



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 02:44 pm BST

PDB ID : 4NHY  
Title : Crystal structure of human OGFOD1, 2-oxoglutarate and iron-dependent oxygenase domain containing 1, in complex with pyridine-2,4-dicarboxylic acid (2,4-PDCA)  
Authors : Horita, S.; McDonough, M.A.; Schofield, C.J.  
Deposited on : 2013-11-05  
Resolution : 2.60 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](mailto: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.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

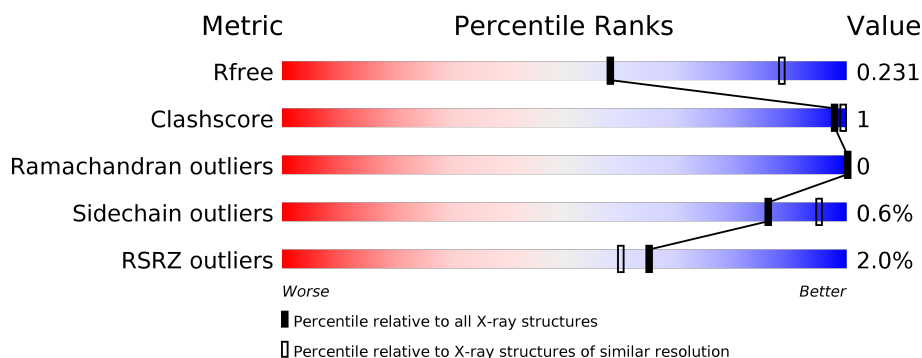
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	562	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 80%, grey 18%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>80%</span> <span>18%</span> </div> </div>
1	B	562	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 1%, green 81%, grey 18%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>81%</span> <span>18%</span> </div> </div>
1	C	562	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 78%, grey 19%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>78%</span> <span>19%</span> </div> </div>
1	D	562	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 3%, yellow 1%, green 80%, grey 18%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>80%</span> <span>18%</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15237 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 2-oxoglutarate and iron-dependent oxygenase domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	1	0
			3788	2448	622	702	16			
1	B	461	Total	C	N	O	S	0	2	0
			3784	2448	621	699	16			
1	C	457	Total	C	N	O	S	0	1	0
			3754	2437	613	688	16			
1	D	461	Total	C	N	O	S	0	1	0
			3758	2434	615	693	16			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	INITIATING METHIONINE	UNP Q8N543
A	-18	GLY	-	EXPRESSION TAG	UNP Q8N543
A	-17	SER	-	EXPRESSION TAG	UNP Q8N543
A	-16	SER	-	EXPRESSION TAG	UNP Q8N543
A	-15	HIS	-	EXPRESSION TAG	UNP Q8N543
A	-14	HIS	-	EXPRESSION TAG	UNP Q8N543
A	-13	HIS	-	EXPRESSION TAG	UNP Q8N543
A	-12	HIS	-	EXPRESSION TAG	UNP Q8N543
A	-11	HIS	-	EXPRESSION TAG	UNP Q8N543
A	-10	HIS	-	EXPRESSION TAG	UNP Q8N543
A	-9	SER	-	EXPRESSION TAG	UNP Q8N543
A	-8	SER	-	EXPRESSION TAG	UNP Q8N543
A	-7	GLY	-	EXPRESSION TAG	UNP Q8N543
A	-6	LEU	-	EXPRESSION TAG	UNP Q8N543
A	-5	VAL	-	EXPRESSION TAG	UNP Q8N543
A	-4	PRO	-	EXPRESSION TAG	UNP Q8N543
A	-3	ARG	-	EXPRESSION TAG	UNP Q8N543
A	-2	GLY	-	EXPRESSION TAG	UNP Q8N543
A	-1	SER	-	EXPRESSION TAG	UNP Q8N543
A	0	HIS	-	EXPRESSION TAG	UNP Q8N543

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	INITIATING METHIONINE	UNP Q8N543
B	-18	GLY	-	EXPRESSION TAG	UNP Q8N543
B	-17	SER	-	EXPRESSION TAG	UNP Q8N543
B	-16	SER	-	EXPRESSION TAG	UNP Q8N543
B	-15	HIS	-	EXPRESSION TAG	UNP Q8N543
B	-14	HIS	-	EXPRESSION TAG	UNP Q8N543
B	-13	HIS	-	EXPRESSION TAG	UNP Q8N543
B	-12	HIS	-	EXPRESSION TAG	UNP Q8N543
B	-11	HIS	-	EXPRESSION TAG	UNP Q8N543
B	-10	HIS	-	EXPRESSION TAG	UNP Q8N543
B	-9	SER	-	EXPRESSION TAG	UNP Q8N543
B	-8	SER	-	EXPRESSION TAG	UNP Q8N543
B	-7	GLY	-	EXPRESSION TAG	UNP Q8N543
B	-6	LEU	-	EXPRESSION TAG	UNP Q8N543
B	-5	VAL	-	EXPRESSION TAG	UNP Q8N543
B	-4	PRO	-	EXPRESSION TAG	UNP Q8N543
B	-3	ARG	-	EXPRESSION TAG	UNP Q8N543
B	-2	GLY	-	EXPRESSION TAG	UNP Q8N543
B	-1	SER	-	EXPRESSION TAG	UNP Q8N543
B	0	HIS	-	EXPRESSION TAG	UNP Q8N543
C	-19	MET	-	INITIATING METHIONINE	UNP Q8N543
C	-18	GLY	-	EXPRESSION TAG	UNP Q8N543
C	-17	SER	-	EXPRESSION TAG	UNP Q8N543
C	-16	SER	-	EXPRESSION TAG	UNP Q8N543
C	-15	HIS	-	EXPRESSION TAG	UNP Q8N543
C	-14	HIS	-	EXPRESSION TAG	UNP Q8N543
C	-13	HIS	-	EXPRESSION TAG	UNP Q8N543
C	-12	HIS	-	EXPRESSION TAG	UNP Q8N543
C	-11	HIS	-	EXPRESSION TAG	UNP Q8N543
C	-10	HIS	-	EXPRESSION TAG	UNP Q8N543
C	-9	SER	-	EXPRESSION TAG	UNP Q8N543
C	-8	SER	-	EXPRESSION TAG	UNP Q8N543
C	-7	GLY	-	EXPRESSION TAG	UNP Q8N543
C	-6	LEU	-	EXPRESSION TAG	UNP Q8N543
C	-5	VAL	-	EXPRESSION TAG	UNP Q8N543
C	-4	PRO	-	EXPRESSION TAG	UNP Q8N543
C	-3	ARG	-	EXPRESSION TAG	UNP Q8N543
C	-2	GLY	-	EXPRESSION TAG	UNP Q8N543
C	-1	SER	-	EXPRESSION TAG	UNP Q8N543
C	0	HIS	-	EXPRESSION TAG	UNP Q8N543
D	-19	MET	-	INITIATING METHIONINE	UNP Q8N543
D	-18	GLY	-	EXPRESSION TAG	UNP Q8N543

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	EXPRESSION TAG	UNP Q8N543
D	-16	SER	-	EXPRESSION TAG	UNP Q8N543
D	-15	HIS	-	EXPRESSION TAG	UNP Q8N543
D	-14	HIS	-	EXPRESSION TAG	UNP Q8N543
D	-13	HIS	-	EXPRESSION TAG	UNP Q8N543
D	-12	HIS	-	EXPRESSION TAG	UNP Q8N543
D	-11	HIS	-	EXPRESSION TAG	UNP Q8N543
D	-10	HIS	-	EXPRESSION TAG	UNP Q8N543
D	-9	SER	-	EXPRESSION TAG	UNP Q8N543
D	-8	SER	-	EXPRESSION TAG	UNP Q8N543
D	-7	GLY	-	EXPRESSION TAG	UNP Q8N543
D	-6	LEU	-	EXPRESSION TAG	UNP Q8N543
D	-5	VAL	-	EXPRESSION TAG	UNP Q8N543
D	-4	PRO	-	EXPRESSION TAG	UNP Q8N543
D	-3	ARG	-	EXPRESSION TAG	UNP Q8N543
D	-2	GLY	-	EXPRESSION TAG	UNP Q8N543
D	-1	SER	-	EXPRESSION TAG	UNP Q8N543
D	0	HIS	-	EXPRESSION TAG	UNP Q8N543

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

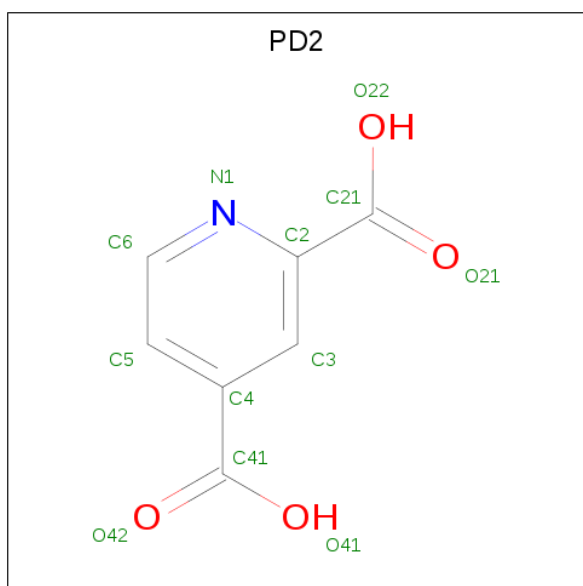
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PYRIDINE-2,4-DICARBOXYLIC ACID (three-letter code: PD2) (formula:  $C_7H_5NO_4$ ).



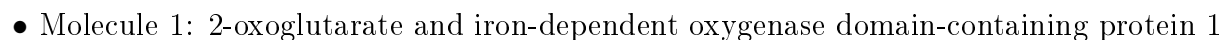
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 12 7 1 4	0	0
4	B	1	Total C N O 12 7 1 4	0	0
4	C	1	Total C N O 12 7 1 4	0	0
4	D	1	Total C N O 12 7 1 4	0	0

- Molecule 5 is water.

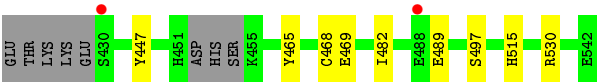
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	36	Total O 36 36	0	0
5	B	18	Total O 18 18	0	0
5	C	23	Total O 23 23	0	0
5	D	6	Total O 6 6	0	0



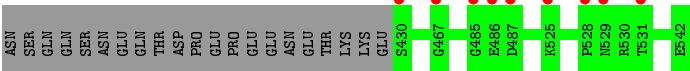
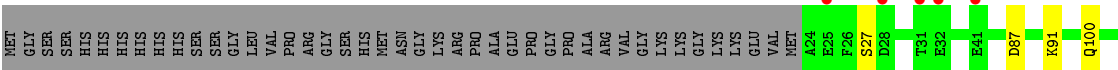
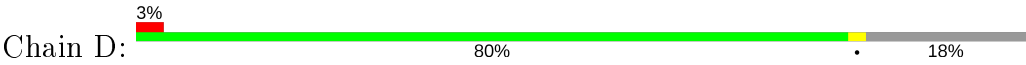
- Molecule 1: 2-oxoglutarate and iron-dependent oxygenase domain-containing protein 1







● Molecule 1: 2-oxoglutarate and iron-dependent oxygenase domain-containing protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.68Å 130.47Å 175.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.24 – 2.60 48.24 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.24-2.60) 94.4 (48.24-2.60)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309, REFMAC	Depositor
R, $R_{free}$	0.190 , 0.226 0.189 , 0.231	Depositor DCC
$R_{free}$ test set	2000 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.5	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15237	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: GOL, MN, PD2

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	0.32	0/3902	0.48	0/5285
1	B	0.30	0/3901	0.47	0/5284
1	C	0.32	0/3868	0.49	0/5239
1	D	0.28	0/3871	0.45	0/5246
All	All	0.31	0/15542	0.47	0/21054

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	3788	0	3638	6	1
1	B	3784	0	3634	3	0
1	C	3754	0	3601	7	0
1	D	3758	0	3599	4	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	0	0
3	D	6	0	8	0	0
4	A	12	0	3	0	0
4	B	12	0	3	0	0
4	C	12	0	3	0	0
4	D	12	0	3	1	0
5	A	36	0	0	0	0
5	B	18	0	0	0	0
5	C	23	0	0	0	0
5	D	6	0	0	0	0
All	All	15237	0	14508	20	1

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 1.

The worst 5 of 20 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:GLU:OE1	1:A:530:ARG:NH1	2.24	0.70
1:C:469:GLU:OE2	1:C:530:ARG:NH1	2.35	0.59
1:C:155:HIS:CD2	1:C:157:ASP:OD1	2.59	0.54
1:D:283:ILE:HG23	1:D:293:ILE:HD13	1.91	0.53
1:D:218:HIS:CD2	4:D:603:PD2:H6	2.48	0.49

All (1) 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)
1:A:108:ARG:NH1	1:D:286:GLU:OE2[4_554]	2.16	0.04

## 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	458/562 (82%)	435 (95%)	23 (5%)	0	100	100
1	B	459/562 (82%)	442 (96%)	17 (4%)	0	100	100
1	C	452/562 (80%)	431 (95%)	21 (5%)	0	100	100
1	D	458/562 (82%)	436 (95%)	22 (5%)	0	100	100
All	All	1827/2248 (81%)	1744 (96%)	83 (4%)	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	416/518 (80%)	414 (100%)	2 (0%)	88	96
1	B	414/518 (80%)	412 (100%)	2 (0%)	88	96
1	C	408/518 (79%)	405 (99%)	3 (1%)	84	94
1	D	408/518 (79%)	405 (99%)	3 (1%)	84	94
All	All	1646/2072 (79%)	1636 (99%)	10 (1%)	86	95

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	207	LEU
1	C	353	LEU
1	D	27	SER
1	B	353	LEU
1	C	497	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	GLN
1	B	258	HIS
1	C	529	ASN

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Mol	Chain	Res	Type
1	D	38	GLN
1	D	258	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	PD2	A	603	2	7,12,12	1.86	1 (14%)	8,16,16	1.59	1 (12%)
4	PD2	C	602	2	7,12,12	1.80	1 (14%)	8,16,16	1.47	1 (12%)
3	GOL	A	602	-	5,5,5	0.40	0	5,5,5	0.23	0
4	PD2	B	603	2	7,12,12	2.09	1 (14%)	8,16,16	1.39	1 (12%)
3	GOL	D	602	-	5,5,5	0.38	0	5,5,5	0.22	0
3	GOL	B	602	-	5,5,5	0.38	0	5,5,5	0.26	0
4	PD2	D	603	2	7,12,12	1.92	1 (14%)	8,16,16	1.41	1 (12%)

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	PD2	A	603	2	-	0/0/8/8	0/1/1/1
4	PD2	C	602	2	-	0/0/8/8	0/1/1/1
3	GOL	A	602	-	-	2/4/4/4	-
4	PD2	B	603	2	-	0/0/8/8	0/1/1/1
3	GOL	D	602	-	-	2/4/4/4	-
3	GOL	B	602	-	-	4/4/4/4	-
4	PD2	D	603	2	-	0/0/8/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	PD2	C4-C41	5.03	1.52	1.47
4	D	603	PD2	C4-C41	4.46	1.51	1.47
4	A	603	PD2	C4-C41	4.30	1.51	1.47
4	C	602	PD2	C4-C41	4.03	1.51	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	PD2	C5-C6-N1	-3.33	119.83	123.96
4	C	602	PD2	C5-C6-N1	-3.30	119.86	123.96
4	B	603	PD2	C5-C6-N1	-3.04	120.18	123.96
4	D	603	PD2	C5-C6-N1	-2.79	120.49	123.96

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	GOL	O1-C1-C2-C3
3	D	602	GOL	O1-C1-C2-C3
3	B	602	GOL	O1-C1-C2-C3
3	B	602	GOL	O2-C2-C3-O3
3	B	602	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	603	PD2	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](#)

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	461/562 (82%)	-0.33	5 (1%) 80 78	27, 46, 91, 139	0
1	B	461/562 (82%)	-0.11	9 (1%) 65 60	30, 56, 109, 132	0
1	C	457/562 (81%)	-0.27	4 (0%) 84 82	25, 49, 95, 120	0
1	D	461/562 (82%)	0.10	19 (4%) 37 30	33, 72, 125, 151	0
All	All	1840/2248 (81%)	-0.15	37 (2%) 65 60	25, 56, 110, 151	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	488	GLU	8.1
1	D	529	ASN	6.8
1	C	430	SER	5.6
1	A	263	HIS	4.4
1	B	529	ASN	4.4

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	D	602	6/6	0.81	0.29	85,89,93,94	0
3	GOL	B	602	6/6	0.89	0.23	64,74,79,81	0
3	GOL	A	602	6/6	0.90	0.22	69,76,81,83	0
4	PD2	C	602	12/12	0.94	0.15	27,41,49,50	0
4	PD2	D	603	12/12	0.94	0.16	54,57,61,62	0
4	PD2	A	603	12/12	0.95	0.15	39,49,55,56	0
4	PD2	B	603	12/12	0.95	0.13	42,51,67,67	0
2	MN	D	601	1/1	0.98	0.10	61,61,61,61	0
2	MN	B	601	1/1	0.99	0.15	46,46,46,46	0
2	MN	A	601	1/1	0.99	0.11	36,36,36,36	0
2	MN	C	601	1/1	0.99	0.14	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.