



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:44 AM GMT

PDB ID : 3FRO  
Title : Crystal structure of Pyrococcus abyssi glycogen synthase with open and closed conformations  
Authors : Diaz, A.; Guinovart, J.J.; Fita, I.; Ferrer, J.C.  
Deposited on : 2009-01-08  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

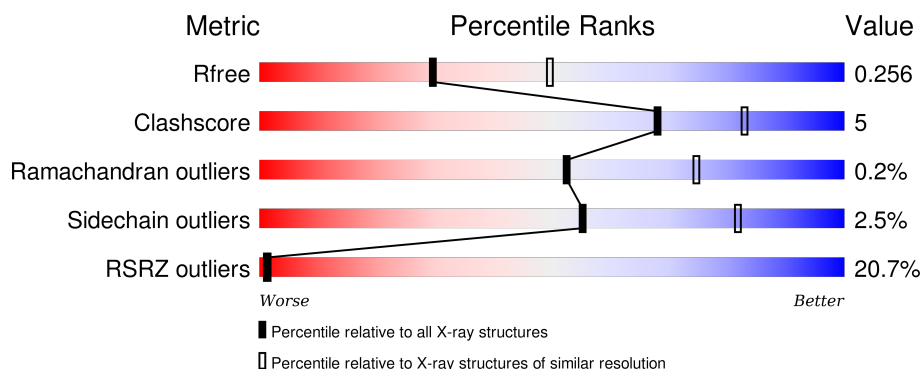
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	439	<div> <div>17%</div> <div>85%</div> <div>14%</div> </div>
1	B	439	<div> <div>27%</div> <div>87%</div> <div>13%</div> </div>
1	C	439	<div> <div>18%</div> <div>91%</div> <div>8%</div> </div>

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
3	TRS	A	7361	-	-	-	X
3	TRS	B	7362	-	-	-	X
4	PO4	A	8000	-	-	-	X
4	PO4	B	8001	-	-	-	X
4	PO4	C	8002	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10635 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.

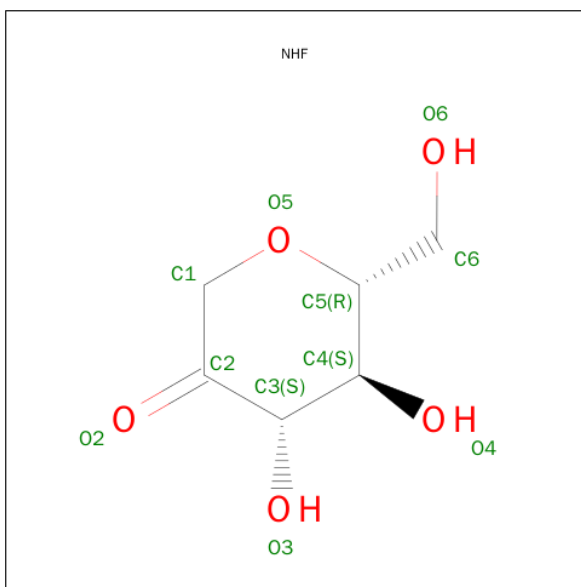
- Molecule 1 is a protein called GlgA glycogen synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	2	0
			3502	2268	589	634	11			
1	B	439	Total	C	N	O	S	0	1	0
			3494	2263	588	633	10			
1	C	439	Total	C	N	O	S	0	1	0
			3494	2263	588	633	10			

There are 6 discrepancies between the modelled and reference sequences:

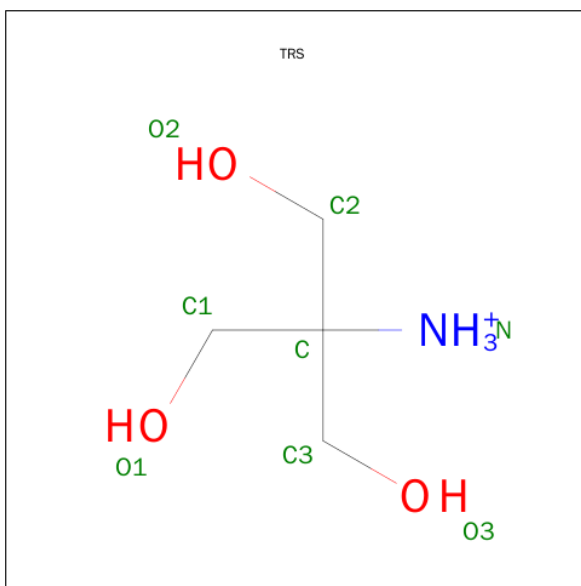
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	EXPRESSION TAG	UNP Q9V2J8
A	0	HIS	-	EXPRESSION TAG	UNP Q9V2J8
B	-1	ARG	-	EXPRESSION TAG	UNP Q9V2J8
B	0	HIS	-	EXPRESSION TAG	UNP Q9V2J8
C	-1	ARG	-	EXPRESSION TAG	UNP Q9V2J8
C	0	HIS	-	EXPRESSION TAG	UNP Q9V2J8

- Molecule 2 is SUGAR (1,5-ANHYDRO-D-FRUCTOSE) (three-letter code: NHF) (formula: C<sub>6</sub>H<sub>10</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



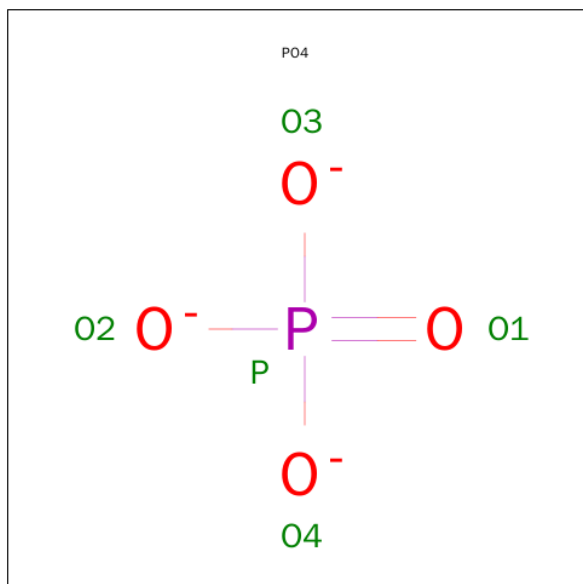
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	A	1	Total	C	N	O	0	0
			8	4	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

- 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	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		

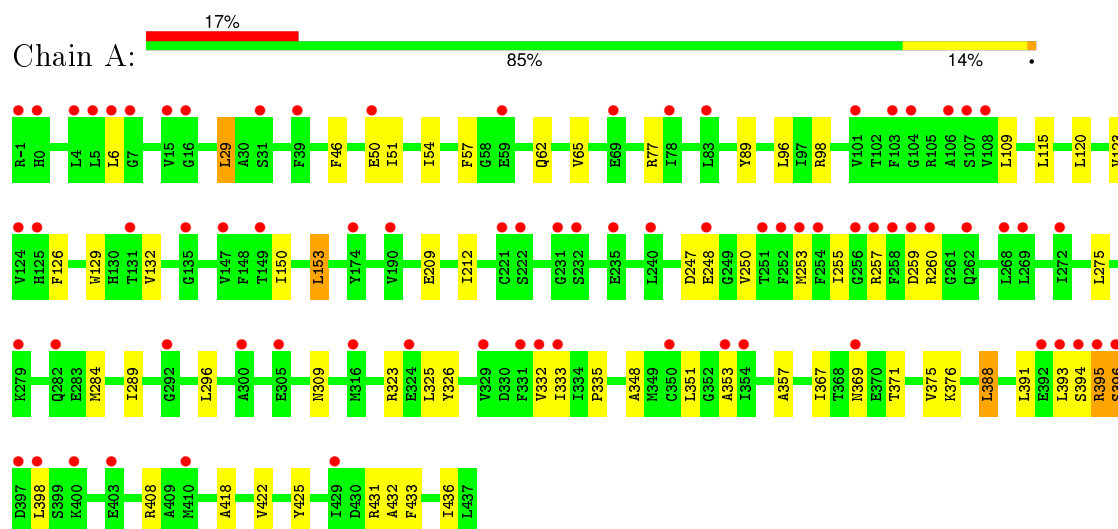
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	40	Total	O	0	0
			40	40		
5	B	30	Total	O	0	0
			30	30		
5	C	25	Total	O	0	0
			25	25		

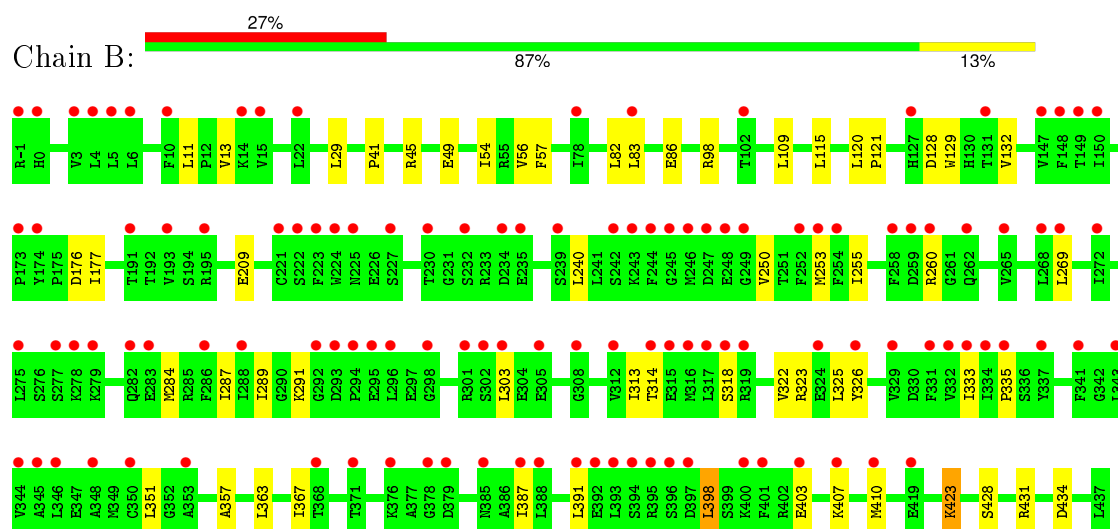
### 3 Residue-property plots [i](#)

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: GlgA glycogen synthase

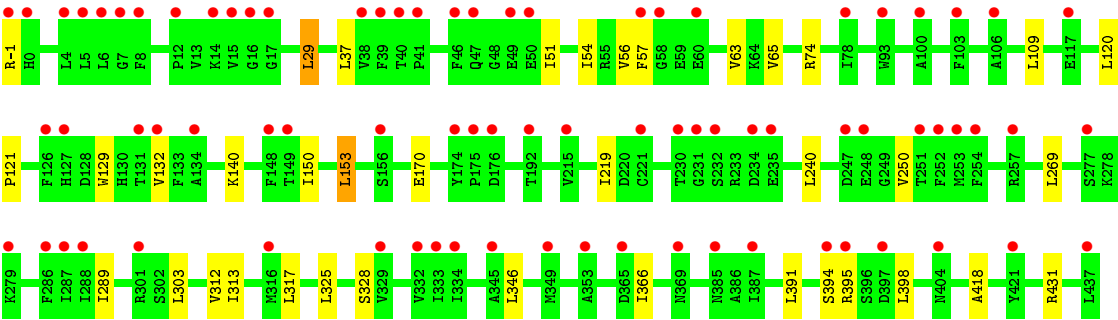


- Molecule 1: GlgA glycogen synthase



- Molecule 1: GlgA glycogen synthase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.00Å 139.91Å 159.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.91 – 2.50 24.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (24.91-2.50) 99.4 (24.90-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.214 , 0.255 0.218 , 0.256	Depositor DCC
$R_{free}$ test set	2950 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.8	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 58364 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10635	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4, NHF, TRS

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	0.31	0/3584	0.47	0/4832
1	B	0.30	0/3576	0.46	0/4822
1	C	0.30	0/3576	0.45	0/4822
All	All	0.30	0/10736	0.46	0/14476

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

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	3502	0	3504	41	0
1	B	3494	0	3496	35	0
1	C	3494	0	3496	22	0
2	B	11	0	10	0	0
3	A	16	0	24	0	0
3	B	8	0	12	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
5	A	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	30	0	0	0	0
5	C	25	0	0	0	0
All	All	10635	0	10542	98	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 (98) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:VAL:HG21	1:A:391:LEU:HD22	1.63	0.79
1:A:150:ILE:HG21	1:A:153:LEU:HD13	1.73	0.70
1:C:150:ILE:HG21	1:C:153:LEU:CD1	2.22	0.69
1:B:269:LEU:HD22	1:B:303:LEU:HD12	1.75	0.69
1:A:433:PHE:HB2	1:A:436:ILE:HD13	1.77	0.67
1:B:287:ILE:HG22	1:B:289:ILE:HD11	1.76	0.67
1:A:323:ARG:HG2	1:A:351:LEU:HD11	1.79	0.64
1:A:29:LEU:HD12	1:A:418:ALA:HB1	1.80	0.63
1:B:253:MET:HE2	1:B:289:ILE:HD13	1.81	0.63
1:C:346:LEU:HD13	1:C:366:ILE:HD13	1.79	0.63
1:C:51:ILE:HD13	1:C:65:VAL:HG21	1.82	0.61
1:A:253:MET:HE2	1:A:289:ILE:HD12	1.84	0.60
1:C:289:ILE:HD13	1:C:317:LEU:HD22	1.85	0.59
1:B:56:VAL:HG12	1:B:57:PHE:CD1	2.38	0.58
1:C:129:TRP:HA	1:C:132:VAL:HG23	1.83	0.58
1:A:29:LEU:CD1	1:A:418:ALA:HB1	2.33	0.58
1:C:150:ILE:HG21	1:C:153:LEU:HD12	1.86	0.58
1:A:433:PHE:CB	1:A:436:ILE:HD13	2.34	0.57
1:A:51:ILE:HD13	1:A:65:VAL:HG21	1.86	0.57
1:B:407:LYS:HA	1:B:410:MET:HE3	1.86	0.57
1:C:37:LEU:HD21	1:C:74:ARG:NH1	2.19	0.56
1:B:287:ILE:HG22	1:B:289:ILE:CD1	2.36	0.56
1:B:129:TRP:HA	1:B:132:VAL:HG23	1.88	0.56
1:B:250:VAL:HG11	1:B:391:LEU:HD13	1.87	0.56
1:B:253:MET:CE	1:B:255:ILE:HD11	2.35	0.56
1:B:250:VAL:HG11	1:B:391:LEU:CD1	2.36	0.56
1:A:393:LEU:C	1:A:395:ARG:H	2.10	0.55
1:C:56:VAL:HG12	1:C:57:PHE:CD1	2.42	0.54
1:A:275:LEU:HD13	1:A:284:MET:CE	2.38	0.54
1:A:253:MET:CE	1:A:289:ILE:HD12	2.38	0.54
1:A:332:VAL:HG23	1:A:353:ALA:HB1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:VAL:C	1:C:313:ILE:HD12	2.28	0.53
1:C:240:LEU:HD22	1:C:328:SER:HB2	1.90	0.53
1:B:13:VAL:HG22	1:B:45:ARG:HG3	1.90	0.53
1:A:326:TYR:HB2	1:A:351:LEU:HD13	1.89	0.53
1:C:219:ILE:HD12	1:C:346:LEU:HB3	1.90	0.52
1:A:333:ILE:HG22	1:A:335:PRO:HD3	1.91	0.52
1:A:371:THR:HG21	1:A:408:ARG:HD3	1.91	0.51
1:C:54:ILE:HG23	1:C:109:LEU:HD22	1.92	0.51
1:B:209:GLU:HG3	1:B:434:ASP:HB2	1.91	0.51
1:C:240:LEU:HD21	1:C:325:LEU:HD23	1.93	0.50
1:A:275:LEU:HD13	1:A:284:MET:HE1	1.92	0.50
1:B:318:SER:O	1:B:322:VAL:HG23	2.11	0.50
1:B:82:LEU:HD12	1:B:98:ARG:HG3	1.93	0.49
1:C:140:LYS:NZ	1:C:170:GLU:OE2	2.43	0.49
1:C:250:VAL:HG21	1:C:391:LEU:HD12	1.95	0.49
1:C:29:LEU:CD1	1:C:418:ALA:HB1	2.43	0.49
1:C:394:SER:HA	1:C:398:LEU:HD11	1.96	0.48
1:A:115:LEU:HD21	1:A:120:LEU:HA	1.96	0.48
1:A:275:LEU:CD2	1:A:388:LEU:HD13	2.44	0.48
1:C:120:LEU:HD12	1:C:121:PRO:HD2	1.96	0.47
1:C:51:ILE:HD13	1:C:65:VAL:CG2	2.44	0.47
1:B:357:ALA:HB1	1:B:363:LEU:HD13	1.96	0.46
1:A:54:ILE:HG23	1:A:109:LEU:HD22	1.96	0.46
1:C:289:ILE:HD13	1:C:317:LEU:CD2	2.46	0.46
1:A:348:ALA:HB1	1:A:353:ALA:HB3	1.98	0.45
1:B:54:ILE:HG23	1:B:109:LEU:HD22	1.98	0.45
1:B:120:LEU:HD12	1:B:121:PRO:HD2	1.97	0.45
1:A:253:MET:HE3	1:A:325:LEU:HD13	1.97	0.45
1:A:357:ALA:HB3	1:A:367:ILE:HD12	1.97	0.45
1:B:176:ASP:C	1:B:177:ILE:HD12	2.37	0.45
1:B:322:VAL:HG12	1:B:326:TYR:CE1	2.52	0.45
1:B:287:ILE:CG2	1:B:289:ILE:HD11	2.45	0.44
1:A:150:ILE:CG2	1:A:153:LEU:HD13	2.46	0.44
1:A:395:ARG:O	1:A:396:SER:CB	2.66	0.44
1:A:129:TRP:HA	1:A:132:VAL:HG23	2.00	0.44
1:B:284:MET:HE3	1:B:387:ILE:CG2	2.47	0.44
1:B:326:TYR:HB2	1:B:351:LEU:HD13	2.00	0.44
1:A:250:VAL:HG23	1:A:250:VAL:O	2.19	0.43
1:A:255:ILE:HG21	1:A:326:TYR:OH	2.19	0.43
1:A:89:TYR:HA	1:A:96:LEU:HD13	2.00	0.43
1:A:257:ARG:HG2	1:A:259:ASP:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:HD21	1:B:120:LEU:HA	2.00	0.42
1:A:50:GLU:HB2	1:A:62:GLN:HE21	1.84	0.42
1:A:212:ILE:HG23	1:A:432:ALA:HB3	2.00	0.42
1:C:63:VAL:HG21	1:C:109:LEU:HD23	2.00	0.42
1:B:291:LYS:CB	1:B:314:THR:HG23	2.50	0.42
1:C:269:LEU:HD22	1:C:303:LEU:HD12	2.01	0.42
1:B:333:ILE:HG22	1:B:335:PRO:HD3	2.02	0.42
1:B:291:LYS:HB3	1:B:314:THR:HG23	2.01	0.42
1:A:123:VAL:HG11	1:A:425:TYR:CG	2.55	0.41
1:B:240:LEU:HD21	1:B:325:LEU:HD23	2.01	0.41
1:B:253:MET:CE	1:B:325:LEU:HD13	2.50	0.41
1:B:398:LEU:HD23	1:B:398:LEU:O	2.20	0.41
1:A:371:THR:HG21	1:A:408:ARG:CD	2.51	0.41
1:A:46:PHE:CE1	1:A:77:ARG:HD3	2.55	0.41
1:B:82:LEU:CD1	1:B:98:ARG:HG3	2.50	0.41
1:B:357:ALA:HB3	1:B:367:ILE:HD12	2.02	0.41
1:B:41:PRO:HB3	1:B:83:LEU:HD22	2.03	0.41
1:B:323:ARG:HG3	1:B:351:LEU:HD11	2.01	0.41
1:A:6:LEU:HD12	1:A:126:PHE:HB3	2.03	0.41
1:A:255:ILE:O	1:A:255:ILE:HG23	2.21	0.40
1:A:375:VAL:HG12	1:A:376:LYS:N	2.37	0.40
1:B:313:ILE:HD12	1:B:313:ILE:N	2.36	0.40
1:A:250:VAL:HG21	1:A:391:LEU:CD2	2.43	0.40
1:A:57:PHE:CZ	1:A:98:ARG:HG2	2.56	0.40
1:A:418:ALA:O	1:A:422:VAL:HG23	2.20	0.40
1:B:423:LYS:HB3	1:B:428:SER:O	2.22	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	Percentiles	
1	A	439/439 (100%)	422 (96%)	15 (3%)	2 (0%)	34	55
1	B	438/439 (100%)	419 (96%)	18 (4%)	1 (0%)	52	75
1	C	438/439 (100%)	425 (97%)	13 (3%)	0	100	100
All	All	1315/1317 (100%)	1266 (96%)	46 (4%)	3 (0%)	52	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	394	SER
1	A	396	SER
1	B	128	ASP

### 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	369/367 (100%)	356 (96%)	13 (4%)	43	70
1	B	368/367 (100%)	359 (98%)	9 (2%)	57	82
1	C	368/367 (100%)	363 (99%)	5 (1%)	74	91
All	All	1105/1101 (100%)	1078 (98%)	27 (2%)	55	82

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	153	LEU
1	A	209	GLU
1	A	247	ASP
1	A	248	GLU
1	A	260	ARG
1	A	296	LEU
1	A	309	ASN
1	A	369	ASN
1	A	388	LEU

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Mol	Chain	Res	Type
1	A	395	ARG
1	A	398	LEU
1	A	431	ARG
1	B	11	LEU
1	B	29	LEU
1	B	49	GLU
1	B	86	GLU
1	B	260	ARG
1	B	398	LEU
1	B	403	GLU
1	B	423	LYS
1	B	431	ARG
1	C	-1	ARG
1	C	29	LEU
1	C	153	LEU
1	C	395	ARG
1	C	431	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	309	ASN
1	B	217	ASN
1	B	369	ASN
1	C	217	ASN
1	C	225	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 carbohydrates in this entry.

## 5.6 Ligand geometry

7 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$
3	TRS	A	7360	-	7,7,7	0.93	1 (14%)	9,9,9	0.43	0
3	TRS	A	7361	-	7,7,7	0.92	1 (14%)	9,9,9	0.30	0
4	PO4	A	8000	-	4,4,4	0.46	0	6,6,6	0.27	0
2	NHF	B	438	-	11,11,11	6.04	2 (18%)	8,15,15	0.84	0
3	TRS	B	7362	-	7,7,7	0.94	1 (14%)	9,9,9	0.59	0
4	PO4	B	8001	-	4,4,4	0.45	0	6,6,6	0.27	0
4	PO4	C	8002	-	4,4,4	0.46	0	6,6,6	0.27	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	TRS	A	7360	-	-	0/9/9/9	0/0/0/0
3	TRS	A	7361	-	-	0/9/9/9	0/0/0/0
4	PO4	A	8000	-	-	0/0/0/0	0/0/0/0
2	NHF	B	438	-	-	0/2/19/19	0/1/1/1
3	TRS	B	7362	-	-	0/9/9/9	0/0/0/0
4	PO4	B	8001	-	-	0/0/0/0	0/0/0/0
4	PO4	C	8002	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	438	NHF	C1-C2	-18.77	1.34	1.51
3	B	7362	TRS	C-N	-2.44	1.47	1.50
3	A	7360	TRS	C-N	-2.41	1.47	1.50
3	A	7361	TRS	C-N	-2.34	1.47	1.50
2	B	438	NHF	O2-C2	6.83	1.33	1.21



There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	439/439 (100%)	1.07	75 (17%) 2 2	38, 42, 52, 58	0
1	B	439/439 (100%)	1.44	118 (26%) 1 1	37, 43, 50, 56	0
1	C	439/439 (100%)	1.14	79 (17%) 2 2	37, 42, 49, 56	0
All	All	1317/1317 (100%)	1.21	272 (20%) 1 1	37, 42, 50, 58	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	395	ARG	11.0
1	B	395	ARG	10.7
1	B	394	SER	10.5
1	B	391	LEU	7.9
1	B	-1	ARG	7.9
1	C	221	CYS	7.0
1	A	259	ASP	6.6
1	B	332	VAL	6.2
1	B	174	TYR	6.0
1	A	394	SER	5.8
1	B	242	SER	5.7
1	B	393	LEU	5.7
1	B	400	LYS	5.5
1	B	371	THR	5.5
1	B	260	ARG	5.4
1	B	259	ASP	5.3
1	C	-1	ARG	5.3
1	C	395	ARG	5.0
1	B	387	ILE	5.0
1	B	275	LEU	5.0
1	B	396	SER	4.9
1	B	243	LYS	4.8
1	C	58	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	279	LYS	4.6
1	B	403	GLU	4.6
1	A	0	HIS	4.6
1	C	394	SER	4.6
1	A	-1	ARG	4.5
1	C	93	TRP	4.5
1	B	244	PHE	4.5
1	A	262	GLN	4.5
1	B	301	ARG	4.5
1	B	316	MET	4.5
1	A	260	ARG	4.4
1	B	407	LYS	4.4
1	C	231	GLY	4.4
1	B	337	TYR	4.3
1	B	401	PHE	4.3
1	B	252	PHE	4.3
1	B	334	ILE	4.3
1	C	6	LEU	4.3
1	A	174	TYR	4.2
1	B	221	CYS	4.2
1	B	222	SER	4.2
1	C	369	ASN	4.2
1	C	39	PHE	4.1
1	B	397	ASP	4.1
1	C	251	THR	4.1
1	C	0	HIS	4.0
1	B	245	GLY	4.0
1	A	78	ILE	4.0
1	A	253	MET	4.0
1	A	106	ALA	4.0
1	B	223	PHE	4.0
1	B	149	THR	3.9
1	B	385	ASN	3.9
1	B	333	ILE	3.9
1	A	333	ILE	3.9
1	A	258	PHE	3.9
1	C	47	GLN	3.9
1	C	134	ALA	3.9
1	A	6	LEU	3.9
1	B	348	ALA	3.8
1	A	251	THR	3.8
1	C	50	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	5	LEU	3.8
1	C	252	PHE	3.8
1	A	248	GLU	3.8
1	C	333	ILE	3.7
1	B	344	VAL	3.7
1	A	282	GLN	3.7
1	B	392	GLU	3.7
1	C	316	MET	3.7
1	C	60	GLU	3.7
1	B	258	PHE	3.7
1	B	318	SER	3.6
1	B	268	LEU	3.6
1	A	410	MET	3.6
1	C	253	MET	3.6
1	B	353	ALA	3.6
1	A	369	ASN	3.6
1	B	234	ASP	3.6
1	B	282	GLN	3.5
1	B	329	VAL	3.5
1	C	38	VAL	3.5
1	C	174	TYR	3.5
1	A	393	LEU	3.5
1	C	103	PHE	3.5
1	B	331	PHE	3.5
1	B	248	GLU	3.5
1	C	397	ASP	3.5
1	C	100	ALA	3.4
1	C	14	LYS	3.4
1	C	353	ALA	3.4
1	B	277	SER	3.4
1	B	272	ILE	3.4
1	B	6	LEU	3.3
1	C	49	GLU	3.3
1	C	332	VAL	3.3
1	A	403	GLU	3.3
1	A	5	LEU	3.3
1	C	131	THR	3.3
1	C	234	ASP	3.2
1	C	254	PHE	3.2
1	C	287	ILE	3.2
1	B	253	MET	3.2
1	B	279	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	15	VAL	3.1
1	C	15	VAL	3.1
1	B	294	PRO	3.1
1	A	252	PHE	3.1
1	C	149	THR	3.0
1	B	254	PHE	3.0
1	B	317	LEU	3.0
1	B	326	TYR	3.0
1	B	150	ILE	3.0
1	C	329	VAL	3.0
1	A	350	CYS	3.0
1	B	278	LYS	3.0
1	C	41	PRO	3.0
1	C	148	PHE	2.9
1	C	247	ASP	2.9
1	B	239	SER	2.9
1	C	301	ARG	2.9
1	B	379	ASP	2.9
1	B	225	ASN	2.9
1	C	46	PHE	2.9
1	B	319	ARG	2.8
1	B	78	ILE	2.8
1	A	254	PHE	2.8
1	A	59	GLU	2.8
1	C	7	GLY	2.8
1	B	302	SER	2.8
1	C	78	ILE	2.8
1	B	324	GLU	2.8
1	B	376	LYS	2.7
1	A	104	GLY	2.7
1	A	103	PHE	2.7
1	A	272	ILE	2.7
1	C	385	ASN	2.7
1	B	293	ASP	2.7
1	C	126	PHE	2.7
1	A	15	VAL	2.7
1	B	247	ASP	2.7
1	B	147	VAL	2.7
1	A	16	GLY	2.7
1	C	16	GLY	2.7
1	B	14	LYS	2.7
1	A	108	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	332	VAL	2.6
1	B	315	GLU	2.6
1	C	230	THR	2.6
1	C	57	PHE	2.6
1	B	249	GLY	2.6
1	C	235	GLU	2.6
1	B	0	HIS	2.6
1	B	235	GLU	2.6
1	B	341	PHE	2.6
1	A	50	GLU	2.6
1	A	398	LEU	2.6
1	C	387	ILE	2.6
1	B	230	THR	2.6
1	C	106	ALA	2.6
1	A	124	VAL	2.6
1	A	397	ASP	2.6
1	A	396	SER	2.5
1	C	12	PRO	2.5
1	B	308	GLY	2.5
1	A	354	ILE	2.5
1	C	334	ILE	2.5
1	B	343	LEU	2.5
1	A	221	CYS	2.5
1	A	235	GLU	2.5
1	B	305	GLU	2.5
1	A	83	LEU	2.5
1	A	331	PHE	2.5
1	C	8	PHE	2.5
1	C	277	SER	2.5
1	B	22	LEU	2.5
1	B	246	MET	2.5
1	B	298	GLY	2.5
1	B	3	VAL	2.4
1	C	156	SER	2.4
1	A	329	VAL	2.4
1	A	131	THR	2.4
1	A	232	SER	2.4
1	C	349	MET	2.4
1	A	31	SER	2.4
1	C	288	ILE	2.4
1	C	404	ASN	2.4
1	A	268	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	5	LEU	2.4
1	A	4	LEU	2.4
1	A	147	VAL	2.4
1	B	312	VAL	2.4
1	C	132	VAL	2.4
1	C	437	LEU	2.4
1	C	40	THR	2.4
1	A	400	LYS	2.4
1	A	300	ALA	2.4
1	B	335	PRO	2.3
1	B	350	CYS	2.3
1	B	83	LEU	2.3
1	B	378	GLY	2.3
1	C	175	PRO	2.3
1	C	257	ARG	2.3
1	C	248	GLU	2.3
1	C	192	THR	2.3
1	C	17	GLY	2.3
1	B	10	PHE	2.3
1	B	4	LEU	2.3
1	A	190	VAL	2.3
1	B	148	PHE	2.3
1	A	392	GLU	2.3
1	B	227	SER	2.3
1	C	232	SER	2.3
1	B	224	TRP	2.3
1	B	410	MET	2.2
1	A	292	GLY	2.2
1	A	69	GLU	2.2
1	B	262	GLN	2.2
1	A	125	HIS	2.2
1	A	429	ILE	2.2
1	A	240	LEU	2.2
1	B	346	LEU	2.2
1	C	421	TYR	2.2
1	B	286	PHE	2.2
1	B	193	VAL	2.2
1	A	135	GLY	2.2
1	B	292	GLY	2.2
1	B	283	GLU	2.2
1	B	295	GLU	2.2
1	B	102	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	7	GLY	2.1
1	A	353	ALA	2.1
1	B	345	ALA	2.1
1	B	314	THR	2.1
1	A	231	GLY	2.1
1	A	305	GLU	2.1
1	B	127	HIS	2.1
1	B	232	SER	2.1
1	A	257	ARG	2.1
1	B	265	VAL	2.1
1	C	345	ALA	2.1
1	C	365	ASP	2.1
1	A	279	LYS	2.1
1	B	131	THR	2.1
1	B	173	PRO	2.1
1	B	288	ILE	2.1
1	B	388	LEU	2.1
1	C	4	LEU	2.1
1	C	286	PHE	2.1
1	A	39	PHE	2.1
1	B	269	LEU	2.1
1	B	296	LEU	2.1
1	B	303	LEU	2.1
1	A	107	SER	2.1
1	B	419	GLU	2.1
1	C	127	HIS	2.1
1	A	149	THR	2.1
1	A	316[A]	MET	2.0
1	C	176	ASP	2.0
1	A	324	GLU	2.0
1	C	215	VAL	2.0
1	A	269	LEU	2.0
1	A	222	SER	2.0
1	B	191	THR	2.0
1	B	195	ARG	2.0
1	C	117	GLU	2.0
1	A	101	VAL	2.0
1	A	256	GLY	2.0
1	B	368	THR	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 carbohydrates 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. 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, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PO4	C	8002	5/5	0.76	0.45	12.46	85,85,85,86	0
4	PO4	A	8000	5/5	0.87	0.49	10.67	81,81,81,82	0
4	PO4	B	8001	5/5	0.91	0.29	6.42	93,93,93,93	0
3	TRS	A	7361	8/8	0.71	0.35	4.88	56,57,57,57	0
3	TRS	B	7362	8/8	0.70	0.34	4.48	84,84,84,84	0
3	TRS	A	7360	8/8	0.78	0.28	1.98	60,61,61,61	0
2	NHF	B	438	11/11	0.80	0.22	-0.51	65,66,66,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.