9-C8	3.69	109.61	105.74
4	B	401	TXA	C4-C5-N7	-3.69	106.37	110.58
4	G	401	TXA	C2-N1-C6	3.36	124.25	118.73
4	G	401	TXA	C5-N7-C8	3.18	108.45	103.45
4	B	401	TXA	C4-N9-C8	3.14	109.03	105.74
4	G	401	TXA	O4'-C1'-N9	3.14	114.11	108.09
4	G	401	TXA	N9-C8-N7	-3.03	109.64	113.94
4	B	401	TXA	C2-N1-C6	3.00	123.66	118.73
4	B	401	TXA	C5-N7-C8	2.85	107.93	103.45
7	D	201	APC	O2B-PB-O1B	2.81	119.09	109.95
7	D	201	APC	O2A-PA-O1A	2.53	118.19	109.95
4	B	401	TXA	N9-C8-N7	-2.47	110.43	113.94
7	E	201	APC	O2A-PA-O1A	2.39	117.74	109.95
4	G	401	TXA	C6-C5-N7	2.37	136.65	132.09
4	G	401	TXA	CBX-CAX-CX	2.31	114.05	110.03
4	B	401	TXA	CBX-CAX-NX	-2.28	105.64	111.70

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	TXA	C5'-O5'-P-OP3
7	D	201	APC	PB-C3A-PA-O1A
7	D	201	APC	PB-C3A-PA-O2A
7	D	201	APC	PB-C3A-PA-O5'
7	E	201	APC	PA-C3A-PB-O1B
7	E	201	APC	PA-C3A-PB-O2B
7	E	201	APC	PA-C3A-PB-O3B
7	E	201	APC	C5'-O5'-PA-O1A
7	E	201	APC	O4'-C4'-C5'-O5'
7	E	201	APC	C3'-C4'-C5'-O5'
7	E	201	APC	PB-O3B-PG-O1G

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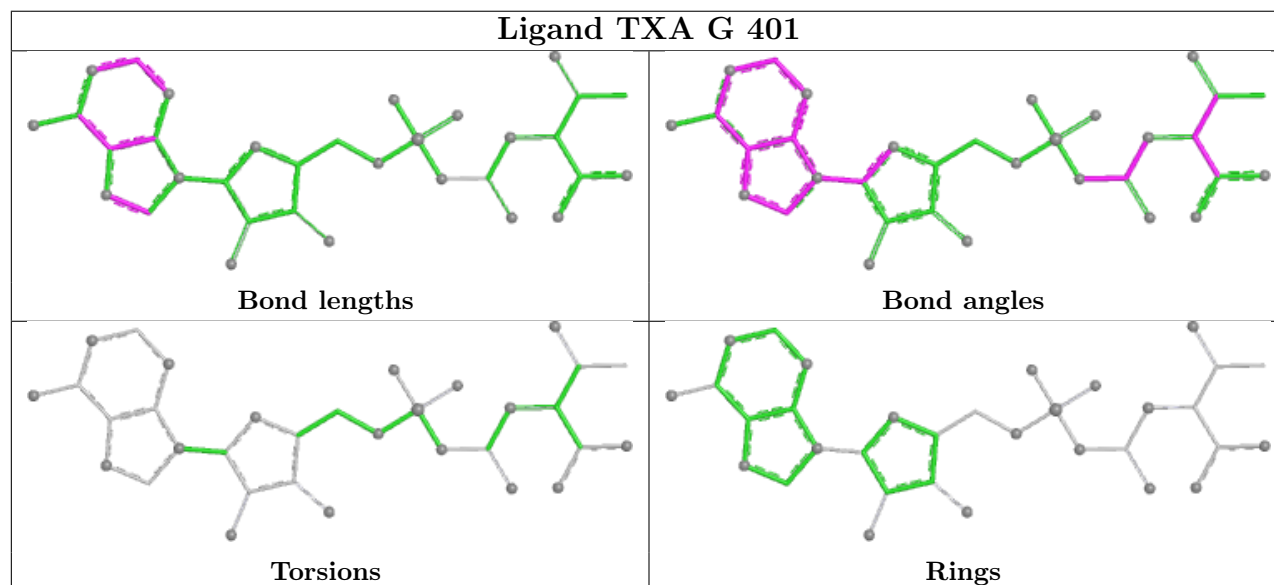
Mol	Chain	Res	Type	Atoms
4	B	401	TXA	C5'-O5'-P-OP2
7	E	201	APC	O4'-C1'-N9-C4
7	E	201	APC	O4'-C1'-N9-C8
7	E	201	APC	C5'-O5'-PA-O2A

There are no ring outliers.

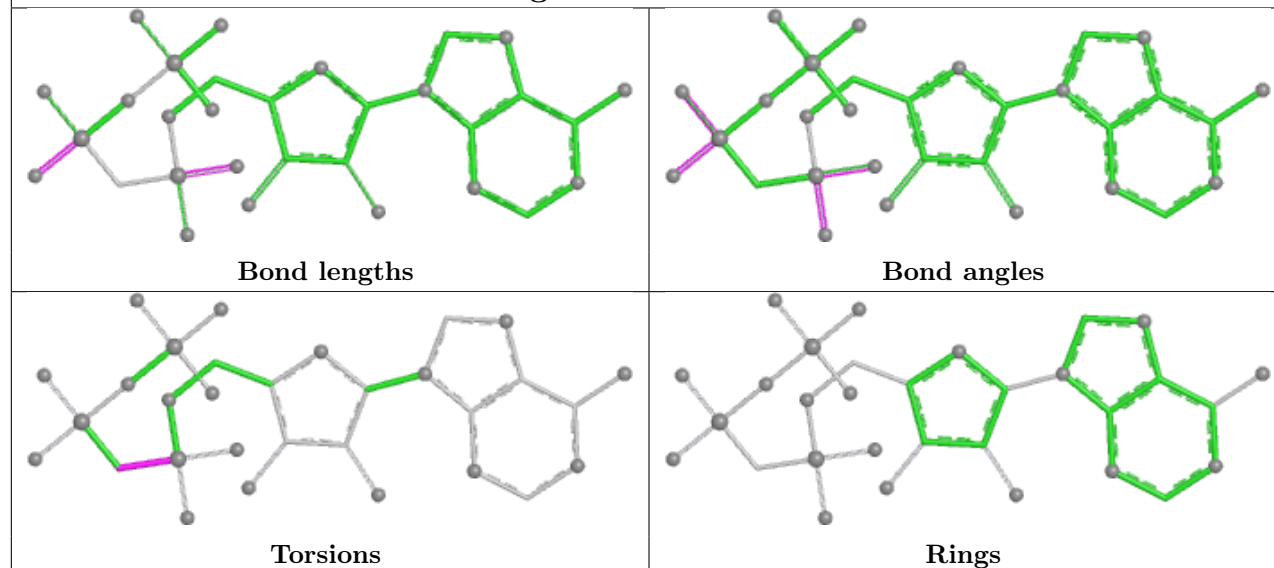
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	201	APC	1	0
7	E	201	APC	2	0
4	B	401	TXA	1	0

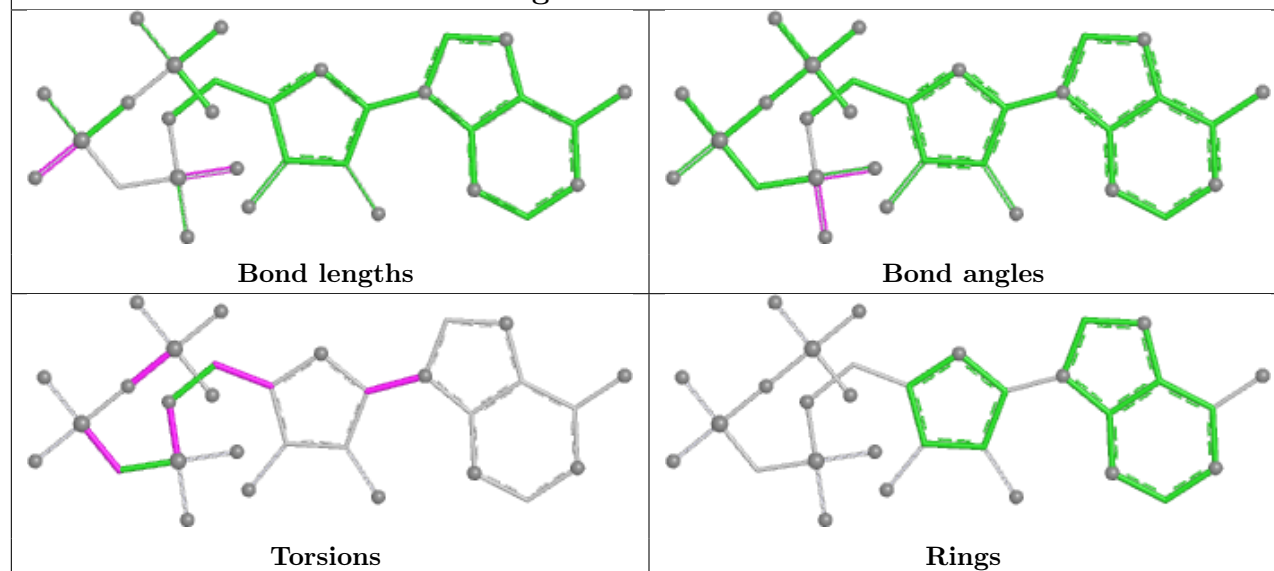
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

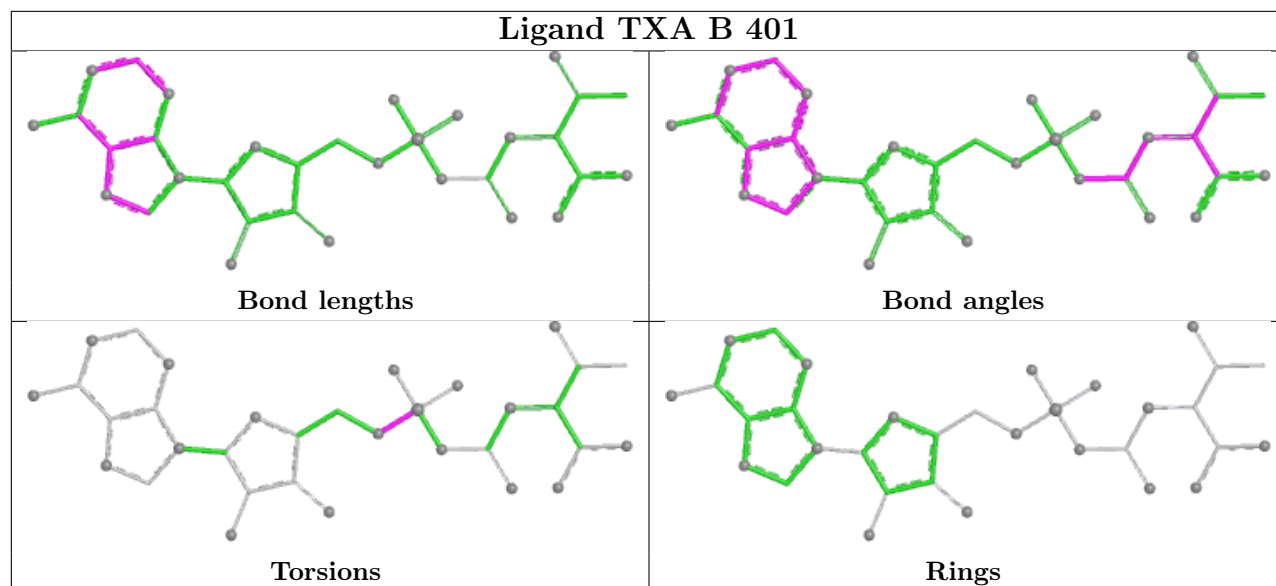


Ligand APC D 201



Ligand APC E 201





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	203/206 (98%)	-0.64	0	100	100	58, 85, 122, 157	0
1	C	206/206 (100%)	-0.69	0	100	100	52, 74, 114, 141	0
2	B	327/327 (100%)	-0.55	0	100	100	71, 99, 145, 205	0
2	G	321/327 (98%)	-0.60	1 (0%)	90	80	56, 84, 135, 187	0
3	D	165/184 (89%)	-0.46	0	100	100	79, 110, 147, 174	0
3	E	161/184 (87%)	-0.76	0	100	100	56, 79, 120, 142	0
All	All	1383/1434 (96%)	-0.61	1 (0%)	92	86	52, 89, 136, 205	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	293	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

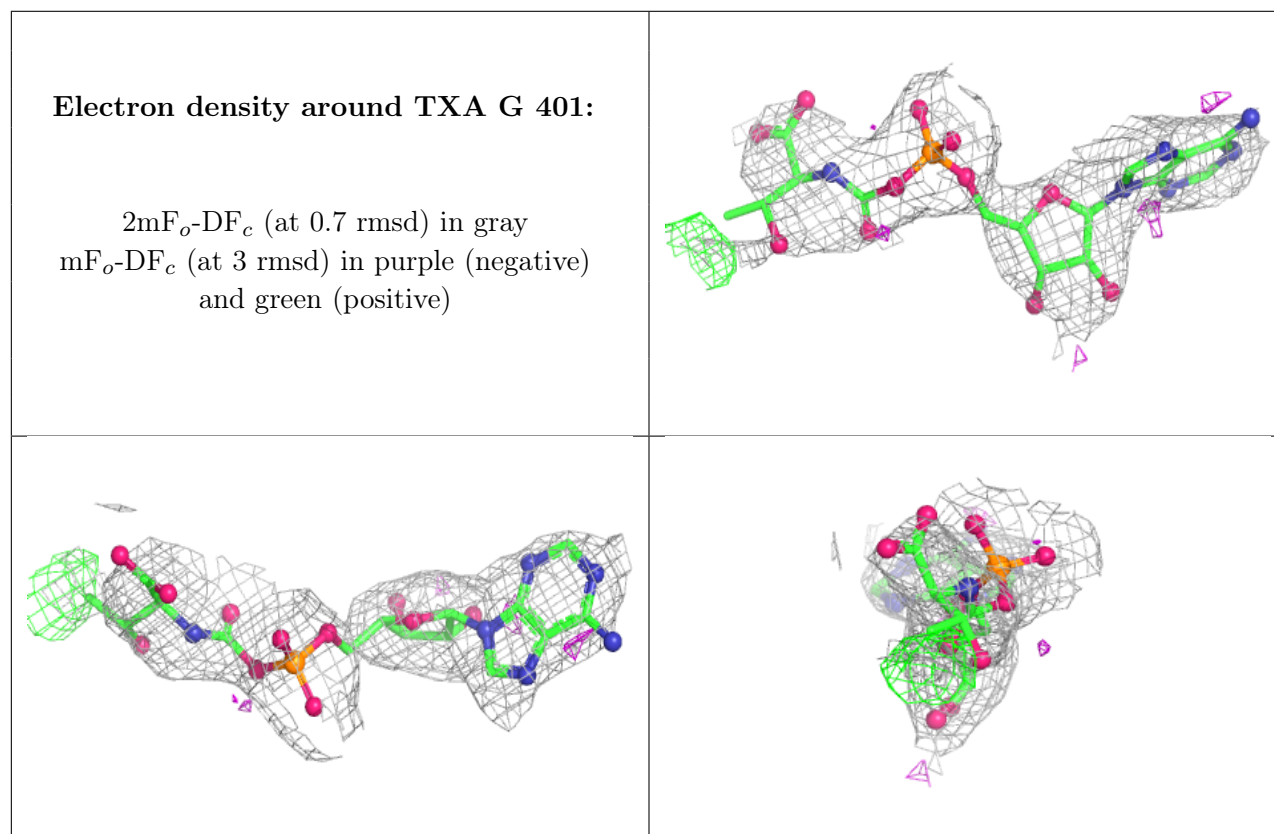
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

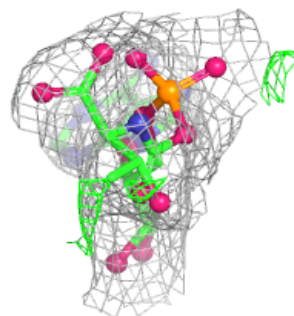
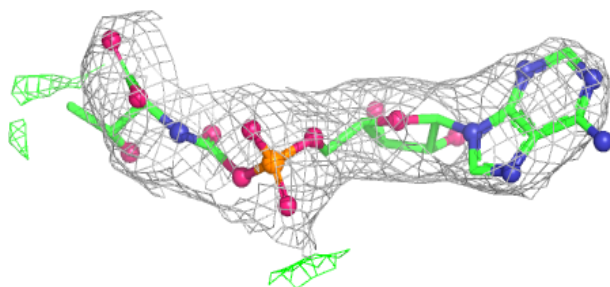
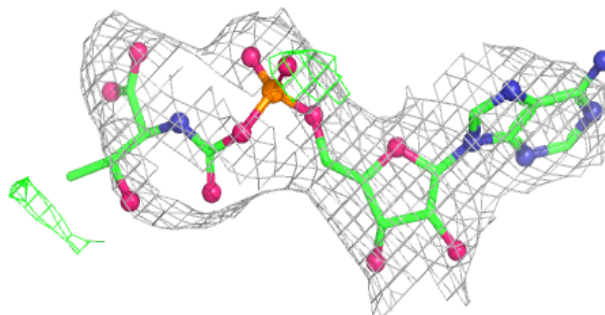
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ZN	G	402	1/1	0.77	0.12	106,106,106,106	1
4	TXA	G	401	33/33	0.85	0.11	83,106,136,140	0
4	TXA	B	401	33/33	0.90	0.08	88,101,121,128	0
5	ZN	B	402	1/1	0.92	0.06	108,108,108,108	1
7	APC	E	201	31/31	0.97	0.06	62,75,88,89	0
7	APC	D	201	31/31	0.98	0.05	77,85,105,108	0
6	MG	D	200	1/1	0.98	0.03	61,61,61,61	0
6	MG	E	200	1/1	0.99	0.02	39,39,39,39	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.

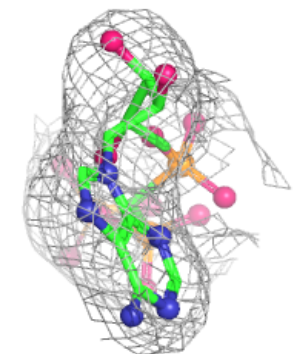
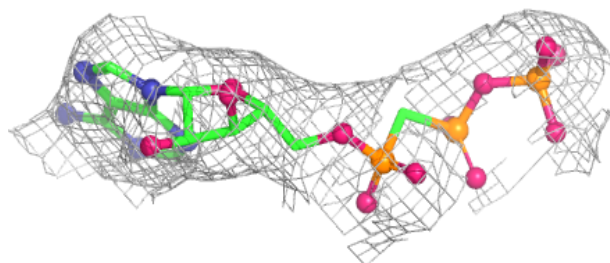
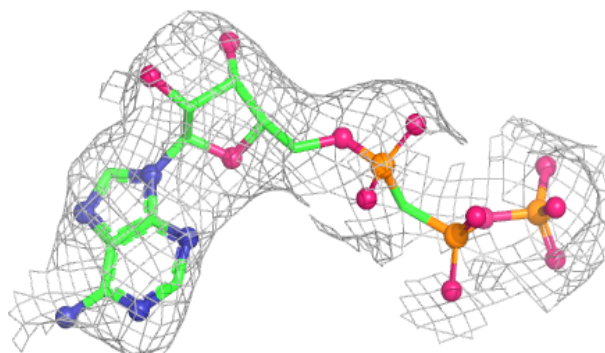


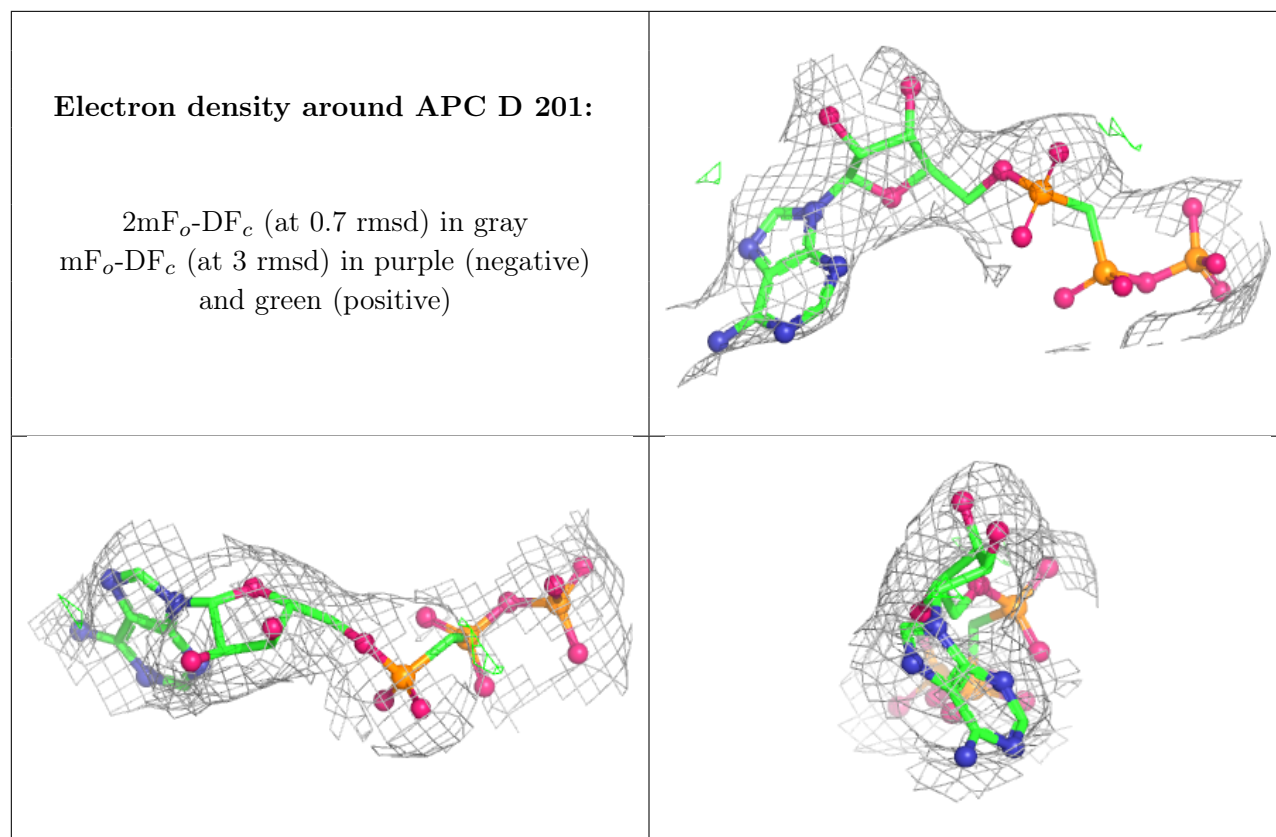
Electron density around TXA B 401:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.