



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:54 PM GMT

PDB ID : 4HGD
Title : Structural insights into yeast Nit2: C169S mutant of yeast Nit2 in complex with an endogenous peptide-like ligand
Authors : Liu, H.; Qiu, X.; Zhang, M.; Gao, Y.; Niu, L.; Teng, M.
Deposited on : 2012-10-08
Resolution : 2.04 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

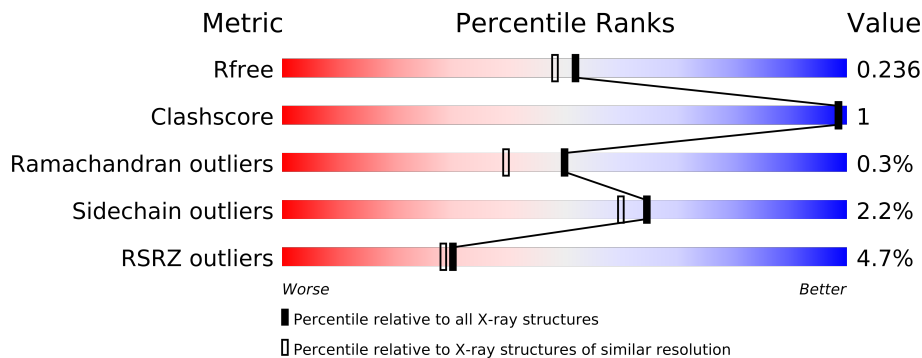
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.04 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}	66092	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	A	403	-	X
2	GOL	A	404	-	X
2	GOL	B	401	-	X
2	GOL	B	402	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	D	401	-	X
2	GOL	D	402	-	X
2	GOL	D	403	-	X
3	CAC	A	406	X	X
3	CAC	B	403	X	X
3	CAC	C	404	X	X
3	CAC	D	404	X	X
4	KGT	A	407	-	X
4	KGT	B	404	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9730 atoms, of which 0 are hydrogen and 0 are deuterium.

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	299	Total	C	N	O	S	0	0	0
			2324	1478	404	433	9			
1	B	300	Total	C	N	O	S	0	0	0
			2347	1492	405	441	9			
1	C	302	Total	C	N	O	S	0	2	0
			2338	1490	407	431	10			
1	D	292	Total	C	N	O	S	0	0	0
			2213	1413	382	411	7			

There are 140 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

Continued on next page...

Continued from previous page...

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
A	169	SER	CYS	ENGINEERED MUTATION	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

Continued on next page...

Continued from previous page...

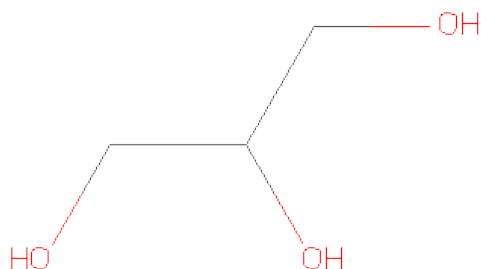
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLN	-	EXPRESSION TAG	UNP P47016
B	-4	MET	-	EXPRESSION TAG	UNP P47016
B	-3	GLY	-	EXPRESSION TAG	UNP P47016
B	-2	ARG	-	EXPRESSION TAG	UNP P47016
B	-1	GLY	-	EXPRESSION TAG	UNP P47016
B	0	SER	-	EXPRESSION TAG	UNP P47016
B	169	SER	CYS	ENGINEERED MUTATION	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
C	169	SER	CYS	ENGINEERED MUTATION	UNP P47016

Continued on next page...

Continued from previous page...

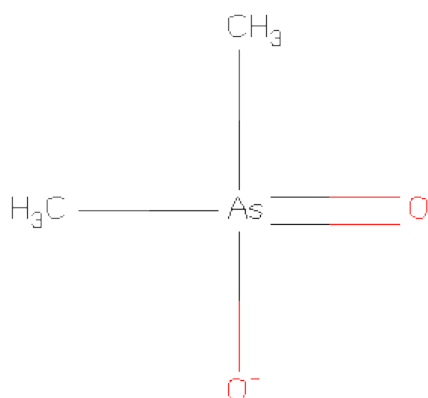
Chain	Residue	Modelled	Actual	Comment	Reference
D	-33	MET	-	EXPRESSION TAG	UNP P47016
D	-32	GLY	-	EXPRESSION TAG	UNP P47016
D	-31	SER	-	EXPRESSION TAG	UNP P47016
D	-30	SER	-	EXPRESSION TAG	UNP P47016
D	-29	HIS	-	EXPRESSION TAG	UNP P47016
D	-28	HIS	-	EXPRESSION TAG	UNP P47016
D	-27	HIS	-	EXPRESSION TAG	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
D	169	SER	CYS	ENGINEERED MUTATION	UNP P47016

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



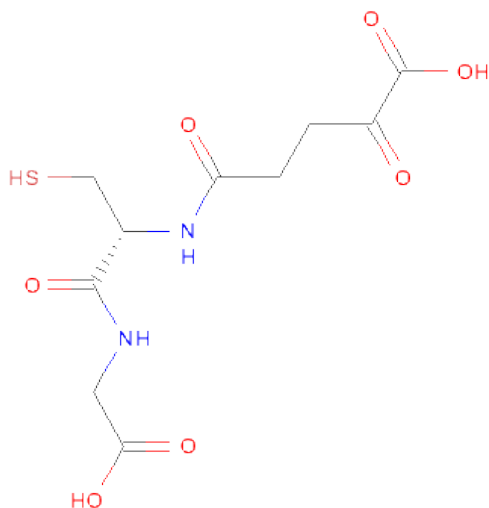
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total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

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



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

- Molecule 4 is N-(4-CARBOXY-4-OXOBUTANOYL)-L-CYSTEINYLGLYCINE (three-letter code: KGT) (formula: $C_{10}H_{14}N_2O_7S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			20	10	2	7	1		
4	B	1	Total	C	N	O	S	0	0
			20	10	2	7	1		
4	C	1	Total	C	N	O	S	0	0
			20	10	2	7	1		
4	D	1	Total	C	N	O	S	0	0
			20	10	2	7	1		

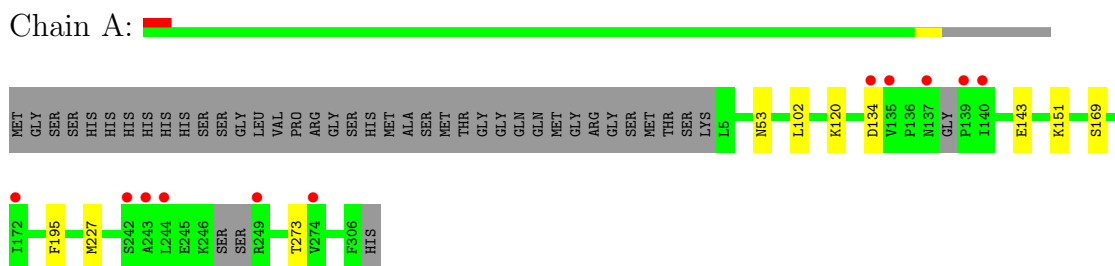
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	92	Total	O	0	0
			92	92		
5	B	111	Total	O	0	0
			111	111		
5	C	77	Total	O	0	0
			77	77		
5	D	50	Total	O	0	0
			50	50		

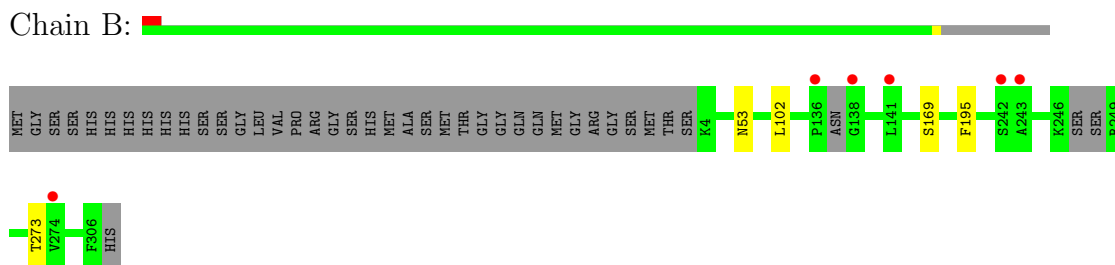
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

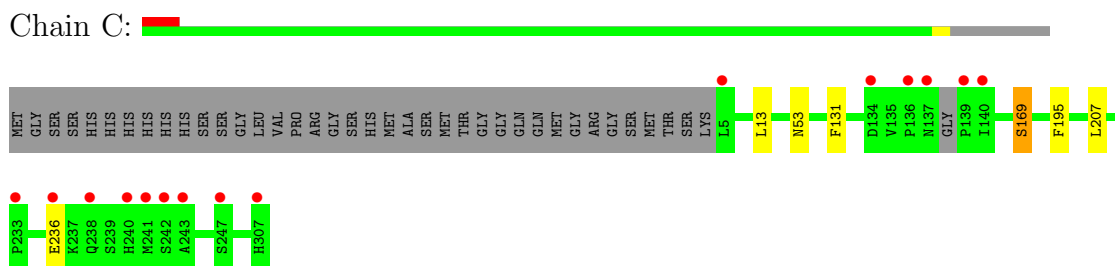
- Molecule 1: Probable hydrolase NIT2



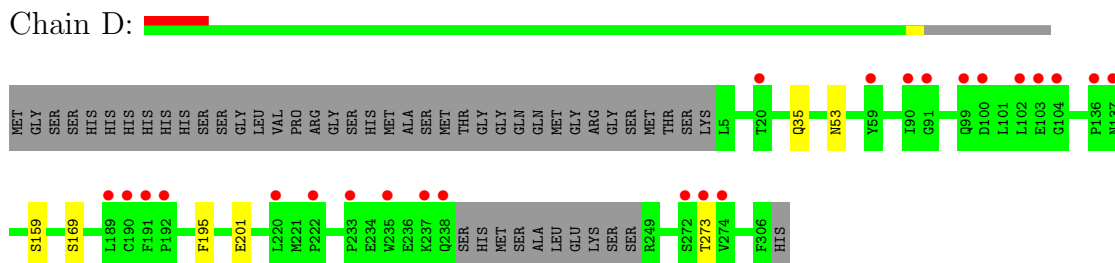
- Molecule 1: Probable hydrolase NIT2



- 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	65.63Å 126.92Å 77.62Å 90.00° 95.61° 90.00°	Depositor
Resolution (Å)	35.51 – 2.04 34.77 – 2.04	Depositor EDS
% Data completeness (in resolution range)	94.4 (35.51-2.04) 94.4 (34.77-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.189 , 0.228 0.201 , 0.236	Depositor DCC
R_{free} test set	3803 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 76017 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9730	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, GOL, KGT

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	0.39	0/2372	0.55	0/3215
1	B	0.42	0/2395	0.55	0/3245
1	C	0.39	0/2395	0.55	0/3252
1	D	0.36	0/2261	0.52	0/3080
All	All	0.39	0/9423	0.54	0/12792

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2324	0	0	2	0
1	B	2347	0	0	0	0
1	C	2338	0	0	2	0
1	D	2213	0	0	1	0
2	A	30	0	0	0	0
2	B	12	0	0	1	0
2	C	18	0	0	0	0
2	D	18	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	20	0	12	1	0
4	B	20	0	12	0	0
4	C	20	0	12	2	0
4	D	20	0	12	0	0
5	A	92	0	0	0	0
5	B	111	0	0	0	0
5	C	77	0	0	0	0
5	D	50	0	0	1	0
All	All	9730	0	48	5	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (5) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:169:SER:CB	4:C:405:KGT:H3	2.25	0.66
1:A:151:LYS:O	2:B:401:GOL:C1	2.48	0.62
1:A:143:GLU:CD	4:A:407:KGT:H8	2.25	0.57
1:C:131:PHE:CD1	4:C:405:KGT:H2	2.49	0.47
1:D:35:GLN:NE2	5:D:533:HOH:O	2.50	0.43

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	293/341 (86%)	290 (99%)	2 (1%)	1 (0%)	50 39
1	B	294/341 (86%)	291 (99%)	2 (1%)	1 (0%)	50 39
1	C	300/341 (88%)	290 (97%)	9 (3%)	1 (0%)	50 39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	288/341 (84%)	279 (97%)	8 (3%)	1 (0%)	50 39
All	All	1175/1364 (86%)	1150 (98%)	21 (2%)	4 (0%)	50 39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	169	SER
1	C	169	SER
1	A	169	SER
1	D	169	SER

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	249/300 (83%)	242 (97%)	7 (3%)	56 50
1	B	251/300 (84%)	247 (98%)	4 (2%)	75 73
1	C	241/300 (80%)	236 (98%)	5 (2%)	66 62
1	D	223/300 (74%)	218 (98%)	5 (2%)	64 60
All	All	964/1200 (80%)	943 (98%)	21 (2%)	64 60

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	102	LEU
1	A	120	LYS
1	A	134	ASP
1	A	195	PHE
1	A	227	MET
1	A	273	THR
1	B	53	ASN
1	B	102	LEU
1	B	195	PHE
1	B	273	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	13	LEU
1	C	53	ASN
1	C	195	PHE
1	C	207	LEU
1	C	236	GLU
1	D	53	ASN
1	D	159	SER
1	D	195	PHE
1	D	201	GLU
1	D	273	THR

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

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

21 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	$\# Z > 2$
2	GOL	A	401	-	5,5,5	0.34	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	402	-	5,5,5	0.32	0	5,5,5	0.47	0
2	GOL	A	403	-	5,5,5	0.35	0	5,5,5	0.13	0
2	GOL	A	404	-	5,5,5	0.31	0	5,5,5	0.61	0
2	GOL	A	405	-	5,5,5	0.44	0	5,5,5	0.38	0
3	CAC	A	406	-	4,4,4	3.96	4 (100%)	6,6,6	5.49	1 (16%)
4	KGT	A	407	-	19,19,19	1.96	2 (10%)	24,24,24	2.40	8 (33%)
2	GOL	B	401	-	5,5,5	0.37	0	5,5,5	0.34	0
2	GOL	B	402	-	5,5,5	0.36	0	5,5,5	0.44	0
3	CAC	B	403	-	4,4,4	3.81	4 (100%)	6,6,6	5.05	1 (16%)
4	KGT	B	404	-	19,19,19	2.04	2 (10%)	24,24,24	1.50	4 (16%)
2	GOL	C	401	-	5,5,5	0.35	0	5,5,5	0.32	0
2	GOL	C	402	-	5,5,5	0.39	0	5,5,5	0.30	0
2	GOL	C	403	-	5,5,5	0.32	0	5,5,5	0.36	0
3	CAC	C	404	-	4,4,4	3.87	4 (100%)	6,6,6	5.92	1 (16%)
4	KGT	C	405	-	19,19,19	2.01	2 (10%)	24,24,24	1.37	3 (12%)
2	GOL	D	401	-	5,5,5	0.40	0	5,5,5	0.34	0
2	GOL	D	402	-	5,5,5	0.35	0	5,5,5	0.32	0
2	GOL	D	403	-	5,5,5	0.32	0	5,5,5	0.25	0
3	CAC	D	404	-	4,4,4	4.03	4 (100%)	6,6,6	4.30	1 (16%)
4	KGT	D	405	-	19,19,19	2.03	2 (10%)	24,24,24	1.40	3 (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
2	GOL	A	401	-	-	0/4/4/4	0/0/0/0
2	GOL	A	402	-	-	0/4/4/4	0/0/0/0
2	GOL	A	403	-	-	0/4/4/4	0/0/0/0
2	GOL	A	404	-	-	0/4/4/4	0/0/0/0
2	GOL	A	405	-	-	0/4/4/4	0/0/0/0
3	CAC	A	406	-	-	0/0/0/0	0/0/0/0
4	KGT	A	407	-	-	0/24/24/24	0/0/0/0
2	GOL	B	401	-	-	0/4/4/4	0/0/0/0
2	GOL	B	402	-	-	0/4/4/4	0/0/0/0
3	CAC	B	403	-	-	0/0/0/0	0/0/0/0
4	KGT	B	404	-	-	0/24/24/24	0/0/0/0
2	GOL	C	401	-	-	0/4/4/4	0/0/0/0
2	GOL	C	402	-	-	0/4/4/4	0/0/0/0
2	GOL	C	403	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CAC	C	404	-	-	0/0/0/0	0/0/0/0
4	KGT	C	405	-	-	0/24/24/24	0/0/0/0
2	GOL	D	401	-	-	0/4/4/4	0/0/0/0
2	GOL	D	402	-	-	0/4/4/4	0/0/0/0
2	GOL	D	403	-	-	0/4/4/4	0/0/0/0
3	CAC	D	404	-	-	0/0/0/0	0/0/0/0
4	KGT	D	405	-	-	0/24/24/24	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	404	KGT	C09-N11	5.89	1.46	1.33
3	D	404	CAC	O2-AS	5.85	1.74	1.68
4	C	405	KGT	C09-N11	5.83	1.46	1.33
4	B	404	KGT	C03-N05	5.79	1.45	1.34
4	D	405	KGT	C09-N11	5.77	1.46	1.33
4	D	405	KGT	C03-N05	5.72	1.45	1.34
4	C	405	KGT	C03-N05	5.70	1.45	1.34
3	A	406	CAC	O2-AS	5.69	1.74	1.68
4	A	407	KGT	C03-N05	5.55	1.45	1.34
4	A	407	KGT	C09-N11	5.52	1.45	1.33
3	C	404	CAC	O2-AS	5.36	1.74	1.68
3	B	403	CAC	O2-AS	5.31	1.74	1.68
3	C	404	CAC	AS-C1	3.63	1.96	1.90
3	A	406	CAC	AS-C1	3.59	1.96	1.90
3	B	403	CAC	AS-C2	3.59	1.96	1.90
3	D	404	CAC	AS-C1	3.57	1.96	1.90
3	D	404	CAC	AS-C2	3.53	1.96	1.90
3	C	404	CAC	AS-C2	3.50	1.96	1.90
3	A	406	CAC	AS-C2	3.42	1.96	1.90
3	B	403	CAC	AS-C1	3.34	1.96	1.90
3	B	403	CAC	O1-AS	2.43	1.74	1.66
3	C	404	CAC	O1-AS	2.39	1.74	1.66
3	A	406	CAC	O1-AS	2.36	1.74	1.66
3	D	404	CAC	O1-AS	2.32	1.74	1.66

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	404	CAC	O2-AS-O1	-14.48	109.41	112.54
3	A	406	CAC	O2-AS-O1	-13.42	109.64	112.54
3	B	403	CAC	O2-AS-O1	-12.23	109.90	112.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	404	CAC	O2-AS-O1	-10.50	110.27	112.54
4	A	407	KGT	C06-C09-N11	5.63	127.73	116.72
4	A	407	KGT	C01-C02-C03	5.34	120.42	112.65
4	B	404	KGT	C02-C01-C16	4.63	123.21	112.43
4	A	407	KGT	O10-C09-N11	-4.14	114.64	123.05
4	C	405	KGT	C01-C02-C03	3.63	117.94	112.65
4	A	407	KGT	C12-N11-C09	3.27	128.54	121.29
4	D	405	KGT	C02-C01-C16	3.20	119.87	112.43
4	D	405	KGT	C01-C02-C03	3.00	117.03	112.65
4	C	405	KGT	C02-C01-C16	2.99	119.39	112.43
4	A	407	KGT	C02-C01-C16	2.95	119.30	112.43
4	A	407	KGT	C06-N05-C03	2.93	129.40	121.53
4	A	407	KGT	C07-C06-C09	2.89	115.98	109.70
4	B	404	KGT	C09-C06-N05	2.79	119.12	111.28
4	D	405	KGT	O18-C17-C16	2.76	120.45	114.37
4	A	407	KGT	O18-C17-C16	2.37	119.60	114.37
4	C	405	KGT	O18-C17-C16	2.25	119.33	114.37
4	B	404	KGT	O18-C17-C16	2.20	119.23	114.37
4	B	404	KGT	O15-C13-C12	2.10	120.62	112.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	299/341 (87%)	0.07	11 (3%) 39 39	18, 25, 42, 56	0
1	B	300/341 (87%)	-0.02	6 (2%) 62 63	15, 23, 38, 55	0
1	C	302/341 (88%)	0.16	15 (4%) 28 26	17, 27, 48, 60	0
1	D	292/341 (85%)	0.59	24 (8%) 12 11	23, 40, 60, 83	0
All	All	1193/1364 (87%)	0.20	56 (4%) 30 28	15, 28, 52, 83	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	233	PRO	6.4
1	C	136	PRO	4.6
1	A	243	ALA	3.9
1	C	240	HIS	3.8
1	D	274	VAL	3.6
1	D	59	TYR	3.6
1	D	272	SER	3.5
1	D	102	LEU	3.5
1	C	140	ILE	3.5
1	D	237	LYS	3.4
1	A	244	LEU	3.3
1	B	243	ALA	3.3
1	C	134	ASP	3.1
1	A	242	SER	3.0
1	C	247	SER	3.0
1	D	136	PRO	3.0
1	C	243	ALA	2.9
1	A	140	ILE	2.8
1	C	139	PRO	2.8
1	C	307	HIS	2.7
1	C	241	MET	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	238	GLN	2.7
1	D	222	PRO	2.6
1	A	137	ASN	2.6
1	D	100	ASP	2.6
1	A	135	VAL	2.6
1	C	137	ASN	2.6
1	D	91	GLY	2.5
1	D	137	ASN	2.4
1	D	235	TRP	2.4
1	A	249	ARG	2.4
1	C	233	PRO	2.4
1	B	141	LEU	2.4
1	B	242	SER	2.4
1	C	242	SER	2.4
1	D	192	PRO	2.4
1	A	134	ASP	2.3
1	B	138	GLY	2.3
1	C	5	LEU	2.3
1	D	190	CYS	2.2
1	D	90	ILE	2.2
1	D	104	GLY	2.2
1	B	136	PRO	2.2
1	C	236	GLU	2.2
1	D	273	THR	2.2
1	D	191	PHE	2.1
1	D	220	LEU	2.1
1	C	238	GLN	2.1
1	A	139	PRO	2.1
1	B	274	VAL	2.1
1	D	99	GLN	2.1
1	D	20	THR	2.0
1	D	189	LEU	2.0
1	D	103	GLU	2.0
1	A	274	VAL	2.0
1	A	172	ILE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CAC	D	404	5/5	0.34	16.25	206,206,215,220	0
3	CAC	B	403	5/5	0.27	14.65	94,97,98,103	5
2	GOL	D	401	6/6	0.28	6.86	42,45,46,47	0
3	CAC	A	406	5/5	0.20	5.67	93,95,96,101	5
2	GOL	D	403	6/6	0.33	3.92	75,76,76,76	0
4	KGT	B	404	20/20	0.28	3.65	28,35,37,39	20
2	GOL	D	402	6/6	0.26	3.64	37,38,39,40	0
2	GOL	A	403	6/6	0.17	3.35	51,52,53,53	0
2	GOL	A	404	6/6	0.21	3.11	49,50,51,51	0
3	CAC	C	404	5/5	0.20	2.82	195,201,206,210	0
2	GOL	B	401	6/6	0.17	2.58	37,40,40,43	0
2	GOL	B	402	6/6	0.23	2.21	57,58,58,58	0
4	KGT	A	407	20/20	0.18	2.02	36,42,48,48	0
2	GOL	A	405	6/6	0.31	1.83	37,38,39,39	0
4	KGT	C	405	20/20	0.17	1.37	39,45,48,49	0
4	KGT	D	405	20/20	0.17	1.10	35,38,40,41	0
2	GOL	A	402	6/6	0.12	1.02	28,29,30,30	0
2	GOL	C	403	6/6	0.12	0.72	45,46,47,47	0
2	GOL	C	401	6/6	0.11	0.16	37,38,38,38	0
2	GOL	C	402	6/6	0.11	-0.07	39,40,40,41	0
2	GOL	A	401	6/6	0.09	-1.36	28,28,28,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.