wwPDB X-ray Structure Validation Summary Report (i)

Sep 16, 2023 – 05:17 PM EDT

PDB ID	:	4TN7
Title	:	Crystal structure of mouse KDM2A-H3K36ME-NO complex
Authors	:	Cheng, Z.
Deposited on	:	2014-06-03
Resolution	:	2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

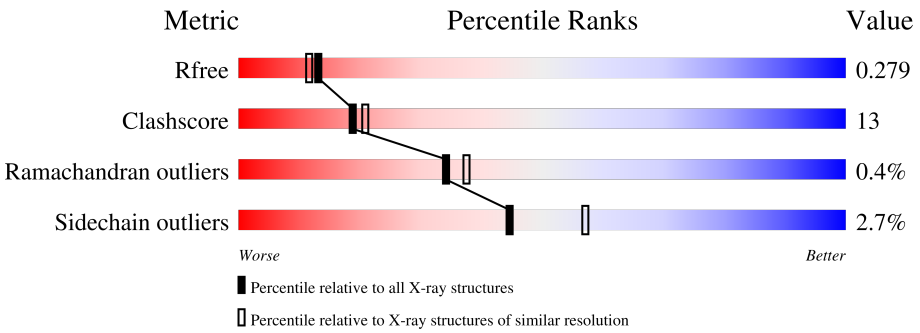
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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%

Mol	Chain	Length	Quality of chain
1	A	329	71% 27% •
1	C	329	72% 27% •
2	B	68	76% 22% •
2	D	68	65% 31% •
3	E	15	47% 13% 7% 33%
3	F	15	33% 27% 7% 33%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7113 atoms, of which 8 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 Lysine-specific demethylase 2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	329	2747	1761	458	507	21	1	1	0
1	C	329	2748	1762	458	507	21	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	ARG	TRP	conflict	UNP P59997
A	202	MET	ILE	conflict	UNP P59997
C	159	ARG	TRP	conflict	UNP P59997
C	202	MET	ILE	conflict	UNP P59997

- Molecule 2 is a protein called Lysine-specific demethylase 2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	68	528	341	85	100	2	2	0	0
2	D	68	528	341	85	100	2	1	0	0

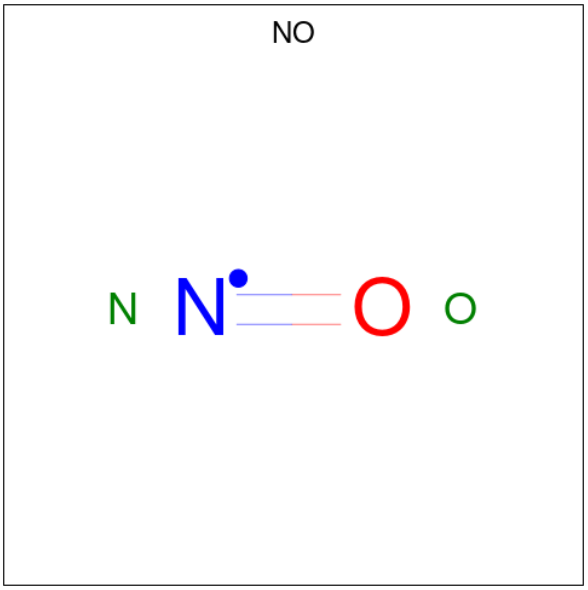
- Molecule 3 is a protein called Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	10	65	42	12	11	0	0	0
3	F	10	65	42	12	11	0	0	0

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

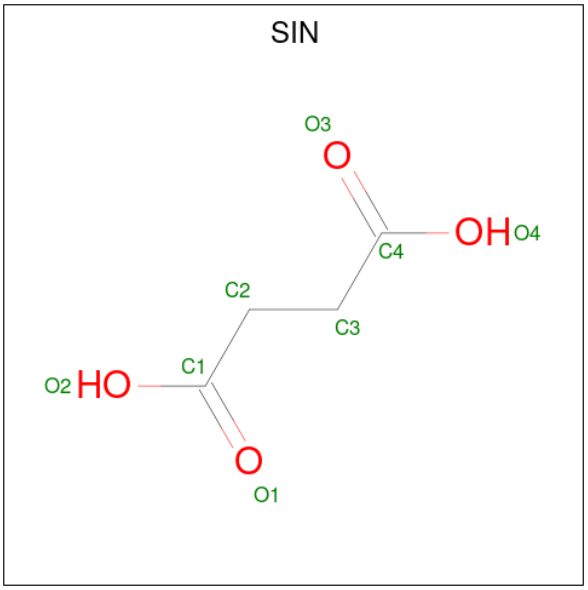
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
4	A	1	1	1	0	0
			Total	Fe		
4	C	1	1	1	0	0

- Molecule 5 is NITRIC OXIDE (three-letter code: NO) (formula: NO).



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

- Molecule 6 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	A	1	12	4	4	4	0	0
			Total	C	H	O		
6	C	1	12	4	4	4	0	0

- Molecule 7 is water.

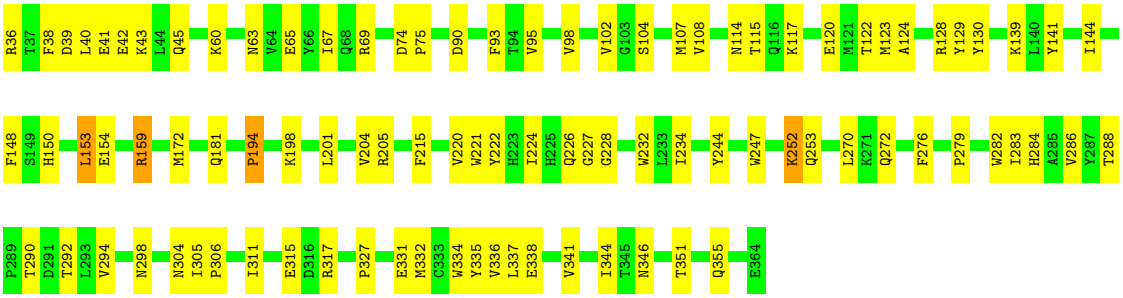
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	159	159	159	0	0
			Total	O		
7	B	40	40	40	0	0
			Total	O		
7	C	168	168	168	0	0
			Total	O		
7	D	29	29	29	0	0
			Total	O		
7	E	3	3	3	0	0
			Total	O		
7	F	5	5	5	0	0

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. 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. 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.

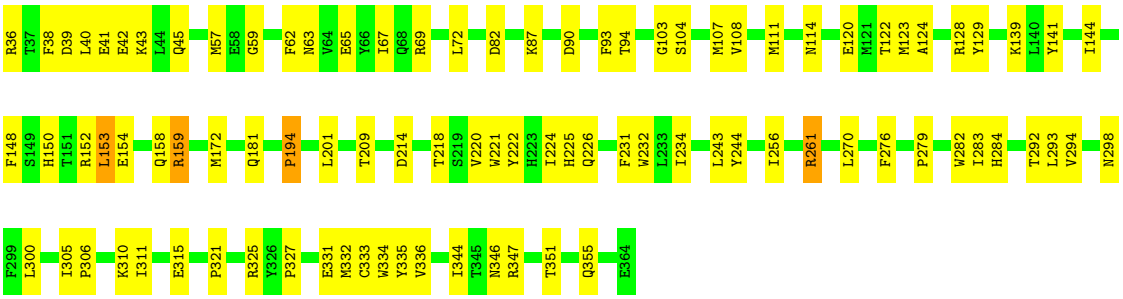
• Molecule 1: Lysine-specific demethylase 2A

Chain A:



• Molecule 1: Lysine-specific demethylase 2A

Chain C:



• Molecule 2: Lysine-specific demethylase 2A

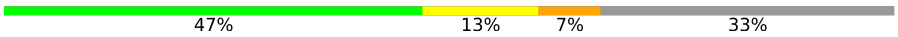
Chain B:

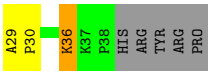
• Molecule 2: Lysine-specific demethylase 2A

Chain D:

- Molecule 3: Peptide

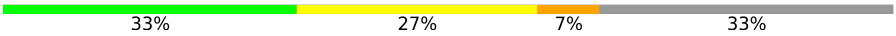
Chain E:





- Molecule 3: Peptide

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.06Å 157.93Å 48.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.17 – 2.20 46.54 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.6 (45.17-2.20) 97.6 (46.54-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1760)	Depositor
R, R_{free}	0.229 , 0.279 0.231 , 0.279	Depositor DCC
R_{free} test set	2067 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 19.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.439 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7113	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NO, MLZ, SIN, FE

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	0.22	0/2826	0.38	0/3827
1	C	0.22	0/2827	0.38	0/3827
2	B	0.20	0/538	0.36	0/733
2	D	0.20	0/538	0.38	0/733
3	E	0.17	0/55	0.39	0/73
3	F	0.18	0/55	0.41	0/73
All	All	0.22	0/6839	0.38	0/9266

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	2747	0	2646	71	0
1	C	2748	0	2648	74	0
2	B	528	0	546	13	0
2	D	528	0	546	23	0
3	E	65	0	71	2	0
3	F	65	0	72	8	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
5	A	2	0	0	0	0
6	A	8	4	4	1	0
6	C	8	4	4	1	0
7	A	159	0	0	7	0
7	B	40	0	0	0	0
7	C	168	0	0	6	0
7	D	29	0	0	0	0
7	E	3	0	0	0	0
7	F	5	0	0	0	0
All	All	7105	8	6537	173	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 13.

The worst 5 of 173 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:111:MET:HE2	3:F:37:LYS:HG3	1.39	1.05
2:D:479:PRO:HG2	2:D:482:ILE:HG12	1.58	0.85
2:B:479:PRO:HG2	2:B:482:ILE:HG12	1.62	0.82
1:C:114:ASN:ND2	1:C:139:LYS:HE2	2.02	0.73
1:A:114:ASN:ND2	1:A:139:LYS:HE2	2.04	0.73

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	328/329 (100%)	320 (98%)	7 (2%)	1 (0%)	41 46
1	C	328/329 (100%)	319 (97%)	8 (2%)	1 (0%)	41 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
2	D	66/68 (97%)	63 (96%)	2 (3%)	1 (2%)	10	8
3	E	7/15 (47%)	7 (100%)	0	0	100	100
3	F	7/15 (47%)	7 (100%)	0	0	100	100
All	All	802/824 (97%)	780 (97%)	19 (2%)	3 (0%)	34	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	451	VAL
1	A	194	PRO
1	C	194	PRO

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	306/305 (100%)	300 (98%)	6 (2%)	55	69
1	C	306/305 (100%)	300 (98%)	6 (2%)	55	69
2	B	61/61 (100%)	57 (93%)	4 (7%)	16	19
2	D	61/61 (100%)	57 (93%)	4 (7%)	16	19
3	E	5/10 (50%)	5 (100%)	0	100	100
3	F	5/10 (50%)	5 (100%)	0	100	100
All	All	744/752 (99%)	724 (97%)	20 (3%)	44	57

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	261	ARG
2	D	473	LEU
2	D	511	VAL
2	D	505	LYS

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Mol	Chain	Res	Type
2	B	464	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
3	MLZ	E	36	3	8,9,10	0.72	0	4,9,11	1.39	1 (25%)
3	MLZ	F	36	3	8,9,10	0.72	0	4,9,11	1.47	1 (25%)

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	MLZ	E	36	3	-	0/7/8/10	-
3	MLZ	F	36	3	-	0/7/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	36	MLZ	CM-NZ-CE	2.79	120.02	111.95
3	E	36	MLZ	CM-NZ-CE	2.62	119.53	111.95

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
3	E	36	MLZ	1	0
3	F	36	MLZ	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
5	NO	A	602	4	0,1,1	-	-	-		
6	SIN	A	603	4	7,7,7	1.03	0	8,8,8	1.60	2 (25%)
6	SIN	C	602	4	7,7,7	1.04	0	8,8,8	1.63	2 (25%)

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
6	SIN	A	603	4	-	5/5/5/5	-
6	SIN	C	602	4	-	2/5/5/5	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	602	SIN	O2-C1-C2	2.17	121.00	114.03
6	A	603	SIN	O4-C4-C3	2.03	120.55	114.03
6	C	602	SIN	O4-C4-C3	2.01	120.49	114.03
6	A	603	SIN	O2-C1-C2	2.01	120.48	114.03

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	603	SIN	C1-C2-C3-C4
6	A	603	SIN	C2-C3-C4-O3
6	A	603	SIN	C2-C3-C4-O4
6	A	603	SIN	O2-C1-C2-C3
6	A	603	SIN	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	SIN	1	0
6	C	602	SIN	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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.