



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 08:14 pm BST

PDB ID : 3RZI  
Title : The structure of 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase from mycobacterium tuberculosis cocrystallized and complexed with phenylalanine and tryptophan  
Authors : Jiao, W.; Jameson, G.B.; Hutton, R.D.; Parker, E.J.  
Deposited on : 2011-05-11  
Resolution : 1.95 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

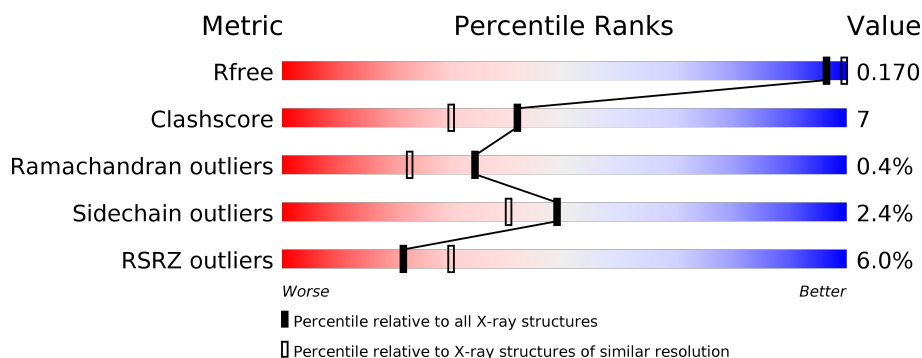
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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	462	
1	B	462	

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
7	GOL	A	471	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7800 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.

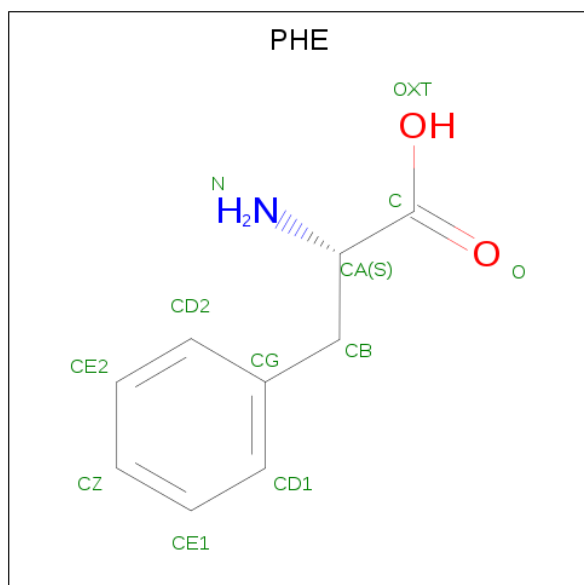
- Molecule 1 is a protein called Probable 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase AroG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	9	0
			3570	2226	655	672	17			
1	B	457	Total	C	N	O	S	0	10	0
			3599	2242	659	680	18			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

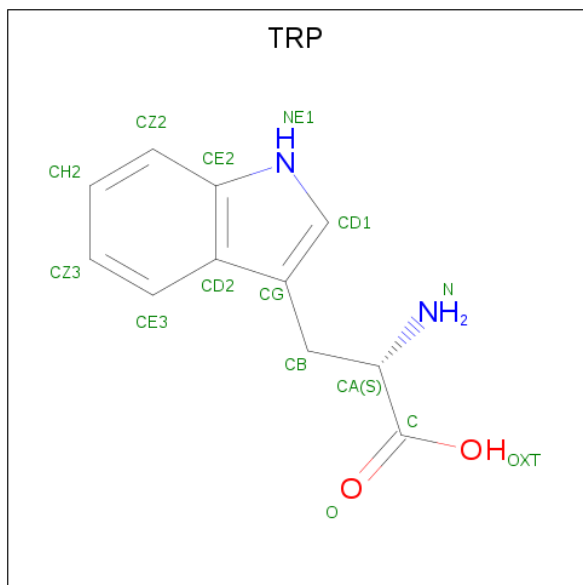
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		

- Molecule 3 is PHENYLALANINE (three-letter code: PHE) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	9	1	2		
3	B	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 4 is TRYPTOPHAN (three-letter code: TRP) (formula:  $C_{11}H_{12}N_2O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	11	2	2		
4	B	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula:  $Cl$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total 1	Cl 1	0	0
8	A	1	Total 1	Cl 1	0	0

- Molecule 9 is water.

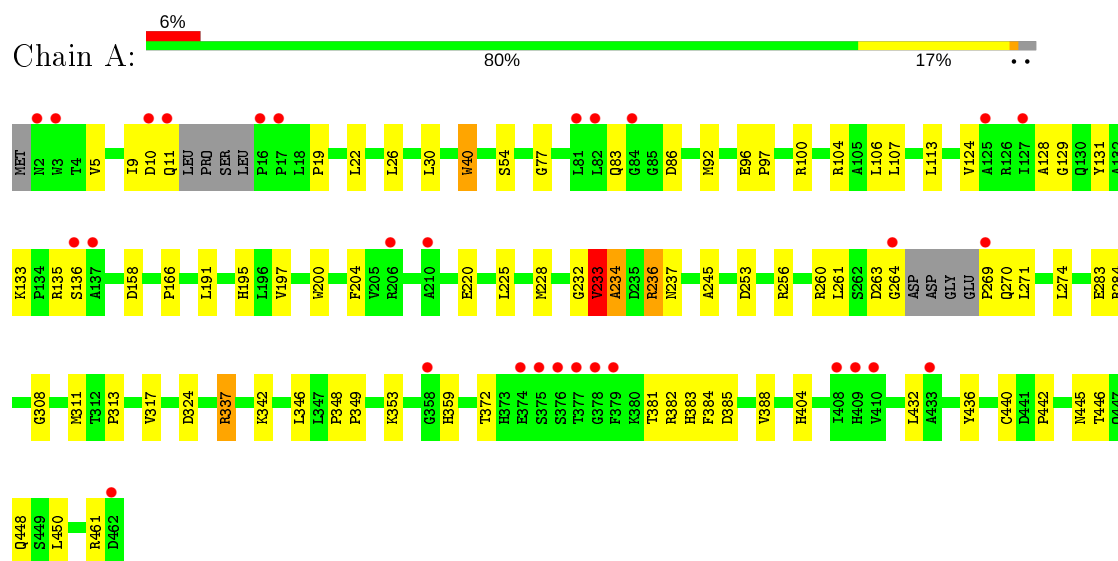
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	229	Total 229	O 229	0	0
9	B	266	Total 266	O 266	0	0



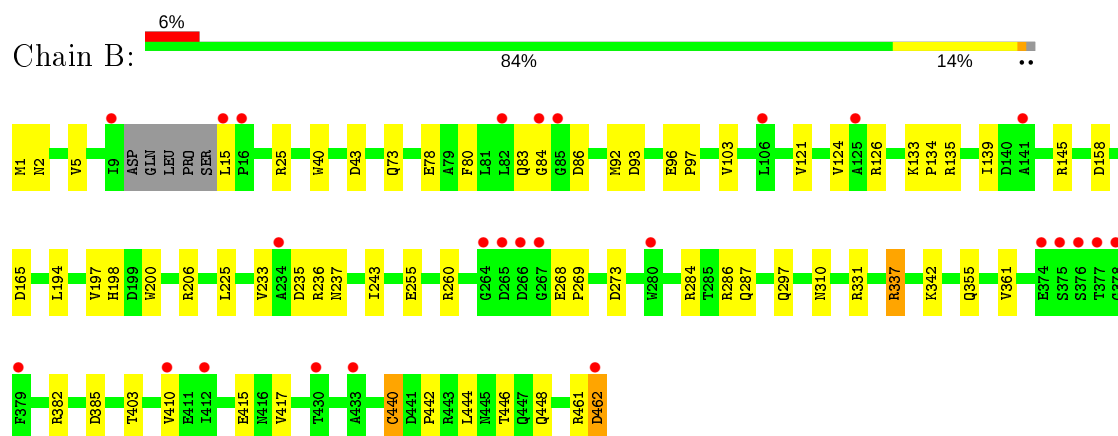
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase AroG



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	207.56 Å   207.56 Å   66.98 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	31.88 – 1.95 31.68 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (31.88-1.95) 99.4 (31.68-1.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	54.24 (at 1.95 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.153 , 0.168 0.154 , 0.170	Depositor DCC
$R_{free}$ test set	6034 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 51.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7800	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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, 0.333 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: GOL, PO4, MN, SO4, CL

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	0.71	2/3642 (0.1%)	1.00	9/4950 (0.2%)
1	B	0.75	0/3672	1.05	15/4994 (0.3%)
All	All	0.73	2/7314 (0.0%)	1.03	24/9944 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	ALA	CA-CB	5.10	1.63	1.52
1	A	128	ALA	CA-CB	5.04	1.63	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	ASP	CB-CG-OD1	9.43	126.78	118.30
1	B	260	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	A	104	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	B	165	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	93	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	B	126	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	A	236	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	B	43	ASP	CB-CG-OD1	5.86	123.58	118.30
1	B	126	ARG	NE-CZ-NH2	-5.82	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	86	ASP	CB-CG-OD1	5.74	123.46	118.30
1	B	25	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	206	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	A	107	LEU	CA-CB-CG	5.59	128.15	115.30
1	A	106	LEU	CB-CG-CD1	-5.52	101.61	111.00
1	A	253	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	337	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	B	25	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	260	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	113	LEU	CB-CG-CD1	-5.27	102.04	111.00
1	B	206	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	A	261	LEU	CB-CG-CD1	-5.17	102.22	111.00
1	A	86	ASP	CB-CG-OD1	5.02	122.82	118.30
1	B	385	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	GLY	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3570	0	3515	66	0
1	B	3599	0	3538	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	12	0	8	0	0
3	B	12	0	8	0	0
4	A	15	0	9	1	0
4	B	15	0	9	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	15	0	0	0	0
7	A	18	0	24	4	0
7	B	30	0	40	2	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	229	0	0	4	0
9	B	266	0	0	6	0
All	All	7800	0	7151	102	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 7.

All (102) 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:233[B]:VAL:CG2	1:A:234[B]:ALA:H	1.38	1.25
1:A:22[B]:LEU:HD11	1:A:271:LEU:HD12	1.26	1.10
1:A:233[B]:VAL:HG23	1:A:234[B]:ALA:N	1.50	1.07
1:A:22[B]:LEU:HD11	1:A:271:LEU:CD1	1.90	0.99
1:B:133:LYS:NZ	1:B:440:CYS:SG	2.42	0.92
1:B:382:ARG:HD2	1:B:442:PRO:HG2	1.50	0.90
1:A:233[B]:VAL:HG23	1:A:234[B]:ALA:H	0.71	0.85
1:A:233[B]:VAL:CG2	1:A:234[B]:ALA:N	2.06	0.84
1:A:225:LEU:HD23	1:A:228:MET:HE3	1.65	0.76
1:B:233[B]:VAL:HG23	1:B:233[B]:VAL:O	1.85	0.74
1:A:233[B]:VAL:HG22	1:A:234[B]:ALA:N	2.03	0.73
1:B:15:LEU:HA	9:B:662:HOH:O	1.88	0.73
1:A:236:ARG:HD2	1:B:236:ARG:CD	2.23	0.68
1:A:233[A]:VAL:HG23	1:A:234[A]:ALA:O	1.94	0.67
1:A:236:ARG:HD2	1:B:236:ARG:HD2	1.77	0.67
1:A:225:LEU:HD23	1:A:228:MET:CE	2.26	0.65
1:A:22[B]:LEU:HD21	1:A:271:LEU:HG	1.80	0.64
1:A:30:LEU:HD13	1:A:256:ARG:CZ	2.29	0.63
1:B:133:LYS:HD2	1:B:135[A]:ARG:HE	1.64	0.61
1:B:194:LEU:CD2	1:B:225:LEU:HD21	2.32	0.60
1:A:136:SER:H	7:A:471:GOL:H31	1.66	0.59
1:A:313:PRO:O	1:A:317:VAL:HG23	2.03	0.58
1:A:264:GLY:HA3	1:A:269:PRO:HD3	1.84	0.58
1:A:348:PRO:HB2	1:A:349:PRO:HD3	1.84	0.58
1:A:195:HIS:ND1	9:A:594:HOH:O	2.31	0.58
1:A:381:THR:HA	1:A:442:PRO:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233[B]:VAL:O	1:A:234[B]:ALA:HB3	2.06	0.56
1:A:133:LYS:HD2	1:A:135:ARG:HD3	1.87	0.56
1:A:204:PHE:CG	1:A:450:LEU:HD23	2.41	0.55
1:B:103:VAL:HG13	1:B:243:ILE:CD1	2.36	0.55
1:A:83:GLN:HA	1:A:124:VAL:O	2.07	0.55
1:B:235[B]:ASP:CG	1:B:237:ASN:H	2.09	0.54
1:B:355:GLN:HG3	1:B:403:THR:HG21	1.90	0.54
1:A:135:ARG:HE	7:A:471:GOL:H32	1.74	0.53
1:B:233[A]:VAL:O	1:B:233[A]:VAL:HG23	2.09	0.53
1:A:135:ARG:NE	7:A:471:GOL:H32	2.23	0.53
1:B:331:ARG:HD2	1:B:331:ARG:O	2.09	0.53
1:B:83:GLN:HA	1:B:124:VAL:O	2.09	0.53
1:A:10:ASP:O	1:A:11:GLN:HB2	2.08	0.53
1:A:283:GLU:OE2	1:A:308:GLY:HA3	2.09	0.53
1:A:311:MET:HA	1:A:311:MET:HE2	1.91	0.52
1:B:96:GLU:HB3	1:B:97:PRO:HD3	1.91	0.52
1:B:134:PRO:O	1:B:135[A]:ARG:HD3	2.09	0.52
1:A:220:GLU:OE2	1:A:461:ARG:NH2	2.40	0.51
1:B:415:GLU:HB2	1:B:417:VAL:HG13	1.92	0.51
1:B:268:GLU:HG2	1:B:269:PRO:CD	2.41	0.51
1:B:382:ARG:CD	1:B:442:PRO:HG2	2.32	0.50
1:A:131:TYR:OH	9:A:547:HOH:O	2.15	0.49
1:A:26:LEU:HD11	1:A:271:LEU:CD1	2.42	0.49
1:B:297:GLN:NE2	7:B:472:GOL:O1	2.46	0.49
1:B:461:ARG:O	1:B:462:ASP:C	2.50	0.49
1:A:237[B]:ASN:HD21	1:B:236:ARG:HH12	1.61	0.49
1:A:19:PRO:HD2	1:A:22[B]:LEU:HD23	1.93	0.49
1:B:194:LEU:HD21	1:B:225:LEU:HD21	1.94	0.49
1:B:342:LYS:NZ	9:B:671:HOH:O	2.46	0.48
1:A:236:ARG:CD	1:B:236:ARG:HD2	2.42	0.48
1:B:198:HIS:ND1	9:B:679:HOH:O	2.30	0.48
1:A:26:LEU:HD11	1:A:271:LEU:HD11	1.96	0.48
1:A:133:LYS:NZ	1:A:440:CYS:SG	2.67	0.48
1:A:92:MET:HE3	9:A:662:HOH:O	2.14	0.48
1:B:268:GLU:HG2	1:B:269:PRO:HD2	1.96	0.48
1:B:268:GLU:HG2	1:B:269:PRO:N	2.29	0.48
1:A:432:LEU:O	1:A:436:TYR:HB2	2.14	0.47
1:B:80:PHE:O	1:B:121:VAL:HA	2.14	0.47
1:A:96:GLU:HB3	1:A:97:PRO:HD3	1.96	0.47
1:A:337:ARG:HD3	1:A:337:ARG:O	2.15	0.47
1:A:22[B]:LEU:HD11	1:A:271:LEU:HD11	1.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:PHE:O	1:A:388:VAL:HG23	2.16	0.46
1:B:1:MET:HG2	1:B:2:ASN:H	1.81	0.45
1:B:84:GLY:HA2	1:B:410:VAL:O	2.17	0.45
1:A:237[A]:ASN:O	4:A:465:TRP:N	2.49	0.45
1:A:77:GLY:HA2	1:A:404:HIS:CD2	2.52	0.45
1:A:5:VAL:CG2	1:B:5:VAL:HG22	2.47	0.45
1:B:255:GLU:OE1	1:B:273:ASP:OD2	2.35	0.45
1:A:445:ASN:OD1	1:A:448:GLN:HG3	2.18	0.44
1:B:73:GLN:NE2	1:B:78:GLU:OE1	2.50	0.44
1:A:204:PHE:CD2	1:A:450:LEU:HD23	2.53	0.44
1:A:271:LEU:HD23	1:A:271:LEU:HA	1.78	0.44
1:B:145:ARG:NH1	9:B:542:HOH:O	2.38	0.44
1:A:100[B]:ARG:NH2	9:A:632:HOH:O	2.51	0.44
1:A:10:ASP:O	1:A:11:GLN:CB	2.66	0.43
1:A:346:LEU:HA	1:A:346:LEU:HD23	1.78	0.43
1:A:342:LYS:HB3	1:A:346:LEU:HD12	2.00	0.43
7:B:472:GOL:H11	9:B:537:HOH:O	2.18	0.43
1:B:361:VAL:HG22	9:B:726:HOH:O	2.19	0.42
1:A:260:ARG:HB2	1:A:274:LEU:HD12	2.00	0.42
1:A:372:THR:HA	1:A:382:ARG:HG2	2.02	0.42
1:A:100[B]:ARG:HE	1:A:191:LEU:HD13	1.84	0.42
1:A:22[B]:LEU:HD12	1:A:22[B]:LEU:C	2.40	0.41
1:A:197:VAL:HA	1:A:200:TRP:CE3	2.55	0.41
1:A:263:ASP:OD2	1:A:263:ASP:C	2.58	0.41
1:A:40:TRP:CZ3	1:A:166:PRO:HA	2.55	0.41
1:A:284:ARG:HH12	7:A:471:GOL:H11	1.85	0.41
1:B:197:VAL:HA	1:B:200:TRP:CE3	2.55	0.41
1:B:444:LEU:HD22	1:B:448:GLN:HB3	2.03	0.41
1:A:383[A]:HIS:HD2	1:A:385:ASP:H	1.67	0.41
1:B:133:LYS:HD2	1:B:135[A]:ARG:NE	2.31	0.41
1:A:324:ASP:O	1:A:359:HIS:HE1	2.03	0.41
1:A:382:ARG:HG3	1:A:442:PRO:HG2	2.03	0.41
1:A:233[B]:VAL:O	1:A:234[B]:ALA:CB	2.66	0.40
1:A:348:PRO:HB2	1:A:349:PRO:CD	2.51	0.40
1:B:286:ARG:O	1:B:287:GLN:C	2.59	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	456/462 (99%)	436 (96%)	15 (3%)	5 (1%)	14	5
1	B	463/462 (100%)	448 (97%)	14 (3%)	1 (0%)	47	38
All	All	919/924 (100%)	884 (96%)	29 (3%)	6 (1%)	34	11

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	GLY
1	A	233[A]	VAL
1	A	233[B]	VAL
1	A	234[A]	ALA
1	A	234[B]	ALA
1	B	440	CYS

### 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	376/376 (100%)	366 (97%)	10 (3%)	44	34
1	B	379/376 (101%)	369 (97%)	10 (3%)	46	36
All	All	755/752 (100%)	735 (97%)	20 (3%)	49	36

All (20) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	9	ILE
1	A	40	TRP
1	A	54	SER
1	A	158	ASP
1	A	233[A]	VAL
1	A	233[B]	VAL
1	A	270	GLN
1	A	337	ARG
1	A	353	LYS
1	A	446	THR
1	B	40	TRP
1	B	92	MET
1	B	139	ILE
1	B	158	ASP
1	B	284	ARG
1	B	310[A]	ASN
1	B	310[B]	ASN
1	B	337	ARG
1	B	446	THR
1	B	462	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	44	GLN
1	B	73	GLN
1	B	297	GLN
1	B	373	HIS

### 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

Of 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	GOL	B	475	-	5,5,5	0.36	0	5,5,5	0.37	0
5	PO4	B	467	-	4,4,4	1.05	0	6,6,6	0.93	0
6	SO4	B	470	-	4,4,4	0.15	0	6,6,6	0.45	0
7	GOL	B	472	-	5,5,5	0.37	0	5,5,5	0.76	0
6	SO4	A	467	-	4,4,4	0.18	0	6,6,6	0.15	0
6	SO4	B	469	-	4,4,4	0.20	0	6,6,6	0.32	0
7	GOL	A	468	-	5,5,5	0.46	0	5,5,5	0.33	0
6	SO4	B	468	-	4,4,4	0.15	0	6,6,6	0.18	0
7	GOL	A	471	-	5,5,5	0.34	0	5,5,5	0.14	0
7	GOL	B	474	-	5,5,5	0.36	0	5,5,5	0.25	0
7	GOL	B	473	-	5,5,5	0.46	0	5,5,5	0.40	0
7	GOL	A	469	-	5,5,5	0.36	0	5,5,5	0.35	0
5	PO4	A	466	-	4,4,4	1.24	0	6,6,6	0.65	0
7	GOL	B	464	-	5,5,5	0.31	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
7	GOL	B	475	-	-	2/4/4/4	-
7	GOL	B	472	-	-	2/4/4/4	-
7	GOL	A	468	-	-	2/4/4/4	-
7	GOL	A	471	-	-	2/4/4/4	-
7	GOL	B	474	-	-	4/4/4/4	-
7	GOL	B	473	-	-	0/4/4/4	-
7	GOL	A	469	-	-	2/4/4/4	-
7	GOL	B	464	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	475	GOL	C1-C2-C3-O3
7	A	471	GOL	O1-C1-C2-C3
7	A	469	GOL	C1-C2-C3-O3
7	A	469	GOL	O2-C2-C3-O3
7	B	474	GOL	O1-C1-C2-C3
7	B	474	GOL	C1-C2-C3-O3
7	B	464	GOL	O1-C1-C2-C3
7	A	471	GOL	O1-C1-C2-O2
7	A	468	GOL	O1-C1-C2-C3
7	B	472	GOL	O1-C1-C2-C3
7	B	475	GOL	O2-C2-C3-O3
7	B	474	GOL	O1-C1-C2-O2
7	B	472	GOL	O1-C1-C2-O2
7	B	464	GOL	O1-C1-C2-O2
7	B	474	GOL	O2-C2-C3-O3
7	A	468	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	472	GOL	2	0
7	A	471	GOL	4	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, 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	453/462 (98%)	0.06	29 (6%)	19 28	19, 31, 51, 76	0
1	B	457/462 (98%)	-0.04	26 (5%)	23 32	18, 28, 50, 83	1 (0%)
All	All	910/924 (98%)	0.01	55 (6%)	21 30	18, 30, 50, 83	1 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	TRP	7.4
1	B	265	ASP	5.8
1	B	15	LEU	5.3
1	B	267	GLY	4.9
1	A	2	ASN	4.5
1	B	376	SER	4.5
1	A	377	THR	4.5
1	A	11	GLN	4.3
1	B	9	ILE	4.3
1	B	266	ASP	4.1
1	A	376	SER	4.0
1	A	462	ASP	4.0
1	B	16	PRO	3.8
1	B	462	ASP	3.7
1	A	16	PRO	3.6
1	A	264	GLY	3.2
1	A	378	GLY	3.1
1	B	378	GLY	3.1
1	A	375	SER	3.1
1	A	17	PRO	3.0
1	A	410	VAL	2.9
1	B	82	LEU	2.8
1	A	374	GLU	2.8
1	A	136	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	206	ARG	2.7
1	A	269	PRO	2.6
1	B	433	ALA	2.5
1	A	379	PHE	2.5
1	A	10	ASP	2.5
1	B	106	LEU	2.4
1	B	141	ALA	2.4
1	B	410	VAL	2.4
1	B	264	GLY	2.4
1	B	374	GLU	2.4
1	A	408	ILE	2.4
1	A	82	LEU	2.3
1	A	137	ALA	2.3
1	B	280	TRP	2.3
1	B	412	ILE	2.2
1	B	377	THR	2.2
1	A	409	HIS	2.2
1	B	375	SER	2.2
1	B	234[A]	ALA	2.2
1	B	84	GLY	2.2
1	A	210	ALA	2.1
1	B	379	PHE	2.1
1	A	358	GLY	2.1
1	A	433	ALA	2.1
1	B	125	ALA	2.1
1	B	85	GLY	2.1
1	A	84	GLY	2.0
1	A	127	ILE	2.0
1	A	125	ALA	2.0
1	A	81	LEU	2.0
1	B	430	THR	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
7	GOL	A	471	6/6	0.41	0.24	75,80,81,83	0
7	GOL	A	468	6/6	0.67	0.36	85,91,92,92	0
7	GOL	B	473	6/6	0.72	0.24	81,86,88,90	0
8	CL	B	471	1/1	0.74	0.14	92,92,92,92	0
7	GOL	A	469	6/6	0.77	0.23	83,87,88,89	0
7	GOL	B	475	6/6	0.78	0.20	76,82,86,88	0
7	GOL	B	474	6/6	0.80	0.18	92,93,93,95	0
7	GOL	B	472	6/6	0.82	0.19	80,86,87,88	0
3	PHE	A	464	12/12	0.84	0.35	37,40,43,43	12
7	GOL	B	464	6/6	0.84	0.14	74,79,81,82	0
3	PHE	B	465	12/12	0.86	0.29	42,45,47,47	12
6	SO4	A	467	5/5	0.92	0.16	90,91,93,93	0
8	CL	A	470	1/1	0.93	0.09	88,88,88,88	0
4	TRP	B	466	15/15	0.94	0.14	39,43,45,46	0
4	TRP	A	465	15/15	0.96	0.15	46,49,51,52	0
6	SO4	B	468	5/5	0.96	0.12	100,101,101,102	0
6	SO4	B	470	5/5	0.98	0.08	46,48,55,56	0
2	MN	A	463	1/1	0.98	0.13	44,44,44,44	1
5	PO4	A	466	5/5	0.99	0.15	58,62,67,70	0
6	SO4	B	469	5/5	0.99	0.16	52,55,56,57	0
5	PO4	B	467	5/5	0.99	0.12	45,46,48,50	0
2	MN	B	463	1/1	1.00	0.05	47,47,47,47	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.