



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:15 PM UTC

PDB ID : 6ICO / pdb_00006ico
Title : Pseudomonas putida CBB5 NdmA with theophylline
Authors : Kim, J.H.; Kim, B.H.; Kang, S.Y.; Song, H.K.
Deposited on : 2018-09-06
Resolution : 1.85 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
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

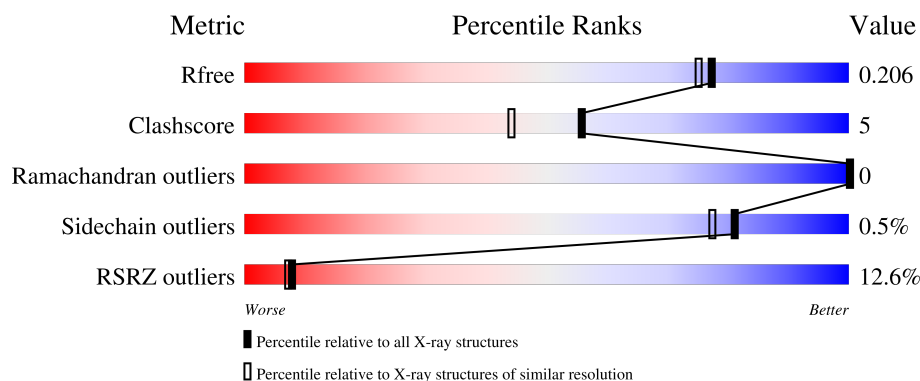
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	369	13% 85% 8% 7%
1	B	369	12% 86% 7% 7%
1	C	369	10% 85% 8% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TEP	B	402	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9621 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 Methylxanthine N1-demethylase NdmA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2782	1771	476	522	13			
1	B	344	Total	C	N	O	S	0	0	0
			2782	1771	476	522	13			
1	C	344	Total	C	N	O	S	0	0	0
			2782	1771	476	522	13			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP H9N289
A	-16	GLY	-	expression tag	UNP H9N289
A	-15	SER	-	expression tag	UNP H9N289
A	-14	SER	-	expression tag	UNP H9N289
A	-13	HIS	-	expression tag	UNP H9N289
A	-12	HIS	-	expression tag	UNP H9N289
A	-11	HIS	-	expression tag	UNP H9N289
A	-10	HIS	-	expression tag	UNP H9N289
A	-9	HIS	-	expression tag	UNP H9N289
A	-8	HIS	-	expression tag	UNP H9N289
A	-7	GLU	-	expression tag	UNP H9N289
A	-6	ASN	-	expression tag	UNP H9N289
A	-5	LEU	-	expression tag	UNP H9N289
A	-4	TYR	-	expression tag	UNP H9N289
A	-3	PHE	-	expression tag	UNP H9N289
A	-2	GLN	-	expression tag	UNP H9N289
A	-1	GLY	-	expression tag	UNP H9N289
A	0	SER	-	expression tag	UNP H9N289
B	-17	MET	-	expression tag	UNP H9N289
B	-16	GLY	-	expression tag	UNP H9N289
B	-15	SER	-	expression tag	UNP H9N289
B	-14	SER	-	expression tag	UNP H9N289
B	-13	HIS	-	expression tag	UNP H9N289

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP H9N289
B	-11	HIS	-	expression tag	UNP H9N289
B	-10	HIS	-	expression tag	UNP H9N289
B	-9	HIS	-	expression tag	UNP H9N289
B	-8	HIS	-	expression tag	UNP H9N289
B	-7	GLU	-	expression tag	UNP H9N289
B	-6	ASN	-	expression tag	UNP H9N289
B	-5	LEU	-	expression tag	UNP H9N289
B	-4	TYR	-	expression tag	UNP H9N289
B	-3	PHE	-	expression tag	UNP H9N289
B	-2	GLN	-	expression tag	UNP H9N289
B	-1	GLY	-	expression tag	UNP H9N289
B	0	SER	-	expression tag	UNP H9N289
C	-17	MET	-	expression tag	UNP H9N289
C	-16	GLY	-	expression tag	UNP H9N289
C	-15	SER	-	expression tag	UNP H9N289
C	-14	SER	-	expression tag	UNP H9N289
C	-13	HIS	-	expression tag	UNP H9N289
C	-12	HIS	-	expression tag	UNP H9N289
C	-11	HIS	-	expression tag	UNP H9N289
C	-10	HIS	-	expression tag	UNP H9N289
C	-9	HIS	-	expression tag	UNP H9N289
C	-8	HIS	-	expression tag	UNP H9N289
C	-7	GLU	-	expression tag	UNP H9N289
C	-6	ASN	-	expression tag	UNP H9N289
C	-5	LEU	-	expression tag	UNP H9N289
C	-4	TYR	-	expression tag	UNP H9N289
C	-3	PHE	-	expression tag	UNP H9N289
C	-2	GLN	-	expression tag	UNP H9N289
C	-1	GLY	-	expression tag	UNP H9N289
C	0	SER	-	expression tag	UNP H9N289

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

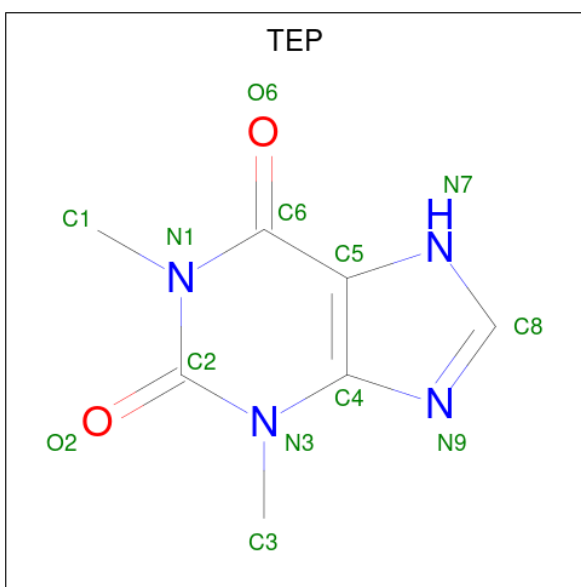


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	C	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Co	0	0
			1	1		
3	B	1	Total	Co	0	0
			1	1		
3	C	1	Total	Co	0	0
			1	1		

- Molecule 4 is THEOPHYLLINE (CCD ID: TEP) (formula: C₇H₈N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			13	7	4	2		
4	B	1	Total	C	N	O	0	0
			13	7	4	2		
4	C	1	Total	C	N	O	0	0
			13	7	4	2		

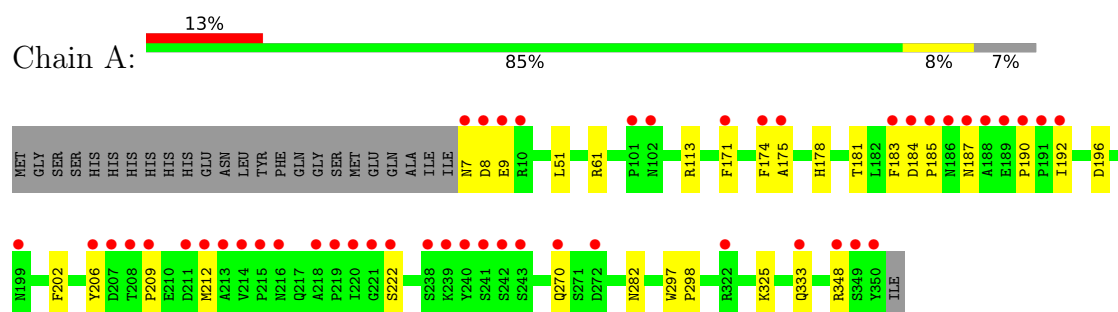
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	397	Total	O	0	0
			397	397		
5	B	404	Total	O	0	0
			404	404		
5	C	420	Total	O	0	0
			420	420		

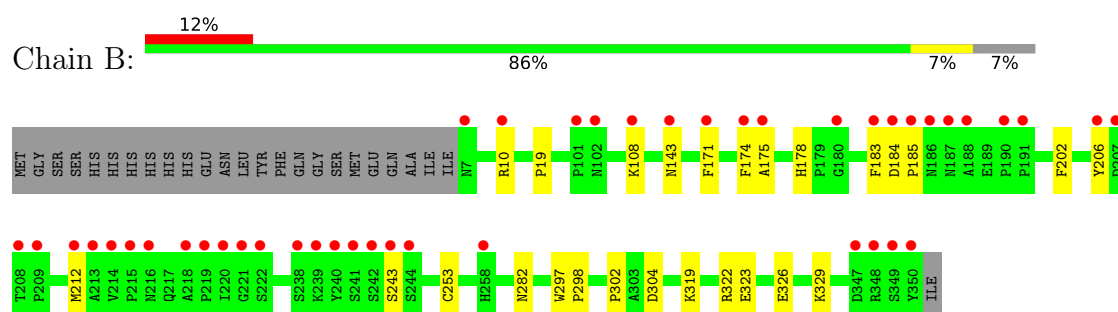
3 Residue-property plots [i](#)

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.

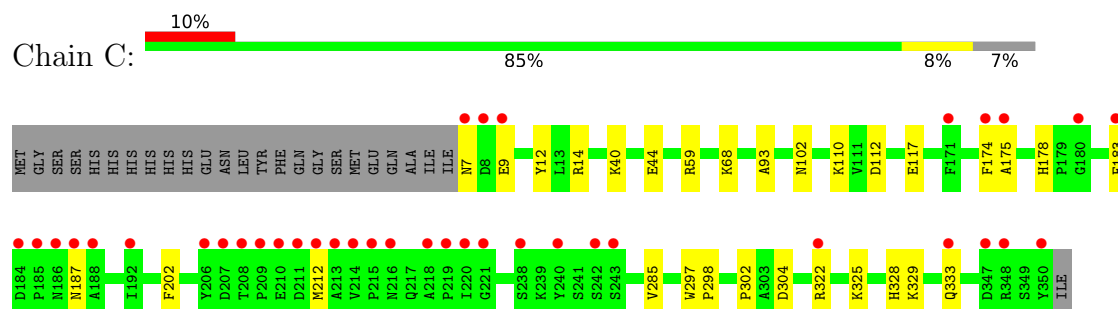
• Molecule 1: Methylxanthine N1-demethylase NdmA



• Molecule 1: Methylxanthine N1-demethylase NdmA



• Molecule 1: Methylxanthine N1-demethylase NdmA



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.88Å 135.88Å 155.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.04 – 1.85 38.04 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.7 (38.04-1.85) 97.4 (38.04-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.35 (at 1.84Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.174 , 0.203 0.181 , 0.206	Depositor DCC
R_{free} test set	2012 reflections (1.41%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9621	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: TEP, CO, FES

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	0.35	0/2867	0.55	0/3907
1	B	0.35	0/2867	0.54	0/3907
1	C	0.34	0/2867	0.54	0/3907
All	All	0.35	0/8601	0.55	0/11721

There are no bond length outliers.

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	2782	0	2640	32	0
1	B	2782	0	2640	21	0
1	C	2782	0	2640	25	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	13	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	13	0	8	1	0
4	C	13	0	8	0	0
5	A	397	0	0	10	2
5	B	404	0	0	7	3
5	C	420	0	0	16	1
All	All	9621	0	7944	76	3

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 5.

All (76) 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:C:329:LYS:NZ	5:C:501:HOH:O	1.77	1.14
1:B:322:ARG:NH1	5:B:501:HOH:O	1.85	1.10
1:A:348:ARG:NH1	5:A:501:HOH:O	2.08	0.87
1:C:110:LYS:NZ	5:C:506:HOH:O	2.07	0.85
1:C:117:GLU:OE2	5:C:502:HOH:O	1.96	0.82
1:B:212:MET:SD	5:B:785:HOH:O	2.40	0.79
1:A:187:ASN:ND2	1:A:209:PRO:HG2	1.99	0.77
1:A:348:ARG:NH1	5:A:504:HOH:O	2.17	0.76
1:C:175:ALA:O	5:C:504:HOH:O	2.06	0.73
1:C:333:GLN:OE1	5:C:505:HOH:O	2.06	0.72
1:B:322:ARG:NH2	5:B:503:HOH:O	2.22	0.72
1:C:7:ASN:N	5:C:508:HOH:O	2.23	0.70
1:C:328:HIS:ND1	5:C:501:HOH:O	2.23	0.70
1:A:174:PHE:HB3	1:A:183:PHE:HB2	1.73	0.70
1:A:333:GLN:H	1:A:333:GLN:CD	2.01	0.69
1:A:9:GLU:HB3	1:A:325:LYS:HZ1	1.59	0.67
1:C:212:MET:SD	5:C:514:HOH:O	2.54	0.65
1:C:68:LYS:NZ	5:C:513:HOH:O	2.30	0.64
1:C:187:ASN:ND2	5:C:514:HOH:O	2.31	0.64
1:C:14:ARG:NH1	1:C:44:GLU:OE1	2.26	0.63
1:C:9:GLU:HG2	1:C:325:LYS:HD3	1.81	0.62
1:C:40:LYS:NZ	5:C:509:HOH:O	2.25	0.61
1:A:348:ARG:NH2	5:A:505:HOH:O	2.19	0.61
1:B:143:ASN:ND2	5:B:504:HOH:O	2.33	0.61
1:A:9:GLU:H	1:A:9:GLU:CD	2.09	0.61
1:B:323:GLU:HG3	5:B:501:HOH:O	2.01	0.60
1:B:174:PHE:HB3	1:B:183:PHE:HB2	1.82	0.60
1:A:7:ASN:CG	1:A:8:ASP:H	2.10	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:SER:O	5:B:502:HOH:O	2.15	0.59
1:A:222:SER:OG	5:A:503:HOH:O	2.17	0.59
1:A:270:GLN:OE1	5:A:502:HOH:O	2.16	0.58
1:B:326:GLU:OE1	1:B:329:LYS:NZ	2.37	0.58
1:A:196:ASP:OD2	5:A:501:HOH:O	2.17	0.57
1:A:171:PHE:CE1	1:A:190:PRO:HB2	2.41	0.55
1:C:102:ASN:OD1	5:C:507:HOH:O	2.18	0.55
1:B:171:PHE:CE2	1:B:206:TYR:CZ	2.96	0.54
1:C:174:PHE:HB3	1:C:183:PHE:HB2	1.91	0.52
1:A:270:GLN:NE2	5:A:512:HOH:O	2.41	0.52
1:A:61:ARG:HD2	1:B:297:TRP:O	2.10	0.52
1:C:302:PRO:HG2	1:C:304:ASP:OD1	2.10	0.51
1:A:9:GLU:CB	1:A:325:LYS:HZ1	2.24	0.51
1:A:282:ASN:OD1	4:A:402:TEP:H8	2.12	0.50
1:A:61:ARG:NH2	1:B:304:ASP:OD2	2.41	0.49
1:A:171:PHE:CE2	1:A:206:TYR:CZ	3.00	0.49
1:A:9:GLU:HB3	1:A:325:LYS:NZ	2.28	0.48
1:A:171:PHE:HE2	1:A:206:TYR:CZ	2.31	0.48
1:B:297:TRP:HA	1:B:298:PRO:C	2.39	0.48
1:C:14:ARG:NH2	5:C:511:HOH:O	2.28	0.48
1:B:175:ALA:HB1	1:B:185:PRO:HA	1.96	0.47
1:C:93:ALA:HA	1:C:110:LYS:HG2	1.96	0.47
1:B:108:LYS:H	1:B:108:LYS:HD2	1.78	0.47
1:A:184:ASP:HB2	5:A:654:HOH:O	2.16	0.46
1:A:9:GLU:OE2	1:A:9:GLU:N	2.32	0.46
1:C:322:ARG:NH2	5:C:524:HOH:O	2.49	0.45
1:C:59:ARG:NH2	1:C:112:ASP:OD2	2.46	0.45
1:A:192:ILE:HD11	5:A:882:HOH:O	2.16	0.45
1:A:192:ILE:HA	5:A:644:HOH:O	2.15	0.45
1:B:184:ASP:OD2	1:B:212:MET:HG2	2.17	0.45
1:A:297:TRP:HA	1:A:298:PRO:C	2.42	0.44
1:A:7:ASN:CG	1:A:8:ASP:N	2.74	0.44
1:B:298:PRO:HG2	1:B:302:PRO:HG3	1.99	0.44
1:A:171:PHE:CE1	1:A:190:PRO:CB	3.01	0.44
1:B:174:PHE:HD1	1:B:178:HIS:HD2	1.67	0.43
1:C:14:ARG:NE	5:C:511:HOH:O	2.38	0.43
1:A:175:ALA:HB1	1:A:185:PRO:HA	2.01	0.43
1:B:282:ASN:OD1	4:B:402:TEP:H8	2.18	0.42
1:C:297:TRP:HA	1:C:298:PRO:C	2.45	0.42
1:B:319:LYS:NZ	5:B:520:HOH:O	2.50	0.42
1:A:183:PHE:CD1	1:A:212:MET:HE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:LYS:HE2	1:C:325:LYS:HB2	1.74	0.41
1:B:10:ARG:HD3	1:B:10:ARG:HA	1.85	0.41
1:A:9:GLU:HA	1:A:325:LYS:NZ	2.35	0.41
1:A:178:HIS:HB3	1:A:181:THR:OG1	2.21	0.40
1:C:12:TYR:HB3	5:C:501:HOH:O	2.19	0.40
1:C:178:HIS:CE1	1:C:285:VAL:HG13	2.56	0.40
1:B:19:PRO:O	1:B:253:CYS:HB2	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:685:HOH:O	5:B:784:HOH:O[5_556]	2.09	0.11
5:B:759:HOH:O	5:C:829:HOH:O[3_665]	2.17	0.03
5:A:866:HOH:O	5:B:902:HOH:O[5_556]	2.18	0.02

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	342/369 (93%)	332 (97%)	10 (3%)	0	100	100
1	B	342/369 (93%)	332 (97%)	10 (3%)	0	100	100
1	C	342/369 (93%)	333 (97%)	9 (3%)	0	100	100
All	All	1026/1107 (93%)	997 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	306/328 (93%)	303 (99%)	3 (1%)	68	60
1	B	306/328 (93%)	305 (100%)	1 (0%)	86	85
1	C	306/328 (93%)	305 (100%)	1 (0%)	86	85
All	All	918/984 (93%)	913 (100%)	5 (0%)	81	77

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	113	ARG
1	A	202	PHE
1	B	202	PHE
1	C	202	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	187	ASN
1	A	250	ASN
1	A	316	GLN
1	B	45	GLN
1	B	216	ASN
1	B	250	ASN
1	B	316	GLN
1	C	45	GLN
1	C	91	HIS
1	C	186	ASN
1	C	258	HIS

5.3.3 RNA ⓘ

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 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FES	B	400	1	0,4,4	-	-	-		
4	TEP	B	402	-	14,14,14	1.44	3 (21%)	21,21,21	3.12	12 (57%)
2	FES	C	400	1	0,4,4	-	-	-		
4	TEP	C	402	-	14,14,14	1.60	3 (21%)	21,21,21	3.10	11 (52%)
2	FES	A	400	1	0,4,4	-	-	-		
4	TEP	A	402	-	14,14,14	1.51	3 (21%)	21,21,21	3.20	9 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FES	B	400	1	-	-	0/1/1/1
4	TEP	B	402	-	-	-	0/2/2/2
2	FES	C	400	1	-	-	0/1/1/1
4	TEP	C	402	-	-	-	0/2/2/2
2	FES	A	400	1	-	-	0/1/1/1
4	TEP	A	402	-	-	-	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402	TEP	C6-N1	-3.48	1.33	1.40
4	A	402	TEP	C6-N1	-3.10	1.34	1.40
4	B	402	TEP	C6-N1	-2.92	1.34	1.40
4	C	402	TEP	C5-N7	-2.21	1.34	1.38
4	B	402	TEP	C5-C6	-2.17	1.38	1.42
4	A	402	TEP	C5-C6	-2.16	1.38	1.42
4	C	402	TEP	C5-C6	-2.10	1.38	1.42
4	B	402	TEP	C5-N7	-2.10	1.35	1.38
4	A	402	TEP	C5-N7	-2.08	1.35	1.38

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	402	TEP	C4-C5-N7	7.04	108.75	105.29
4	B	402	TEP	C4-C5-N7	6.59	108.53	105.29
4	A	402	TEP	C4-C5-N7	6.58	108.52	105.29
4	A	402	TEP	C8-N9-C4	6.05	107.50	103.45
4	C	402	TEP	C5-C6-N1	5.60	119.58	112.07
4	B	402	TEP	C8-N9-C4	5.55	107.17	103.45
4	A	402	TEP	C5-C6-N1	5.42	119.35	112.07
4	A	402	TEP	C5-C4-N9	-5.39	107.85	111.63
4	B	402	TEP	C5-C6-N1	5.32	119.21	112.07
4	C	402	TEP	C8-N9-C4	4.91	106.74	103.45
4	B	402	TEP	C5-C4-N9	-4.83	108.24	111.63
4	C	402	TEP	C5-C4-N9	-4.57	108.43	111.63
4	C	402	TEP	C6-C5-C4	-4.26	119.77	123.13
4	A	402	TEP	C6-C5-C4	-4.19	119.82	123.13
4	B	402	TEP	O6-C6-C5	-3.71	119.07	126.64
4	B	402	TEP	C6-C5-C4	-3.64	120.26	123.13
4	A	402	TEP	O6-C6-C5	-3.44	119.62	126.64
4	A	402	TEP	N3-C4-N9	3.35	131.54	126.27
4	C	402	TEP	O6-C6-C5	-3.30	119.91	126.64
4	A	402	TEP	N7-C8-N9	-3.30	109.15	112.98
4	C	402	TEP	N3-C4-N9	3.26	131.39	126.27
4	B	402	TEP	N3-C4-N9	3.24	131.36	126.27
4	B	402	TEP	C6-N1-C2	-3.12	120.58	125.66
4	B	402	TEP	N7-C8-N9	-3.09	109.40	112.98
4	C	402	TEP	C6-N1-C2	-2.99	120.79	125.66
4	A	402	TEP	C6-N1-C2	-2.99	120.80	125.66
4	C	402	TEP	N7-C8-N9	-2.97	109.54	112.98
4	C	402	TEP	C5-C4-N3	-2.78	120.16	121.73
4	B	402	TEP	C5-C4-N3	-2.37	120.39	121.73
4	B	402	TEP	N3-C2-N1	2.17	119.85	117.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	402	TEP	N3-C2-N1	2.03	119.67	117.14
4	B	402	TEP	C3-N3-C2	2.01	120.84	117.33

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
4	B	402	TEP	1	0
4	A	402	TEP	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, 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	344/369 (93%)	0.42	48 (13%) 6 6	17, 25, 56, 67	0
1	B	344/369 (93%)	0.32	44 (12%) 7 7	17, 24, 53, 63	0
1	C	344/369 (93%)	0.28	38 (11%) 10 10	17, 25, 51, 63	0
All	All	1032/1107 (93%)	0.34	130 (12%) 8 7	17, 25, 53, 67	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	TYR	8.5
1	A	171	PHE	7.5
1	B	206	TYR	6.9
1	A	350	TYR	6.5
1	A	187	ASN	6.5
1	B	171	PHE	6.4
1	A	208	THR	6.1
1	A	185	PRO	5.9
1	B	220	ILE	5.3
1	B	208	THR	5.3
1	A	221	GLY	5.2
1	B	183	PHE	5.2
1	A	186	ASN	5.2
1	C	213	ALA	5.2
1	B	240	TYR	5.0
1	C	206	TYR	5.0
1	C	171	PHE	4.9
1	A	240	TYR	4.8
1	A	183	PHE	4.7
1	A	209	PRO	4.7
1	B	185	PRO	4.7
1	C	221	GLY	4.7
1	C	185	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	209	PRO	4.6
1	A	188	ALA	4.5
1	B	143	ASN	4.5
1	C	183	PHE	4.5
1	A	7	ASN	4.4
1	B	221	GLY	4.3
1	A	213	ALA	4.3
1	A	242	SER	4.2
1	A	215	PRO	4.2
1	A	207	ASP	4.1
1	C	240	TYR	4.0
1	C	350	TYR	4.0
1	B	188	ALA	3.9
1	A	191	PRO	3.8
1	C	184	ASP	3.8
1	B	350	TYR	3.8
1	A	214	VAL	3.8
1	C	186	ASN	3.7
1	C	220	ILE	3.7
1	C	214	VAL	3.7
1	A	218	ALA	3.6
1	B	174	PHE	3.6
1	A	101	PRO	3.6
1	B	242	SER	3.6
1	A	190	PRO	3.5
1	B	219	PRO	3.4
1	A	216	ASN	3.4
1	C	208	THR	3.4
1	B	348	ARG	3.4
1	B	215	PRO	3.4
1	A	241	SER	3.3
1	A	211	ASP	3.2
1	B	213	ALA	3.2
1	B	7	ASN	3.2
1	A	192	ILE	3.2
1	B	186	ASN	3.2
1	C	187	ASN	3.2
1	C	209	PRO	3.1
1	C	215	PRO	3.1
1	C	219	PRO	3.1
1	A	333	GLN	3.1
1	C	192	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	187	ASN	3.0
1	B	184	ASP	3.0
1	C	7	ASN	3.0
1	A	174	PHE	3.0
1	B	239	LYS	3.0
1	B	241	SER	2.9
1	C	211	ASP	2.9
1	B	214	VAL	2.9
1	C	174	PHE	2.9
1	A	220	ILE	2.9
1	B	218	ALA	2.9
1	C	188	ALA	2.9
1	A	348	ARG	2.9
1	A	222	SER	2.8
1	B	212	MET	2.8
1	A	349	SER	2.8
1	B	243	SER	2.8
1	B	216	ASN	2.8
1	A	8	ASP	2.7
1	C	218	ALA	2.7
1	B	190	PRO	2.7
1	A	189	GLU	2.6
1	C	238	SER	2.6
1	C	242	SER	2.6
1	C	216	ASN	2.6
1	B	191	PRO	2.6
1	A	184	ASP	2.5
1	A	243	SER	2.5
1	A	238	SER	2.5
1	C	210	GLU	2.5
1	A	219	PRO	2.5
1	C	243	SER	2.5
1	C	9	GLU	2.5
1	B	10	ARG	2.4
1	A	175	ALA	2.4
1	A	10	ARG	2.4
1	B	102	ASN	2.4
1	B	222	SER	2.4
1	B	238	SER	2.4
1	A	322	ARG	2.4
1	A	272	ASP	2.3
1	B	244	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	349	SER	2.3
1	B	207	ASP	2.3
1	B	258	HIS	2.3
1	C	212	MET	2.3
1	C	180	GLY	2.3
1	A	102	ASN	2.3
1	A	212	MET	2.2
1	C	207	ASP	2.2
1	B	175	ALA	2.2
1	B	347	ASP	2.2
1	C	8	ASP	2.2
1	B	101	PRO	2.2
1	C	348	ARG	2.2
1	A	9	GLU	2.1
1	A	199	ASN	2.1
1	C	333	GLN	2.1
1	B	180	GLY	2.1
1	A	270	GLN	2.1
1	B	108	LYS	2.0
1	C	175	ALA	2.0
1	C	322	ARG	2.0
1	C	347	ASP	2.0
1	A	239	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	TEP	B	402	13/13	0.84	0.13	29,34,36,36	0
4	TEP	A	402	13/13	0.87	0.12	30,35,39,39	0
4	TEP	C	402	13/13	0.87	0.12	31,34,36,36	0
3	CO	A	401	1/1	0.99	0.02	23,23,23,23	0
3	CO	B	401	1/1	0.99	0.02	22,22,22,22	0
3	CO	C	401	1/1	0.99	0.02	23,23,23,23	0
2	FES	A	400	4/4	1.00	0.03	18,18,19,19	0
2	FES	B	400	4/4	1.00	0.02	18,19,19,19	0
2	FES	C	400	4/4	1.00	0.02	18,18,19,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.