



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:21 PM UTC

PDB ID : 4NHY / pdb_00004nhy
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 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

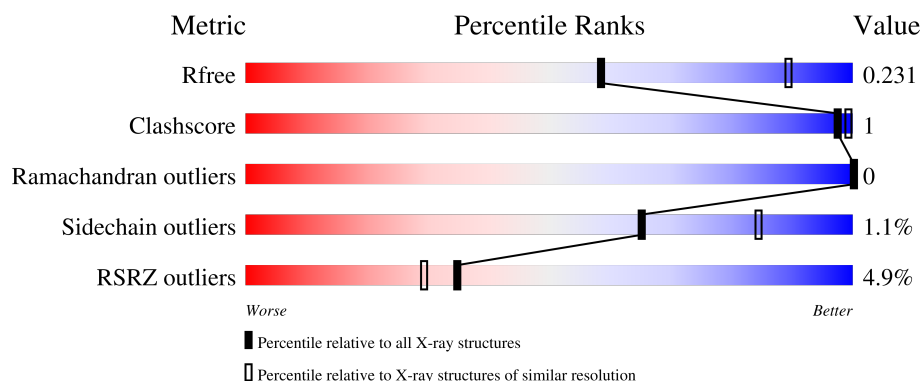
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	562	
1	B	562	
1	C	562	
1	D	562	

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 (CCD ID: MN) (formula: Mn).

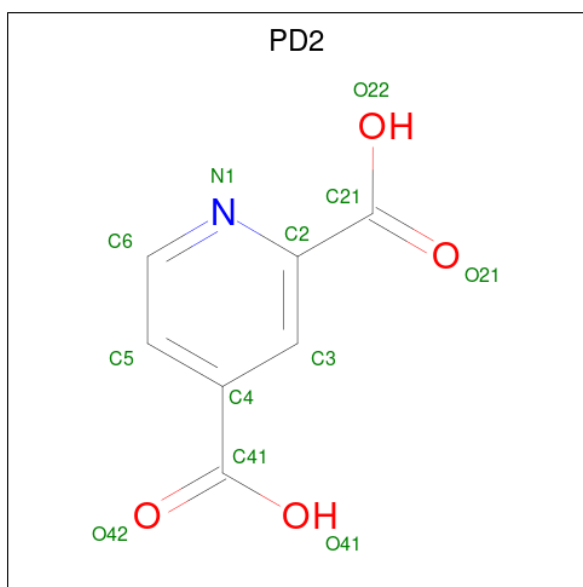
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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 (CCD ID: PD2) (formula: $C_7H_5NO_4$).



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

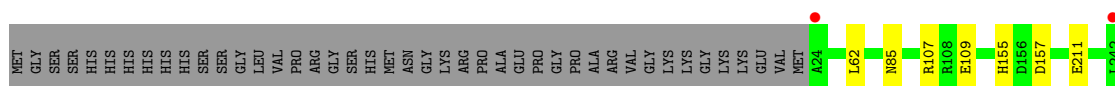
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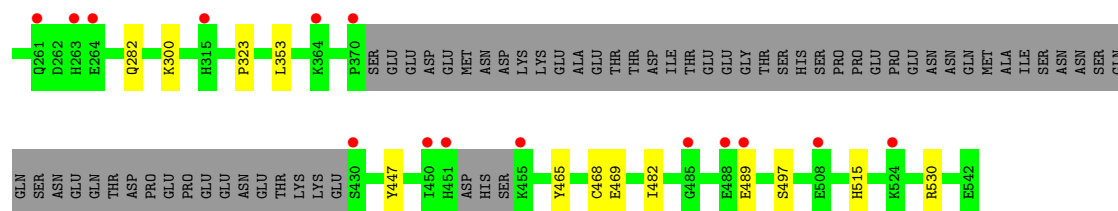
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			12	7	1	4		
4	C	1	Total	C	N	O	0	0
			12	7	1	4		
4	D	1	Total	C	N	O	0	0
			12	7	1	4		

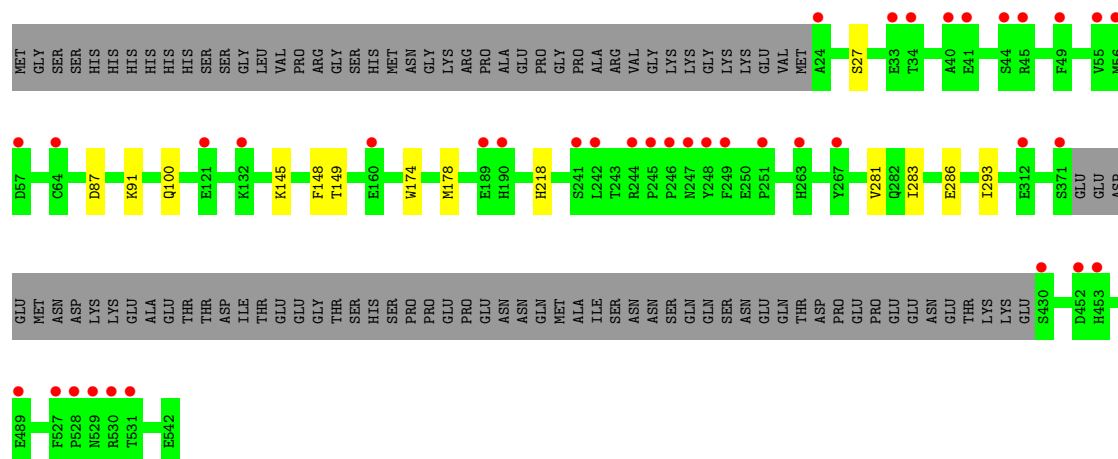
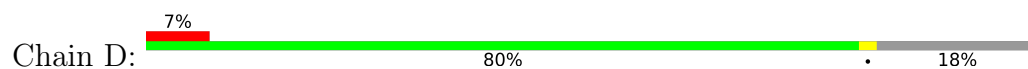
- Molecule 5 is water.

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





- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	41.5	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, GOL, 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	0.40	0/3902	0.67	2/5285 (0.0%)
1	B	0.38	0/3901	0.66	0/5284
1	C	0.39	0/3868	0.69	2/5239 (0.0%)
1	D	0.35	0/3871	0.65	0/5246
All	All	0.38	0/15542	0.67	4/21054 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	323	PRO	CA-C-N	5.72	127.00	119.84
1	C	323	PRO	C-N-CA	5.72	127.00	119.84
1	A	323	PRO	CA-C-N	5.45	125.12	119.56
1	A	323	PRO	C-N-CA	5.45	125.12	119.56

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	3788	0	3638	8	1
1	B	3784	0	3634	3	0
1	C	3754	0	3601	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3758	0	3599	5	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
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	23	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.

All (23) 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
1:B:109:GLU:N	1:B:109:GLU:OE1	2.47	0.47
1:A:261:GLN:NE2	1:A:264:GLU:OE1	2.46	0.47
1:A:247:ASN:ND2	1:A:452:ASP:OD2	2.49	0.46
1:B:348:PHE:HA	1:B:353:LEU:HD22	1.98	0.45
1:A:348:PHE:HA	1:A:353:LEU:HD22	1.98	0.45
1:D:174:TRP:HA	1:D:178:MET:SD	2.57	0.45
1:B:283:ILE:HG23	1:B:293:ILE:HD13	1.99	0.45
1:C:465:TYR:HB3	1:C:468:CYS:SG	2.58	0.43
1:C:62:LEU:HB3	1:C:211:GLU:HG2	2.00	0.43
1:C:482:ILE:HG22	1:C:489:GLU:HA	2.01	0.43
1:A:39:VAL:HG13	1:A:56:MET:HE1	2.01	0.42
1:D:148:PHE:O	1:D:149:THR:OG1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLU:OE2	1:A:517:ASN:HB2	2.20	0.41
1:D:91:LYS:HD3	1:D:100:GLN:HB2	2.03	0.41
1:A:213:SER:HB2	1:A:214:PRO:HD2	2.03	0.41
1:A:42:ALA:HB3	1:A:56:MET:HE3	2.03	0.41
1:C:107:ARG:HG3	1:C:109:GLU:OE1	2.21	0.40
1:C:447:TYR:HB3	1:C:515:HIS:HA	2.04	0.40

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 [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	416/518 (80%)	412 (99%)	4 (1%)	68	86
1	B	414/518 (80%)	409 (99%)	5 (1%)	63	83
1	C	408/518 (79%)	403 (99%)	5 (1%)	63	83
1	D	408/518 (79%)	404 (99%)	4 (1%)	68	86
All	All	1646/2072 (79%)	1628 (99%)	18 (1%)	65	84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	LYS
1	A	187	ILE
1	A	353	LEU
1	A	492	THR
1	B	145	LYS
1	B	281	VAL
1	B	305	THR
1	B	353	LEU
1	B	508	GLU
1	C	85	ASN
1	C	282	GLN
1	C	300	LYS
1	C	353	LEU
1	C	497	SER
1	D	27	SER
1	D	87	ASP
1	D	145	LYS
1	D	281	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	89	HIS
1	B	258	HIS
1	B	451	HIS
1	B	453	HIS
1	B	494	ASN
1	C	38	GLN
1	C	89	HIS

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Mol	Chain	Res	Type
1	C	190	HIS
1	C	261	GLN
1	D	38	GLN
1	D	190	HIS
1	D	238	HIS
1	D	258	HIS
1	D	282	GLN
1	D	494	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	GOL	D	602	-	5,5,5	0.39	0	5,5,5	0.24	0
4	PD2	D	603	2	12,12,12	1.23	0	16,16,16	1.55	3 (18%)
4	PD2	C	602	2	12,12,12	1.20	0	16,16,16	1.38	1 (6%)
3	GOL	B	602	-	5,5,5	0.38	0	5,5,5	0.30	0
3	GOL	A	602	-	5,5,5	0.41	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PD2	B	603	2	12,12,12	1.19	0	16,16,16	1.48	3 (18%)
4	PD2	A	603	2	12,12,12	1.19	0	16,16,16	1.51	4 (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	GOL	D	602	-	-	2/4/4/4	-
4	PD2	D	603	2	-	0/8/8/8	0/1/1/1
4	PD2	C	602	2	-	0/8/8/8	0/1/1/1
3	GOL	B	602	-	-	4/4/4/4	-
3	GOL	A	602	-	-	2/4/4/4	-
4	PD2	B	603	2	-	0/8/8/8	0/1/1/1
4	PD2	A	603	2	-	0/8/8/8	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	PD2	C5-C6-N1	-3.38	119.83	123.97
4	C	602	PD2	C5-C6-N1	-3.35	119.86	123.97
4	B	603	PD2	C5-C6-N1	-3.09	120.18	123.97
4	D	603	PD2	C5-C6-N1	-2.84	120.49	123.97
4	D	603	PD2	C3-C2-N1	-2.63	120.12	123.27
4	B	603	PD2	C3-C2-N1	-2.42	120.37	123.27
4	D	603	PD2	O22-C21-C2	2.31	120.20	114.71
4	A	603	PD2	C3-C2-N1	-2.24	120.59	123.27
4	A	603	PD2	C6-N1-C2	2.22	119.79	116.93
4	A	603	PD2	O22-C21-C2	2.15	119.82	114.71
4	B	603	PD2	C6-N1-C2	2.09	119.62	116.93

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

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

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 ⓘ

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	461/562 (82%)	-0.18	17 (3%)	45 39	27, 46, 91, 139	1 (0%)
1	B	461/562 (82%)	0.07	17 (3%)	45 39	30, 56, 109, 132	2 (0%)
1	C	457/562 (81%)	-0.05	17 (3%)	45 39	25, 49, 95, 120	1 (0%)
1	D	461/562 (82%)	0.51	39 (8%)	16 13	33, 72, 125, 151	1 (0%)
All	All	1840/2248 (81%)	0.09	90 (4%)	35 29	25, 55, 110, 151	5 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	430	SER	6.3
1	C	430	SER	5.8
1	C	488	GLU	5.2
1	D	430	SER	4.9
1	A	430	SER	4.8
1	D	245	PRO	4.4
1	D	242	LEU	4.1
1	D	247	ASN	4.1
1	B	242	LEU	3.9
1	C	264	GLU	3.8
1	D	371	SER	3.8
1	C	451	HIS	3.6
1	D	56	MET	3.6
1	B	488	GLU	3.5
1	D	246	PRO	3.4
1	B	371	SER	3.3
1	D	248	TYR	3.3
1	D	530	ARG	3.3
1	A	263	HIS	3.3
1	D	312	GLU	3.2
1	D	527	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	529	ASN	3.1
1	D	267	TYR	3.0
1	A	189	GLU	3.0
1	B	431	SER	3.0
1	A	371	SER	3.0
1	B	263	HIS	3.0
1	C	263	HIS	3.0
1	D	34	THR	3.0
1	D	44	SER	3.0
1	B	246	PRO	3.0
1	C	364	LYS	3.0
1	A	264	GLU	2.9
1	D	241	SER	2.9
1	D	529	ASN	2.9
1	D	121	GLU	2.9
1	A	261	GLN	2.8
1	C	24	ALA	2.8
1	D	33	GLU	2.7
1	A	24	ALA	2.7
1	C	455	LYS	2.7
1	B	528	PRO	2.7
1	D	64	CYS	2.6
1	B	244	ARG	2.6
1	B	455	LYS	2.5
1	C	261	GLN	2.5
1	D	24	ALA	2.5
1	C	370	PRO	2.5
1	A	242	LEU	2.5
1	D	41	GLU	2.5
1	D	49	PHE	2.5
1	A	243	THR	2.4
1	D	132	LYS	2.4
1	D	190	HIS	2.4
1	C	242	LEU	2.4
1	D	528	PRO	2.4
1	D	45	ARG	2.4
1	D	57	ASP	2.4
1	B	262	ASP	2.3
1	B	89	HIS	2.3
1	C	508	GLU	2.3
1	D	263	HIS	2.3
1	C	489	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	160	GLU	2.3
1	D	189	GLU	2.3
1	D	489	GLU	2.3
1	C	450	ILE	2.2
1	D	531	THR	2.2
1	B	527	PHE	2.2
1	D	249	PHE	2.2
1	A	526	THR	2.2
1	A	431	SER	2.2
1	A	527	PHE	2.2
1	C	315	HIS	2.2
1	B	245	PRO	2.2
1	B	247	ASN	2.2
1	C	485	GLY	2.2
1	D	452	ASP	2.2
1	B	24	ALA	2.1
1	D	40	ALA	2.1
1	B	529	ASN	2.1
1	D	244	ARG	2.1
1	D	453	HIS	2.1
1	C	524	LYS	2.1
1	D	251	PRO	2.1
1	A	487	ASP	2.1
1	A	244	ARG	2.1
1	D	55	VAL	2.1
1	A	247	ASN	2.0
1	A	485	GLY	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	D	602	6/6	0.85	0.17	85,89,93,94	0
3	GOL	B	602	6/6	0.86	0.13	64,74,79,81	0
4	PD2	C	602	12/12	0.90	0.10	27,41,49,50	0
4	PD2	A	603	12/12	0.91	0.10	39,49,55,56	0
4	PD2	D	603	12/12	0.91	0.10	54,57,61,62	0
3	GOL	A	602	6/6	0.92	0.14	69,76,81,83	0
4	PD2	B	603	12/12	0.92	0.10	42,51,67,67	0
2	MN	D	601	1/1	0.98	0.04	61,61,61,61	0
2	MN	B	601	1/1	0.99	0.03	46,46,46,46	0
2	MN	C	601	1/1	0.99	0.02	45,45,45,45	0
2	MN	A	601	1/1	1.00	0.02	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.