Full wwPDB X-ray Structure Validation Report (i)

Mar 18, 2024 – 12:52 PM JST

PDB ID	:	6ICQ
Title	:	Pseudomonas putida CBB5 NdmA QL mutant with theobromine
Authors	:	Kim, J.H.; Kim, B.H.; Kang, S.Y.; Song, H.K.
Deposited on	:	2018-09-06
Resolution	:	1.90 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 (i) 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 (1)) were used in the production of this report:

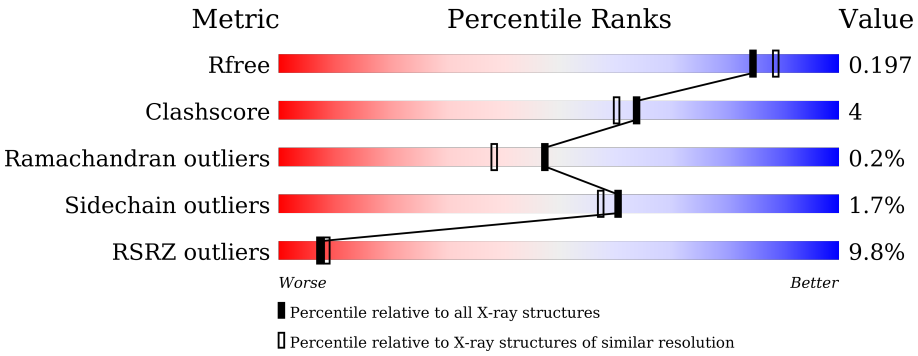
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	9% 84% 6% 9%
1	B	369	9% 81% 9% 10%
1	C	369	9% 83% 8% 9%

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	37T	A	402	-	X	-	-
4	37T	B	402	-	X	-	-
4	37T	C	402	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8997 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	334	Total	C	N	O	S	0	0	0
			2705	1724	464	505	12			
1	B	333	Total	C	N	O	S	0	0	0
			2700	1721	463	504	12			
1	C	334	Total	C	N	O	S	0	0	0
			2707	1725	464	506	12			

There are 60 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
A	282	GLN	ASN	engineered mutation	UNP H9N289
A	286	LEU	PHE	engineered mutation	UNP H9N289
B	-17	MET	-	expression tag	UNP H9N289
B	-16	GLY	-	expression tag	UNP H9N289
B	-15	SER	-	expression tag	UNP H9N289

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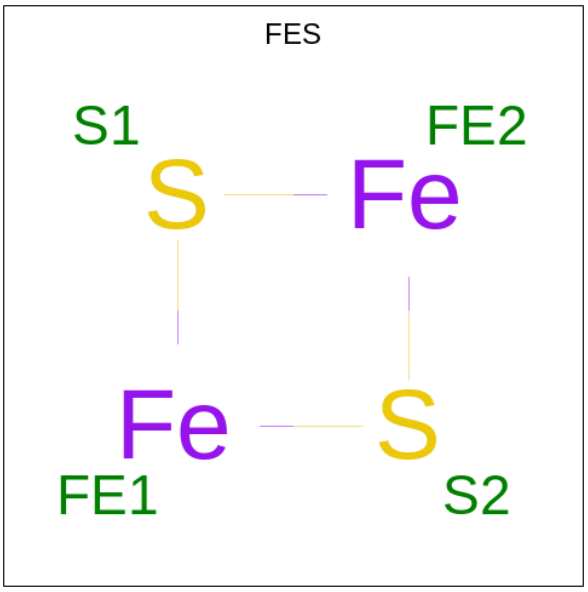
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	SER	-	expression tag	UNP H9N289
B	-13	HIS	-	expression tag	UNP H9N289
B	-12	HIS	-	expression tag	UNP H9N289
B	-11	HIS	-	expression tag	UNP H9N289
B	-10	HIS	-	expression tag	UNP H9N289
B	-9	HIS	-	expression tag	UNP H9N289
B	-8	HIS	-	expression tag	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
B	282	GLN	ASN	engineered mutation	UNP H9N289
B	286	LEU	PHE	engineered mutation	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
C	282	GLN	ASN	engineered mutation	UNP H9N289
C	286	LEU	PHE	engineered mutation	UNP H9N289

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

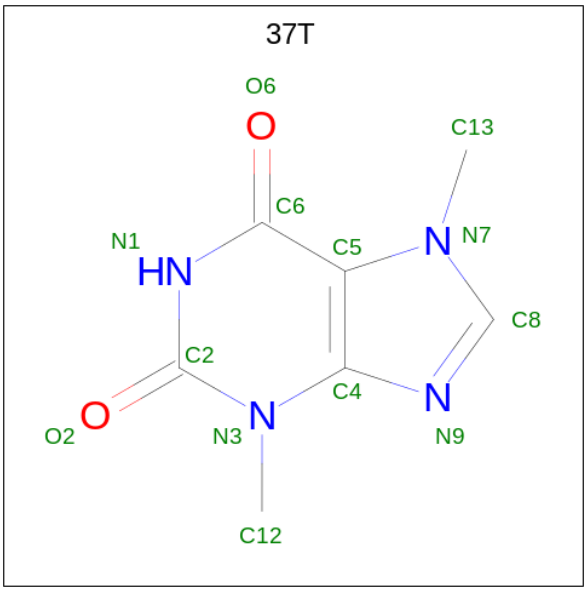


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 4 2 2	0	0
2	B	1	Total Fe S 4 2 2	0	0
2	C	1	Total Fe S 4 2 2	0	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 4 is THEOBROMINE (three-letter code: 37T) (formula: $C_7H_8N_4O_2$).



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

- Molecule 5 is water.

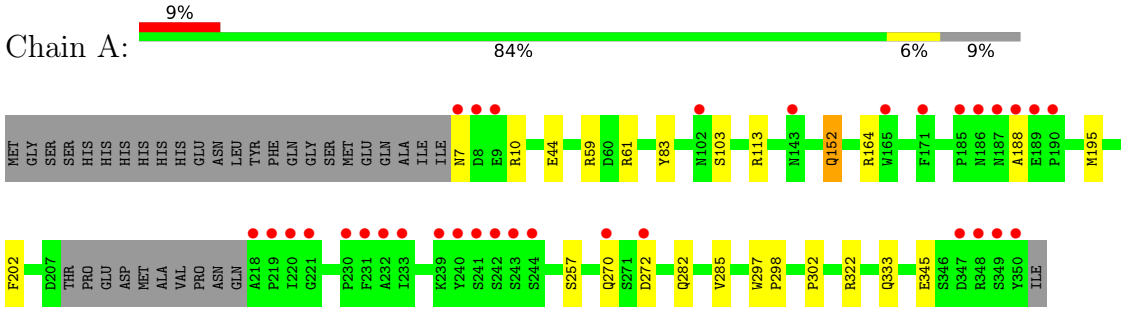
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	287	Total O 287 287	0	0
5	B	279	Total O 279 279	0	0
5	C	265	Total O 265 265	0	0

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.

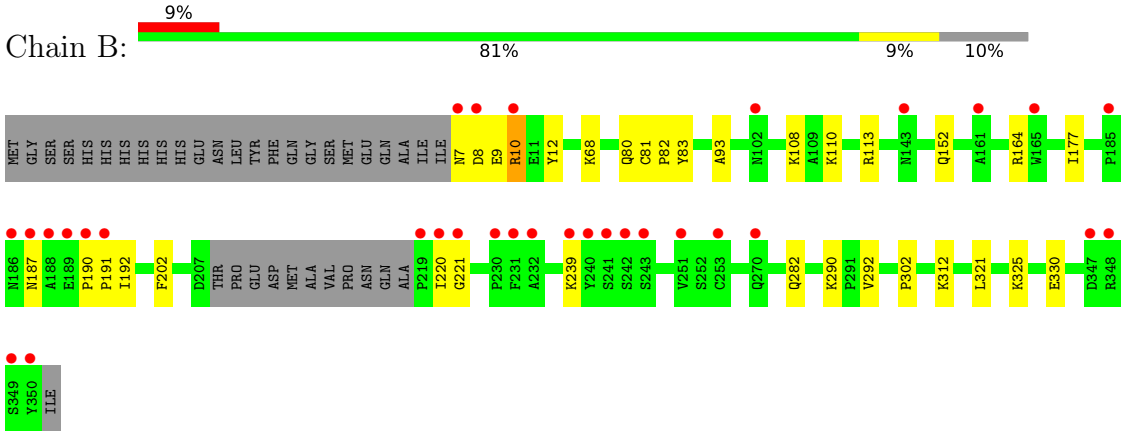
• Molecule 1: Methylxanthine N1-demethylase NdmA

Chain A:



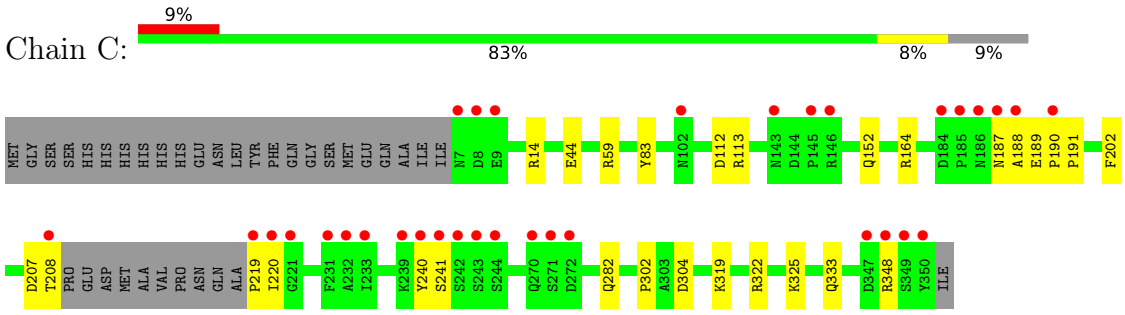
• Molecule 1: Methylxanthine N1-demethylase NdmA

Chain B:



• Molecule 1: Methylxanthine N1-demethylase NdmA

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	135.95Å 135.95Å 155.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.04 – 1.90 35.04 – 1.89	Depositor EDS
% Data completeness (in resolution range)	98.9 (35.04-1.90) 98.9 (35.04-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 1.89Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.170 , 0.196 0.169 , 0.197	Depositor DCC
R_{free} test set	2000 reflections (1.53%)	wwPDB-VP
Wilson B-factor (Å^2)	30.3	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8997	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, 37T, 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	0.43	0/2786	0.56	0/3793
1	B	0.44	0/2781	0.59	0/3785
1	C	0.45	0/2788	0.60	0/3795
All	All	0.44	0/8355	0.58	0/11373

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

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	2705	0	2575	15	0
1	B	2700	0	2571	31	0
1	C	2707	0	2578	22	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	0	0
4	C	13	0	8	2	0
5	A	287	0	0	4	0
5	B	279	0	0	5	0
5	C	265	0	0	4	0
All	All	8997	0	7748	67	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 4.

All (67) 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:108:LYS:NZ	5:B:501:HOH:O	1.82	1.12
1:B:68:LYS:NZ	5:B:502:HOH:O	1.91	1.03
1:A:322:ARG:NH2	5:A:501:HOH:O	2.07	0.87
1:B:152:GLN:NE2	1:B:282:GLN:OE1	2.12	0.81
1:B:220:ILE:HB	1:B:239:LYS:HZ3	1.52	0.74
1:B:7:ASN:N	1:B:9:GLU:OE2	2.21	0.73
1:C:333:GLN:O	5:C:501:HOH:O	2.06	0.73
1:A:270:GLN:OE1	1:A:272:ASP:OD1	2.08	0.72
1:C:348:ARG:HG2	1:C:348:ARG:HH11	1.53	0.72
1:B:220:ILE:C	1:B:239:LYS:HZ1	1.93	0.72
1:B:220:ILE:HD12	1:B:239:LYS:NZ	2.04	0.71
1:C:59:ARG:NH2	1:C:112:ASP:OD2	2.23	0.71
1:A:10:ARG:NH2	1:A:257:SER:HA	2.06	0.70
1:B:220:ILE:HB	1:B:239:LYS:NZ	2.11	0.64
1:B:220:ILE:HD12	1:B:239:LYS:HZ3	1.62	0.63
1:B:220:ILE:HG13	1:B:221:GLY:N	2.16	0.60
1:C:348:ARG:HG2	1:C:348:ARG:NH1	2.17	0.59
1:C:14:ARG:NH1	1:C:44:GLU:OE1	2.22	0.59
1:B:12:TYR:CE1	1:B:325:LYS:HG2	2.37	0.58
1:A:152:GLN:OE1	1:A:282:GLN:NE2	2.34	0.58
1:A:103:SER:OG	5:A:502:HOH:O	2.16	0.57
1:C:208:THR:HB	1:C:220:ILE:HG13	1.85	0.57
1:A:10:ARG:HH22	1:A:257:SER:HA	1.71	0.55
1:A:7:ASN:ND2	5:A:507:HOH:O	2.41	0.53
1:C:322:ARG:NH1	5:C:502:HOH:O	2.24	0.53
1:B:80:GLN:NE2	5:B:508:HOH:O	2.40	0.53
1:C:152:GLN:OE1	1:C:282:GLN:NE2	2.39	0.53
1:B:321:LEU:O	1:B:325:LYS:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:GLN:H	1:A:333:GLN:CD	2.14	0.52
1:C:207:ASP:HB3	1:C:219:PRO:HB3	1.92	0.52
1:B:9:GLU:HG2	1:B:10:ARG:HD3	1.92	0.51
1:C:220:ILE:HA	1:C:240:TYR:CZ	2.45	0.50
1:B:220:ILE:CB	1:B:239:LYS:NZ	2.75	0.50
1:C:282:GLN:CG	4:C:402:37T:H8	2.43	0.48
1:C:325:LYS:NZ	5:C:511:HOH:O	2.47	0.47
1:A:44:GLU:OE1	1:A:59:ARG:NH1	2.39	0.47
1:C:302:PRO:HG2	1:C:304:ASP:OD1	2.15	0.47
1:C:187:ASN:O	1:C:189:GLU:N	2.47	0.46
1:A:61:ARG:NH2	1:B:302:PRO:HG2	2.30	0.46
1:B:220:ILE:C	1:B:239:LYS:NZ	2.65	0.46
1:C:219:PRO:O	1:C:240:TYR:CE2	2.68	0.46
1:B:177:ILE:CD1	1:B:292:VAL:HG21	2.46	0.46
1:B:93:ALA:HA	1:B:110:LYS:HG2	1.97	0.45
1:C:282:GLN:HG3	4:C:402:37T:H8	1.99	0.45
1:A:298:PRO:HG2	1:A:302:PRO:HG3	1.99	0.45
1:B:220:ILE:HG13	1:B:221:GLY:H	1.82	0.44
1:C:319:LYS:HG3	1:C:322:ARG:HH22	1.81	0.44
1:C:220:ILE:HA	1:C:240:TYR:OH	2.18	0.44
1:B:220:ILE:HD12	1:B:239:LYS:HZ2	1.80	0.44
1:B:81:CYS:SG	1:B:82:PRO:HD2	2.58	0.43
1:A:195:MET:O	1:A:345:GLU:HG2	2.17	0.43
1:A:10:ARG:NH2	5:A:515:HOH:O	2.50	0.43
1:B:177:ILE:HD11	1:B:292:VAL:HG21	2.00	0.43
1:C:190:PRO:HA	1:C:191:PRO:HD3	1.85	0.43
1:C:219:PRO:O	1:C:240:TYR:HE2	2.02	0.42
1:B:190:PRO:HA	1:B:191:PRO:HD3	1.90	0.42
1:B:220:ILE:CD1	1:B:239:LYS:NZ	2.78	0.42
1:A:297:TRP:HA	1:A:298:PRO:C	2.39	0.42
1:B:8:ASP:O	1:B:8:ASP:OD1	2.37	0.42
1:B:220:ILE:CD1	1:B:239:LYS:HZ3	2.30	0.42
1:C:240:TYR:O	1:C:241:SER:OG	2.34	0.42
1:C:59:ARG:HG3	5:C:616:HOH:O	2.20	0.42
1:A:285:VAL:HG11	4:A:402:37T:H122	2.02	0.41
1:B:290:LYS:HE2	5:B:741:HOH:O	2.20	0.41
1:B:192:ILE:HG23	1:B:312:LYS:HD2	2.03	0.40
1:B:330:GLU:OE1	5:B:503:HOH:O	2.21	0.40
1:B:220:ILE:CG1	1:B:239:LYS:NZ	2.85	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	330/369 (89%)	320 (97%)	9 (3%)	1 (0%)	41 31
1	B	329/369 (89%)	316 (96%)	13 (4%)	0	100 100
1	C	330/369 (89%)	318 (96%)	11 (3%)	1 (0%)	41 31
All	All	989/1107 (89%)	954 (96%)	33 (3%)	2 (0%)	47 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	ALA
1	C	188	ALA

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	297/328 (90%)	292 (98%)	5 (2%)	60 57
1	B	297/328 (90%)	291 (98%)	6 (2%)	55 51
1	C	298/328 (91%)	294 (99%)	4 (1%)	69 68
All	All	892/984 (91%)	877 (98%)	15 (2%)	60 57

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	TYR

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Mol	Chain	Res	Type
1	A	113	ARG
1	A	152	GLN
1	A	164	ARG
1	A	202	PHE
1	B	10	ARG
1	B	83	TYR
1	B	113	ARG
1	B	164	ARG
1	B	187	ASN
1	B	202	PHE
1	C	83	TYR
1	C	113	ARG
1	C	164	ARG
1	C	202	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	ASN
1	B	80	GLN
1	B	102	ASN
1	B	143	ASN
1	B	152	GLN
1	B	187	ASN
1	B	282	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 monosaccharides 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	$\#\|Z\| > 2$
4	37T	A	402	-	14,14,14	3.98	10 (71%)	21,21,21	2.31	7 (33%)
4	37T	B	402	-	14,14,14	3.72	11 (78%)	21,21,21	2.61	8 (38%)
4	37T	C	402	-	14,14,14	3.75	10 (71%)	21,21,21	2.40	6 (28%)
2	FES	A	400	1	0,4,4	-	-	-		
2	FES	C	400	1	0,4,4	-	-	-		
2	FES	B	400	1	0,4,4	-	-	-		

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
4	37T	A	402	-	-	-	0/2/2/2
4	37T	B	402	-	-	-	0/2/2/2
4	37T	C	402	-	-	-	0/2/2/2
2	FES	A	400	1	-	-	0/1/1/1
2	FES	C	400	1	-	-	0/1/1/1
2	FES	B	400	1	-	-	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	402	37T	C2-N1	6.73	1.50	1.38
4	C	402	37T	C2-N1	6.01	1.48	1.38
4	A	402	37T	C5-N7	5.91	1.48	1.38
4	B	402	37T	C2-N1	5.66	1.48	1.38
4	C	402	37T	C5-N7	5.49	1.47	1.38
4	C	402	37T	C8-N7	5.37	1.49	1.35
4	A	402	37T	C4-N3	5.35	1.47	1.38
4	B	402	37T	C5-N7	5.25	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	402	37T	C8-N7	5.16	1.49	1.35
4	B	402	37T	C8-N7	5.16	1.49	1.35
4	B	402	37T	C4-N3	4.71	1.46	1.38
4	A	402	37T	C2-N3	4.66	1.48	1.38
4	C	402	37T	C4-N3	4.53	1.45	1.38
4	A	402	37T	C6-N1	4.35	1.46	1.38
4	B	402	37T	C4-N9	4.25	1.44	1.35
4	C	402	37T	C2-N3	4.14	1.47	1.38
4	A	402	37T	C4-N9	4.11	1.44	1.35
4	C	402	37T	C6-N1	3.98	1.46	1.38
4	C	402	37T	C4-N9	3.96	1.44	1.35
4	B	402	37T	C6-N1	3.91	1.46	1.38
4	B	402	37T	C2-N3	3.91	1.47	1.38
4	C	402	37T	C5-C6	3.41	1.52	1.43
4	A	402	37T	C5-C6	3.39	1.52	1.43
4	B	402	37T	C5-C6	3.33	1.52	1.43
4	B	402	37T	O2-C2	-2.79	1.17	1.23
4	B	402	37T	O6-C6	-2.58	1.18	1.23
4	A	402	37T	C8-N9	2.51	1.39	1.32
4	C	402	37T	O6-C6	-2.50	1.18	1.23
4	B	402	37T	C8-N9	2.45	1.39	1.32
4	C	402	37T	C8-N9	2.24	1.38	1.32
4	A	402	37T	O6-C6	-2.01	1.19	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	402	37T	C6-N1-C2	-7.21	118.02	127.35
4	C	402	37T	C6-N1-C2	-6.51	118.92	127.35
4	A	402	37T	C6-N1-C2	-5.81	119.83	127.35
4	B	402	37T	C5-C6-N1	5.31	120.35	110.99
4	C	402	37T	C5-C6-N1	5.23	120.21	110.99
4	A	402	37T	C5-C6-N1	4.75	119.36	110.99
4	B	402	37T	N3-C4-N9	3.78	132.51	126.32
4	B	402	37T	N7-C8-N9	-3.27	107.55	113.40
4	A	402	37T	C8-N9-C4	3.26	111.14	103.06
4	A	402	37T	N7-C8-N9	-3.19	107.70	113.40
4	A	402	37T	N3-C4-N9	3.12	131.44	126.32
4	C	402	37T	N7-C8-N9	-3.06	107.93	113.40
4	A	402	37T	O6-C6-C5	-3.02	120.13	127.54
4	C	402	37T	N3-C4-N9	2.95	131.16	126.32
4	B	402	37T	C8-N9-C4	2.91	110.29	103.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	402	37T	O6-C6-C5	-2.88	120.49	127.54
4	C	402	37T	C8-N9-C4	2.84	110.10	103.06
4	B	402	37T	O6-C6-C5	-2.68	120.96	127.54
4	B	402	37T	O2-C2-N3	-2.45	118.22	121.83
4	B	402	37T	N1-C2-N3	2.37	120.76	116.68
4	A	402	37T	C5-C4-N9	-2.36	107.10	112.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	37T	1	0
4	C	402	37T	2	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	334/369 (90%)	0.30	33 (9%)	7	8	23, 33, 70, 94	0
1	B	333/369 (90%)	0.20	32 (9%)	8	9	23, 31, 66, 88	0
1	C	334/369 (90%)	0.33	33 (9%)	7	8	23, 31, 68, 98	0
All	All	1001/1107 (90%)	0.28	98 (9%)	7	8	23, 32, 69, 98	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	240	TYR	13.2
1	C	241	SER	10.5
1	A	241	SER	9.9
1	C	220	ILE	8.7
1	B	241	SER	8.3
1	B	240	TYR	8.2
1	A	240	TYR	7.5
1	C	219	PRO	7.4
1	A	219	PRO	7.2
1	C	243	SER	7.2
1	A	218	ALA	7.1
1	A	349	SER	6.9
1	A	350	TYR	6.4
1	A	187	ASN	6.0
1	A	221	GLY	6.0
1	A	243	SER	5.8
1	B	219	PRO	5.8
1	A	242	SER	5.7
1	C	242	SER	5.6
1	C	186	ASN	5.4
1	C	221	GLY	5.1
1	B	221	GLY	5.0
1	B	220	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	143	ASN	4.8
1	C	239	LYS	4.7
1	A	188	ALA	4.7
1	C	188	ALA	4.7
1	B	350	TYR	4.7
1	B	7	ASN	4.6
1	A	186	ASN	4.6
1	A	270	GLN	4.4
1	A	220	ILE	4.4
1	C	185	PRO	4.0
1	A	102	ASN	3.9
1	B	239	LYS	3.9
1	C	7	ASN	3.9
1	B	186	ASN	3.9
1	A	348	ARG	3.8
1	A	239	LYS	3.8
1	B	243	SER	3.8
1	C	208	THR	3.7
1	B	242	SER	3.7
1	B	190	PRO	3.7
1	A	8	ASP	3.7
1	A	272	ASP	3.7
1	C	350	TYR	3.5
1	B	188	ALA	3.5
1	C	143	ASN	3.5
1	B	347	ASP	3.5
1	C	270	GLN	3.5
1	C	8	ASP	3.4
1	A	233	ILE	3.3
1	B	187	ASN	3.3
1	B	189	GLU	3.3
1	B	349	SER	3.2
1	A	185	PRO	3.2
1	A	231	PHE	3.1
1	C	347	ASP	3.1
1	A	347	ASP	3.1
1	C	244	SER	3.0
1	C	187	ASN	3.0
1	B	185	PRO	3.0
1	C	349	SER	2.9
1	C	145	PRO	2.9
1	C	190	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	191	PRO	2.8
1	B	102	ASN	2.8
1	B	251	VAL	2.8
1	A	143	ASN	2.8
1	B	348	ARG	2.7
1	B	231	PHE	2.7
1	C	272	ASP	2.7
1	A	7	ASN	2.7
1	A	189	GLU	2.6
1	C	146	ARG	2.6
1	C	184	ASP	2.6
1	A	190	PRO	2.6
1	A	244	SER	2.6
1	C	9	GLU	2.6
1	B	270	GLN	2.6
1	C	231	PHE	2.5
1	B	10	ARG	2.5
1	B	8	ASP	2.5
1	C	348	ARG	2.5
1	C	102	ASN	2.5
1	C	233	ILE	2.5
1	B	232	ALA	2.4
1	C	232	ALA	2.4
1	B	165	TRP	2.3
1	C	271	SER	2.3
1	B	161	ALA	2.2
1	A	171	PHE	2.2
1	A	165	TRP	2.2
1	A	9	GLU	2.1
1	B	230	PRO	2.1
1	B	253	CYS	2.1
1	A	232	ALA	2.1
1	A	230	PRO	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	37T	A	402	13/13	0.61	0.27	52,57,62,65	0
4	37T	C	402	13/13	0.85	0.16	45,49,55,55	0
4	37T	B	402	13/13	0.87	0.17	45,53,58,59	0
3	FE	C	401	1/1	0.99	0.10	28,28,28,28	0
3	FE	B	401	1/1	1.00	0.10	28,28,28,28	0
2	FES	A	400	4/4	1.00	0.09	23,24,24,24	0
2	FES	B	400	4/4	1.00	0.10	24,24,24,27	0
2	FES	C	400	4/4	1.00	0.10	23,24,24,25	0
3	FE	A	401	1/1	1.00	0.09	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.