WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2023 – 01:14 pm GMT

PDB ID	:	2W2I
Title	:	Crystal structure of the human 2-oxoglutarate oxygenase LOC390245
Authors	:	Yue, W.W.; Ng, S.; Shafqat, N.; Ugochukwu, E.; McDonough, M.; Pike, A.C.W.; Filippakopoulos, P.; von Delft, F.; Arrowsmith, C.; Weigelt, J.; Edwards, A.; Bountra, C.; Schofield, C.; Oppermann, U.
Deposited on	:	2008-10-31
Resolution	:	2.10 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, 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 ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	Percentile Ranks	Value
Rfree		0.248
Clashscore		5
Ramachandran outliers		0.3%
Sidechain outliers		4.4%
RSRZ outliers		5.5%

Worse ——————————————————— *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
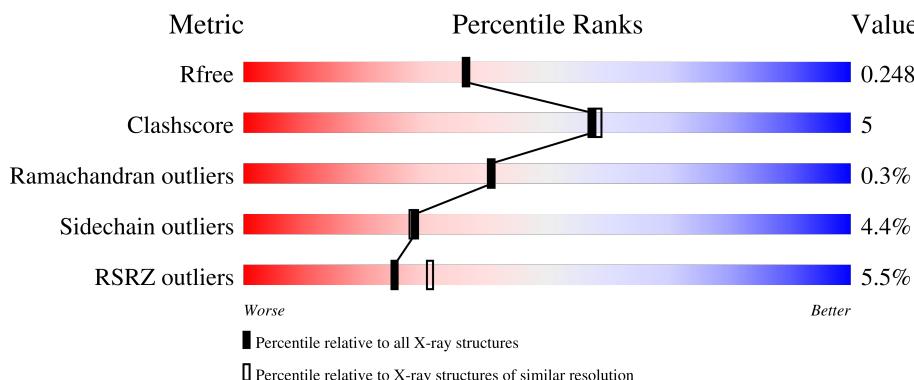
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	358	4% / 74% / 10% · 15%
1	B	358	4% / 75% / 9% · 15%
1	C	358	6% / 78% / 8% · 12%
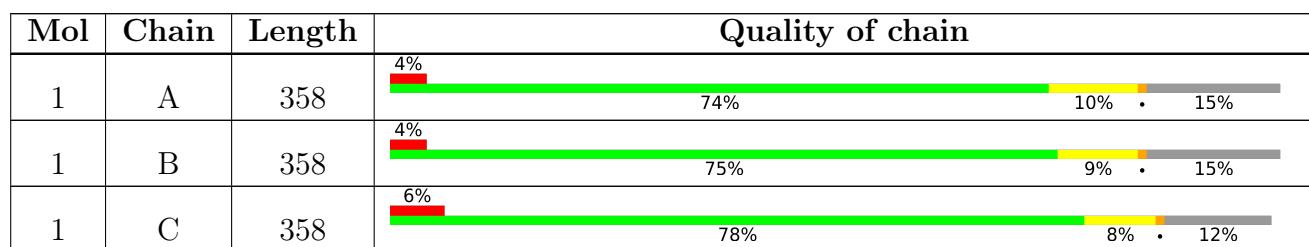
2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 7717 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 OXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	1	0
			2396	1561	387	434	14			
1	B	306	Total	C	N	O	S	0	2	0
			2435	1583	399	440	13			
1	C	314	Total	C	N	O	S	0	2	0
			2476	1611	407	443	15			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP B2RXH2
A	-20	HIS	-	expression tag	UNP B2RXH2
A	-19	HIS	-	expression tag	UNP B2RXH2
A	-18	HIS	-	expression tag	UNP B2RXH2
A	-17	HIS	-	expression tag	UNP B2RXH2
A	-16	HIS	-	expression tag	UNP B2RXH2
A	-15	HIS	-	expression tag	UNP B2RXH2
A	-14	SER	-	expression tag	UNP B2RXH2
A	-13	SER	-	expression tag	UNP B2RXH2
A	-12	GLY	-	expression tag	UNP B2RXH2
A	-11	VAL	-	expression tag	UNP B2RXH2
A	-10	ASP	-	expression tag	UNP B2RXH2
A	-9	LEU	-	expression tag	UNP B2RXH2
A	-8	GLY	-	expression tag	UNP B2RXH2
A	-7	THR	-	expression tag	UNP B2RXH2
A	-6	GLU	-	expression tag	UNP B2RXH2
A	-5	ASN	-	expression tag	UNP B2RXH2
A	-4	LEU	-	expression tag	UNP B2RXH2
A	-3	TYR	-	expression tag	UNP B2RXH2
A	-2	PHE	-	expression tag	UNP B2RXH2
A	-1	GLN	-	expression tag	UNP B2RXH2
A	0	SER	-	expression tag	UNP B2RXH2
B	-21	MET	-	expression tag	UNP B2RXH2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	expression tag	UNP B2RXH2
B	-19	HIS	-	expression tag	UNP B2RXH2
B	-18	HIS	-	expression tag	UNP B2RXH2
B	-17	HIS	-	expression tag	UNP B2RXH2
B	-16	HIS	-	expression tag	UNP B2RXH2
B	-15	HIS	-	expression tag	UNP B2RXH2
B	-14	SER	-	expression tag	UNP B2RXH2
B	-13	SER	-	expression tag	UNP B2RXH2
B	-12	GLY	-	expression tag	UNP B2RXH2
B	-11	VAL	-	expression tag	UNP B2RXH2
B	-10	ASP	-	expression tag	UNP B2RXH2
B	-9	LEU	-	expression tag	UNP B2RXH2
B	-8	GLY	-	expression tag	UNP B2RXH2
B	-7	THR	-	expression tag	UNP B2RXH2
B	-6	GLU	-	expression tag	UNP B2RXH2
B	-5	ASN	-	expression tag	UNP B2RXH2
B	-4	LEU	-	expression tag	UNP B2RXH2
B	-3	TYR	-	expression tag	UNP B2RXH2
B	-2	PHE	-	expression tag	UNP B2RXH2
B	-1	GLN	-	expression tag	UNP B2RXH2
B	0	SER	-	expression tag	UNP B2RXH2
C	-21	MET	-	expression tag	UNP B2RXH2
C	-20	HIS	-	expression tag	UNP B2RXH2
C	-19	HIS	-	expression tag	UNP B2RXH2
C	-18	HIS	-	expression tag	UNP B2RXH2
C	-17	HIS	-	expression tag	UNP B2RXH2
C	-16	HIS	-	expression tag	UNP B2RXH2
C	-15	HIS	-	expression tag	UNP B2RXH2
C	-14	SER	-	expression tag	UNP B2RXH2
C	-13	SER	-	expression tag	UNP B2RXH2
C	-12	GLY	-	expression tag	UNP B2RXH2
C	-11	VAL	-	expression tag	UNP B2RXH2
C	-10	ASP	-	expression tag	UNP B2RXH2
C	-9	LEU	-	expression tag	UNP B2RXH2
C	-8	GLY	-	expression tag	UNP B2RXH2
C	-7	THR	-	expression tag	UNP B2RXH2
C	-6	GLU	-	expression tag	UNP B2RXH2
C	-5	ASN	-	expression tag	UNP B2RXH2
C	-4	LEU	-	expression tag	UNP B2RXH2
C	-3	TYR	-	expression tag	UNP B2RXH2
C	-2	PHE	-	expression tag	UNP B2RXH2
C	-1	GLN	-	expression tag	UNP B2RXH2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP B2RXH2

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 3 is PYRIDINE-2,4-DICARBOXYLIC ACID (three-letter code: PD2) (formula: $C_7H_5NO_4$).
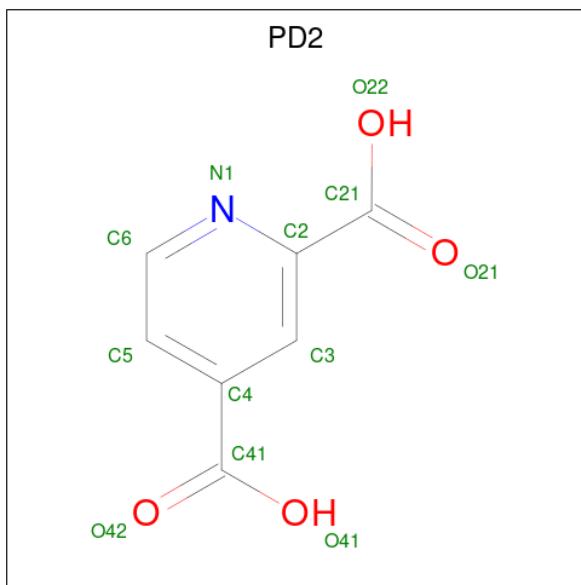
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 12	C 7	N 1	O 4	0	0
3	B	1	Total 12	C 7	N 1	O 4	0	0
3	C	1	Total 12	C 7	N 1	O 4	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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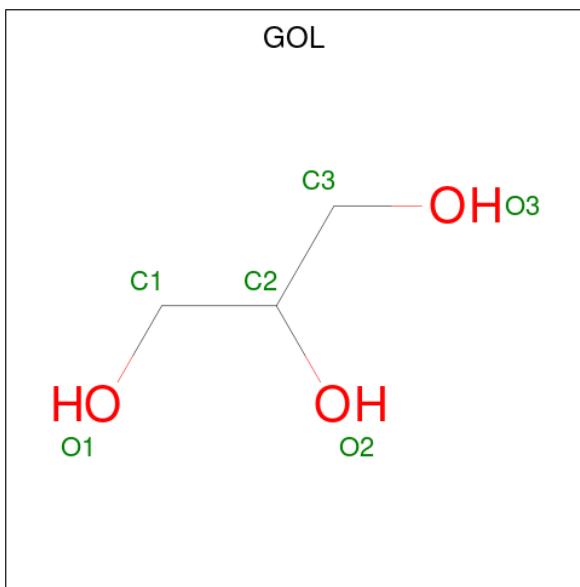
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	115	Total 115	O 115	0	0
5	B	122	Total 122	O 122	0	0
5	C	104	Total 104	O 104	0	0

3 Residue-property plots ⓘ

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: 2-OXOGLUTARATE OXYGENASE
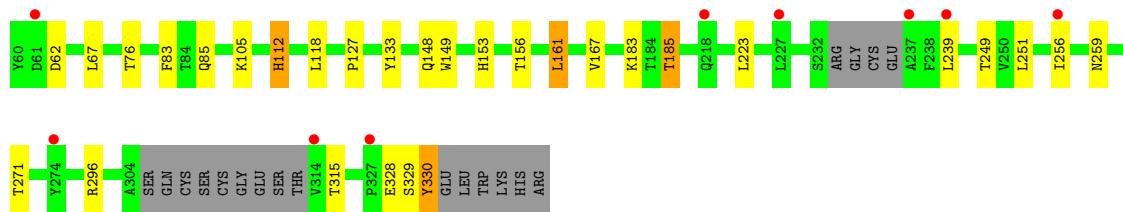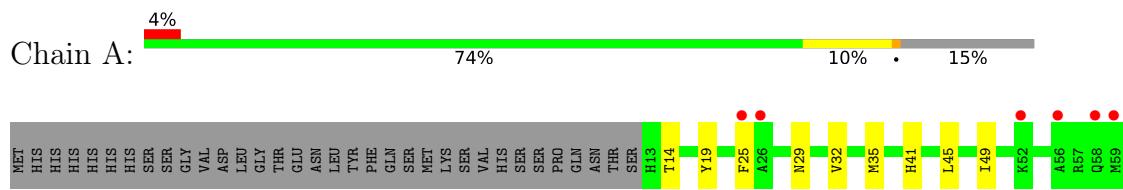
Chain A:

- Molecule 1: 2-OXOGLUTARATE OXYGENASE

Chain B:

- Molecule 1: 2-OXOGLUTARATE OXYGENASE

Chain C:
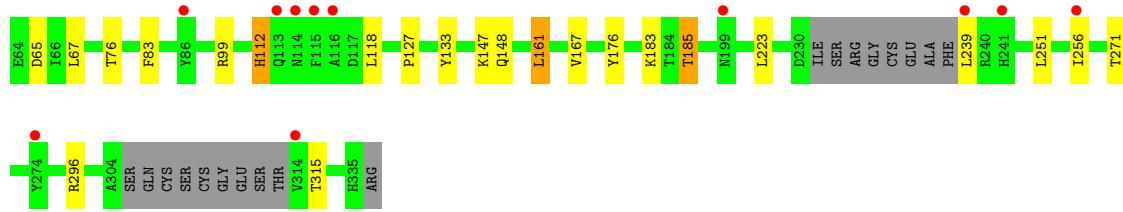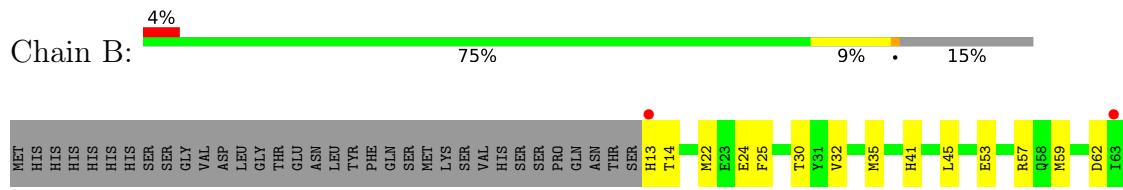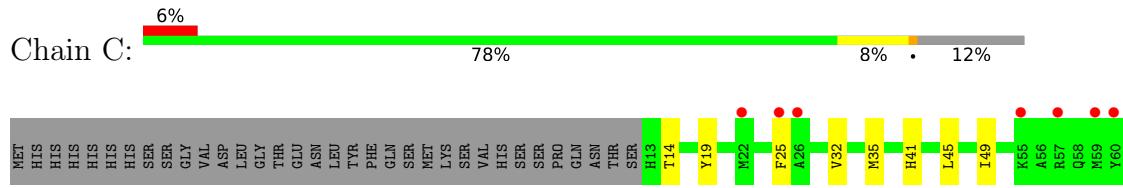
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	90.90Å 111.01Å 224.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	111.80 – 2.10 41.34 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (111.80-2.10) 99.9 (41.34-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0055	Depositor
R, R_{free}	0.210 , 0.236 0.234 , 0.248	Depositor DCC
R_{free} test set	3333 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	35.4	Xtriage
Anisotropy	0.647	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7717	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: NI, 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	0.64	2/2478 (0.1%)	0.66	1/3379 (0.0%)
1	B	0.61	0/2522	0.65	1/3439 (0.0%)
1	C	0.57	0/2564	0.65	3/3494 (0.1%)
All	All	0.60	2/7564 (0.0%)	0.65	5/10312 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	GLN	CD-NE2	-5.46	1.19	1.32
1	A	259	ASN	CG-OD1	-5.13	1.12	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	296	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	B	296	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	C	177	LEU	CB-CG-CD1	6.49	122.04	111.00
1	C	296	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	C	296	ARG	NE-CZ-NH1	-5.29	117.66	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	GLN	Peptide
1	B	148	GLN	Peptide
1	C	148	GLN	Peptide

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	2396	0	2208	28	0
1	B	2435	0	2254	25	0
1	C	2476	0	2302	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	12	0	3	0	0
3	B	12	0	3	0	0
3	C	12	0	3	0	0
4	A	12	0	16	3	0
4	B	18	0	24	1	0
5	A	115	0	0	0	0
5	B	122	0	0	2	0
5	C	104	0	0	1	0
All	All	7717	0	6813	70	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 5.

All (70) 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:161:LEU:HD22	1:C:167:VAL:HB	1.58	0.85
1:A:161:LEU:HD22	1:A:167:VAL:HB	1.63	0.79
1:B:161:LEU:HD22	1:B:167:VAL:HB	1.65	0.79
1:C:112:HIS:ND1	1:C:118:LEU:HD13	2.05	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:SER:O	1:A:330:TYR:O	2.10	0.70
1:A:112:HIS:ND1	1:A:118:LEU:HD13	2.10	0.67
1:B:112:HIS:ND1	1:B:118:LEU:HD13	2.10	0.67
1:A:105:LYS:CE	1:B:30:THR:HG22	2.26	0.66
1:A:112:HIS:CE1	1:A:118:LEU:HD22	2.31	0.66
1:B:112:HIS:CE1	1:B:118:LEU:HD22	2.31	0.65
1:A:328:GLU:HG2	1:A:329:SER:OG	1.97	0.63
1:C:223:LEU:CD2	1:C:256:ILE:HD12	2.32	0.60
1:B:223:LEU:CD2	1:B:256:ILE:HD12	2.32	0.59
1:A:223:LEU:CD2	1:A:256:ILE:HD12	2.35	0.57
1:B:223:LEU:HD23	1:B:256:ILE:HD12	1.88	0.56
1:B:32:VAL:HA	1:B:35:MET:CE	2.36	0.55
1:B:22:MET:HE3	1:B:53:GLU:HB2	1.88	0.55
1:B:32:VAL:HA	1:B:35:MET:HE3	1.90	0.53
1:B:32:VAL:HG22	1:B:35:MET:HE3	1.89	0.53
1:B:22:MET:CE	1:B:53:GLU:HB2	2.39	0.53
1:C:239:LEU:HD12	1:C:239:LEU:N	2.23	0.53
1:C:112:HIS:CE1	1:C:118:LEU:HD22	2.44	0.53
1:C:223:LEU:HD23	1:C:256:ILE:HD12	1.91	0.53
1:B:41:HIS:H	1:B:41:HIS:CD2	2.27	0.52
1:A:153:HIS:O	4:A:1331:GOL:H31	2.10	0.52
1:A:105:LYS:CE	1:B:30:THR:CG2	2.88	0.51
1:A:223:LEU:HD23	1:A:256:ILE:HD12	1.91	0.51
1:C:45:LEU:HD13	1:C:271:THR:HG22	1.93	0.51
1:A:149:TRP:N	4:A:1331:GOL:O3	2.44	0.50
1:B:62:ASP:OD1	1:B:62:ASP:N	2.45	0.50
1:B:239:LEU:N	1:B:239:LEU:HD12	2.27	0.50
1:A:249:THR:HB	4:A:1332:GOL:H12	1.94	0.50
1:A:45:LEU:HD13	1:A:271:THR:HG22	1.94	0.49
1:C:32:VAL:HA	1:C:35:MET:CE	2.41	0.49
1:A:41:HIS:CD2	1:A:41:HIS:H	2.29	0.49
1:C:62:ASP:N	1:C:62:ASP:OD1	2.44	0.49
1:A:32:VAL:HA	1:A:35:MET:CE	2.42	0.49
1:B:99:ARG:NH1	5:B:2042:HOH:O	2.45	0.49
1:B:76:THR:CG2	1:B:83:PHE:HB3	2.43	0.48
1:B:112:HIS:ND1	1:B:118:LEU:HB2	2.28	0.48
1:A:105:LYS:HB3	1:B:24:GLU:HG2	1.96	0.47
1:A:62:ASP:N	1:A:62:ASP:OD1	2.46	0.47
1:C:223:LEU:HD22	1:C:256:ILE:HD12	1.95	0.47
1:A:183:LYS:O	1:A:185:THR:HG22	2.15	0.47
1:A:76:THR:CG2	1:A:83:PHE:HB3	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:LYS:O	1:C:335:HIS:CB	2.63	0.47
1:C:32:VAL:HA	1:C:35:MET:HE2	1.97	0.46
1:C:32:VAL:HG22	1:C:35:MET:HE3	1.97	0.46
1:A:32:VAL:HG22	1:A:35:MET:HE3	1.98	0.46
1:A:239:LEU:HD12	1:A:239:LEU:N	2.30	0.46
1:B:183:LYS:O	1:B:185:THR:HG22	2.14	0.46
1:C:41:HIS:H	1:C:41:HIS:CD2	2.33	0.46
1:C:76:THR:CG2	1:C:83:PHE:HB3	2.46	0.45
1:A:29:ASN:OD1	1:A:156:THR:HG22	2.15	0.45
1:B:45:LEU:HD13	1:B:271:THR:HG22	1.97	0.45
1:B:223:LEU:HD22	1:B:256:ILE:HD12	1.98	0.44
1:B:57:ARG:HD3	1:B:59:MET:O	2.18	0.44
1:A:112:HIS:ND1	1:A:118:LEU:HB2	2.32	0.44
1:A:223:LEU:HD22	1:A:256:ILE:HD12	2.00	0.43
1:C:183:LYS:O	1:C:185:THR:HG22	2.18	0.42
1:C:112:HIS:ND1	1:C:118:LEU:HB2	2.34	0.42
1:C:331:GLU:O	1:C:334:LYS:O	2.37	0.42
1:A:32:VAL:HA	1:A:35:MET:HE2	2.00	0.42
1:A:76:THR:HG23	1:A:83:PHE:HB3	2.01	0.42
1:B:147:LYS:O	4:B:1336:GOL:H32	2.20	0.42
1:B:65:ASP:HB2	5:B:2028:HOH:O	2.20	0.41
1:C:19:TYR:CE2	1:C:49:ILE:HD12	2.55	0.41
1:A:19:TYR:CE2	1:A:49:ILE:HD12	2.56	0.41
1:A:112:HIS:ND1	1:A:118:LEU:HD22	2.35	0.41
1:C:259:ASN:ND2	5:C:2075:HOH:O	2.53	0.41

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	300/358 (84%)	291 (97%)	8 (3%)	1 (0%)	41	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	302/358 (84%)	294 (97%)	7 (2%)	1 (0%)	41	41
1	C	312/358 (87%)	302 (97%)	9 (3%)	1 (0%)	41	41
All	All	914/1074 (85%)	887 (97%)	24 (3%)	3 (0%)	41	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	PRO
1	B	127	PRO
1	C	127	PRO

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	238/311 (76%)	228 (96%)	10 (4%)	30	30
1	B	245/311 (79%)	234 (96%)	11 (4%)	27	27
1	C	247/311 (79%)	236 (96%)	11 (4%)	27	27
All	All	730/933 (78%)	698 (96%)	32 (4%)	28	28

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	25	PHE
1	A	67	LEU
1	A	112	HIS
1	A	133	TYR
1	A	161	LEU
1	A	185	THR
1	A	251	LEU
1	A	315	THR
1	A	330	TYR
1	B	13	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	14	THR
1	B	25	PHE
1	B	67	LEU
1	B	112	HIS
1	B	133	TYR
1	B	161	LEU
1	B	176	TYR
1	B	185	THR
1	B	251	LEU
1	B	315	THR
1	C	14	THR
1	C	25	PHE
1	C	67	LEU
1	C	112	HIS
1	C	133	TYR
1	C	161	LEU
1	C	176	TYR
1	C	177	LEU
1	C	185	THR
1	C	251	LEU
1	C	315	THR

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	41	HIS
1	B	41	HIS
1	B	259	ASN
1	C	41	HIS
1	C	103	ASN
1	C	113	GLN
1	C	259	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	PD2	B	402	2	12,12,12	1.09	0	16,16,16	1.76	5 (31%)
4	GOL	B	1338	-	5,5,5	0.41	0	5,5,5	0.22	0
3	PD2	C	502	2	12,12,12	1.33	3 (25%)	16,16,16	1.57	4 (25%)
4	GOL	B	1337	-	5,5,5	0.38	0	5,5,5	0.18	0
4	GOL	B	1336	-	5,5,5	0.63	0	5,5,5	0.44	0
3	PD2	A	602	2	12,12,12	1.17	1 (8%)	16,16,16	2.51	4 (25%)
4	GOL	A	1332	-	5,5,5	0.27	0	5,5,5	0.75	0
4	GOL	A	1331	-	5,5,5	0.59	0	5,5,5	0.95	0

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	PD2	B	402	2	-	4/8/8/8	0/1/1/1
4	GOL	B	1338	-	-	4/4/4/4	-
3	PD2	C	502	2	-	7/8/8/8	0/1/1/1
4	GOL	B	1337	-	-	2/4/4/4	-
4	GOL	B	1336	-	-	2/4/4/4	-
3	PD2	A	602	2	-	4/8/8/8	0/1/1/1
4	GOL	A	1332	-	-	2/4/4/4	-
4	GOL	A	1331	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	PD2	C2-C21	2.40	1.54	1.50
3	C	502	PD2	C4-C41	2.40	1.54	1.49
3	A	602	PD2	O41-C41	-2.17	1.23	1.30
3	C	502	PD2	O41-C41	-2.00	1.24	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	PD2	C6-N1-C2	5.94	124.64	116.93
3	A	602	PD2	C4-C3-C2	-4.79	115.28	118.92
3	A	602	PD2	C5-C6-N1	-4.71	118.11	123.96
3	B	402	PD2	C6-N1-C2	3.74	121.79	116.93
3	C	502	PD2	C6-N1-C2	3.41	121.35	116.93
3	B	402	PD2	O21-C21-C2	-3.04	115.08	121.24
3	C	502	PD2	C3-C2-N1	-2.68	119.81	123.19
3	B	402	PD2	C5-C6-N1	-2.45	120.92	123.96
3	A	602	PD2	C3-C2-N1	-2.35	120.24	123.19
3	C	502	PD2	O21-C21-C2	-2.32	116.54	121.24
3	B	402	PD2	C3-C2-N1	-2.27	120.34	123.19
3	B	402	PD2	O22-C21-C2	2.21	119.71	114.69
3	C	502	PD2	O22-C21-C2	2.18	119.66	114.69

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1331	GOL	C1-C2-C3-O3
4	A	1332	GOL	O1-C1-C2-C3
4	B	1336	GOL	C1-C2-C3-O3
4	B	1337	GOL	C1-C2-C3-O3
4	B	1338	GOL	O1-C1-C2-C3
3	B	402	PD2	C5-C4-C41-O41
3	C	502	PD2	C5-C4-C41-O41
3	B	402	PD2	C3-C4-C41-O41
3	A	602	PD2	C5-C4-C41-O41
3	C	502	PD2	C3-C4-C41-O41
4	B	1338	GOL	O2-C2-C3-O3
3	B	402	PD2	C5-C4-C41-O42
3	A	602	PD2	C3-C4-C41-O41
3	B	402	PD2	C3-C4-C41-O42
3	C	502	PD2	C5-C4-C41-O42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	1338	GOL	C1-C2-C3-O3
3	A	602	PD2	C5-C4-C41-O42
4	A	1332	GOL	O1-C1-C2-O2
4	B	1336	GOL	O2-C2-C3-O3
4	B	1337	GOL	O2-C2-C3-O3
3	C	502	PD2	C3-C4-C41-O42
3	A	602	PD2	C3-C4-C41-O42
4	A	1331	GOL	O2-C2-C3-O3
3	C	502	PD2	C3-C2-C21-O22
3	C	502	PD2	N1-C2-C21-O22
4	B	1338	GOL	O1-C1-C2-O2
3	C	502	PD2	C3-C2-C21-O21

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1336	GOL	1	0
4	A	1332	GOL	1	0
4	A	1331	GOL	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, 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(Å²)	Q<0.9
1	A	305/358 (85%)	0.55	15 (4%)	29	35	2, 15, 40, 65	0
1	B	306/358 (85%)	0.48	13 (4%)	36	42	2, 15, 37, 61	0
1	C	314/358 (87%)	0.56	23 (7%)	15	19	2, 15, 41, 75	0
All	All	925/1074 (86%)	0.53	51 (5%)	25	31	2, 15, 40, 75	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	235	CYS	5.3
1	B	274	TYR	4.7
1	C	274	TYR	3.9
1	C	239	LEU	3.8
1	A	274	TYR	3.8
1	C	61	ASP	3.7
1	A	314	VAL	3.4
1	A	237	ALA	3.3
1	C	237	ALA	3.3
1	A	61	ASP	3.3
1	B	239	LEU	3.3
1	C	238	PHE	3.3
1	C	115[A]	PHE	3.2
1	C	22	MET	3.2
1	A	239	LEU	3.1
1	C	251	LEU	3.1
1	C	60	TYR	3.1
1	A	59	MET	3.1
1	C	219	HIS	3.0
1	B	314	VAL	2.9
1	B	13	HIS	2.9
1	A	52	LYS	2.7
1	A	327	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	116	ALA	2.6
1	C	26	ALA	2.6
1	C	220	LEU	2.6
1	A	25	PHE	2.6
1	B	114	ASN	2.5
1	A	256	ILE	2.5
1	B	63	ILE	2.5
1	C	80	GLY	2.5
1	A	56	ALA	2.5
1	A	218	GLN	2.4
1	B	113	GLN	2.4
1	C	234	GLY	2.4
1	C	227	LEU	2.3
1	B	256	ILE	2.3
1	C	59	MET	2.3
1	C	222	ARG	2.3
1	B	115	PHE	2.3
1	A	227	LEU	2.2
1	C	82	VAL	2.2
1	C	55	LYS	2.2
1	B	241	HIS	2.2
1	B	199[A]	ASN	2.2
1	A	26	ALA	2.1
1	C	25	PHE	2.1
1	A	58	GLN	2.0
1	C	246	ILE	2.0
1	C	57	ARG	2.0
1	B	86	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
4	GOL	B	1338	6/6	0.67	0.28	57,67,70,74	0
4	GOL	B	1337	6/6	0.73	0.30	55,66,69,78	0
4	GOL	A	1332	6/6	0.73	0.19	61,65,66,69	0
4	GOL	A	1331	6/6	0.80	0.27	40,48,57,58	0
4	GOL	B	1336	6/6	0.92	0.22	44,49,52,58	0
3	PD2	C	502	12/12	0.94	0.19	30,34,45,46	0
3	PD2	B	402	12/12	0.95	0.26	25,29,36,41	0
3	PD2	A	602	12/12	0.96	0.22	21,24,32,36	0
2	NI	B	401	1/1	0.97	0.28	30,30,30,30	0
2	NI	C	501	1/1	0.98	0.28	35,35,35,35	0
2	NI	A	601	1/1	0.99	0.27	26,26,26,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.