



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:20 AM GMT

PDB ID : 3I3W  
Title : Structure of a phosphoglucosamine mutase from Francisella tularensis  
Authors : Brunzelle, J.S.; Wawrzak, Z.; Skarina, T.; Onopriyenko, O.; Savchenko, A.; Anderson, W.F.  
Deposited on : 2009-07-01  
Resolution : 2.30 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

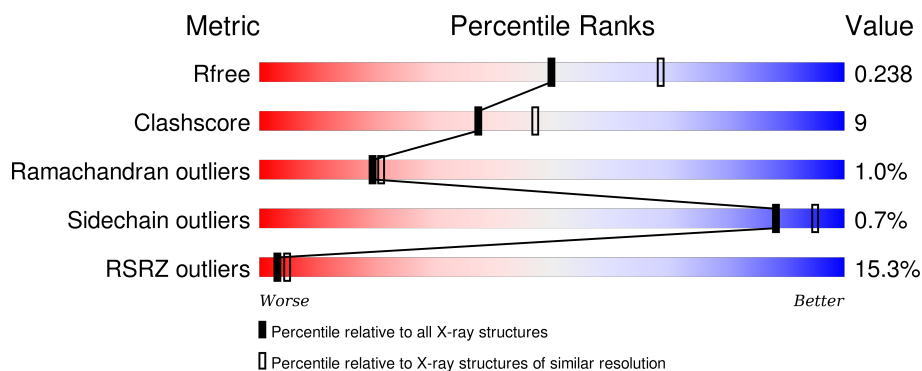
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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. 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	443	 16% 80% 19%
1	B	443	 14% 82% 16% ..

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7026 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 Phosphoglucosamine mutase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	P	S	Se	0	0	0
			3383	2141	572	659	1	4	6			
1	B	440	Total	C	N	O	P	S	Se	0	0	0
			3376	2136	571	658	1	4	6			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

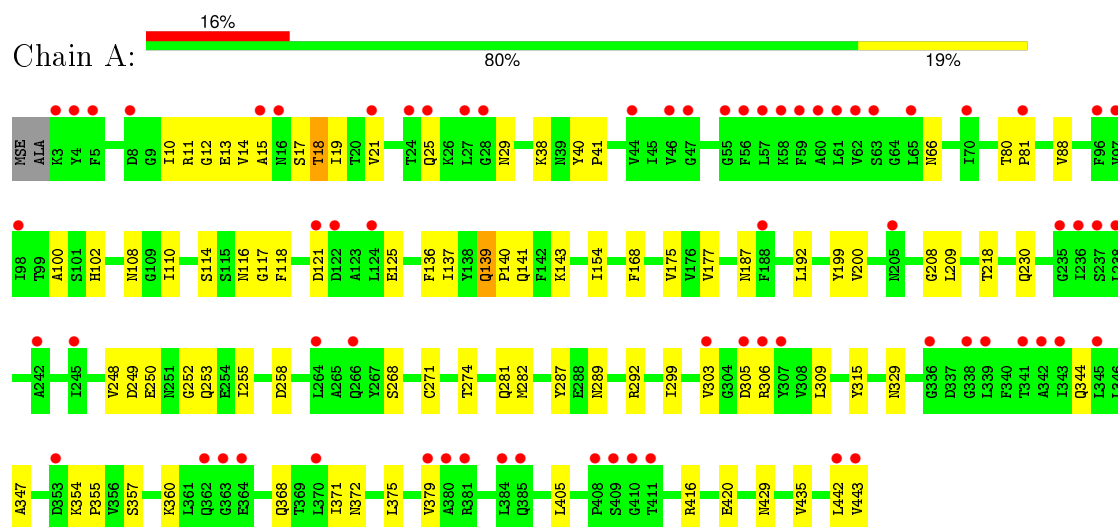
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	132	Total	O	0	0
			132	132		
3	B	133	Total	O	0	0
			133	133		

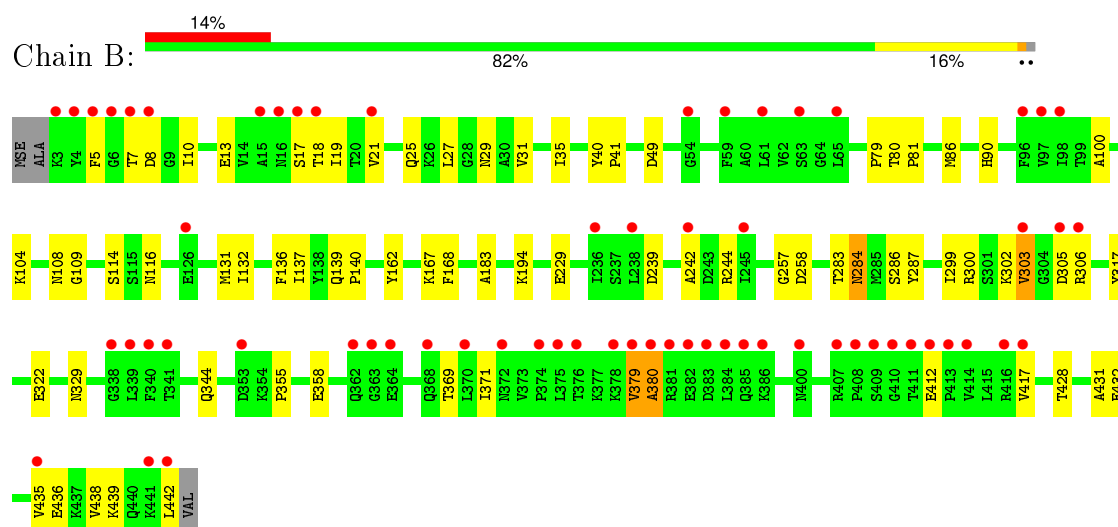
### 3 Residue-property plots [i](#)

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: Phosphoglucosamine mutase



#### • Molecule 1: Phosphoglucosamine mutase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.43 Å   206.68 Å   44.76 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.16 – 2.30 29.16 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.16-2.30) 99.3 (29.16-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.34 (at 2.31 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.194   ,   0.236 0.197   ,   0.238	Depositor DCC
$R_{free}$ test set	2216 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	1.016	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 43865 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7026	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.66 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.6332e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.34	0/3418	0.51	0/4603
1	B	0.36	1/3411 (0.0%)	0.50	0/4593
All	All	0.35	1/6829 (0.0%)	0.50	0/9196

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	412	GLU	CD-OE2	7.97	1.34	1.25

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	3383	0	3383	73	0
1	B	3376	0	3374	56	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	132	0	0	3	0
3	B	133	0	0	4	0
All	All	7026	0	6757	125	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 9.

All (125) 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:329:ASN:HD22	1:A:344:GLN:HE22	1.19	0.87
1:A:329:ASN:ND2	1:A:344:GLN:HE22	1.74	0.85
1:B:29:ASN:HD21	1:B:137:ILE:H	1.25	0.83
1:A:282:MSE:HA	1:A:282:MSE:HE2	1.62	0.80
1:A:306:ARG:HG2	1:A:306:ARG:O	1.87	0.75
1:B:284:ASN:HD22	1:B:286:SER:H	1.37	0.72
1:B:299:ILE:HD13	1:B:317:TYR:HE2	1.54	0.71
1:A:429:ASN:HB3	3:A:540:HOH:O	1.90	0.69
1:A:282:MSE:CE	1:A:405:LEU:CD2	2.70	0.69
1:B:306:ARG:HA	3:B:573:HOH:O	1.95	0.67
1:B:7:THR:O	1:B:8:ASP:HB2	1.94	0.67
1:A:118:PHE:HD1	1:A:309:LEU:HD21	1.60	0.66
1:A:139:GLN:NE2	1:A:141:GLN:H	1.94	0.65
1:B:329:ASN:HD22	1:B:344:GLN:HE22	1.44	0.65
1:B:299:ILE:HD13	1:B:317:TYR:CE2	2.33	0.63
1:B:131:MSE:HA	1:B:131:MSE:HE2	1.81	0.63
1:A:100:ALA:HB2	1:A:108:ASN:HA	1.80	0.62
1:A:139:GLN:HE21	1:A:143:LYS:H	1.47	0.62
1:A:139:GLN:HE22	1:A:141:GLN:H	1.45	0.62
1:B:432:GLU:O	1:B:436:GLU:HG2	1.98	0.62
1:A:289:ASN:OD1	1:A:292:ARG:NH2	2.33	0.61
1:A:88:VAL:CG2	1:A:117:GLY:HA3	2.30	0.61
1:A:17:SER:OG	1:A:18:THR:N	2.34	0.61
1:A:13:GLU:O	1:A:17:SER:HB3	2.01	0.61
1:B:379:VAL:O	1:B:380:ALA:HB3	2.01	0.60
1:B:299:ILE:CD1	1:B:317:TYR:HE2	2.13	0.60
1:B:417:VAL:HG11	1:B:435:VAL:HG22	1.84	0.60
1:B:114:SER:OG	1:B:116:ASN:OD1	2.20	0.59
1:B:379:VAL:O	1:B:380:ALA:CB	2.50	0.59
1:A:282:MSE:HE3	1:A:405:LEU:CD2	2.32	0.59
1:A:255:ILE:HG12	1:A:360:LYS:HD3	1.84	0.58
1:A:19:ILE:HD13	1:A:108:ASN:O	2.04	0.58
1:A:80:THR:N	1:A:81:PRO:HD2	2.18	0.57
1:A:12:GLY:N	1:A:19:ILE:HD12	2.19	0.57
1:A:29:ASN:HD21	1:A:137:ILE:H	1.50	0.57
1:B:167:LYS:HE3	1:B:168:PHE:CE2	2.39	0.57
1:A:21:VAL:HG21	1:B:136:PHE:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:PHE:CD1	1:A:309:LEU:HD21	2.38	0.56
1:A:282:MSE:HE1	1:A:405:LEU:HD23	1.89	0.55
1:B:29:ASN:ND2	1:B:137:ILE:H	2.00	0.55
1:B:100:ALA:HB2	1:B:108:ASN:HA	1.89	0.54
1:A:250:GLU:OE2	1:A:357:SER:OG	2.16	0.54
1:A:282:MSE:CE	1:A:282:MSE:HA	2.37	0.54
1:A:100:ALA:HB2	1:A:108:ASN:CA	2.38	0.54
1:B:35:ILE:HG23	1:B:40:TYR:HB2	1.88	0.54
1:A:114:SER:OG	1:A:116:ASN:OD1	2.23	0.53
1:B:80:THR:N	1:B:81:PRO:HD2	2.22	0.53
1:A:14:VAL:O	1:A:15:ALA:HB3	2.08	0.53
1:B:17:SER:OG	1:B:18:THR:N	2.40	0.53
1:B:104:LYS:HD2	3:B:522:HOH:O	2.09	0.53
1:A:139:GLN:NE2	1:A:143:LYS:H	2.06	0.52
1:A:29:ASN:ND2	1:A:137:ILE:H	2.08	0.52
1:B:329:ASN:HD22	1:B:344:GLN:NE2	2.09	0.51
1:A:19:ILE:CD1	1:A:108:ASN:O	2.58	0.51
1:A:66:ASN:ND2	3:A:459:HOH:O	2.43	0.51
1:A:175:VAL:O	1:A:199:TYR:HA	2.10	0.51
1:A:136:PHE:CZ	1:B:21:VAL:HG11	2.45	0.51
1:B:431:ALA:O	1:B:435:VAL:HG23	2.11	0.50
1:A:271:CYS:CB	1:A:344:GLN:HE21	2.25	0.50
1:A:38:LYS:HD3	1:A:40:TYR:CE2	2.47	0.50
1:A:282:MSE:CE	1:A:405:LEU:HD23	2.41	0.49
1:B:40:TYR:HB3	1:B:41:PRO:HD2	1.94	0.49
1:A:116:ASN:CG	1:A:118:PHE:HD2	2.15	0.49
1:B:257:GLY:HA3	1:B:322:GLU:O	2.12	0.49
1:A:121:ASP:O	1:A:125:GLU:HG3	2.13	0.49
1:A:306:ARG:O	1:A:306:ARG:CG	2.58	0.49
1:A:11:ARG:CA	1:A:19:ILE:HD11	2.44	0.48
1:B:258:ASP:HB3	1:B:287:TYR:CE2	2.48	0.48
1:A:25:GLN:OE1	1:B:21:VAL:HG22	2.14	0.48
1:A:40:TYR:HB3	1:A:41:PRO:HD2	1.95	0.48
1:B:79:PRO:HB3	1:B:242:ALA:HB3	1.95	0.47
1:B:439:LYS:HE2	3:B:548:HOH:O	2.14	0.47
1:A:12:GLY:N	1:A:19:ILE:CD1	2.78	0.47
1:A:168:PHE:HB3	1:A:347:ALA:HB1	1.97	0.47
1:A:442:LEU:O	1:A:443:VAL:HB	2.15	0.47
1:A:139:GLN:HE22	1:A:141:GLN:N	2.12	0.47
1:B:371:ILE:O	1:B:417:VAL:HG12	2.14	0.47
1:A:258:ASP:HB3	1:A:287:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:MSE:CE	1:B:90:HIS:HE1	2.28	0.46
1:B:86:MSE:CE	1:B:90:HIS:CE1	2.98	0.46
1:B:13:GLU:O	1:B:17:SER:HB3	2.16	0.46
1:B:283:THR:O	1:B:300:ARG:NH2	2.30	0.46
1:B:302:LYS:O	1:B:303:VAL:HG12	2.16	0.46
1:A:372:ASN:ND2	1:A:416:ARG:HG2	2.31	0.46
1:A:299:ILE:HD12	1:A:315:TYR:CD2	2.51	0.45
1:B:139:GLN:HA	1:B:140:PRO:HD3	1.84	0.45
1:B:306:ARG:HG2	1:B:306:ARG:O	2.17	0.45
1:B:31:VAL:O	1:B:35:ILE:HG13	2.15	0.45
1:A:282:MSE:HE1	1:A:405:LEU:CD2	2.45	0.45
1:B:100:ALA:HB2	1:B:108:ASN:CA	2.47	0.44
1:A:371:ILE:HG21	1:A:435:VAL:HG21	1.98	0.44
1:A:102:HIS:HB2	1:A:218:THR:HG21	1.98	0.44
1:A:11:ARG:HA	1:A:19:ILE:HD11	2.00	0.44
1:B:379:VAL:HG23	1:B:380:ALA:H	1.83	0.43
1:B:27:LEU:CD1	1:B:132:ILE:HD11	2.48	0.43
1:B:306:ARG:CA	3:B:573:HOH:O	2.60	0.43
1:A:248:VAL:CG1	1:A:252:GLY:HA2	2.48	0.43
1:B:239:ASP:CG	1:B:244:ARG:HB3	2.39	0.43
1:A:271:CYS:HB3	1:A:344:GLN:NE2	2.34	0.43
1:A:177:VAL:HG11	1:A:192:LEU:HD11	2.01	0.43
1:A:40:TYR:HB3	1:A:41:PRO:CD	2.49	0.43
1:A:268:SER:HB2	1:A:274:THR:HG22	2.00	0.43
1:A:249:ASP:OD2	1:A:253:GLN:HB2	2.19	0.42
1:B:355:PRO:HG2	1:B:358:GLU:HG3	2.01	0.42
1:B:417:VAL:HG11	1:B:435:VAL:CG2	2.49	0.42
1:B:86:MSE:HE1	1:B:90:HIS:HE1	1.84	0.42
1:B:369:THR:HG21	1:B:428:THR:HA	2.01	0.42
1:B:229:GLU:OE1	1:B:229:GLU:HA	2.19	0.42
1:A:139:GLN:HA	1:A:140:PRO:HD3	1.82	0.42
1:B:27:LEU:HD12	1:B:132:ILE:HD11	2.02	0.42
1:A:282:MSE:HE3	1:A:405:LEU:HD21	2.00	0.42
1:A:354:LYS:HB2	1:A:355:PRO:HD2	2.02	0.42
1:B:162:TYR:CD1	1:B:194:LYS:HG3	2.55	0.42
1:A:368:GLN:HG3	1:A:420:GLU:HG3	2.02	0.41
1:A:139:GLN:HE22	1:A:141:GLN:HB2	1.85	0.41
1:A:200:VAL:HG11	1:A:230:GLN:NE2	2.35	0.41
1:A:375:LEU:HD22	1:A:443:VAL:HG23	2.03	0.41
1:B:19:ILE:HD12	1:B:109:GLY:HA2	2.03	0.41
1:A:208:GLY:O	1:A:209:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ASP:HA	1:B:183:ALA:HB2	2.03	0.41
1:B:438:VAL:HG23	1:B:442:LEU:HD12	2.02	0.41
1:A:121:ASP:HB3	1:A:306:ARG:NH2	2.36	0.41
1:A:154:ILE:CD1	1:A:187:ASN:HB3	2.51	0.41
1:A:21:VAL:HB	1:B:25:GLN:OE1	2.21	0.40
1:A:281:GLN:HG3	3:A:552:HOH:O	2.21	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	438/443 (99%)	416 (95%)	19 (4%)	3 (1%)	26	31
1	B	437/443 (99%)	410 (94%)	21 (5%)	6 (1%)	14	13
All	All	875/886 (99%)	826 (94%)	40 (5%)	9 (1%)	19	21

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	ASP
1	B	380	ALA
1	B	10	ILE
1	B	305	ASP
1	B	5	PHE
1	A	303	VAL
1	B	303	VAL
1	B	379	VAL
1	A	10	ILE

### 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	364/358 (102%)	360 (99%)	4 (1%)	80	90
1	B	363/358 (101%)	362 (100%)	1 (0%)	94	98
All	All	727/716 (102%)	722 (99%)	5 (1%)	88	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	110	ILE
1	A	139	GLN
1	A	379	VAL
1	B	284	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	66	ASN
1	A	90	HIS
1	A	139	GLN
1	A	141	GLN
1	A	187	ASN
1	A	251	ASN
1	A	262	ASN
1	A	275	ASN
1	A	290	HIS
1	A	331	ASN
1	A	344	GLN
1	A	362	GLN
1	A	372	ASN
1	B	29	ASN
1	B	90	HIS
1	B	187	ASN

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Mol	Chain	Res	Type
1	B	230	GLN
1	B	262	ASN
1	B	275	ASN
1	B	281	GLN
1	B	284	ASN
1	B	290	HIS
1	B	331	ASN
1	B	344	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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$
1	SEP	A	101	1,2	8,9,10	1.55	1 (12%)	8,12,14	2.01	1 (12%)
1	SEP	B	101	1,2	8,9,10	1.63	2 (25%)	8,12,14	2.01	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	101	1,2	-	0/6/8/10	0/0/0/0
1	SEP	B	101	1,2	-	0/6/8/10	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	101	SEP	P-O3P	2.03	1.62	1.54
1	A	101	SEP	P-O1P	3.11	1.61	1.51
1	B	101	SEP	P-O1P	3.38	1.62	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	SEP	OG-CB-CA	4.80	112.37	108.27
1	A	101	SEP	OG-CB-CA	4.90	112.45	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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 [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	434/443 (97%)	0.77	69 (15%) 3 4	30, 40, 45, 69	0
1	B	433/443 (97%)	0.70	64 (14%) 3 5	32, 41, 46, 78	0
All	All	867/886 (97%)	0.73	133 (15%) 3 5	30, 40, 46, 78	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	413	PRO	8.5
1	A	443	VAL	8.2
1	B	381	ARG	7.1
1	B	7	THR	7.0
1	A	411	THR	6.5
1	A	353	ASP	6.4
1	B	4	TYR	5.9
1	A	410	GLY	5.6
1	B	409	SER	5.6
1	B	382	GLU	5.4
1	B	6	GLY	5.3
1	B	362	GLN	4.9
1	B	380	ALA	4.9
1	A	121	ASP	4.7
1	A	8	ASP	4.6
1	B	383	ASP	4.6
1	B	414	VAL	4.5
1	A	5	PHE	4.4
1	A	98	ILE	4.3
1	A	303	VAL	4.3
1	A	60	ALA	4.3
1	B	416	ARG	4.2
1	A	306	ARG	4.1
1	B	363	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	245	ILE	4.1
1	A	4	TYR	4.1
1	A	339	LEU	4.0
1	A	62	VAL	3.9
1	A	305	ASP	3.9
1	B	442	LEU	3.8
1	A	342	ALA	3.8
1	B	339	LEU	3.8
1	A	381	ARG	3.7
1	B	408	PRO	3.7
1	A	380	ALA	3.7
1	B	379	VAL	3.7
1	A	59	PHE	3.6
1	A	122	ASP	3.6
1	B	370	LEU	3.5
1	A	56	PHE	3.5
1	B	242	ALA	3.5
1	A	3	LYS	3.4
1	A	409	SER	3.4
1	B	340	PHE	3.4
1	B	353	ASP	3.4
1	A	24	THR	3.3
1	B	5	PHE	3.3
1	B	15	ALA	3.3
1	A	61	LEU	3.3
1	B	306	ARG	3.3
1	B	378	LYS	3.3
1	A	238	LEU	3.2
1	B	417	VAL	3.2
1	B	364	GLU	3.2
1	A	44	VAL	3.1
1	A	46	VAL	3.1
1	A	57	LEU	3.1
1	A	236	ILE	3.0
1	B	16	ASN	3.0
1	A	364	GLU	3.0
1	A	363	GLY	3.0
1	A	21	VAL	3.0
1	A	336	GLY	3.0
1	B	8	ASP	2.9
1	B	441	LYS	2.9
1	A	27	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	65	LEU	2.9
1	B	238	LEU	2.9
1	A	242	ALA	2.9
1	B	338	GLY	2.9
1	B	303	VAL	2.8
1	A	55	GLY	2.8
1	A	28	GLY	2.8
1	A	338	GLY	2.8
1	B	236	ILE	2.8
1	B	410	GLY	2.8
1	A	16	ASN	2.8
1	A	63	SER	2.7
1	B	59	PHE	2.7
1	A	70	ILE	2.7
1	B	374	PRO	2.7
1	B	63	SER	2.7
1	A	370	LEU	2.7
1	A	97	VAL	2.7
1	B	21	VAL	2.7
1	A	47	GLY	2.6
1	B	18	THR	2.6
1	A	384	LEU	2.6
1	A	362	GLN	2.6
1	B	411	THR	2.6
1	A	25	GLN	2.6
1	A	15	ALA	2.6
1	A	408	PRO	2.5
1	A	235	GLY	2.5
1	A	188	PHE	2.5
1	B	375	LEU	2.4
1	B	98	ILE	2.4
1	A	96	PHE	2.4
1	B	386	LYS	2.4
1	B	17	SER	2.4
1	B	126	GLU	2.4
1	B	384	LEU	2.4
1	A	237	SER	2.4
1	B	376	THR	2.4
1	A	124	LEU	2.4
1	B	97	VAL	2.4
1	B	407	ARG	2.4
1	A	245	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	61	LEU	2.3
1	B	65	LEU	2.3
1	A	81	PRO	2.3
1	A	379	VAL	2.3
1	B	305	ASP	2.3
1	A	343	ILE	2.2
1	A	205	ASN	2.2
1	A	266	GLN	2.2
1	A	442	LEU	2.2
1	B	412	GLU	2.2
1	A	341	THR	2.2
1	B	368	GLN	2.2
1	A	264	LEU	2.2
1	B	341	THR	2.2
1	A	345	LEU	2.1
1	A	58	LYS	2.1
1	B	435	VAL	2.1
1	A	307	TYR	2.1
1	B	54	GLY	2.1
1	B	400	ASN	2.0
1	B	96	PHE	2.0
1	A	385	GLN	2.0
1	B	385	GLN	2.0
1	B	372	ASN	2.0
1	B	3	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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(Å <sup>2</sup> )	Q<0.9
1	SEP	B	101	10/11	0.93	0.12	-	37,41,42,42	0
1	SEP	A	101	10/11	0.93	0.11	-	40,42,44,45	0

## 6.3 Carbohydrates ⓘ

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
2	ZN	A	900	1/1	0.96	0.26	1.02	68,68,68,68	1
2	ZN	B	900	1/1	0.93	0.24	0.67	57,57,57,57	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.