



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:02 am GMT

PDB ID : 3OUY
Title : How the CCA-adding Enzyme Selects Adenine Over Cytosine at Position 76 of tRNA
Authors : Pan, B.C.; Xiong, Y.; Steitz, T.A.
Deposited on : 2010-09-15
Resolution : 2.69 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

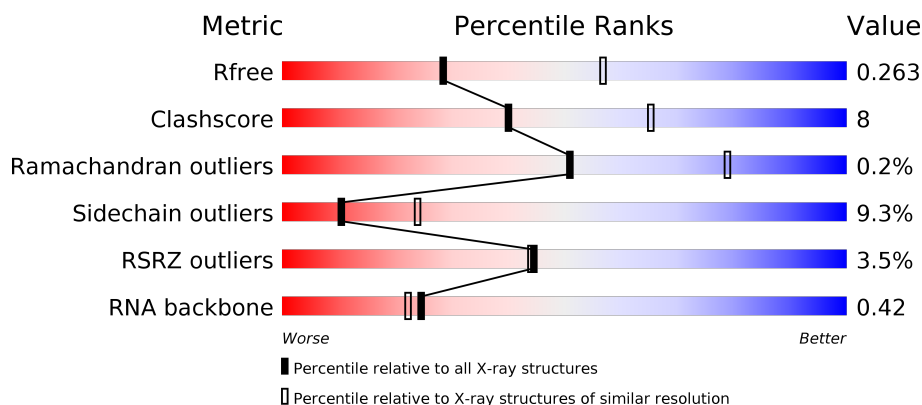
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)
RNA backbone	2435	1011 (3.06-2.34)

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. 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	441	<div> <div>76%</div> <div>23%</div> <div>.</div> </div>
2	B	437	<div> <div>6%</div> <div>72%</div> <div>25%</div> <div>.</div> </div>
3	C	35	<div> <div>9%</div> <div>54%</div> <div>26%</div> <div>17%</div> <div>.</div> </div>
3	D	35	<div> <div>11%</div> <div>49%</div> <div>26%</div> <div>20%</div> <div>6%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8942 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 CCA-Adding Enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3655	2347	636	655	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	438	CYS	-	EXPRESSION TAG	UNP O28126
A	439	CYS	-	EXPRESSION TAG	UNP O28126
A	440	CYS	-	EXPRESSION TAG	UNP O28126
A	441	MET	-	EXPRESSION TAG	UNP O28126

- Molecule 2 is a protein called CCA-Adding Enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	437	Total	C	N	O	S	0	0	0
			3629	2333	632	651	13			

- Molecule 3 is a RNA chain called RNA (35-MER).

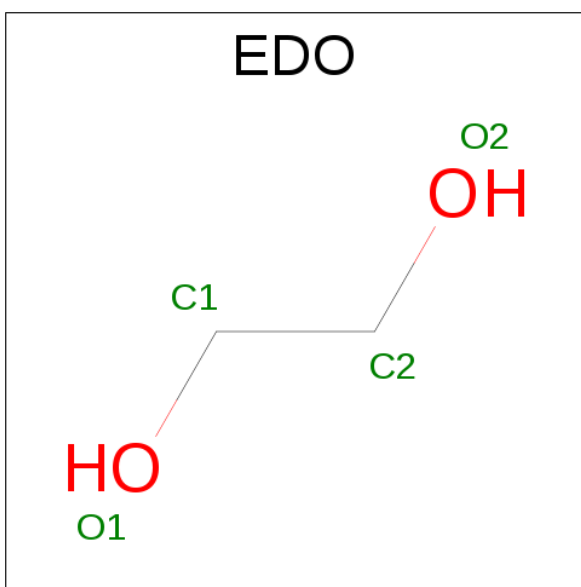
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	35	Total	C	N	O	P	3	0	0
			742	332	129	246	35			
3	D	35	Total	C	N	O	P	3	0	0
			742	332	129	246	35			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



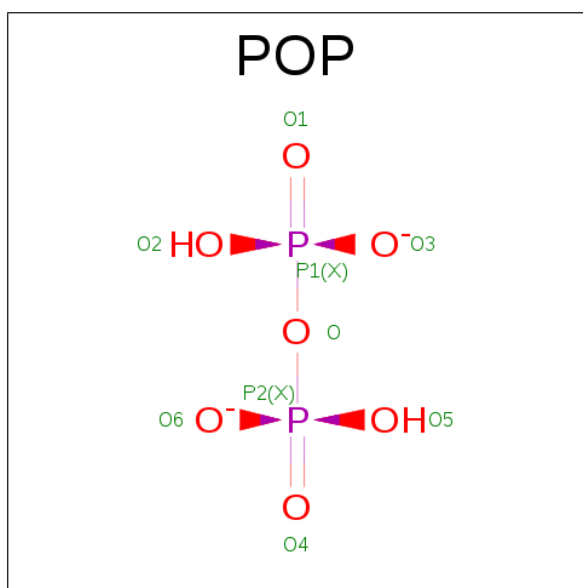
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			9	7	2		
6	C	1	Total	O	P	0	0
			9	7	2		

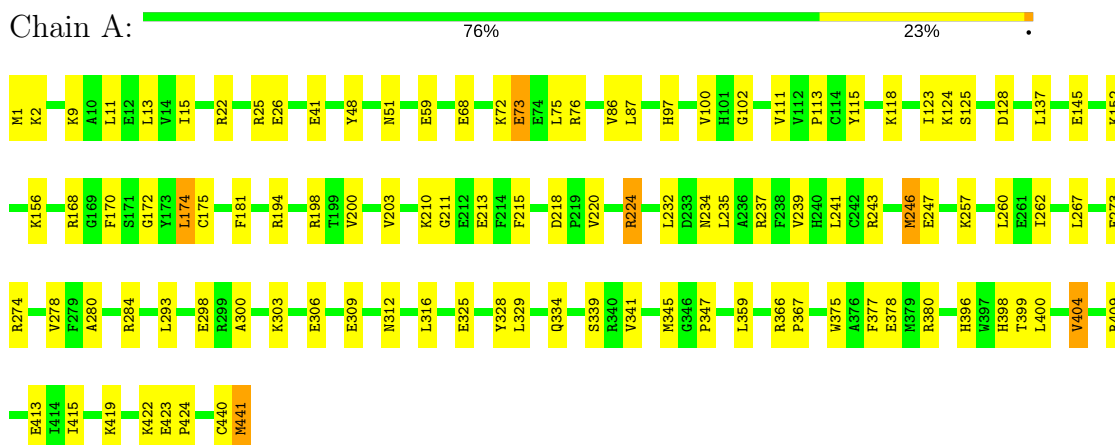
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	101	Total	O	0	0
			101	101		
7	B	26	Total	O	0	0
			26	26		
7	C	8	Total	O	0	0
			8	8		
7	D	2	Total	O	0	0
			2	2		

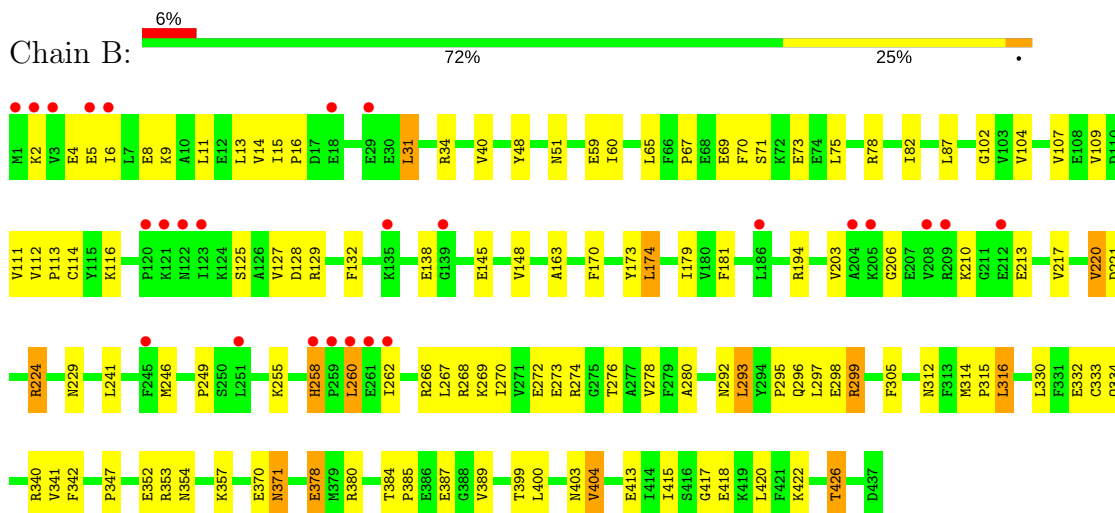
3 Residue-property plots

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.

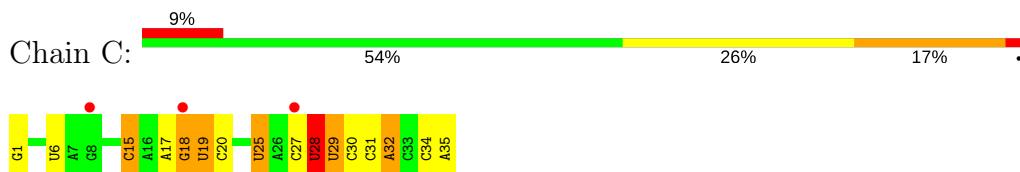
• Molecule 1: CCA-Adding Enzyme



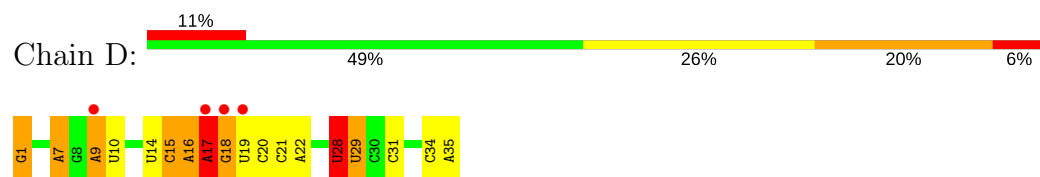
• Molecule 2: CCA-Adding Enzyme



• Molecule 3: RNA (35-MER)



● Molecule 3: RNA (35-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	111.22Å 228.07Å 58.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.69 49.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.69) 91.2 (49.98-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.264 0.204 , 0.263	Depositor DCC
R_{free} test set	1968 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8942	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, POP, EDO

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	0.64	0/3738	0.72	0/5021
2	B	0.53	0/3712	0.64	0/4987
3	C	0.95	2/828 (0.2%)	1.58	14/1285 (1.1%)
3	D	1.38	2/828 (0.2%)	1.61	11/1285 (0.9%)
All	All	0.74	4/9106 (0.0%)	0.94	25/12578 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	G	P-O5'	30.87	1.90	1.59
3	D	1	G	OP3-P	-12.36	1.46	1.61
3	C	1	G	OP3-P	6.20	1.68	1.61
3	C	18	G	C3'-O3'	5.06	1.49	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	G	O5'-P-OP1	-20.23	86.42	110.70
3	D	1	G	O5'-P-OP2	18.95	133.44	110.70
3	D	1	G	P-O5'-C5'	9.76	136.51	120.90
3	C	1	G	P-O5'-C5'	9.40	135.94	120.90
3	C	30	C	O4'-C1'-N1	8.90	115.32	108.20
3	D	15	C	O4'-C1'-N1	8.85	115.28	108.20
3	C	1	G	O5'-P-OP2	6.62	118.65	110.70
3	D	28	U	O4'-C1'-N1	6.43	113.35	108.20
3	D	17	A	C1'-O4'-C4'	-6.30	104.86	109.90
3	C	28	U	O4'-C1'-N1	6.15	113.12	108.20
3	C	15	C	O4'-C1'-N1	6.00	113.00	108.20
3	D	15	C	C6-N1-C2	-5.99	117.91	120.30
3	C	31	C	N1-C2-O2	5.91	122.45	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	19	U	C1'-O4'-C4'	-5.77	105.28	109.90
3	C	27	C	O4'-C1'-N1	5.74	112.79	108.20
3	C	19	U	O4'-C1'-N1	5.72	112.78	108.20
3	D	21	C	O4'-C1'-N1	5.67	112.74	108.20
3	C	30	C	C4'-C3'-C2'	-5.56	97.04	102.60
3	D	22	A	O4'-C1'-N9	5.48	112.58	108.20
3	D	9	A	C3'-C2'-C1'	-5.43	97.16	101.50
3	C	34	C	C4'-C3'-C2'	-5.16	97.44	102.60
3	C	25	U	O4'-C1'-N1	5.08	112.26	108.20
3	D	15	C	C2-N1-C1'	5.07	124.38	118.80
3	C	32	A	N1-C2-N3	-5.06	126.77	129.30
3	C	6	U	O4'-C1'-N1	5.03	112.22	108.20

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	3655	0	3657	70	0
2	B	3629	0	3633	70	0
3	C	742	0	376	7	0
3	D	742	0	376	12	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
5	A	4	0	6	1	0
6	B	9	0	0	0	0
6	C	9	0	0	1	0
7	A	101	0	0	5	0
7	B	26	0	0	1	0
7	C	8	0	0	3	0
7	D	2	0	0	0	0
All	All	8942	0	8048	140	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 8.

All (140) 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:A:246:MET:HA	1:A:246:MET:CE	1.86	1.04
1:A:246:MET:HA	1:A:246:MET:HE3	1.41	1.03
1:A:380:ARG:HH22	2:B:334:GLN:NE2	1.66	0.93
1:A:380:ARG:HH22	2:B:334:GLN:HE22	1.11	0.93
2:B:132:PHE:HB3	2:B:220:VAL:HG11	1.55	0.87
3:C:15:C:H5	7:C:106:HOH:O	1.65	0.79
1:A:423:GLU:HG3	1:A:424:PRO:HD2	1.68	0.75
1:A:334:GLN:HE21	2:B:380:ARG:HH12	1.39	0.69
2:B:296:GLN:HE22	2:B:403:ASN:HD22	1.41	0.67
3:D:16:A:H3'	3:D:17:A:H5''	1.76	0.66
1:A:339:SER:CB	2:B:276:THR:HG22	2.27	0.65
2:B:278:VAL:HG12	2:B:332:GLU:HG3	1.78	0.65
2:B:347:PRO:HB3	3:D:15:C:C5	2.32	0.65
2:B:400:LEU:O	2:B:404:VAL:HG23	1.97	0.64
3:C:35:A:H5''	6:C:701:POP:O4	1.96	0.64
1:A:123:ILE:CG2	1:A:125:SER:O	2.45	0.64
1:A:123:ILE:HG23	1:A:125:SER:O	1.98	0.63
3:C:28:U:H2'	3:C:29:U:O4'	2.00	0.62
1:A:409:ARG:HD3	7:A:480:HOH:O	1.99	0.62
1:A:1:MET:HE3	1:A:9:LYS:HE2	1.82	0.61
1:A:246:MET:HA	1:A:246:MET:HE2	1.77	0.61
2:B:170:PHE:HD2	2:B:174:LEU:HD13	1.64	0.61
3:D:14:U:C2	3:D:16:A:OP2	2.54	0.61
3:C:25:U:O5'	3:C:25:U:H6	1.85	0.60
1:A:339:SER:HB2	2:B:276:THR:HG22	1.84	0.60
1:A:312:ASN:HB3	2:B:314:MET:HE2	1.85	0.59
2:B:221:ASP:HB3	2:B:224:ARG:HB2	1.83	0.59
1:A:400:LEU:O	1:A:404:VAL:CG2	2.51	0.58
2:B:305:PHE:CE1	2:B:315:PRO:HB2	2.38	0.58
2:B:342:PHE:CE2	2:B:378:GLU:HB3	2.39	0.58
1:A:400:LEU:O	1:A:404:VAL:HG22	2.04	0.58
1:A:312:ASN:HB3	2:B:314:MET:CE	2.34	0.57
2:B:14:VAL:HG23	2:B:15:ILE:HD12	1.86	0.57
2:B:2:LYS:O	2:B:5:GLU:HB2	2.04	0.57
1:A:41:GLU:H	5:A:801:EDO:H21	1.70	0.57
2:B:173:TYR:HB2	3:D:35:A:H2'	1.87	0.57
2:B:270:ILE:O	2:B:274:ARG:HG3	2.05	0.56
1:A:243:ARG:HD3	2:B:352:GLU:HG3	1.86	0.56
1:A:224:ARG:HD2	7:A:493:HOH:O	2.05	0.56
1:A:334:GLN:NE2	2:B:380:ARG:HH22	2.04	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:MET:HB2	1:A:375:TRP:CZ3	2.42	0.54
1:A:328:TYR:CE2	1:A:423:GLU:HG2	2.42	0.54
2:B:370:GLU:HG2	2:B:371:ASN:ND2	2.21	0.54
2:B:181:PHE:HE1	2:B:206:GLY:HA2	1.73	0.54
2:B:87:LEU:HD13	2:B:102:GLY:HA3	1.89	0.54
1:A:306:GLU:HA	1:A:309:GLU:CG	2.38	0.53
2:B:60:ILE:HB	2:B:109:VAL:HG13	1.90	0.53
1:A:87:LEU:HD13	1:A:102:GLY:HA3	1.91	0.53
1:A:396:HIS:O	1:A:399:THR:HG22	2.09	0.52
2:B:276:THR:HB	2:B:333:CYS:O	2.10	0.51
2:B:4:GLU:O	2:B:8:GLU:HG2	2.11	0.51
2:B:258:HIS:HB3	2:B:260:LEU:HD12	1.90	0.51
2:B:170:PHE:CD2	2:B:174:LEU:HD13	2.46	0.51
2:B:129:ARG:NE	2:B:224:ARG:HG3	2.26	0.51
2:B:65:LEU:HD22	2:B:116:LYS:HG3	1.93	0.51
2:B:293:LEU:HD22	2:B:297:LEU:HG	1.94	0.50
2:B:354:ASN:HB3	3:D:15:C:H6	1.76	0.50
2:B:280:ALA:HB2	2:B:330:LEU:HD23	1.94	0.50
2:B:270:ILE:O	2:B:273:GLU:HB3	2.12	0.49
1:A:334:GLN:HE22	2:B:380:ARG:HH22	1.59	0.49
1:A:366:ARG:HH11	1:A:367:PRO:HD2	1.77	0.49
3:D:17:A:H4'	3:D:18:G:OP1	2.12	0.49
1:A:300:ALA:HB1	1:A:329:LEU:HD11	1.94	0.49
1:A:168:ARG:NH2	1:A:298:GLU:OE1	2.45	0.48
3:D:7:A:O5'	3:D:7:A:H8	1.95	0.48
2:B:48:TYR:HB2	2:B:59:GLU:O	2.14	0.48
1:A:257:LYS:HA	1:A:440:CYS:O	2.14	0.48
1:A:306:GLU:HA	1:A:309:GLU:HG3	1.94	0.48
2:B:293:LEU:O	2:B:296:GLN:HB2	2.13	0.48
1:A:339:SER:O	1:A:380:ARG:NH1	2.47	0.47
1:A:22:ARG:O	1:A:26:GLU:HG2	2.13	0.47
3:D:16:A:H3'	3:D:17:A:C5'	2.42	0.47
2:B:34:ARG:HH21	2:B:104:VAL:HG13	1.79	0.47
1:A:152:LYS:HE2	1:A:172:GLY:HA2	1.97	0.47
1:A:200:VAL:HA	1:A:215:PHE:O	2.15	0.47
1:A:224:ARG:HH22	3:C:32:A:P	2.38	0.47
2:B:127:VAL:HG12	3:D:34:C:C2	2.49	0.47
2:B:246:MET:CE	2:B:246:MET:HA	2.44	0.47
1:A:168:ARG:HD3	7:A:453:HOH:O	2.14	0.47
1:A:22:ARG:HB3	1:A:22:ARG:NH1	2.30	0.47
1:A:262:ILE:HD13	1:A:267:LEU:HD13	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:LEU:HD13	2:B:104:VAL:HG21	1.96	0.47
1:A:234:ASN:ND2	1:A:237:ARG:HH11	2.13	0.46
2:B:31:LEU:HD21	2:B:109:VAL:HG11	1.97	0.46
1:A:347:PRO:HB3	3:C:15:C:C5	2.51	0.46
2:B:246:MET:HA	2:B:246:MET:HE3	1.97	0.46
1:A:218:ASP:HB2	1:A:224:ARG:HB3	1.97	0.46
1:A:246:MET:HE3	1:A:246:MET:CA	2.29	0.46
1:A:415:ILE:HG23	1:A:419:LYS:HD3	1.97	0.46
2:B:296:GLN:OE1	2:B:404:VAL:HG22	2.16	0.46
1:A:123:ILE:HG23	1:A:128:ASP:HB2	1.98	0.45
2:B:114:CYS:HB2	2:B:128:ASP:OD1	2.16	0.45
1:A:73:GLU:OE1	1:A:76:ARG:HD3	2.17	0.45
2:B:385:PRO:O	2:B:389:VAL:HG12	2.17	0.45
1:A:413:GLU:HG3	1:A:415:ILE:HD11	1.99	0.45
2:B:148:VAL:HA	2:B:179:ILE:HG13	1.99	0.45
3:C:15:C:C5	7:C:106:HOH:O	2.50	0.44
1:A:172:GLY:O	1:A:175:CYS:HB2	2.17	0.44
1:A:339:SER:HB2	2:B:276:THR:CG2	2.47	0.44
2:B:316:LEU:HD12	2:B:316:LEU:HA	1.53	0.44
2:B:357:LYS:HB3	2:B:357:LYS:HE2	1.86	0.44
2:B:417:GLY:O	2:B:420:LEU:HB3	2.18	0.43
1:A:198:ARG:HD3	7:A:486:HOH:O	2.18	0.43
2:B:67:PRO:HG2	2:B:70:PHE:CE1	2.54	0.43
2:B:312:ASN:ND2	7:B:460:HOH:O	2.49	0.43
1:A:380:ARG:NH2	2:B:334:GLN:HE22	1.94	0.43
2:B:78:ARG:HE	2:B:82:ILE:HD11	1.83	0.43
1:A:170:PHE:CD2	1:A:174:LEU:HD13	2.54	0.42
3:D:28:U:H2'	3:D:29:U:O4'	2.18	0.42
1:A:232:LEU:O	1:A:235:LEU:HB3	2.18	0.42
1:A:243:ARG:O	1:A:247:GLU:HG3	2.19	0.42
2:B:11:LEU:HD22	2:B:15:ILE:CD1	2.49	0.42
2:B:299:ARG:NH1	2:B:399:THR:O	2.53	0.42
2:B:6:ILE:HG13	2:B:249:PRO:HB2	2.01	0.42
1:A:398:HIS:HB3	7:C:41:HOH:O	2.20	0.42
2:B:71:SER:OG	2:B:73:GLU:HB3	2.20	0.42
1:A:303:LYS:HA	1:A:303:LYS:HD2	1.82	0.42
2:B:163:ALA:O	2:B:229:ASN:ND2	2.51	0.42
2:B:262:ILE:HD11	2:B:266:ARG:HD3	2.02	0.42
1:A:1:MET:CE	1:A:9:LYS:HE2	2.50	0.42
1:A:115:TYR:CD1	1:A:124:LYS:HB3	2.55	0.41
2:B:267:LEU:HD22	2:B:426:THR:HG22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:14:U:O5'	3:D:14:U:H6	2.02	0.41
1:A:198:ARG:NE	1:A:211:GLY:O	2.52	0.41
2:B:295:PRO:O	2:B:298:GLU:HB2	2.21	0.41
2:B:112:VAL:HA	2:B:113:PRO:HD2	1.94	0.41
1:A:11:LEU:HB3	1:A:15:ILE:HD13	2.02	0.41
1:A:145:GLU:H	1:A:145:GLU:CD	2.24	0.41
1:A:440:CYS:SG	1:A:441:MET:N	2.93	0.41
1:A:59:GLU:HB3	7:A:490:HOH:O	2.21	0.41
1:A:280:ALA:HA	1:A:329:LEU:O	2.20	0.41
2:B:413:GLU:HG3	2:B:415:ILE:HD11	2.03	0.41
2:B:292:ASN:OD1	3:D:1:G:H1'	2.21	0.41
2:B:15:ILE:HA	2:B:16:PRO:HD3	1.91	0.40
2:B:384:THR:HG23	2:B:387:GLU:OE2	2.21	0.40
1:A:246:MET:CE	1:A:246:MET:CA	2.74	0.40
1:A:341:VAL:CG2	1:A:377:PHE:HB3	2.52	0.40
1:A:25:ARG:NH1	1:A:48:TYR:OH	2.55	0.40
1:A:181:PHE:HD1	1:A:203:VAL:HG13	1.85	0.40
1:A:97:HIS:HE1	1:A:113:PRO:O	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	439/441 (100%)	419 (95%)	20 (5%)	0	100	100
2	B	435/437 (100%)	399 (92%)	34 (8%)	2 (0%)	32	60
All	All	874/878 (100%)	818 (94%)	54 (6%)	2 (0%)	51	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	138	GLU
2	B	260	LEU

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	391/391 (100%)	356 (91%)	35 (9%)	11	25
2	B	387/387 (100%)	350 (90%)	37 (10%)	10	22
All	All	778/778 (100%)	706 (91%)	72 (9%)	10	24

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	13	LEU
1	A	51	ASN
1	A	68	GLU
1	A	72	LYS
1	A	73	GLU
1	A	75	LEU
1	A	86	VAL
1	A	100	VAL
1	A	111	VAL
1	A	118	LYS
1	A	137	LEU
1	A	156	LYS
1	A	174	LEU
1	A	194	ARG
1	A	210	LYS
1	A	213	GLU
1	A	220	VAL
1	A	224	ARG
1	A	239	VAL
1	A	241	LEU
1	A	246	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	260	LEU
1	A	273	GLU
1	A	274	ARG
1	A	278	VAL
1	A	284	ARG
1	A	293	LEU
1	A	316	LEU
1	A	325	GLU
1	A	359	LEU
1	A	378	GLU
1	A	404	VAL
1	A	422	LYS
1	A	441	MET
2	B	9	LYS
2	B	13	LEU
2	B	31	LEU
2	B	40	VAL
2	B	51	ASN
2	B	69	GLU
2	B	75	LEU
2	B	107	VAL
2	B	111	VAL
2	B	125	SER
2	B	145	GLU
2	B	174	LEU
2	B	194	ARG
2	B	203	VAL
2	B	210	LYS
2	B	213	GLU
2	B	217	VAL
2	B	220	VAL
2	B	224	ARG
2	B	241	LEU
2	B	255	LYS
2	B	258	HIS
2	B	268	ARG
2	B	269	LYS
2	B	272	GLU
2	B	293	LEU
2	B	299	ARG
2	B	316	LEU
2	B	340	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	341	VAL
2	B	353	ARG
2	B	371	ASN
2	B	378	GLU
2	B	404	VAL
2	B	418	GLU
2	B	422	LYS
2	B	426	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	234	ASN
1	A	312	ASN
1	A	334	GLN
1	A	348	GLN
1	A	396	HIS
1	A	403	ASN
2	B	146	ASN
2	B	234	ASN
2	B	334	GLN
2	B	371	ASN
2	B	396	HIS
2	B	403	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	34/35 (97%)	6 (17%)	0
3	D	34/35 (97%)	11 (32%)	0
All	All	68/70 (97%)	17 (25%)	0

All (17) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	17	A
3	C	18	G
3	C	19	U
3	C	20	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	28	U
3	C	29	U
3	D	7	A
3	D	9	A
3	D	10	U
3	D	16	A
3	D	17	A
3	D	18	G
3	D	19	U
3	D	20	C
3	D	28	U
3	D	29	U
3	D	31	C

There are no RNA pucker outliers to report.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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	SO4	A	601	-	4,4,4	0.19	0	6,6,6	0.41	0
4	SO4	A	602	-	4,4,4	0.10	0	6,6,6	0.22	0
5	EDO	A	801	-	3,3,3	0.41	0	2,2,2	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	603	-	4,4,4	0.18	0	6,6,6	0.15	0
6	POP	B	702	-	8,8,8	1.16	1 (12%)	8,13,13	0.39	0
6	POP	C	701	-	8,8,8	1.53	2 (25%)	8,13,13	0.64	0

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	SO4	A	601	-	-	0/0/0/0	0/0/0/0
4	SO4	A	602	-	-	0/0/0/0	0/0/0/0
5	EDO	A	801	-	-	0/1/1/1	0/0/0/0
4	SO4	B	603	-	-	0/0/0/0	0/0/0/0
6	POP	B	702	-	-	0/6/6/6	0/0/0/0
6	POP	C	701	-	-	0/6/6/6	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	702	POP	P2-O	2.13	1.63	1.60
6	C	701	POP	P1-O	2.64	1.64	1.60
6	C	701	POP	P2-O	2.98	1.64	1.60

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	801	EDO	1	0
6	C	701	POP	1	0

5.7 Other polymers [i](#)

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, 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	441/441 (100%)	-0.22	0 100 100	19, 33, 65, 103	0
2	B	437/437 (100%)	0.22	26 (5%) 23 21	22, 68, 110, 135	0
3	C	35/35 (100%)	0.05	3 (8%) 11 9	22, 69, 106, 119	1 (2%)
3	D	35/35 (100%)	0.57	4 (11%) 6 4	54, 85, 142, 146	1 (2%)
All	All	948/948 (100%)	0.02	33 (3%) 44 44	19, 44, 106, 146	2 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	260	LEU	6.1
3	D	18	G	4.9
2	B	121	LYS	4.1
2	B	1	MET	4.0
2	B	139	GLY	4.0
2	B	204	ALA	4.0
2	B	135	LYS	3.7
3	D	17	A	3.7
2	B	2	LYS	3.7
2	B	262	ILE	3.6
2	B	261	GLU	3.5
3	C	18	G	3.3
2	B	258	HIS	3.3
2	B	245	PHE	3.2
3	D	19	U	3.1
2	B	5	GLU	3.0
2	B	212	GLU	2.9
2	B	6	ILE	2.9
2	B	259	PRO	2.8
3	D	9	A	2.8
2	B	122	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	208	VAL	2.7
2	B	205	LYS	2.6
2	B	251	LEU	2.6
2	B	123	ILE	2.5
3	C	8	G	2.4
2	B	29	GLU	2.3
2	B	186	LEU	2.2
2	B	120	PRO	2.2
2	B	209	ARG	2.1
2	B	3	VAL	2.1
2	B	18	GLU	2.0
3	C	27	C	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
6	POP	C	701	9/9	0.91	0.18	1.71	63,64,64,65	0
5	EDO	A	801	4/4	0.90	0.19	1.65	40,41,42,43	0
4	SO4	B	603	5/5	0.92	0.14	-0.30	89,89,90,90	0
6	POP	B	702	9/9	0.92	0.13	-1.09	97,98,98,99	0
4	SO4	A	601	5/5	0.96	0.09	-5.58	51,52,53,54	0
4	SO4	A	602	5/5	0.93	0.21	-	97,97,97,97	0

6.5 Other polymers [i](#)

There are no such residues in this entry.