



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:56 AM UTC

PDB ID : 4HG3 / pdb_00004hg3
Title : Structural insights into yeast Nit2: wild-type yeast Nit2 in complex with alpha-ketoglutarate
Authors : Liu, H.; Qiu, X.; Zhang, M.; Gao, Y.; Niu, L.; Teng, M.
Deposited on : 2012-10-06
Resolution : 1.93 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

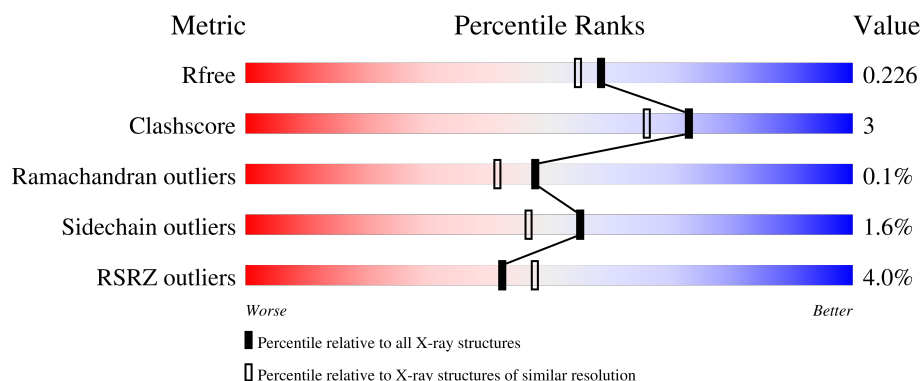
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

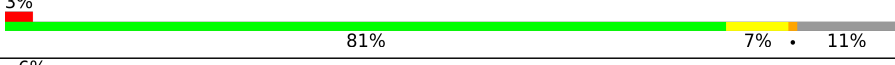
The reported resolution of this entry is 1.93 Å.

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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	341	
1	B	341	
1	C	341	
1	D	341	

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
2	AKG	A	401	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10264 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 Probable hydrolase NIT2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	2	0
			2393	1523	417	441	12			
1	B	303	Total	C	N	O	S	0	1	0
			2391	1520	418	442	11			
1	C	303	Total	C	N	O	S	0	1	0
			2380	1510	415	445	10			
1	D	292	Total	C	N	O	S	0	1	0
			2317	1473	403	431	10			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	expression tag	UNP P47016
A	-32	GLY	-	expression tag	UNP P47016
A	-31	SER	-	expression tag	UNP P47016
A	-30	SER	-	expression tag	UNP P47016
A	-29	HIS	-	expression tag	UNP P47016
A	-28	HIS	-	expression tag	UNP P47016
A	-27	HIS	-	expression tag	UNP P47016
A	-26	HIS	-	expression tag	UNP P47016
A	-25	HIS	-	expression tag	UNP P47016
A	-24	HIS	-	expression tag	UNP P47016
A	-23	SER	-	expression tag	UNP P47016
A	-22	SER	-	expression tag	UNP P47016
A	-21	GLY	-	expression tag	UNP P47016
A	-20	LEU	-	expression tag	UNP P47016
A	-19	VAL	-	expression tag	UNP P47016
A	-18	PRO	-	expression tag	UNP P47016
A	-17	ARG	-	expression tag	UNP P47016
A	-16	GLY	-	expression tag	UNP P47016
A	-15	SER	-	expression tag	UNP P47016
A	-14	HIS	-	expression tag	UNP P47016
A	-13	MET	-	expression tag	UNP P47016

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	ALA	-	expression tag	UNP P47016
A	-11	SER	-	expression tag	UNP P47016
A	-10	MET	-	expression tag	UNP P47016
A	-9	THR	-	expression tag	UNP P47016
A	-8	GLY	-	expression tag	UNP P47016
A	-7	GLY	-	expression tag	UNP P47016
A	-6	GLN	-	expression tag	UNP P47016
A	-5	GLN	-	expression tag	UNP P47016
A	-4	MET	-	expression tag	UNP P47016
A	-3	GLY	-	expression tag	UNP P47016
A	-2	ARG	-	expression tag	UNP P47016
A	-1	GLY	-	expression tag	UNP P47016
A	0	SER	-	expression tag	UNP P47016
B	-33	MET	-	expression tag	UNP P47016
B	-32	GLY	-	expression tag	UNP P47016
B	-31	SER	-	expression tag	UNP P47016
B	-30	SER	-	expression tag	UNP P47016
B	-29	HIS	-	expression tag	UNP P47016
B	-28	HIS	-	expression tag	UNP P47016
B	-27	HIS	-	expression tag	UNP P47016
B	-26	HIS	-	expression tag	UNP P47016
B	-25	HIS	-	expression tag	UNP P47016
B	-24	HIS	-	expression tag	UNP P47016
B	-23	SER	-	expression tag	UNP P47016
B	-22	SER	-	expression tag	UNP P47016
B	-21	GLY	-	expression tag	UNP P47016
B	-20	LEU	-	expression tag	UNP P47016
B	-19	VAL	-	expression tag	UNP P47016
B	-18	PRO	-	expression tag	UNP P47016
B	-17	ARG	-	expression tag	UNP P47016
B	-16	GLY	-	expression tag	UNP P47016
B	-15	SER	-	expression tag	UNP P47016
B	-14	HIS	-	expression tag	UNP P47016
B	-13	MET	-	expression tag	UNP P47016
B	-12	ALA	-	expression tag	UNP P47016
B	-11	SER	-	expression tag	UNP P47016
B	-10	MET	-	expression tag	UNP P47016
B	-9	THR	-	expression tag	UNP P47016
B	-8	GLY	-	expression tag	UNP P47016
B	-7	GLY	-	expression tag	UNP P47016
B	-6	GLN	-	expression tag	UNP P47016
B	-5	GLN	-	expression tag	UNP P47016

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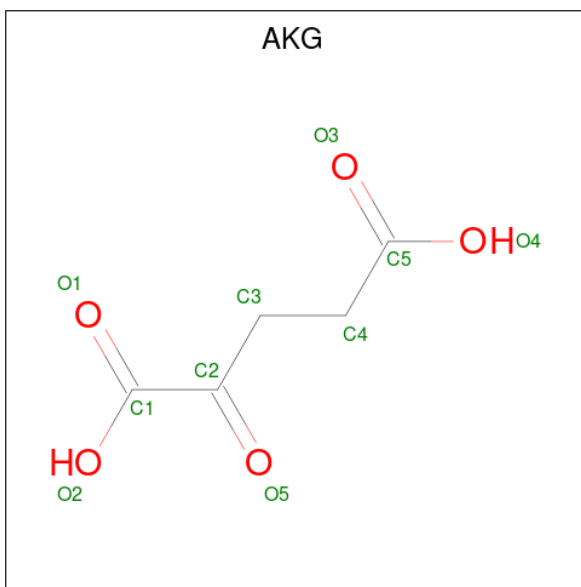
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	expression tag	UNP P47016
B	-3	GLY	-	expression tag	UNP P47016
B	-2	ARG	-	expression tag	UNP P47016
B	-1	GLY	-	expression tag	UNP P47016
B	0	SER	-	expression tag	UNP P47016
C	-33	MET	-	expression tag	UNP P47016
C	-32	GLY	-	expression tag	UNP P47016
C	-31	SER	-	expression tag	UNP P47016
C	-30	SER	-	expression tag	UNP P47016
C	-29	HIS	-	expression tag	UNP P47016
C	-28	HIS	-	expression tag	UNP P47016
C	-27	HIS	-	expression tag	UNP P47016
C	-26	HIS	-	expression tag	UNP P47016
C	-25	HIS	-	expression tag	UNP P47016
C	-24	HIS	-	expression tag	UNP P47016
C	-23	SER	-	expression tag	UNP P47016
C	-22	SER	-	expression tag	UNP P47016
C	-21	GLY	-	expression tag	UNP P47016
C	-20	LEU	-	expression tag	UNP P47016
C	-19	VAL	-	expression tag	UNP P47016
C	-18	PRO	-	expression tag	UNP P47016
C	-17	ARG	-	expression tag	UNP P47016
C	-16	GLY	-	expression tag	UNP P47016
C	-15	SER	-	expression tag	UNP P47016
C	-14	HIS	-	expression tag	UNP P47016
C	-13	MET	-	expression tag	UNP P47016
C	-12	ALA	-	expression tag	UNP P47016
C	-11	SER	-	expression tag	UNP P47016
C	-10	MET	-	expression tag	UNP P47016
C	-9	THR	-	expression tag	UNP P47016
C	-8	GLY	-	expression tag	UNP P47016
C	-7	GLY	-	expression tag	UNP P47016
C	-6	GLN	-	expression tag	UNP P47016
C	-5	GLN	-	expression tag	UNP P47016
C	-4	MET	-	expression tag	UNP P47016
C	-3	GLY	-	expression tag	UNP P47016
C	-2	ARG	-	expression tag	UNP P47016
C	-1	GLY	-	expression tag	UNP P47016
C	0	SER	-	expression tag	UNP P47016
D	-33	MET	-	expression tag	UNP P47016
D	-32	GLY	-	expression tag	UNP P47016
D	-31	SER	-	expression tag	UNP P47016

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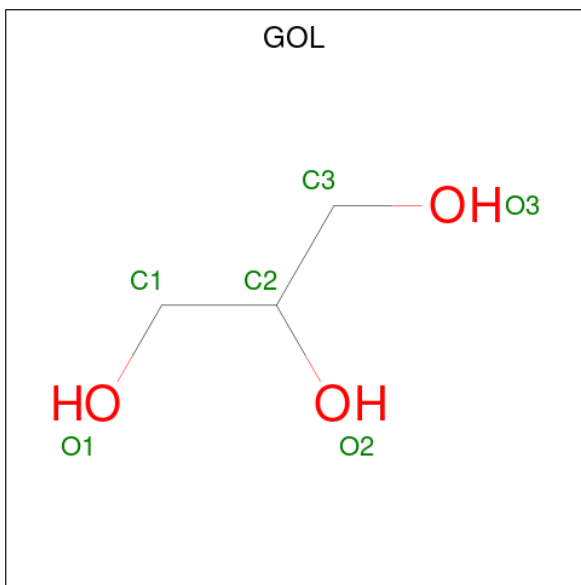
Chain	Residue	Modelled	Actual	Comment	Reference
D	-30	SER	-	expression tag	UNP P47016
D	-29	HIS	-	expression tag	UNP P47016
D	-28	HIS	-	expression tag	UNP P47016
D	-27	HIS	-	expression tag	UNP P47016
D	-26	HIS	-	expression tag	UNP P47016
D	-25	HIS	-	expression tag	UNP P47016
D	-24	HIS	-	expression tag	UNP P47016
D	-23	SER	-	expression tag	UNP P47016
D	-22	SER	-	expression tag	UNP P47016
D	-21	GLY	-	expression tag	UNP P47016
D	-20	LEU	-	expression tag	UNP P47016
D	-19	VAL	-	expression tag	UNP P47016
D	-18	PRO	-	expression tag	UNP P47016
D	-17	ARG	-	expression tag	UNP P47016
D	-16	GLY	-	expression tag	UNP P47016
D	-15	SER	-	expression tag	UNP P47016
D	-14	HIS	-	expression tag	UNP P47016
D	-13	MET	-	expression tag	UNP P47016
D	-12	ALA	-	expression tag	UNP P47016
D	-11	SER	-	expression tag	UNP P47016
D	-10	MET	-	expression tag	UNP P47016
D	-9	THR	-	expression tag	UNP P47016
D	-8	GLY	-	expression tag	UNP P47016
D	-7	GLY	-	expression tag	UNP P47016
D	-6	GLN	-	expression tag	UNP P47016
D	-5	GLN	-	expression tag	UNP P47016
D	-4	MET	-	expression tag	UNP P47016
D	-3	GLY	-	expression tag	UNP P47016
D	-2	ARG	-	expression tag	UNP P47016
D	-1	GLY	-	expression tag	UNP P47016
D	0	SER	-	expression tag	UNP P47016

- Molecule 2 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅).



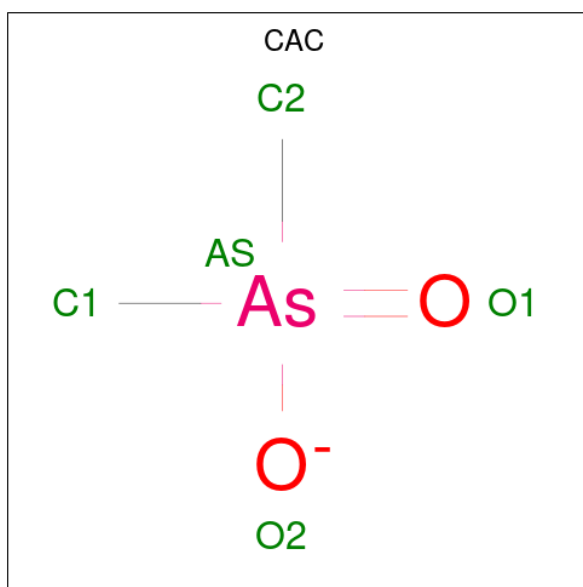
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	5	4		
2	B	1	Total	C	O	0	0
			9	5	4		
2	C	1	Total	C	O	0	0
			9	5	4		
2	D	1	Total	C	O	0	0
			9	5	4		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is CACODYLATE ION (CCD ID: CAC) (formula: $\text{C}_2\text{H}_6\text{AsO}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	C	1	Total	As	C	O	0	0
			5	1	2	2		
4	C	1	Total	As	C	O	0	0
			5	1	2	2		
4	D	1	Total	As	C	O	0	0
			5	1	2	2		

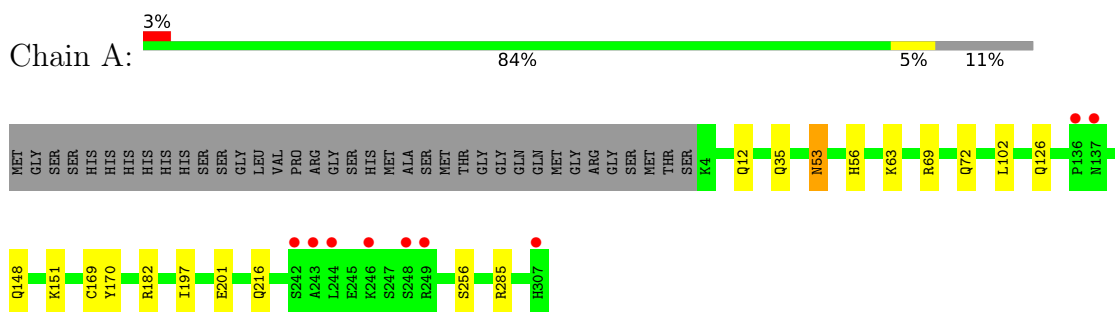
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	176	Total	O	0	0
			176	176		
5	B	163	Total	O	0	0
			163	163		
5	C	166	Total	O	0	0
			166	166		
5	D	111	Total	O	0	0
			111	111		

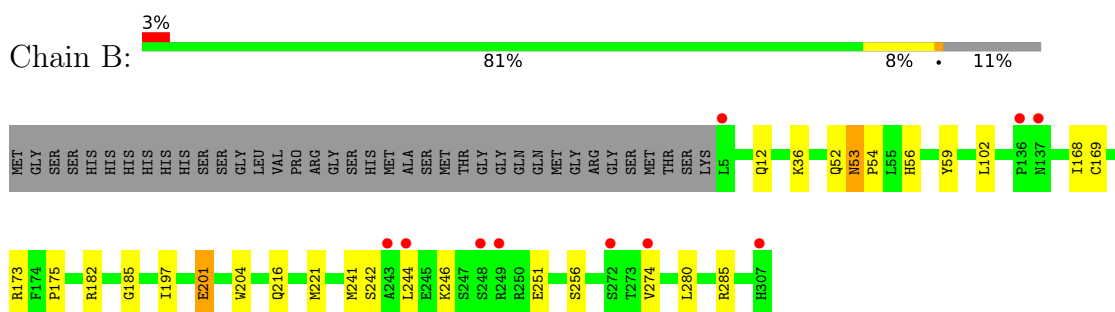
3 Residue-property plots [i](#)

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.

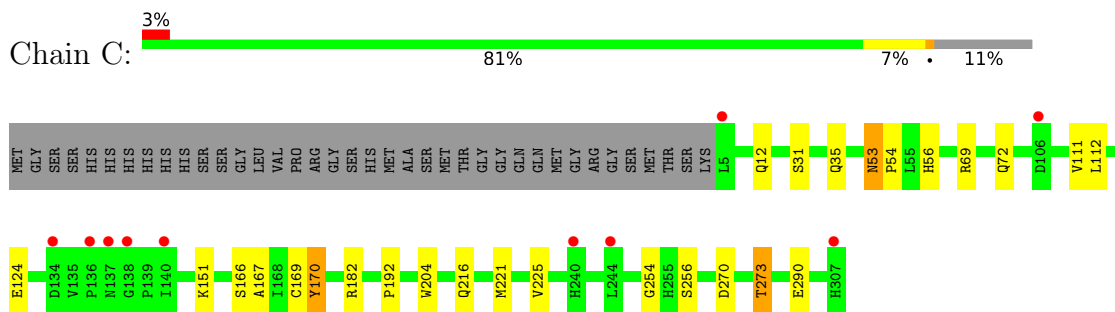
- Molecule 1: Probable hydrolase NIT2



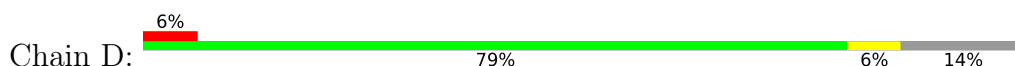
- Molecule 1: Probable hydrolase NIT2

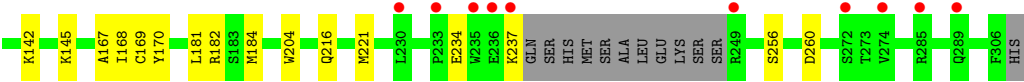
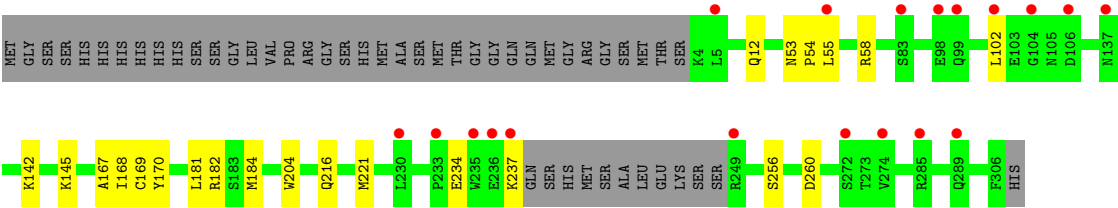


- Molecule 1: Probable hydrolase NIT2



- Molecule 1: Probable hydrolase NIT2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.21Å 125.65Å 77.96Å 90.00° 95.30° 90.00°	Depositor
Resolution (Å)	48.84 – 1.93 48.84 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.84-1.93) 99.3 (48.84-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.197 , 0.227 0.196 , 0.226	Depositor DCC
R_{free} test set	4671 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10264	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.25% 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: CAC, AKG, GOL

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	0.55	3/2449 (0.1%)	0.78	1/3315 (0.0%)
1	B	0.56	3/2445 (0.1%)	0.87	5/3312 (0.2%)
1	C	0.51	1/2433 (0.0%)	0.79	2/3299 (0.1%)
1	D	0.58	4/2368 (0.2%)	0.82	2/3208 (0.1%)
All	All	0.55	11/9695 (0.1%)	0.82	10/13134 (0.1%)

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	D	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	169	CYS	C-N	9.92	1.47	1.34
1	A	169	CYS	C-N	9.51	1.47	1.33
1	D	169	CYS	C-N	7.10	1.43	1.33
1	A	170	TYR	N-CA	6.75	1.54	1.46
1	D	169	CYS	CA-CB	-6.62	1.42	1.53
1	B	169	CYS	CA-C	-6.43	1.44	1.52
1	D	170	TYR	C-O	-6.22	1.16	1.24
1	D	167	ALA	C-O	-5.86	1.16	1.23
1	A	169	CYS	N-CA	5.54	1.53	1.46
1	C	169	CYS	N-CA	-5.33	1.39	1.46
1	B	168	ILE	C-N	5.05	1.40	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	CYS	O-C-N	-11.39	107.44	122.59
1	B	169	CYS	CA-C-N	10.51	135.41	120.28
1	B	169	CYS	C-N-CA	10.51	135.41	120.28
1	B	168	ILE	O-C-N	7.13	130.60	123.18
1	D	169	CYS	CA-C-N	7.06	135.02	121.54
1	D	169	CYS	C-N-CA	7.06	135.02	121.54
1	B	168	ILE	N-CA-C	5.51	115.93	107.77
1	A	169	CYS	N-CA-C	5.35	122.20	110.80
1	C	170	TYR	N-CA-C	5.20	121.87	110.80
1	C	169	CYS	N-CA-C	5.00	121.45	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	168	ILE	Mainchain

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	2393	0	2395	11	0
1	B	2391	0	2387	18	0
1	C	2380	0	2354	16	0
1	D	2317	0	2315	17	0
2	A	9	0	4	0	0
2	B	9	0	4	0	0
2	C	9	0	4	0	0
2	D	9	0	4	0	0
3	A	42	0	56	1	0
3	B	30	0	40	4	0
3	C	12	0	16	0	0
3	D	12	0	16	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	5	0	0	0	0
5	A	176	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	163	0	0	0	0
5	C	166	0	0	0	0
5	D	111	0	0	0	0
All	All	10264	0	9595	62	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 3.

All (62) 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:D:234:GLU:O	1:D:237:LYS:HB2	1.75	0.86
1:A:151:LYS:O	3:B:406:GOL:H31	1.82	0.80
1:D:181:LEU:HD23	1:D:184:MET:CE	2.15	0.75
1:D:182:ARG:HH12	1:D:216:GLN:HE21	1.36	0.73
1:B:182:ARG:HH12	1:B:216:GLN:HE21	1.39	0.70
1:C:182:ARG:HH12	1:C:216:GLN:HE21	1.39	0.69
1:D:181:LEU:HD23	1:D:184:MET:HE1	1.74	0.69
1:A:182:ARG:HH12	1:A:216:GLN:HE21	1.39	0.68
1:D:181:LEU:HA	1:D:184:MET:CE	2.25	0.67
1:C:31:SER:O	1:C:35:GLN:HG2	1.97	0.65
1:B:52:GLN:HE22	1:B:241:MET:HE1	1.62	0.64
1:C:53:ASN:ND2	1:C:56:HIS:H	1.98	0.61
1:C:53:ASN:HB2	1:C:54:PRO:HD2	1.83	0.60
1:B:53:ASN:ND2	1:B:56:HIS:H	1.99	0.60
1:D:181:LEU:HA	1:D:184:MET:HE3	1.83	0.59
1:B:197:ILE:O	1:B:201:GLU:HG2	2.04	0.58
1:D:53:ASN:HB2	1:D:54:PRO:HD2	1.85	0.57
1:A:53:ASN:ND2	1:A:56:HIS:H	2.03	0.56
1:C:53:ASN:HB2	1:C:54:PRO:CD	2.37	0.55
1:D:142:LYS:HD3	1:D:145:LYS:HG3	1.91	0.52
1:B:53:ASN:HB2	1:B:54:PRO:CD	2.40	0.52
1:B:52:GLN:NE2	1:B:241:MET:HE1	2.24	0.52
1:C:12:GLN:NE2	1:C:256:SER:H	2.08	0.52
1:A:12:GLN:NE2	1:A:256:SER:H	2.08	0.52
1:C:12:GLN:HE22	1:C:256:SER:H	1.57	0.52
1:D:12:GLN:NE2	1:D:256:SER:H	2.08	0.51
1:B:12:GLN:NE2	1:B:256:SER:H	2.09	0.51
1:C:53:ASN:C	1:C:53:ASN:HD22	2.18	0.51
1:B:12:GLN:HE22	1:B:256:SER:H	1.59	0.50
1:A:12:GLN:HE22	1:A:256:SER:H	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:VAL:HG11	1:C:124[B]:GLU:HG3	1.93	0.49
1:A:126:GLN:HE22	1:A:148:GLN:HE21	1.59	0.49
1:C:53:ASN:HD22	1:C:56:HIS:H	1.59	0.48
1:A:151:LYS:O	3:B:406:GOL:C3	2.58	0.48
1:D:12:GLN:HE22	1:D:256:SER:H	1.60	0.48
1:D:181:LEU:HA	1:D:184:MET:HE2	1.95	0.48
1:B:197:ILE:HD11	1:B:251:GLU:HG2	1.94	0.48
1:B:53:ASN:C	1:B:53:ASN:HD22	2.22	0.48
1:C:270:ASP:HB3	1:C:273:THR:CG2	2.44	0.48
1:D:181:LEU:HD23	1:D:184:MET:HE3	1.95	0.47
1:A:63:LYS:HE3	3:A:408:GOL:H32	1.96	0.47
1:B:36:LYS:HD3	1:B:280:LEU:HD11	1.96	0.46
1:A:69:ARG:HA	1:A:72:GLN:HE21	1.80	0.46
1:D:204:TRP:CZ2	1:D:221[A]:MET:HB3	2.50	0.46
1:B:242:SER:O	1:B:246:LYS:HG3	2.16	0.46
1:C:204:TRP:CZ2	1:C:221:MET:HB3	2.51	0.45
1:C:69:ARG:HA	1:C:72:GLN:HE21	1.81	0.45
1:A:197:ILE:O	1:A:201:GLU:HG2	2.16	0.45
1:B:53:ASN:HB2	1:B:54:PRO:HD2	1.98	0.44
1:A:53:ASN:HD22	1:A:53:ASN:C	2.26	0.43
1:D:53:ASN:HB2	1:D:54:PRO:CD	2.48	0.43
1:D:204:TRP:CZ2	1:D:221[B]:MET:HB3	2.52	0.43
1:D:53:ASN:HD22	1:D:55:LEU:H	1.65	0.42
1:D:260:ASP:OD1	1:D:260:ASP:C	2.63	0.42
1:B:204:TRP:CZ2	1:B:221[B]:MET:HB3	2.55	0.42
1:C:112:LEU:HD23	1:C:166:SER:HB3	2.01	0.42
1:B:173:ARG:O	1:B:175:PRO:HD3	2.19	0.41
1:B:185:GLY:O	3:B:404:GOL:H31	2.19	0.41
1:B:204:TRP:CZ2	1:B:221[A]:MET:HB3	2.55	0.41
1:C:167:ALA:O	1:C:192:PRO:HD2	2.21	0.41
1:C:225:VAL:HG23	1:C:254:GLY:HA3	2.01	0.41
1:B:59:TYR:OH	3:B:406:GOL:H32	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	304/341 (89%)	300 (99%)	4 (1%)	0	100	100
1	B	302/341 (89%)	298 (99%)	4 (1%)	0	100	100
1	C	302/341 (89%)	295 (98%)	6 (2%)	1 (0%)	36	30
1	D	289/341 (85%)	285 (99%)	4 (1%)	0	100	100
All	All	1197/1364 (88%)	1178 (98%)	18 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	170	TYR

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	263/300 (88%)	259 (98%)	4 (2%)	57	49
1	B	262/300 (87%)	256 (98%)	6 (2%)	44	33
1	C	257/300 (86%)	253 (98%)	4 (2%)	55	46
1	D	253/300 (84%)	251 (99%)	2 (1%)	73	71
All	All	1035/1200 (86%)	1019 (98%)	16 (2%)	55	49

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	53	ASN
1	A	102	LEU
1	A	285	ARG
1	B	53	ASN

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Mol	Chain	Res	Type
1	B	102	LEU
1	B	201	GLU
1	B	244	LEU
1	B	274	VAL
1	B	285	ARG
1	C	53	ASN
1	C	151	LYS
1	C	273	THR
1	C	290	GLU
1	D	58	ARG
1	D	102	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	52	GLN
1	A	53	ASN
1	A	148	GLN
1	A	216	GLN
1	A	268	HIS
1	A	293	ASN
1	B	12	GLN
1	B	52	GLN
1	B	53	ASN
1	B	70	GLN
1	B	148	GLN
1	B	216	GLN
1	B	238	GLN
1	B	240	HIS
1	B	268	HIS
1	B	293	ASN
1	C	12	GLN
1	C	52	GLN
1	C	53	ASN
1	C	72	GLN
1	C	99	GLN
1	C	148	GLN
1	C	216	GLN
1	C	240	HIS
1	C	268	HIS
1	C	293	ASN

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Mol	Chain	Res	Type
1	D	12	GLN
1	D	52	GLN
1	D	53	ASN
1	D	117	HIS
1	D	148	GLN
1	D	216	GLN
1	D	268	HIS
1	D	293	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](#)

27 ligands 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	$\# Z > 2$
4	CAC	C	404	-	2,4,4	2.70	2 (100%)	4,6,6	1.64	0
4	CAC	B	407	-	2,4,4	2.65	2 (100%)	4,6,6	1.59	0
4	CAC	A	409	-	2,4,4	2.62	2 (100%)	4,6,6	1.60	1 (25%)
3	GOL	A	402	-	5,5,5	0.38	0	5,5,5	0.33	0
3	GOL	A	404	-	5,5,5	0.31	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CAC	D	404	-	2,4,4	2.58	2 (100%)	4,6,6	1.17	0
3	GOL	B	404	-	5,5,5	0.32	0	5,5,5	0.34	0
3	GOL	C	402	-	5,5,5	0.37	0	5,5,5	0.40	0
2	AKG	C	401	1	7,8,9	1.77	2 (28%)	9,9,11	3.66	3 (33%)
3	GOL	B	406	-	5,5,5	0.43	0	5,5,5	0.42	0
2	AKG	B	401	1	7,8,9	2.47	4 (57%)	9,9,11	3.94	3 (33%)
3	GOL	C	403	-	5,5,5	0.37	0	5,5,5	0.39	0
4	CAC	A	410	-	2,4,4	2.51	2 (100%)	4,6,6	1.72	1 (25%)
3	GOL	A	406	-	5,5,5	0.39	0	5,5,5	0.35	0
3	GOL	D	403	-	5,5,5	0.37	0	5,5,5	0.31	0
4	CAC	C	405	-	2,4,4	2.39	2 (100%)	4,6,6	1.41	0
3	GOL	B	405	-	5,5,5	0.35	0	5,5,5	0.37	0
4	CAC	B	408	-	2,4,4	2.54	2 (100%)	4,6,6	1.76	1 (25%)
3	GOL	A	405	-	5,5,5	0.42	0	5,5,5	0.48	0
3	GOL	A	403	-	5,5,5	0.38	0	5,5,5	0.38	0
3	GOL	B	403	-	5,5,5	0.33	0	5,5,5	0.52	0
2	AKG	D	401	1	7,8,9	2.15	4 (57%)	9,9,11	2.91	4 (44%)
2	AKG	A	401	1	8,8,9	2.53	5 (62%)	9,9,11	2.63	4 (44%)
3	GOL	B	402	-	5,5,5	0.37	0	5,5,5	0.30	0
3	GOL	D	402	-	5,5,5	0.41	0	5,5,5	0.29	0
3	GOL	A	408	-	5,5,5	0.42	0	5,5,5	0.28	0
3	GOL	A	407	-	5,5,5	0.41	0	5,5,5	0.32	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	GOL	A	402	-	-	0/4/4/4	-
3	GOL	A	404	-	-	0/4/4/4	-
3	GOL	B	404	-	-	2/4/4/4	-
3	GOL	C	402	-	-	2/4/4/4	-
2	AKG	C	401	1	-	2/8/8/9	-
3	GOL	B	406	-	-	4/4/4/4	-
2	AKG	B	401	1	-	1/8/8/9	-
3	GOL	C	403	-	-	0/4/4/4	-
3	GOL	A	406	-	-	2/4/4/4	-
3	GOL	D	403	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	405	-	-	4/4/4/4	-
3	GOL	A	405	-	-	4/4/4/4	-
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	B	403	-	-	4/4/4/4	-
2	AKG	D	401	1	-	0/8/8/9	-
2	AKG	A	401	1	-	1/8/8/9	-
3	GOL	B	402	-	-	0/4/4/4	-
3	GOL	D	402	-	-	0/4/4/4	-
3	GOL	A	408	-	-	2/4/4/4	-
3	GOL	A	407	-	-	2/4/4/4	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	AKG	O4-C5	-4.42	1.19	1.42
2	B	401	AKG	O5-C2	-3.67	1.15	1.23
2	B	401	AKG	O2-C1	-3.19	1.21	1.30
2	D	401	AKG	O2-C1	-3.08	1.22	1.30
2	C	401	AKG	O2-C1	-3.03	1.22	1.30
2	A	401	AKG	O5-C2	-3.01	1.17	1.23
2	B	401	AKG	C3-C2	-2.84	1.47	1.51
2	A	401	AKG	C2-C1	-2.77	1.49	1.53
2	D	401	AKG	O5-C2	-2.72	1.17	1.23
2	A	401	AKG	O2-C1	-2.72	1.23	1.30
4	B	407	CAC	AS-C2	2.72	1.96	1.90
4	C	404	CAC	AS-C1	2.71	1.96	1.90
4	B	408	CAC	AS-C2	2.70	1.96	1.90
4	D	404	CAC	AS-C2	2.70	1.96	1.90
4	A	409	CAC	AS-C1	2.69	1.96	1.90
4	C	404	CAC	AS-C2	2.68	1.96	1.90
2	C	401	AKG	O5-C2	-2.68	1.17	1.23
2	B	401	AKG	C2-C1	-2.61	1.49	1.53
4	B	407	CAC	AS-C1	2.58	1.96	1.90
2	D	401	AKG	C2-C1	-2.58	1.49	1.53
4	A	410	CAC	AS-C1	2.57	1.96	1.90
4	A	409	CAC	AS-C2	2.56	1.96	1.90
4	C	405	CAC	AS-C1	2.49	1.96	1.90
4	D	404	CAC	AS-C1	2.45	1.96	1.90
4	A	410	CAC	AS-C2	2.45	1.96	1.90
2	A	401	AKG	C3-C2	-2.39	1.48	1.51
4	B	408	CAC	AS-C1	2.38	1.95	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	405	CAC	AS-C2	2.29	1.95	1.90
2	D	401	AKG	C3-C4	-2.16	1.46	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	AKG	C4-C3-C2	10.42	125.24	112.67
2	C	401	AKG	C4-C3-C2	9.64	124.30	112.67
2	D	401	AKG	C4-C3-C2	6.88	120.97	112.67
2	A	401	AKG	O1-C1-C2	-5.93	114.43	121.81
2	B	401	AKG	O1-C1-C2	-4.39	116.35	121.81
2	A	401	AKG	C4-C3-C2	3.59	120.58	113.58
2	D	401	AKG	O2-C1-C2	3.35	122.87	113.59
2	C	401	AKG	O1-C1-C2	-3.26	117.76	121.81
2	C	401	AKG	O2-C1-C2	3.03	122.00	113.59
2	D	401	AKG	O2-C1-O1	-3.01	116.74	123.90
4	A	410	CAC	O1-AS-C2	-2.84	107.96	111.50
2	A	401	AKG	O5-C2-C1	2.82	123.69	119.67
2	D	401	AKG	O5-C2-C1	2.36	123.04	119.67
2	A	401	AKG	O2-C1-C2	2.12	119.47	113.59
2	B	401	AKG	O2-C1-C2	2.08	119.36	113.59
4	B	408	CAC	O1-AS-C1	-2.08	108.92	111.50
4	A	409	CAC	O1-AS-C2	-2.06	108.94	111.50

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	AKG	C3-C4-C5-O3
2	C	401	AKG	C3-C4-C5-O3
3	A	403	GOL	C1-C2-C3-O3
3	A	403	GOL	O2-C2-C3-O3
3	B	403	GOL	O1-C1-C2-C3
3	B	404	GOL	O2-C2-C3-O3
3	B	405	GOL	C1-C2-C3-O3
3	B	406	GOL	O1-C1-C2-O2
3	B	406	GOL	O1-C1-C2-C3
3	B	406	GOL	C1-C2-C3-O3
3	A	405	GOL	O2-C2-C3-O3
3	A	405	GOL	O1-C1-C2-C3
3	A	405	GOL	C1-C2-C3-O3
3	A	406	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	407	GOL	C1-C2-C3-O3
3	A	408	GOL	C1-C2-C3-O3
3	B	403	GOL	C1-C2-C3-O3
3	B	404	GOL	C1-C2-C3-O3
3	B	405	GOL	O1-C1-C2-C3
3	C	402	GOL	C1-C2-C3-O3
3	B	403	GOL	O1-C1-C2-O2
3	B	403	GOL	O2-C2-C3-O3
3	B	405	GOL	O2-C2-C3-O3
3	B	406	GOL	O2-C2-C3-O3
3	A	407	GOL	O2-C2-C3-O3
3	B	405	GOL	O1-C1-C2-O2
2	C	401	AKG	C2-C3-C4-C5
3	A	408	GOL	O2-C2-C3-O3
2	A	401	AKG	C3-C4-C5-O4
3	A	405	GOL	O1-C1-C2-O2
3	A	406	GOL	O2-C2-C3-O3
3	C	402	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	404	GOL	1	0
3	B	406	GOL	3	0
3	A	408	GOL	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	304/341 (89%)	-0.06	9 (2%)	52	58	4, 9, 19, 30	2 (0%)
1	B	303/341 (88%)	0.02	10 (3%)	49	55	4, 10, 22, 30	1 (0%)
1	C	303/341 (88%)	0.06	10 (3%)	49	55	5, 11, 24, 35	1 (0%)
1	D	292/341 (85%)	0.47	19 (6%)	25	28	7, 18, 28, 47	1 (0%)
All	All	1202/1364 (88%)	0.12	48 (3%)	42	47	4, 12, 25, 47	5 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	LEU	5.7
1	D	235	TRP	4.2
1	D	237	LYS	3.9
1	B	137	ASN	3.7
1	B	136	PRO	3.7
1	D	5	LEU	3.7
1	A	137	ASN	3.5
1	A	307	HIS	3.5
1	B	274	VAL	3.4
1	D	274	VAL	3.4
1	A	248	SER	3.3
1	D	83	SER	3.3
1	B	244	LEU	3.2
1	B	248	SER	3.1
1	D	98	GLU	2.9
1	A	243	ALA	2.9
1	C	106	ASP	2.8
1	C	140	ILE	2.8
1	A	249	ARG	2.8
1	B	243	ALA	2.8
1	A	246	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	272	SER	2.7
1	A	136	PRO	2.6
1	A	244	LEU	2.6
1	A	242	SER	2.5
1	D	106	ASP	2.5
1	B	272	SER	2.5
1	C	307	HIS	2.4
1	D	285	ARG	2.4
1	C	136	PRO	2.4
1	D	55	LEU	2.4
1	C	5	LEU	2.3
1	D	233	PRO	2.3
1	C	134	ASP	2.3
1	D	102	LEU	2.3
1	C	137	ASN	2.3
1	D	137	ASN	2.3
1	D	99	GLN	2.2
1	D	249	ARG	2.2
1	C	240	HIS	2.2
1	C	244	LEU	2.2
1	D	104	GLY	2.2
1	D	236	GLU	2.1
1	B	307	HIS	2.1
1	B	249	ARG	2.1
1	D	230	LEU	2.1
1	C	138	GLY	2.0
1	D	289	GLN	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	A	406	6/6	0.57	0.23	43,43,43,43	0
3	GOL	A	405	6/6	0.71	0.20	34,35,36,37	0
3	GOL	A	403	6/6	0.79	0.14	26,28,28,29	0
3	GOL	B	404	6/6	0.79	0.17	30,31,31,33	0
4	CAC	C	404	5/5	0.79	0.31	48,48,48,48	5
4	CAC	A	409	5/5	0.82	0.27	48,48,48,49	5
3	GOL	B	402	6/6	0.82	0.13	29,30,31,31	0
4	CAC	B	407	5/5	0.83	0.33	54,54,54,54	5
3	GOL	A	408	6/6	0.83	0.19	23,27,27,28	0
3	GOL	B	403	6/6	0.84	0.17	41,42,42,42	0
3	GOL	B	406	6/6	0.85	0.16	15,19,19,21	0
2	AKG	C	401	9/10	0.87	0.11	11,12,13,14	0
3	GOL	B	405	6/6	0.88	0.13	21,24,25,26	0
3	GOL	C	403	6/6	0.88	0.09	17,18,18,18	0
3	GOL	D	402	6/6	0.88	0.14	18,21,22,23	0
3	GOL	C	402	6/6	0.90	0.09	16,17,17,18	0
2	AKG	D	401	9/10	0.90	0.10	14,15,16,16	0
2	AKG	A	401	9/10	0.90	0.09	10,11,13,13	0
4	CAC	C	405	5/5	0.91	0.20	32,32,32,32	5
3	GOL	A	407	6/6	0.92	0.10	22,24,24,25	0
3	GOL	D	403	6/6	0.93	0.09	19,20,21,21	0
3	GOL	A	402	6/6	0.94	0.08	8,10,10,11	0
3	GOL	A	404	6/6	0.96	0.06	9,11,11,12	0
2	AKG	B	401	9/10	0.96	0.08	8,10,11,12	0
4	CAC	A	410	5/5	0.98	0.12	23,23,24,24	0
4	CAC	D	404	5/5	0.98	0.13	19,19,20,20	5
4	CAC	B	408	5/5	0.99	0.08	18,18,18,18	5

6.5 Other polymers ⓘ

There are no such residues in this entry.