



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:21 pm GMT

PDB ID : 1U7W  
Title : Phosphopantothenoylcysteine synthetase from E. coli, CTP-complex  
Authors : Stanitzek, S.; Augustin, M.A.; Huber, R.; Kupke, T.; Steinbacher, S.  
Deposited on : 2004-08-04  
Resolution : 2.50 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](mailto: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.

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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

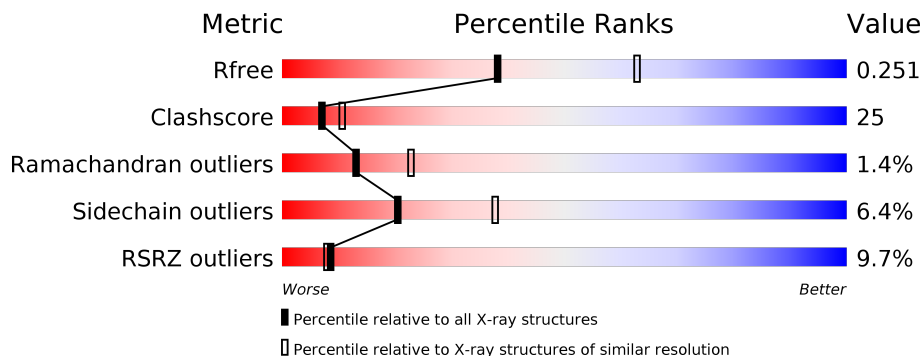
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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  $\geq 3$ , 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	226	<div> <div>10%</div> <div> <div></div> <div>58%</div> <div>30%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	226	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>23%</div> <div>• •</div> <div>10%</div> </div> </div>
1	C	226	<div> <div>13%</div> <div> <div></div> <div>55%</div> <div>30%</div> <div>5%</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4958 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 Coenzyme A biosynthesis bifunctional protein coaBC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1562	985	279	291	7			
1	B	203	Total	C	N	O	S	0	0	0
			1569	989	283	290	7			
1	C	204	Total	C	N	O	S	0	0	0
			1572	989	281	295	7			

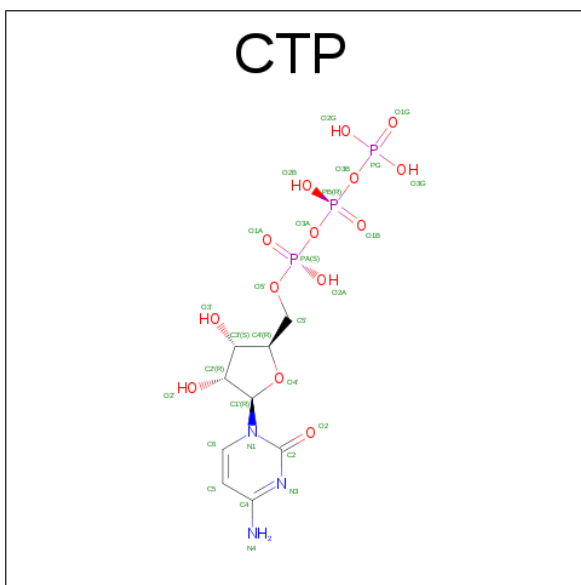
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	210	ASP	ASN	ENGINEERED	UNP P0ABQ0
B	210	ASP	ASN	ENGINEERED	UNP P0ABQ0
C	210	ASP	ASN	ENGINEERED	UNP P0ABQ0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>14</sub>P<sub>3</sub>).

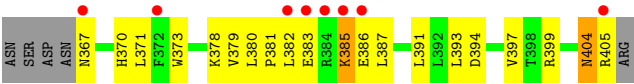


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 29	C 9	N 3	O 14	P 3	0	0
3	B	1	Total 29	C 9	N 3	O 14	P 3	0	0
3	C	1	Total 29	C 9	N 3	O 14	P 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	51	Total O 51 51	0	0
4	B	68	Total O 68 68	0	0
4	C	46	Total O 46 46	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.93Å 144.41Å 246.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-2.50) 99.5 (20.00-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.211 , 0.258 0.206 , 0.251	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	70.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4958	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA, CTP

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	0.51	0/1586	0.73	0/2150
1	B	0.55	0/1594	0.78	0/2159
1	C	0.52	2/1597 (0.1%)	0.73	0/2167
All	All	0.53	2/4777 (0.0%)	0.75	0/6476

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	274	CYS	CB-SG	-5.96	1.72	1.81
1	C	192	MET	SD-CE	-5.27	1.48	1.77

There are no bond angle outliers.

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	1562	0	1591	80	0
1	B	1569	0	1604	83	0
1	C	1572	0	1592	83	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	29	0	12	1	0
3	B	29	0	12	5	0
3	C	29	0	12	1	0
4	A	51	0	0	26	0
4	B	68	0	0	36	0
4	C	46	0	0	27	0
All	All	4958	0	4823	244	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 25.

All (244) 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:B:184:ASN:HB2	4:B:55:HOH:O	1.60	0.99
1:B:401:ASP:HB3	4:B:90:HOH:O	1.62	0.99
1:A:190:ASN:H	1:A:269:ASN:HD22	1.03	0.97
1:B:205:VAL:HB	4:B:153:HOH:O	1.64	0.97
1:B:405:ARG:HH21	1:B:405:ARG:HB2	1.29	0.94
1:C:183:VAL:HG12	1:C:184:ASN:H	1.36	0.90
1:B:370:HIS:HB2	4:B:42:HOH:O	1.70	0.89
1:A:353:ASN:HB3	1:A:369:LEU:HD23	1.56	0.87
1:B:190:ASN:H	1:B:269:ASN:HD22	1.22	0.87
1:A:351:CYS:HB3	4:A:125:HOH:O	1.75	0.86
1:C:190:ASN:H	1:C:269:ASN:HD22	1.24	0.85
1:A:252:MET:HG3	4:A:95:HOH:O	1.76	0.84
1:C:354:ASP:HB2	4:C:84:HOH:O	1.78	0.83
1:C:187:LYS:HA	1:C:228:GLY:O	1.78	0.83
1:C:200:GLU:HB2	1:C:208:ILE:HG22	1.60	0.83
1:C:257:MET:HE2	4:C:71:HOH:O	1.80	0.82
1:A:338:ALA:HB3	4:A:113:HOH:O	1.79	0.81
1:C:200:GLU:HB2	1:C:208:ILE:CG2	2.10	0.81
1:A:324:VAL:HG21	4:A:91:HOH:O	1.80	0.80
1:A:285:VAL:HA	4:A:155:HOH:O	1.81	0.79
1:B:405:ARG:HH21	1:B:405:ARG:CB	1.97	0.78
1:C:381:PRO:HD3	4:C:136:HOH:O	1.85	0.75
1:C:192:MET:SD	4:C:63:HOH:O	2.45	0.73
1:A:327:PHE:O	3:A:500:CTP:H5'1	1.88	0.73
1:B:339:ARG:HG3	1:B:339:ARG:HH11	1.53	0.72
1:A:190:ASN:H	1:A:269:ASN:ND2	1.84	0.71
1:A:336:GLU:HB3	4:A:132:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:GLN:HG2	4:B:24:HOH:O	1.89	0.71
1:A:383:GLU:CD	1:A:387:LEU:HD23	2.11	0.70
1:C:386:GLU:HB2	4:C:111:HOH:O	1.89	0.70
1:B:322:PRO:HG2	4:B:156:HOH:O	1.91	0.70
1:B:215:LYS:HE2	4:B:92:HOH:O	1.91	0.70
1:A:353:ASN:HB2	4:A:109:HOH:O	1.90	0.69
1:A:200:GLU:HB2	1:A:208:ILE:HG22	1.74	0.69
1:A:186:LEU:HD22	1:A:189:LEU:HD12	1.75	0.69
1:A:331:THR:N	4:A:106:HOH:O	2.25	0.69
1:C:378:LYS:HD2	4:C:5:HOH:O	1.93	0.69
1:C:211:HIS:HA	4:C:97:HOH:O	1.94	0.68
1:A:247:LYS:HB3	4:A:7:HOH:O	1.94	0.66
1:C:304:MET:SD	4:C:43:HOH:O	2.52	0.66
1:C:210:ASP:O	4:C:97:HOH:O	2.14	0.66
1:A:304:MET:HE2	4:B:44:HOH:O	1.95	0.65
1:C:183:VAL:HG12	1:C:184:ASN:N	2.10	0.65
1:A:335:GLU:HB3	4:A:3:HOH:O	1.97	0.65
1:B:202:LEU:HD23	1:B:282:ALA:HB2	1.79	0.64
1:B:323:TYR:O	4:B:156:HOH:O	2.15	0.64
1:B:345:LYS:HG3	4:B:17:HOH:O	1.98	0.63
1:C:385:LYS:HE3	4:C:60:HOH:O	1.98	0.63
1:A:383:GLU:HG3	1:A:384:ARG:H	1.63	0.63
1:C:373:TRP:HD1	4:C:52:HOH:O	1.80	0.63
1:B:255:LEU:HG	4:B:120:HOH:O	1.98	0.63
1:C:327:PHE:O	3:C:2500:CTP:H5'1	1.98	0.62
1:B:190:ASN:H	1:B:269:ASN:ND2	1.96	0.62
1:A:336:GLU:O	1:A:340:GLN:HG3	1.99	0.62
1:A:203:ASP:HB2	1:A:204:PRO:CD	2.31	0.61
1:B:302:ILE:HD11	4:B:44:HOH:O	2.00	0.61
1:B:382:LEU:HD12	1:B:383:GLU:H	1.65	0.61
1:B:405:ARG:HH21	1:B:405:ARG:CG	2.14	0.61
1:A:334:VAL:HG21	1:A:354:ASP:HB2	1.81	0.61
1:B:405:ARG:HB3	4:B:54:HOH:O	2.01	0.60
1:C:203:ASP:HB3	1:C:286:ALA:HB3	1.82	0.60
1:C:370:HIS:HD2	1:C:378:LYS:O	1.84	0.60
1:B:182:PRO:HG2	1:B:226:ARG:O	2.02	0.59
1:B:327:PHE:O	3:B:1500:CTP:H5'1	2.02	0.59
1:B:255:LEU:CG	4:B:120:HOH:O	2.50	0.59
1:B:281:ARG:NH1	4:B:120:HOH:O	2.34	0.59
1:B:406:ARG:HB2	4:B:90:HOH:O	2.01	0.59
1:C:205:VAL:HB	4:C:130:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ARG:HH11	1:A:307:ASN:ND2	2.01	0.59
1:C:281:ARG:NH1	1:C:305:VAL:CG1	2.66	0.59
1:C:387:LEU:O	1:C:391:LEU:HD13	2.02	0.59
1:A:304:MET:HG3	4:B:44:HOH:O	2.03	0.59
1:B:183:VAL:HG22	1:B:184:ASN:N	2.18	0.58
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.68	0.58
1:C:182:PRO:HG2	4:C:129:HOH:O	2.02	0.58
1:B:405:ARG:NH2	1:B:405:ARG:HB2	2.11	0.58
1:C:281:ARG:NH1	1:C:305:VAL:HG11	2.19	0.58
3:B:1500:CTP:N4	4:B:126:HOH:O	2.37	0.58
1:C:310:ILE:HA	4:C:53:HOH:O	2.05	0.57
1:C:199:ARG:HG2	1:C:199:ARG:HH21	1.69	0.57
1:B:330:GLU:OE2	1:B:341:LYS:NZ	2.38	0.56
1:A:190:ASN:N	1:A:269:ASN:HD22	1.88	0.56
1:C:234:VAL:O	4:C:71:HOH:O	2.17	0.56
1:C:244:PRO:O	1:C:245:PHE:HB2	2.05	0.56
1:A:383:GLU:HG2	1:A:387:LEU:HB3	1.87	0.56
1:B:350:ILE:HG13	4:B:78:HOH:O	2.06	0.56
1:C:404:ASN:O	1:C:405:ARG:HB2	2.05	0.56
1:C:205:VAL:HG23	1:C:206:ARG:HG3	1.88	0.56
1:A:281:ARG:HH11	1:A:307:ASN:HD22	1.53	0.55
1:B:371:LEU:HD23	1:B:371:LEU:N	2.22	0.55
1:A:349:LEU:HD12	1:A:372:PHE:O	2.07	0.55
1:C:300:LEU:O	1:C:301:THR:HB	2.07	0.55
1:B:328:ALA:HB2	1:B:350:ILE:HD11	1.88	0.54
1:C:309:ASP:HB3	1:C:312:ALA:HB3	1.88	0.54
1:B:184:ASN:N	1:B:184:ASN:HD22	2.05	0.54
1:B:307:ASN:HB3	4:B:126:HOH:O	2.06	0.54
1:A:383:GLU:OE2	1:A:387:LEU:HD23	2.06	0.54
1:B:339:ARG:HG3	1:B:339:ARG:NH1	2.20	0.54
1:B:184:ASN:ND2	1:B:184:ASN:N	2.56	0.54
1:B:347:LEU:CD1	4:B:78:HOH:O	2.55	0.54
1:A:381:PRO:HB2	4:A:101:HOH:O	2.07	0.54
1:C:200:GLU:HG3	1:C:280:TYR:O	2.08	0.54
1:A:197:PRO:O	1:A:236:GLY:HA3	2.08	0.53
1:C:203:ASP:HB2	1:C:204:PRO:CD	2.38	0.53
1:C:213:SER:OG	1:C:215:LYS:HG2	2.08	0.53
1:A:331:THR:HG22	1:A:355:VAL:HG13	1.90	0.53
1:C:334:VAL:HG22	4:C:35:HOH:O	2.09	0.53
1:C:367:ASN:N	1:C:382:LEU:HD12	2.23	0.53
1:C:379:VAL:O	1:C:380:LEU:HD23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:LEU:HB2	4:A:29:HOH:O	2.08	0.53
1:B:190:ASN:N	1:B:269:ASN:HD22	2.01	0.52
1:A:315:ALA:N	4:A:91:HOH:O	2.40	0.52
1:B:198:THR:CG2	1:B:200:GLU:OE2	2.58	0.52
1:B:322:PRO:CG	4:B:156:HOH:O	2.54	0.52
1:A:324:VAL:CG2	4:A:91:HOH:O	2.50	0.52
1:A:398:THR:HG22	1:A:399:ARG:HH12	1.75	0.52
1:A:202:LEU:HD23	1:A:282:ALA:HB2	1.92	0.52
1:A:266:GLN:HG3	4:A:4:HOH:O	2.08	0.52
1:C:192:MET:HE1	1:C:261:VAL:HG13	1.91	0.51
1:B:341:LYS:CB	4:B:17:HOH:O	2.58	0.51
1:B:341:LYS:HB3	4:B:17:HOH:O	2.10	0.51
1:C:202:LEU:HB3	4:C:105:HOH:O	2.09	0.51
1:B:404:ASN:O	1:B:405:ARG:HB2	2.10	0.51
1:C:370:HIS:CD2	1:C:378:LYS:O	2.64	0.51
1:B:183:VAL:C	1:B:184:ASN:HD22	2.15	0.51
1:B:383:GLU:OE1	1:B:391:LEU:HD12	2.11	0.51
1:A:199:ARG:HD2	4:A:36:HOH:O	2.10	0.51
1:C:186:LEU:O	1:C:229:ALA:HA	2.10	0.51
1:A:345:LYS:HD3	4:A:135:HOH:O	2.11	0.51
1:C:383:GLU:CG	1:C:387:LEU:HD23	2.41	0.51
1:C:367:ASN:CA	1:C:382:LEU:HD12	2.41	0.50
1:A:341:LYS:O	1:A:345:LYS:HB2	2.11	0.50
1:A:331:THR:HG23	4:A:106:HOH:O	2.11	0.50
1:A:392:LEU:O	1:A:396:ILE:HG13	2.12	0.50
1:A:399:ARG:HG2	1:A:399:ARG:NH1	2.27	0.50
1:B:405:ARG:CB	4:B:54:HOH:O	2.59	0.49
1:C:216:MET:HG2	4:C:134:HOH:O	2.12	0.49
1:C:333:ASN:HB3	1:C:337:TYR:CD1	2.46	0.49
1:C:201:PRO:HG3	4:C:122:HOH:O	2.12	0.49
1:A:381:PRO:HD2	4:A:16:HOH:O	2.11	0.49
1:A:204:PRO:HG2	1:A:288:GLU:HA	1.94	0.49
1:C:281:ARG:HH12	1:C:305:VAL:HG11	1.77	0.49
1:C:181:SER:N	1:C:182:PRO:HD2	2.28	0.48
1:B:307:ASN:CB	4:B:126:HOH:O	2.59	0.48
1:C:334:VAL:HG21	4:C:84:HOH:O	2.12	0.48
1:A:399:ARG:HH11	1:A:399:ARG:HG2	1.77	0.48
1:A:369:LEU:C	4:A:29:HOH:O	2.51	0.48
1:A:328:ALA:O	1:A:352:ALA:HA	2.14	0.48
1:B:194:THR:OG1	1:B:273:GLY:HA2	2.14	0.48
1:A:203:ASP:HB2	1:A:204:PRO:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:GLU:HG2	1:A:402:GLU:O	2.13	0.48
4:A:40:HOH:O	1:B:289:LYS:HD2	2.12	0.48
1:A:203:ASP:HB3	1:A:286:ALA:HB3	1.96	0.48
1:A:387:LEU:N	4:A:22:HOH:O	2.45	0.48
1:C:287:PRO:O	1:C:288:GLU:HG3	2.13	0.48
1:C:373:TRP:CD1	4:C:52:HOH:O	2.56	0.48
1:C:215:LYS:HD2	4:C:89:HOH:O	2.14	0.47
1:B:322:PRO:HB2	4:B:156:HOH:O	2.12	0.47
1:A:355:VAL:HB	4:A:67:HOH:O	2.15	0.47
1:A:371:LEU:HD23	4:A:125:HOH:O	2.14	0.47
1:A:302:ILE:CD1	1:B:304:MET:HE1	2.45	0.47
1:B:383:GLU:HB2	4:B:50:HOH:O	2.15	0.47
1:C:213:SER:OG	1:C:215:LYS:CG	2.63	0.47
1:A:345:LYS:CD	4:A:135:HOH:O	2.62	0.47
1:B:226:ARG:HD2	4:B:13:HOH:O	2.15	0.47
1:A:187:LYS:HA	1:A:228:GLY:O	2.14	0.47
1:B:268:GLN:O	1:B:322:PRO:HB3	2.14	0.47
1:C:380:LEU:HA	4:C:136:HOH:O	2.14	0.47
1:C:257:MET:CE	4:C:71:HOH:O	2.49	0.47
1:C:224:ALA:HA	1:C:393:LEU:HD21	1.97	0.47
1:A:383:GLU:CG	1:A:384:ARG:N	2.78	0.46
1:B:382:LEU:O	1:B:383:GLU:CB	2.62	0.46
1:A:186:LEU:HD22	1:A:189:LEU:CD1	2.42	0.46
1:A:185:ASP:OD2	1:A:186:LEU:HG	2.14	0.46
1:B:405:ARG:HD3	1:B:405:ARG:HA	1.76	0.46
1:C:330:GLU:HB2	4:C:35:HOH:O	2.16	0.46
1:A:186:LEU:HD12	1:A:227:ARG:HB2	1.97	0.46
1:B:281:ARG:CZ	4:B:120:HOH:O	2.63	0.46
1:B:277:VAL:HB	3:B:1500:CTP:C5	2.50	0.46
1:B:271:PHE:N	4:B:156:HOH:O	2.48	0.46
1:B:322:PRO:CB	4:B:156:HOH:O	2.64	0.46
1:B:345:LYS:HE3	4:B:17:HOH:O	2.15	0.45
1:B:352:ALA:O	1:B:369:LEU:HD23	2.16	0.45
1:A:289:LYS:HE3	3:B:1500:CTP:O1G	2.16	0.45
1:C:203:ASP:HB2	1:C:204:PRO:HD2	1.98	0.45
1:C:319:ASP:O	1:C:320:HIS:HB2	2.15	0.45
1:B:341:LYS:HE2	3:B:1500:CTP:O3A	2.16	0.45
1:B:267:GLN:CG	4:B:24:HOH:O	2.57	0.45
1:B:281:ARG:HD3	1:B:307:ASN:HD21	1.81	0.45
1:C:187:LYS:N	4:C:18:HOH:O	2.49	0.45
1:B:198:THR:HG23	1:B:200:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:ASN:H	1:C:269:ASN:ND2	2.03	0.45
1:C:257:MET:HG3	4:C:71:HOH:O	2.16	0.45
1:B:183:VAL:CG2	1:B:184:ASN:N	2.80	0.45
1:A:200:GLU:HB2	1:A:208:ILE:CG2	2.44	0.45
1:A:211:HIS:HB3	4:A:119:HOH:O	2.17	0.45
1:B:383:GLU:CB	4:B:50:HOH:O	2.64	0.45
1:A:371:LEU:O	1:A:377:ASP:HA	2.17	0.45
1:B:307:ASN:ND2	4:B:120:HOH:O	2.49	0.45
1:B:371:LEU:HD12	1:B:395:GLU:HG2	1.99	0.45
1:C:197:PRO:O	1:C:236:GLY:HA3	2.17	0.45
1:C:281:ARG:NH1	1:C:305:VAL:HG13	2.32	0.45
1:B:198:THR:HG22	1:B:278:ALA:HB2	2.00	0.44
1:A:383:GLU:CG	1:A:384:ARG:H	2.26	0.44
1:A:183:VAL:HG13	1:A:183:VAL:O	2.18	0.44
1:A:321:ARG:NH1	1:A:321:ARG:HG2	2.33	0.44
1:A:330:GLU:HB2	1:A:334:VAL:HA	2.00	0.44
1:C:383:GLU:CD	1:C:387:LEU:HD23	2.38	0.44
1:C:192:MET:CE	1:C:261:VAL:HG13	2.48	0.44
1:C:309:ASP:OD2	1:C:345:LYS:NZ	2.43	0.43
1:C:404:ASN:N	1:C:404:ASN:HD22	2.15	0.43
1:B:406:ARG:HH21	1:B:406:ARG:HG3	1.81	0.43
1:C:321:ARG:HH11	1:C:321:ARG:HG2	1.83	0.43
1:B:194:THR:O	1:B:274:CYS:HB2	2.19	0.43
1:C:333:ASN:HB3	1:C:337:TYR:CE1	2.54	0.43
1:A:399:ARG:HH11	1:A:399:ARG:CG	2.31	0.43
1:A:399:ARG:HA	1:A:399:ARG:HD3	1.84	0.43
1:C:383:GLU:HG2	1:C:387:LEU:HB3	2.01	0.43
1:B:373:TRP:CD2	1:B:399:ARG:HD3	2.54	0.43
1:B:393:LEU:HG	1:B:393:LEU:O	2.17	0.43
1:C:383:GLU:HG2	1:C:387:LEU:HD23	2.00	0.42
1:C:187:LYS:HB3	1:C:187:LYS:NZ	2.34	0.42
1:C:224:ALA:HA	1:C:393:LEU:CD2	2.50	0.42
1:C:371:LEU:N	1:C:371:LEU:HD23	2.34	0.42
1:C:192:MET:HB2	1:C:268:GLN:HG3	2.02	0.42
1:C:199:ARG:CG	1:C:199:ARG:HH21	2.33	0.42
1:A:188:HIS:N	1:A:188:HIS:ND1	2.68	0.42
1:C:261:VAL:O	1:C:265:VAL:HB	2.20	0.42
1:A:261:VAL:O	1:A:265:VAL:HB	2.19	0.42
1:A:398:THR:CG2	1:A:399:ARG:HH12	2.33	0.42
1:B:351:CYS:HB3	1:B:369:LEU:HD22	2.02	0.41
1:C:393:LEU:O	1:C:397:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:TYR:OH	1:A:399:ARG:HB3	2.20	0.41
1:B:404:ASN:O	1:B:405:ARG:CB	2.68	0.41
1:B:192:MET:HB2	1:B:268:GLN:HG3	2.02	0.41
1:A:302:ILE:HD11	1:B:304:MET:CE	2.51	0.41
1:C:386:GLU:H	1:C:386:GLU:CD	2.24	0.41
1:C:300:LEU:O	1:C:301:THR:CB	2.69	0.41
1:B:370:HIS:C	1:B:371:LEU:HD23	2.41	0.41
1:B:378:LYS:HE2	1:B:395:GLU:OE1	2.21	0.41
1:B:405:ARG:CG	1:B:405:ARG:NH2	2.77	0.41
1:A:302:ILE:CD1	1:B:304:MET:CE	2.99	0.41
1:A:192:MET:HB2	1:A:268:GLN:HG3	2.02	0.41
1:B:339:ARG:CG	1:B:339:ARG:NH1	2.84	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	196/226 (87%)	181 (92%)	14 (7%)	1 (0%)	32	53
1	B	197/226 (87%)	182 (92%)	12 (6%)	3 (2%)	12	21
1	C	198/226 (88%)	181 (91%)	13 (7%)	4 (2%)	9	14
All	All	591/678 (87%)	544 (92%)	39 (7%)	8 (1%)	13	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	383	GLU
1	B	405	ARG
1	C	183	VAL
1	C	334	VAL
1	A	203	ASP

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Mol	Chain	Res	Type
1	B	382	LEU
1	C	182	PRO
1	C	301	THR

### 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	167/187 (89%)	161 (96%)	6 (4%)	40	67
1	B	167/187 (89%)	152 (91%)	15 (9%)	11	21
1	C	168/187 (90%)	157 (94%)	11 (6%)	20	37
All	All	502/561 (90%)	470 (94%)	32 (6%)	20	38

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	LYS
1	A	197	PRO
1	A	317	LEU
1	A	332	ASN
1	A	394	ASP
1	A	399	ARG
1	B	189	LEU
1	B	197	PRO
1	B	198	THR
1	B	205	VAL
1	B	230	ASN
1	B	239	SER
1	B	304	MET
1	B	331	THR
1	B	339	ARG
1	B	375	ASP
1	B	382	LEU
1	B	394	ASP
1	B	399	ARG

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Mol	Chain	Res	Type
1	B	405	ARG
1	B	406	ARG
1	C	184	ASN
1	C	187	LYS
1	C	197	PRO
1	C	198	THR
1	C	300	LEU
1	C	317	LEU
1	C	333	ASN
1	C	385	LYS
1	C	394	ASP
1	C	399	ARG
1	C	404	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	ASN
1	A	307	ASN
1	A	332	ASN
1	A	333	ASN
1	A	346	ASN
1	A	370	HIS
1	A	374	GLN
1	B	184	ASN
1	B	230	ASN
1	B	269	ASN
1	B	307	ASN
1	B	346	ASN
1	B	370	HIS
1	C	184	ASN
1	C	190	ASN
1	C	230	ASN
1	C	262	ASN
1	C	269	ASN
1	C	307	ASN
1	C	333	ASN
1	C	370	HIS
1	C	374	GLN
1	C	404	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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$
3	CTP	A	500	2	24,30,30	1.31	3 (12%)	24,47,47	0.91	0
3	CTP	B	1500	2	24,30,30	1.31	3 (12%)	24,47,47	0.89	1 (4%)
3	CTP	C	2500	2	24,30,30	1.29	2 (8%)	24,47,47	0.92	1 (4%)

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
3	CTP	A	500	2	-	0/18/38/38	0/2/2/2
3	CTP	B	1500	2	-	0/18/38/38	0/2/2/2
3	CTP	C	2500	2	-	0/18/38/38	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	CTP	O4'-C1'	2.07	1.44	1.41
3	B	1500	CTP	O4'-C1'	2.17	1.44	1.41
3	B	1500	CTP	C4-N3	2.99	1.40	1.35
3	A	500	CTP	C4-N3	3.03	1.40	1.35
3	C	2500	CTP	C4-N3	3.06	1.40	1.35
3	C	2500	CTP	C6-N1	3.46	1.40	1.35
3	B	1500	CTP	C6-N1	3.61	1.40	1.35
3	A	500	CTP	C6-N1	3.70	1.40	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1500	CTP	N4-C4-N3	2.02	120.03	116.64
3	C	2500	CTP	N4-C4-N3	2.27	120.46	116.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	CTP	1	0
3	B	1500	CTP	5	0
3	C	2500	CTP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	202/226 (89%)	0.44	22 (10%) <b>6</b> <b>6</b>	43, 71, 115, 125	0
1	B	203/226 (89%)	0.03	7 (3%) 46 48	36, 58, 96, 119	0
1	C	204/226 (90%)	0.54	30 (14%) <b>3</b> <b>2</b>	44, 74, 120, 128	0
All	All	609/678 (89%)	0.34	59 (9%) <b>8</b> <b>8</b>	36, 67, 116, 128	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	406	ARG	7.7
1	C	181	SER	7.6
1	A	382	LEU	6.9
1	C	183	VAL	6.0
1	B	181	SER	5.8
1	C	285	VAL	5.5
1	C	286	ALA	5.5
1	C	382	LEU	5.3
1	C	182	PRO	5.3
1	C	367	ASN	5.3
1	A	386	GLU	5.3
1	A	385	LYS	5.2
1	C	287	PRO	5.1
1	A	383	GLU	4.8
1	A	288	GLU	4.2
1	A	355	VAL	4.2
1	C	298	ASP	4.1
1	C	337	TYR	4.1
1	C	405	ARG	4.1
1	A	298	ASP	3.9
1	C	288	GLU	3.9
1	A	354	ASP	3.6
1	C	354	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	287	PRO	3.5
1	B	182	PRO	3.5
1	C	385	LYS	3.4
1	A	325	VAL	3.4
1	C	284	THR	3.3
1	C	303	LYS	3.2
1	C	245	PHE	3.1
1	C	386	GLU	3.1
1	A	183	VAL	3.1
1	C	336	GLU	3.0
1	C	331	THR	3.0
1	A	286	ALA	2.8
1	B	382	LEU	2.7
1	B	319	ASP	2.7
1	C	333	ASN	2.6
1	C	383	GLU	2.6
1	C	193	ILE	2.5
1	C	353	ASN	2.5
1	A	331	THR	2.5
1	A	336	GLU	2.4
1	B	375	ASP	2.4
1	A	329	ALA	2.3
1	A	384	ARG	2.3
1	A	349	LEU	2.3
1	C	372	PHE	2.3
1	A	335	GLU	2.3
1	A	404	ASN	2.2
1	C	299	GLU	2.2
1	A	226	ARG	2.2
1	A	289	LYS	2.2
1	C	384	ARG	2.2
1	A	318	LYS	2.2
1	B	272	ILE	2.1
1	C	272	ILE	2.1
1	C	211	HIS	2.1
1	C	233	LEU	2.1

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

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	CTP	C	2500	29/29	0.92	0.14	-0.40	55,64,90,96	0
3	CTP	B	1500	29/29	0.96	0.11	-0.91	43,56,104,107	0
3	CTP	A	500	29/29	0.98	0.09	-1.18	47,57,74,80	0
2	CA	B	1501	1/1	0.85	0.06	-	83,83,83,83	0
2	CA	C	2501	1/1	0.82	0.05	-	78,78,78,78	0
2	CA	A	501	1/1	0.96	0.03	-	67,67,67,67	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.