

# Full wwPDB X-ray Structure Validation Report (i)

#### Nov 14, 2023 – 04:11 PM JST

PDB ID : 6A0H

Title: Crystal structure of human protein N-terminal asparagine amidohydrolase

(NTAN1) C75S mutant with Asn-Leu-Ala-Ala-Arg peptide

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Deposited on : 2018-06-05

Resolution : 3.19 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 (i) 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 (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{--}467$ 

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

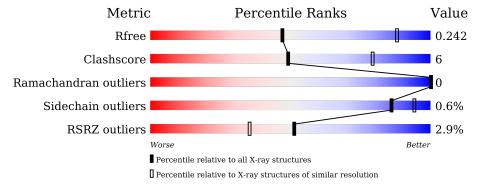
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.19 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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 chai	n		
1	A	318	2%	81%		14%	5%
1	В	318	4%	80%		15%	5%
2	С	5	40%	20%	20%	20%	
2	D	5	40%	20%	409	%	



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4895 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 Protein N-terminal asparagine amidohydrolase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	302	Total	С	N	О	S	0	0	0
1	A	A 302	2389	1499	428	455	7	0	U	0
1	R	302	Total	С	N	О	S	0	0	0
1	Ъ	302	2386	1498	428	453	7		U	

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	SER	CYS	engineered mutation	UNP Q96AB6
A	311	LEU	-	expression tag	UNP Q96AB6
A	312	GLU	-	expression tag	UNP Q96AB6
A	313	HIS	-	expression tag	UNP Q96AB6
A	314	HIS	-	expression tag	UNP Q96AB6
A	315	HIS	-	expression tag	UNP Q96AB6
A	316	HIS	-	expression tag	UNP Q96AB6
A	317	HIS	-	expression tag	UNP Q96AB6
A	318	HIS	-	expression tag	UNP Q96AB6
В	75	SER	CYS	engineered mutation	UNP Q96AB6
В	311	LEU	-	expression tag	UNP Q96AB6
В	312	GLU	-	expression tag	UNP Q96AB6
В	313	HIS	-	expression tag	UNP Q96AB6
В	314	HIS	-	expression tag	UNP Q96AB6
В	315	HIS	_	expression tag	UNP Q96AB6
В	316	HIS	-	expression tag	UNP Q96AB6
В	317	HIS	-	expression tag	UNP Q96AB6
В	318	HIS	_	expression tag	UNP Q96AB6

• Molecule 2 is a protein called 5-mer peptide ASN-LEU-ALA-ALA-ARG.

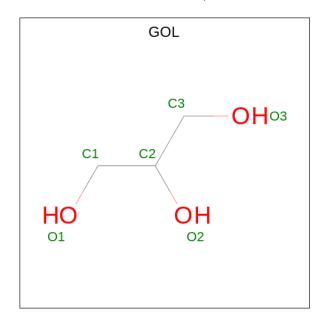
Mo	l Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	С	4	Total 26	C 16	N 5	O 5	0	0	0



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total 21	C 13	N 4	O 4	0	0	0

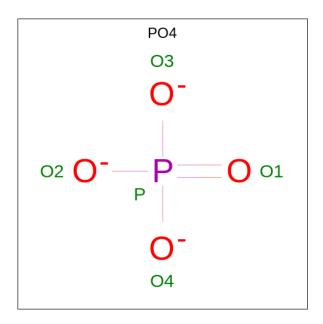
• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O	0	0
	Λ	1	6 3 3	U	U
3	A	1	Total C O	0	0
J	Λ	1	6 3 3	U	U
3	Δ	1	Total C O	0	0
J	А	1	6 3 3	U	U
3	В	1	Total C O	0	0
J	D	1	6 3 3	U	U
3	R	1	Total C O	0	0
3	ע	1	6 3 3	U	

• Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	В	1	Total O P 5 4 1	0	0
4	В	1	Total O P 5 4 1	0	0
4	В	1	Total O P 5 4 1	0	0

### • Molecule 5 is water.

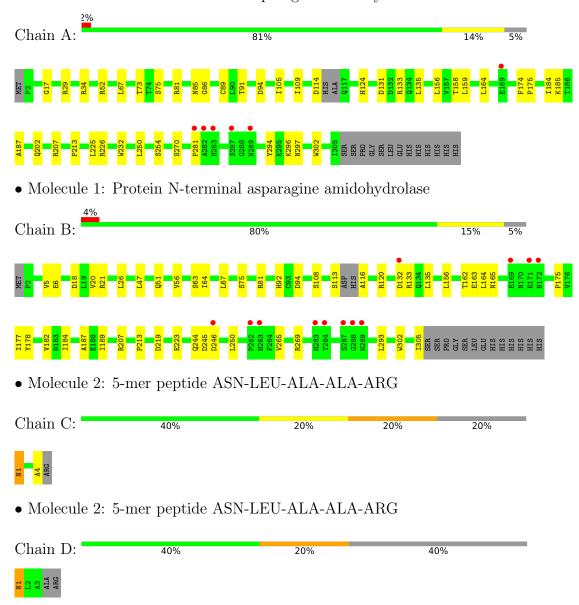
$\mathbf{N}$	$\mathbf{lol}$	Chain	Residues	Atoms	ZeroOcc	AltConf
	5	A	6	Total O 6 6	0	0
	5	В	7	Total O 7 7	0	0



## 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: Protein N-terminal asparagine amidohydrolase





## 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	84.00Å 85.88Å 88.09Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	35.52 - 3.19	Depositor	
Resolution (A)	35.52 - 3.19	EDS	
% Data completeness	99.8 (35.52-3.19)	Depositor	
(in resolution range)	99.8 (35.52-3.19)	EDS	
$R_{merge}$	(Not available)	Depositor	
$\frac{\mathrm{R}_{sym}}{\langle I/\sigma(I)\rangle^{-1}}$	0.17	Depositor	
$< I/\sigma(I) > 1$	2.92  (at  3.18Å)	Xtriage	
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor	
$R, R_{free}$	0.185 , $0.242$	Depositor	
it, it free	0.185 , $0.242$	DCC	
$R_{free}$ test set	541 reflections (4.87%)	wwPDB-VP	
Wilson B-factor $(\mathring{A}^2)$	50.6	Xtriage	
Anisotropy	0.817	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.33, 42.4	EDS	
L-test for twinning <sup>2</sup>	$< L > = 0.47, < L^2> = 0.30$	Xtriage	
	0.023 for -h,l,k		
	0.028  for -l,-k,-h		
Estimated twinning fraction	0.036  for k,h,-l	Xtriage	
	0.009  for  k,l,h		
	0.009  for  l,h,k		
$F_o, F_c$ correlation	0.93	EDS	
Total number of atoms	4895	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4

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		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.24	0/2441	0.43	0/3311	
1	В	0.25	0/2438	0.43	0/3307	
2	С	0.20	0/25	0.35	0/33	
2	D	0.18	0/20	0.39	0/26	
All	All	0.25	0/4924	0.43	0/6677	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2389	0	2354	27	0
1	В	2386	0	2356	30	0
2	С	26	0	29	3	0
2	D	21	0	24	1	0
3	A	18	0	23	1	0
3	В	12	0	16	2	0
4	A	15	0	0	0	0
4	В	15	0	0	1	0
5	A	6	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	В	7	0	0	0	0
All	All	4895	0	4802	57	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 6.

All (57) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:A:67:LEU:HG	1:A:184:ILE:HD11	1.64	0.78
1:B:18:ASP:OD1	1:B:21:ARG:NH1	2.20	0.74
1:A:156:LEU:HD21	1:A:159:LEU:HD22	1.74	0.69
1:B:182:VAL:HG22	1:B:189:ILE:HG12	1.75	0.67
1:B:67:LEU:HG	1:B:184:ILE:HD11	1.75	0.65
1:B:250:LEU:HD11	1:B:265:VAL:HG22	1.77	0.64
1:B:113:SER:HG	1:B:116:ALA:N	1.96	0.63
1:B:244:GLN:O	1:B:269:ARG:NH1	2.31	0.63
1:B:20:VAL:HG22	1:B:26:LEU:HB3	1.84	0.60
1:A:225:LEU:HB3	1:A:294:TYR:HB2	1.84	0.59
1:B:63:SER:OG	1:B:223:GLU:OE1	2.21	0.59
1:A:52:ARG:HH22	2:C:4:ALA:HB2	1.67	0.58
1:A:17:GLY:HA2	1:A:164:LEU:HD21	1.86	0.57
1:A:207:ARG:NH1	1:A:213:PRO:O	2.32	0.56
1:A:85:ASN:OD1	1:A:86:GLY:N	2.40	0.54
1:B:56:VAL:HG11	1:B:108:SER:HB3	1.90	0.54
1:B:246:ASP:OD1	1:B:269:ARG:NH2	2.39	0.54
1:A:81:ARG:CZ	1:A:187:ALA:HB2	2.39	0.52
1:B:245:ASP:OD1	1:B:245:ASP:N	2.40	0.52
1:A:91:THR:HG21	1:A:105:ILE:HG12	1.91	0.52
1:B:120:ARG:HH12	3:B:401:GOL:H2	1.75	0.52
1:B:81:ARG:CZ	1:B:187:ALA:HB2	2.42	0.50
1:B:165:ASN:HD21	1:B:177:ILE:HB	1.77	0.49
1:B:47:LEU:HB2	1:B:64:ILE:HD12	1.94	0.49
1:B:132:ASP:OD1	1:B:132:ASP:N	2.43	0.49
1:A:89:CYS:HB2	1:A:109:ILE:HD11	1.96	0.48
1:A:131:ASP:OD1	1:A:131:ASP:N	2.44	0.48
1:A:297:ASN:OD1	3:A:401:GOL:O1	2.31	0.48
1:B:207:ARG:NH1	1:B:213:PRO:O	2.46	0.48
1:B:175:PRO:HG2	1:B:178:TYR:CZ	2.49	0.47
1:A:202:GLN:NE2	1:A:270:SER:OG	2.47	0.47
1:A:124:HIS:ND1	1:A:158:THR:OG1	2.33	0.47



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A		Interatomic	Clash
Atom-1	Atom-2	${\rm distance}(\mathring{\rm A})$	overlap (Å)
1:A:29:ARG:HG2	1:A:158:THR:HG23	1.97	0.47
1:B:6:GLU:HA	3:B:401:GOL:H11	1.97	0.47
1:B:20:VAL:HG21	1:B:164:LEU:HD11	1.97	0.47
1:A:75:SER:OG	2:C:1:ASN:ND2	2.32	0.47
1:B:302:TRP:N	4:B:404:PO4:O4	2.36	0.45
1:A:226:ARG:NH2	1:B:219:ASP:OD1	2.50	0.45
1:B:5:VAL:HG22	1:B:156:LEU:HB3	1.97	0.45
1:A:133:ARG:HB2	1:A:135:LEU:HG	1.98	0.45
1:A:296:LYS:HE2	1:A:302:TRP:CE2	2.52	0.44
1:B:51:GLN:HE21	1:B:94:ASP:HB3	1.82	0.44
1:A:232:TRP:CZ2	1:A:281:PRO:HG3	2.53	0.44
1:B:133:ARG:HH11	1:B:135:LEU:HD11	1.83	0.43
1:B:133:ARG:HB3	1:B:135:LEU:HG	1.99	0.43
1:B:163:GLU:H	1:B:163:GLU:HG2	1.66	0.43
1:B:293:LEU:HB2	1:B:305:ILE:HD11	2.01	0.43
1:A:73:THR:OG1	2:C:1:ASN:HB2	2.18	0.43
1:B:75:SER:HG	1:B:92:HIS:CD2	2.35	0.42
1:A:34:ARG:HD3	1:A:164:LEU:O	2.20	0.41
1:A:250:LEU:O	1:A:254:SER:HB3	2.20	0.41
2:D:1:ASN:HD22	2:D:1:ASN:HA	1.66	0.41
1:A:52:ARG:NE	1:A:94:ASP:OD2	2.53	0.41
1:A:185:LYS:HE2	1:A:185:LYS:HB2	1.98	0.41
1:A:225:LEU:HB2	1:A:302:TRP:CZ3	2.56	0.41
1:B:162:THR:HB	1:B:163:GLU:H	1.67	0.40
1:A:174:PHE:HB2	1:A:175:PRO:HD2	2.03	0.40

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	Percentile	s
1	A	298/318 (94%)	292 (98%)	6 (2%)	0	100 100	



- 1	Continued	trom	mromonie	maaa
- 1		110116	DICULUUS	pauc

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	В	298/318 (94%)	292 (98%)	6 (2%)	0	100	100
2	С	2/5 (40%)	2 (100%)	0	0	100	100
2	D	1/5 (20%)	1 (100%)	0	0	100	100
All	All	599/646 (93%)	587 (98%)	12 (2%)	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	265/279~(95%)	264 (100%)	1 (0%)	91	96	
1	В	$264/279 \ (95\%)$	264 (100%)	0	100	100	
2	$\mathbf{C}$	2/3~(67%)	1 (50%)	1 (50%)	0	0	
2	D	2/3~(67%)	1 (50%)	1 (50%)	0	0	
All	All	533/564 (94%)	530 (99%)	3 (1%)	86	94	

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ASP
2	С	1	ASN
2	D	1	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN



#### 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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

11 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	Trino	Chain	Res	Link	В	ond leng	gths	В	ond ang	gles
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PO4	В	405	-	4,4,4	0.88	0	6,6,6	0.44	0
4	PO4	В	403	-	4,4,4	0.93	0	6,6,6	0.44	0
4	PO4	A	405	-	4,4,4	0.97	0	6,6,6	0.43	0
4	PO4	В	404	-	4,4,4	0.89	0	6,6,6	0.43	0
3	GOL	В	402	-	5,5,5	0.35	0	5,5,5	0.26	0
3	GOL	A	401	-	5,5,5	0.38	0	5,5,5	0.15	0
3	GOL	A	402	-	5,5,5	0.36	0	5,5,5	0.35	0
3	GOL	В	401	-	5,5,5	0.36	0	5,5,5	0.25	0
4	PO4	A	406	-	4,4,4	0.88	0	6,6,6	0.46	0
4	PO4	A	404	-	4,4,4	0.87	0	6,6,6	0.44	0
3	GOL	A	403	1	5,5,5	0.36	0	5,5,5	0.30	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	В	402	-	-	2/4/4/4	-
3	GOL	A	401	-	-	4/4/4/4	-
3	GOL	A	402	-	-	2/4/4/4	_
3	GOL	В	401	-	-	0/4/4/4	-
3	GOL	A	403	1	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	GOL	O1-C1-C2-C3
3	A	402	GOL	O1-C1-C2-C3
3	A	403	GOL	O1-C1-C2-O2
3	A	401	GOL	C1-C2-C3-O3
3	A	403	GOL	O1-C1-C2-C3
3	A	401	GOL	O1-C1-C2-O2
3	A	402	GOL	O1-C1-C2-O2
3	В	402	GOL	O1-C1-C2-O2
3	A	401	GOL	O2-C2-C3-O3
3	В	402	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	404	PO4	1	0
3	A	401	GOL	1	0
3	В	401	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 (i)

### 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	$302/318 \; (94\%)$	-0.23	6 (1%) 65 50	23, 41, 70, 97	0
1	В	302/318 (94%)	0.13	12 (3%) 38 24	24, 51, 81, 101	0
2	С	4/5 (80%)	-0.07	0 100 100	45, 47, 50, 61	0
2	D	3/5 (60%)	0.09	0 100 100	60, 60, 63, 68	0
All	All	611/646 (94%)	-0.05	18 (2%) 51 35	23, 45, 75, 101	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	289	ASN	5.6
1	В	287	SER	5.1
1	В	288	GLY	4.7
1	В	263	HIS	4.7
1	В	283	HIS	4.4
1	A	283	HIS	3.7
1	A	282	ALA	2.8
1	В	262	PRO	2.8
1	A	281	PRO	2.6
1	В	284	THR	2.4
1	В	132	ASP	2.3
1	В	172	ASN	2.3
1	В	171	GLU	2.2
1	A	289	ASN	2.1
1	В	169	GLU	2.1
1	A	287	SER	2.1
1	В	246	ASP	2.1
1	A	169	GLU	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 monosaccharides in this entry.

### 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	GOL	В	402	6/6	0.67	0.34	63,72,74,79	0
3	GOL	A	401	6/6	0.70	0.30	42,50,60,68	0
3	GOL	В	401	6/6	0.77	0.27	21,40,45,48	0
3	GOL	A	403	6/6	0.79	0.24	54,57,58,62	0
3	GOL	A	402	6/6	0.84	0.33	37,56,59,61	0
4	PO4	В	404	5/5	0.90	0.25	77,80,89,98	0
4	PO4	В	405	5/5	0.91	0.42	81,84,95,104	0
4	PO4	A	404	5/5	0.93	0.19	52,56,62,73	0
4	PO4	A	406	5/5	0.94	0.21	46,50,55,62	0
4	PO4	A	405	5/5	0.95	0.22	44,51,62,67	0
4	PO4	В	403	5/5	0.96	0.26	63,64,78,81	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

