



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:13 PM GMT

PDB ID : 2B7O  
Title : The Structure of 3-Deoxy-D-Arabino-Heptulosonate7-Phosphate Synthase from Mycobacterium tuberculosis  
Authors : Webby, C.J.; Baker, H.M.; Lott, J.S.; Baker, E.N.; Parker, E.J.; Mycobacterium Tuberculosis Structural Proteomics Project (XMTB)  
Deposited on : 2005-10-05  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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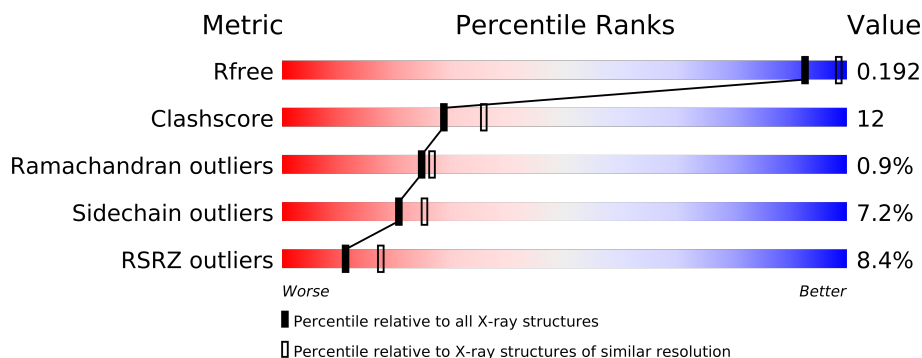
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. 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	464	
1	B	464	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	PEP	A	702	-	X
4	PEP	B	703	-	X
5	CE1	A	1001	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7329 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 3-deoxy-D-arabino-heptulosonate7-phosphate synthase AroG.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	Se	0	0	0
			3468	2170	630	651	4	13			
1	B	451	Total	C	N	O	S	Se	0	0	0
			3468	2172	629	650	4	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP O53512
A	0	ALA	-	EXPRESSION TAG	UNP O53512
B	-1	GLY	-	EXPRESSION TAG	UNP O53512
B	0	ALA	-	EXPRESSION TAG	UNP O53512

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

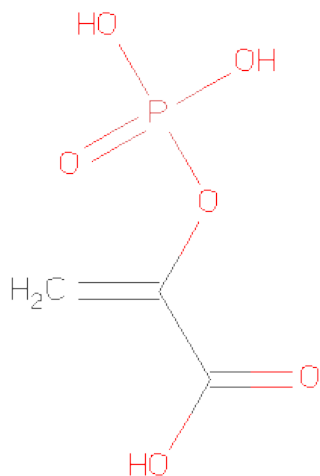
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



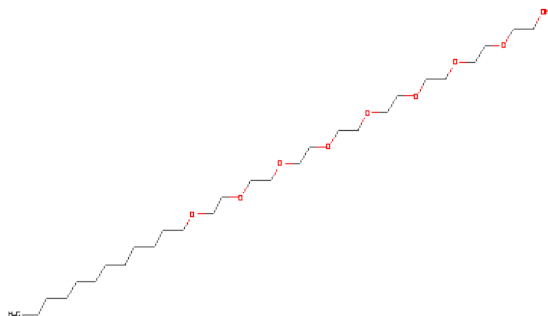
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula:  $C_3H_5O_6P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			10	3	6	1		
4	B	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 5 is O-DODECANYL OCTAETHYLENE GLYCOL (three-letter code: CE1) (formula:  $C_{28}H_{58}O_9$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	25	20	5	0	0

- Molecule 6 is water.

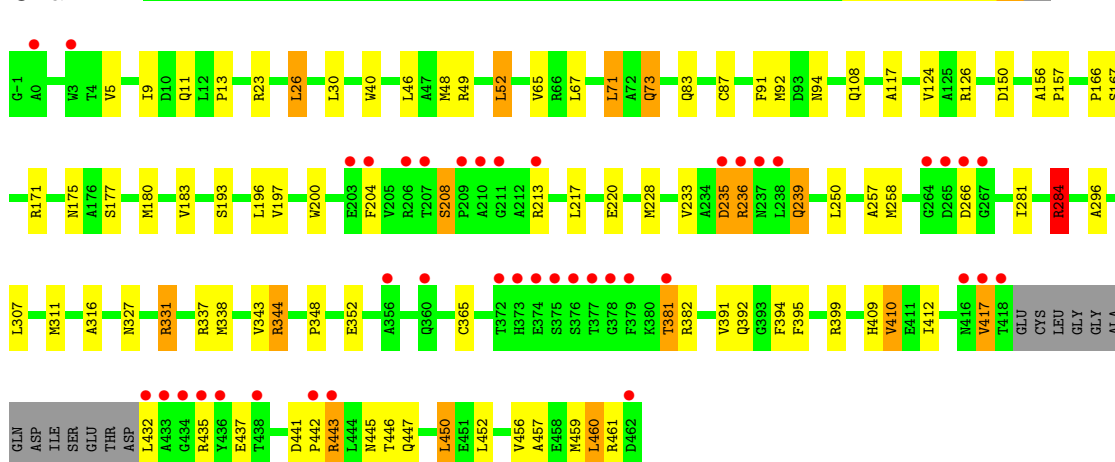
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	151	Total	O	0	0
			151	151		
6	B	185	Total	O	0	0
			185	185		

### 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.

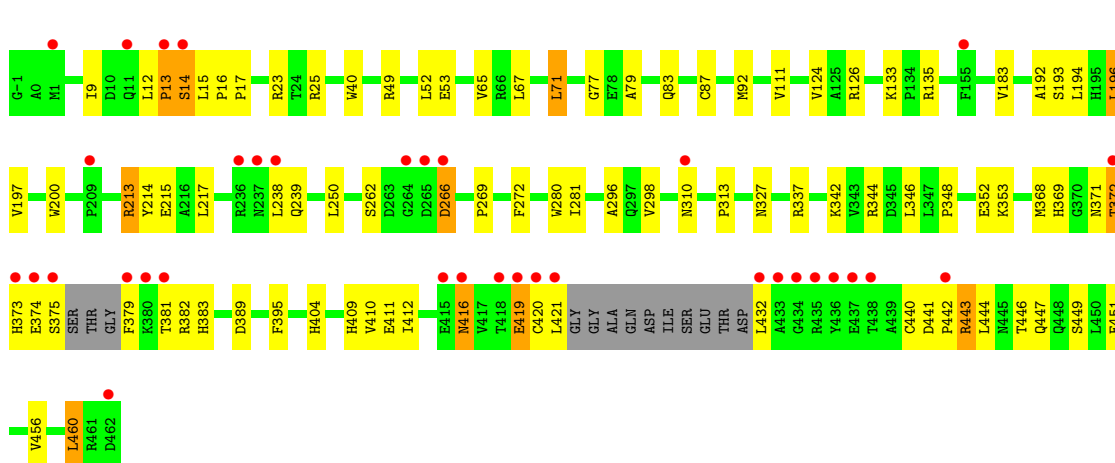
- Molecule 1: 3-deoxy-D-arabino-heptulosonate7-phosphate synthase AroG

Chain A:



- Molecule 1: 3-deoxy-D-arabino-heptulosonate7-phosphate synthase AroG

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.09Å 204.09Å 66.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.04 – 2.30 47.03 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.04-2.30) 100.0 (47.03-2.30)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.67 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.188 , 0.224 0.190 , 0.192	Depositor DCC
$R_{free}$ test set	3567 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 40.7	EDS
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 70361 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7329	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 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: MN, PEP, SO4, CE1

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	0.67	0/3528	0.75	3/4780 (0.1%)
1	B	0.73	0/3527	0.78	4/4777 (0.1%)
All	All	0.70	0/7055	0.77	7/9557 (0.1%)

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

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	B	25	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	A	284	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	183	VAL	CG1-CB-CG2	6.09	120.65	110.90
1	A	331	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	331	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	444	LEU	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	GLN	Peptide



## 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	3468	0	3425	100	0
1	B	3468	0	3421	70	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	10	0	2	0	0
4	B	10	0	2	2	0
5	A	25	0	41	12	0
6	A	151	0	0	8	0
6	B	185	0	0	5	0
All	All	7329	0	6891	173	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 12.

All (173) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:48:MSE:CE	1:A:167:SER:HA	1.41	1.46
1:A:48:MSE:HE2	1:A:167:SER:CA	1.61	1.28
1:A:344:ARG:HG2	1:A:344:ARG:HH11	1.20	1.03
1:A:344:ARG:HD2	6:A:2030:HOH:O	1.59	1.02
1:A:171:ARG:HH21	5:A:1001:CE1:H171	1.22	1.02
1:A:52:LEU:HB3	1:A:258:MSE:CE	1.90	1.00
1:A:311:MSE:HE3	1:A:316:ALA:HB2	1.41	1.00
1:B:197:VAL:HA	1:B:200:TRP:CE3	2.05	0.90
1:A:52:LEU:HB3	1:A:258:MSE:HE1	1.54	0.88
1:A:311:MSE:HE3	1:A:316:ALA:CB	2.02	0.88
1:A:344:ARG:HH11	1:A:344:ARG:CG	1.91	0.84
5:A:1001:CE1:C18	5:A:1001:CE1:H232	2.08	0.83
1:B:133:LYS:HD2	1:B:440:CYS:SG	2.19	0.82
1:A:311:MSE:HE3	1:A:316:ALA:CA	2.09	0.82
1:B:133:LYS:HE3	1:B:135:ARG:HD3	1.59	0.82
1:B:443:ARG:HB2	1:B:443:ARG:NH1	1.96	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:48:MSE:HE2	1:A:167:SER:HA	0.81	0.79
1:B:213:ARG:HG2	1:B:213:ARG:HH11	1.48	0.78
1:B:369:HIS:CE1	1:B:411:GLU:OE2	2.36	0.78
1:A:197:VAL:HA	1:A:200:TRP:CE3	2.19	0.78
1:A:48:MSE:CE	1:A:167:SER:CA	2.38	0.78
1:B:12:LEU:N	1:B:13:PRO:HD3	1.99	0.77
1:B:410:VAL:HG13	1:B:412:ILE:HG23	1.67	0.75
1:A:52:LEU:HB3	1:A:258:MSE:HE3	1.68	0.74
5:A:1001:CE1:H232	5:A:1001:CE1:H181	1.70	0.74
1:A:311:MSE:CE	1:A:316:ALA:HA	2.19	0.72
1:A:392:GLN:HA	1:A:459:MSE:CE	2.19	0.72
1:A:48:MSE:HE3	1:A:167:SER:HA	1.63	0.72
1:B:369:HIS:NE2	1:B:411:GLU:OE2	2.22	0.72
1:A:284:ARG:HG3	1:A:284:ARG:HH11	1.55	0.72
1:B:49:ARG:NH1	6:B:2084:HOH:O	2.24	0.71
1:A:395:PHE:CG	1:A:459:MSE:HE2	2.26	0.70
1:B:197:VAL:HA	1:B:200:TRP:CZ3	2.28	0.69
1:B:9:ILE:O	1:B:12:LEU:HB2	1.93	0.68
1:A:311:MSE:CE	1:A:316:ALA:CA	2.70	0.68
1:A:9:ILE:HD13	1:A:48:MSE:HE1	1.75	0.67
1:A:395:PHE:CD1	1:A:459:MSE:HE2	2.29	0.67
1:A:228:MSE:HE3	1:A:233:VAL:HG11	1.75	0.67
1:B:266:ASP:HB2	6:B:2075:HOH:O	1.93	0.66
1:A:392:GLN:HA	1:A:459:MSE:HE3	1.78	0.66
1:B:213:ARG:CG	1:B:213:ARG:HH11	2.08	0.65
1:A:52:LEU:O	1:A:258:MSE:HE1	1.97	0.65
1:A:9:ILE:CD1	1:A:48:MSE:HE1	2.27	0.65
1:A:23:ARG:NH1	6:A:2144:HOH:O	2.29	0.64
1:A:52:LEU:CB	1:A:258:MSE:HE1	2.27	0.64
1:B:313:PRO:HB3	1:B:353:LYS:HG3	1.81	0.63
1:A:443:ARG:HE	1:A:443:ARG:H	1.47	0.62
1:A:126:ARG:HH11	1:A:409:HIS:CE1	2.16	0.62
1:B:410:VAL:CG1	1:B:412:ILE:HG23	2.29	0.61
1:B:410:VAL:HG13	1:B:412:ILE:CG2	2.30	0.61
1:A:49:ARG:NE	6:A:2015:HOH:O	2.32	0.61
1:A:410:VAL:HG13	1:A:412:ILE:HG23	1.82	0.61
1:A:307:LEU:HD22	1:A:311:MSE:HE2	1.83	0.61
1:B:280:TRP:HE1	4:B:703:PEP:C3	2.14	0.61
5:A:1001:CE1:H182	5:A:1001:CE1:H232	1.82	0.60
1:B:421:LEU:H	1:B:421:LEU:HD23	1.64	0.60
1:A:126:ARG:HH11	1:A:409:HIS:HE1	1.48	0.60
1:B:126:ARG:HH11	1:B:409:HIS:CE1	2.21	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:213:ARG:HH11	1:A:213:ARG:HB2	1.67	0.59
1:A:197:VAL:HA	1:A:200:TRP:CZ3	2.37	0.59
1:B:395:PHE:CE2	1:B:460:LEU:HD13	2.37	0.59
1:A:365:CYS:HB2	1:A:394:PHE:CD1	2.39	0.58
1:B:87:CYS:SG	1:B:441:ASP:HB2	2.44	0.57
1:A:382:ARG:HD2	1:A:442:PRO:HG2	1.87	0.57
1:B:383:HIS:CD2	1:B:421:LEU:C	2.78	0.57
1:A:171:ARG:NH2	5:A:1001:CE1:H171	2.07	0.57
1:A:443:ARG:HE	1:A:443:ARG:N	2.03	0.56
1:B:126:ARG:HH11	1:B:409:HIS:HE1	1.51	0.56
1:A:92:MSE:O	5:A:1001:CE1:O25	2.24	0.56
1:A:87:CYS:SG	1:A:441:ASP:HB2	2.45	0.56
1:B:262:SER:HB3	1:B:272:PHE:CE1	2.40	0.56
1:B:371:ASN:O	1:B:372:THR:HG23	2.06	0.55
1:A:395:PHE:HB2	1:A:459:MSE:CE	2.36	0.55
1:A:311:MSE:HE1	1:A:316:ALA:HA	1.88	0.55
1:A:395:PHE:CD1	1:A:459:MSE:CE	2.90	0.54
1:B:395:PHE:HE2	1:B:460:LEU:HD13	1.73	0.54
1:A:220:GLU:CD	1:A:461:ARG:HH22	2.11	0.54
1:B:67:LEU:HG	1:B:71:LEU:HD22	1.90	0.54
1:B:281:ILE:HD11	1:B:296:ALA:HB2	1.89	0.53
1:B:410:VAL:CG1	1:B:412:ILE:CG2	2.85	0.53
1:A:365:CYS:HB2	1:A:394:PHE:CG	2.43	0.53
1:B:443:ARG:CZ	1:B:443:ARG:HB2	2.37	0.53
1:A:67:LEU:HG	1:A:71:LEU:HD22	1.89	0.53
1:B:443:ARG:HH11	1:B:443:ARG:HB2	1.71	0.53
1:A:437:GLU:H	1:A:443:ARG:HH12	1.56	0.52
1:B:79:ALA:O	1:B:404:HIS:HE1	1.92	0.52
1:A:175:ASN:HD21	5:A:1001:CE1:H151	1.74	0.52
1:B:12:LEU:N	1:B:13:PRO:CD	2.70	0.52
1:A:257:ALA:C	1:A:258:MSE:HE2	2.29	0.52
1:B:13:PRO:O	1:B:14:SER:HB2	2.09	0.52
1:B:280:TRP:HE1	4:B:703:PEP:H31	1.75	0.52
1:A:220:GLU:OE1	1:A:461:ARG:NH2	2.43	0.52
1:A:457:ALA:O	1:A:461:ARG:HG3	2.10	0.52
1:A:344:ARG:CD	6:A:2030:HOH:O	2.34	0.51
1:A:443:ARG:H	1:A:443:ARG:NE	2.07	0.51
1:B:196:LEU:HD13	1:B:200:TRP:CZ2	2.44	0.51
1:A:13:PRO:HD2	1:B:92:MSE:HG3	1.91	0.51
1:B:375:SER:HA	1:B:379:PHE:O	2.10	0.51
1:A:83:GLN:HA	1:A:124:VAL:O	2.11	0.50
1:B:421:LEU:HD21	1:B:432:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:213:ARG:NH1	1:B:213:ARG:CG	2.74	0.50
1:A:48:MSE:HE2	1:A:167:SER:CB	2.39	0.50
1:B:262:SER:HB3	1:B:272:PHE:HE1	1.77	0.50
1:A:410:VAL:HG13	1:A:412:ILE:CG2	2.42	0.50
1:A:126:ARG:HD2	1:A:409:HIS:HE1	1.76	0.50
1:B:310:ASN:ND2	1:B:310:ASN:H	2.09	0.50
1:B:49:ARG:O	1:B:53:GLU:HG3	2.11	0.49
1:A:344:ARG:NH1	1:A:344:ARG:CG	2.61	0.49
1:B:342:LYS:HB3	1:B:346:LEU:HD12	1.96	0.48
5:A:1001:CE1:H142	5:A:1001:CE1:H201	1.96	0.48
1:A:284:ARG:HG3	1:A:284:ARG:NH1	2.27	0.48
1:A:49:ARG:NH2	6:A:2015:HOH:O	2.46	0.48
1:A:52:LEU:CB	1:A:258:MSE:CE	2.78	0.47
1:A:5:VAL:HG13	1:B:9:ILE:HD11	1.96	0.47
1:B:382:ARG:HD2	1:B:442:PRO:HG2	1.96	0.47
1:A:409:HIS:HD2	6:A:2081:HOH:O	1.96	0.47
1:B:416:ASN:ND2	1:B:416:ASN:H	2.12	0.47
1:A:410:VAL:CG1	1:A:412:ILE:HG23	2.42	0.47
1:A:171:ARG:HH21	5:A:1001:CE1:C17	2.09	0.47
1:A:26:LEU:HD13	1:A:30:LEU:HD12	1.97	0.47
1:A:281:ILE:HD11	1:A:296:ALA:HB2	1.95	0.47
1:A:204:PHE:O	1:A:208:SER:HB3	2.15	0.46
1:A:395:PHE:O	1:A:399:ARG:HG2	2.16	0.45
1:A:73:GLN:HA	1:A:73:GLN:HE21	1.82	0.45
1:A:417:VAL:HG22	1:A:435:ARG:O	2.17	0.45
1:A:331:ARG:O	1:A:331:ARG:HD2	2.17	0.45
1:A:392:GLN:HA	1:A:459:MSE:HE1	1.96	0.44
1:B:13:PRO:O	1:B:14:SER:CB	2.65	0.44
1:A:311:MSE:HE3	1:A:316:ALA:N	2.32	0.44
1:A:417:VAL:HG12	1:A:445:ASN:HB3	1.98	0.44
1:B:269:PRO:HD2	6:B:2076:HOH:O	2.17	0.44
1:A:108:GLN:NE2	1:A:450:LEU:HD21	2.33	0.44
1:B:111:VAL:HG12	1:B:194:LEU:HD22	2.00	0.44
1:B:456:VAL:O	1:B:460:LEU:HD22	2.18	0.43
1:A:48:MSE:HE2	1:A:167:SER:N	2.25	0.43
1:B:77:GLY:HA2	1:B:404:HIS:CG	2.53	0.43
1:A:381:THR:HA	1:A:442:PRO:HG3	2.00	0.43
1:A:338:MSE:HG3	1:A:343:VAL:HG23	2.01	0.43
1:B:373:HIS:CE1	1:B:381:THR:HG23	2.54	0.43
1:B:313:PRO:CB	1:B:353:LYS:HG3	2.46	0.43
1:B:381:THR:HA	1:B:442:PRO:HG3	2.00	0.43
1:A:395:PHE:CE2	1:A:460:LEU:HD13	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:87:CYS:H	1:B:443:ARG:HD2	1.84	0.43
1:B:126:ARG:HD2	1:B:409:HIS:HE1	1.83	0.43
1:B:12:LEU:H	1:B:13:PRO:HD3	1.82	0.42
1:A:94:ASN:O	5:A:1001:CE1:C21	2.67	0.42
1:A:180:MSE:HE3	1:A:183:VAL:HG22	2.00	0.42
1:B:443:ARG:H	1:B:443:ARG:HH11	1.67	0.42
1:B:83:GLN:HA	1:B:124:VAL:O	2.20	0.42
1:A:410:VAL:CG1	1:A:412:ILE:CG2	2.98	0.42
1:A:48:MSE:HG3	1:A:166:PRO:O	2.20	0.42
1:B:214:TYR:CZ	1:B:451:GLU:HG3	2.54	0.41
1:A:91:PHE:CE2	1:A:150:ASP:HB3	2.55	0.41
1:A:391:VAL:O	1:A:459:MSE:HE1	2.20	0.41
1:B:16:PRO:HA	1:B:17:PRO:HD3	1.91	0.41
1:B:213:ARG:HD3	1:B:214:TYR:CZ	2.56	0.41
1:B:412:ILE:CG2	1:B:449:SER:OG	2.68	0.41
1:A:409:HIS:CD2	6:A:2081:HOH:O	2.73	0.41
1:B:348:PRO:O	1:B:352:GLU:HG3	2.20	0.41
1:B:23:ARG:HD2	6:B:2082:HOH:O	2.21	0.41
1:A:156:ALA:HA	1:A:157:PRO:HD3	1.96	0.41
1:A:348:PRO:O	1:A:352:GLU:HG3	2.21	0.41
1:A:94:ASN:O	5:A:1001:CE1:H211	2.21	0.41
1:B:368:MSE:HE2	1:B:411:GLU:HB2	2.03	0.41
1:B:344:ARG:NH2	1:B:389:ASP:OD2	2.54	0.41
1:A:452:LEU:O	1:A:456:VAL:HG23	2.20	0.41
1:A:213:ARG:NH1	1:A:213:ARG:HB2	2.34	0.41
5:A:1001:CE1:C18	5:A:1001:CE1:C23	2.90	0.40
1:A:399:ARG:NH2	1:A:459:MSE:O	2.53	0.40
1:B:192:ALA:HB3	6:B:2065:HOH:O	2.21	0.40
1:A:117:ALA:HB2	1:A:460:LEU:HG	2.03	0.40
1:A:49:ARG:CZ	6:A:2015:HOH:O	2.69	0.40
1:A:235:ASP:OD2	1:A:236:ARG:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	447/464 (96%)	432 (97%)	12 (3%)	3 (1%)	30	34
1	B	445/464 (96%)	422 (95%)	18 (4%)	5 (1%)	21	21
All	All	892/928 (96%)	854 (96%)	30 (3%)	8 (1%)	25	26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	ASP
1	A	239	GLN
1	A	266	ASP
1	B	14	SER
1	B	419	GLU
1	B	420	CYS
1	B	13	PRO
1	B	374	GLU

### 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	364/363 (100%)	336 (92%)	28 (8%)	18	22
1	B	363/363 (100%)	339 (93%)	24 (7%)	24	29
All	All	727/726 (100%)	675 (93%)	52 (7%)	21	25

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	26	LEU
1	A	40	TRP
1	A	46	LEU
1	A	52	LEU
1	A	65	VAL
1	A	71	LEU
1	A	73	GLN
1	A	177	SER

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Mol	Chain	Res	Type
1	A	193	SER
1	A	196	LEU
1	A	208	SER
1	A	217	LEU
1	A	236	ARG
1	A	250	LEU
1	A	284	ARG
1	A	327	ASN
1	A	337	ARG
1	A	344	ARG
1	A	381	THR
1	A	410	VAL
1	A	417	VAL
1	A	432	LEU
1	A	443	ARG
1	A	446	THR
1	A	447	GLN
1	A	450	LEU
1	A	460	LEU
1	B	15	LEU
1	B	40	TRP
1	B	52	LEU
1	B	65	VAL
1	B	71	LEU
1	B	193	SER
1	B	196	LEU
1	B	213	ARG
1	B	215	GLU
1	B	217	LEU
1	B	238	LEU
1	B	239	GLN
1	B	250	LEU
1	B	266	ASP
1	B	298	VAL
1	B	327	ASN
1	B	337	ARG
1	B	372	THR
1	B	416	ASN
1	B	419	GLU
1	B	443	ARG
1	B	446	THR
1	B	447	GLN

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Mol	Chain	Res	Type
1	B	460	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	73	GLN
1	A	383	HIS
1	A	409	HIS
1	A	447	GLN
1	B	68	GLN
1	B	239	GLN
1	B	327	ASN
1	B	404	HIS
1	B	409	HIS
1	B	416	ASN

### 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 ⓘ

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
5	CE1	A	1001	-	24,24,36	0.58	0	23,23,35	0.83	1 (4%)
3	SO4	A	2001	-	4,4,4	0.12	0	6,6,6	0.32	0
4	PEP	A	702	-	9,9,9	4.11	1 (11%)	13,13,13	3.61	5 (38%)
3	SO4	B	2002	-	4,4,4	0.20	0	6,6,6	0.12	0
4	PEP	B	703	-	9,9,9	3.00	3 (33%)	13,13,13	3.75	7 (53%)

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
5	CE1	A	1001	-	-	0/22/22/34	0/0/0/0
3	SO4	A	2001	-	-	0/0/0/0	0/0/0/0
4	PEP	A	702	-	-	0/9/9/9	0/0/0/0
3	SO4	B	2002	-	-	0/0/0/0	0/0/0/0
4	PEP	B	703	-	-	0/9/9/9	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	PEP	C2-C1	-12.06	1.37	1.49
4	B	703	PEP	P-O2	-7.51	1.48	1.60
4	B	703	PEP	O2-C2	-3.28	1.30	1.39
4	B	703	PEP	C2-C1	2.95	1.52	1.49

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	PEP	P-O2-C2	9.72	145.83	123.31
4	A	702	PEP	C3-C2-C1	-7.14	109.17	122.72
4	A	702	PEP	O2-C2-C1	6.94	126.82	111.69
4	B	703	PEP	O2-C2-C1	5.95	124.67	111.69
4	A	702	PEP	O2'-C1-C2	4.91	122.48	113.90
4	A	702	PEP	O1-C1-C2	-4.65	114.63	121.81
4	B	703	PEP	O2-C2-C3	-4.53	116.25	124.74
4	A	702	PEP	P-O2-C2	3.90	132.36	123.31
4	B	703	PEP	O2'-C1-O1	-2.98	116.57	123.62
5	A	1001	CE1	O25-C24-C23	-2.89	104.81	114.71
4	B	703	PEP	O1-C1-C2	2.65	125.90	121.81
4	B	703	PEP	O2P-P-O1P	2.52	118.68	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	PEP	C3-C2-C1	-2.04	118.84	122.72

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, 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	451/464 (97%)	0.35	41 (9%) 9 15	25, 41, 80, 97	0
1	B	451/464 (97%)	0.19	35 (7%) 13 19	23, 36, 77, 95	0
All	All	902/928 (97%)	0.27	76 (8%) 11 17	23, 38, 79, 97	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	421	LEU	10.8
1	B	379	PHE	8.5
1	A	379	PHE	7.7
1	B	434	GLY	7.1
1	B	375	SER	6.7
1	A	416	ASN	6.7
1	B	432	LEU	6.3
1	A	418	THR	6.2
1	A	377	THR	6.2
1	B	436	TYR	5.7
1	A	375	SER	5.7
1	A	436	TYR	5.6
1	B	418	THR	5.3
1	A	267	GLY	5.1
1	A	434	GLY	5.1
1	A	376	SER	4.9
1	B	374	GLU	4.6
1	A	210	ALA	4.6
1	B	373	HIS	4.5
1	B	14	SER	4.5
1	B	265	ASP	4.5
1	A	432	LEU	4.4
1	B	433	ALA	4.4
1	A	0	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	13	PRO	4.4
1	B	11	GLN	4.3
1	B	380	LYS	4.3
1	B	435	ARG	4.1
1	A	266	ASP	4.1
1	A	433	ALA	4.1
1	A	417	VAL	4.1
1	A	3	TRP	3.8
1	A	438	THR	3.7
1	B	237	ASN	3.7
1	B	416	ASN	3.4
1	A	435	ARG	3.4
1	A	378	GLY	3.3
1	B	372	THR	3.3
1	A	206	ARG	3.3
1	A	238	LEU	3.2
1	A	374	GLU	3.1
1	A	443	ARG	3.0
1	B	381	THR	3.0
1	A	264	GLY	3.0
1	A	373	HIS	3.0
1	B	209	PRO	2.9
1	A	265	ASP	2.9
1	A	381	THR	2.8
1	B	1	MSE	2.8
1	B	238	LEU	2.7
1	B	420	CYS	2.7
1	A	372	THR	2.6
1	B	415	GLU	2.6
1	A	236	ARG	2.5
1	A	360	GLN	2.5
1	A	237	ASN	2.5
1	B	419	GLU	2.4
1	A	211	GLY	2.4
1	B	236	ARG	2.3
1	A	462	ASP	2.3
1	B	264	GLY	2.3
1	B	437	GLU	2.3
1	A	209	PRO	2.3
1	B	266	ASP	2.3
1	B	462	ASP	2.3
1	B	438	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	213	ARG	2.2
1	A	235	ASP	2.1
1	A	442	PRO	2.1
1	A	204	PHE	2.1
1	A	203	GLU	2.1
1	A	207	THR	2.1
1	B	155	PHE	2.1
1	A	356	ALA	2.1
1	B	310	ASN	2.0
1	B	442	PRO	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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	CE1	A	1001	25/37	0.24	4.11	50,56,65,66	0
4	PEP	B	703	10/10	0.22	4.02	34,40,43,44	10
4	PEP	A	702	10/10	0.23	2.22	45,48,50,52	10
3	SO4	A	2001	5/5	0.24	1.28	53,54,55,56	5
3	SO4	B	2002	5/5	0.23	0.37	68,68,69,69	5
2	MN	B	701	1/1	0.08	-1.46	57,57,57,57	1
2	MN	A	700	1/1	0.06	-2.18	55,55,55,55	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.