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Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2014 – 11:47 PM 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)

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	Percentile Ranks	Value
Rfree		0.238
Clashscore		9
Ramachandran outliers		1.0%
Sidechain outliers		0.7%
RSRZ outliers		19.7%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
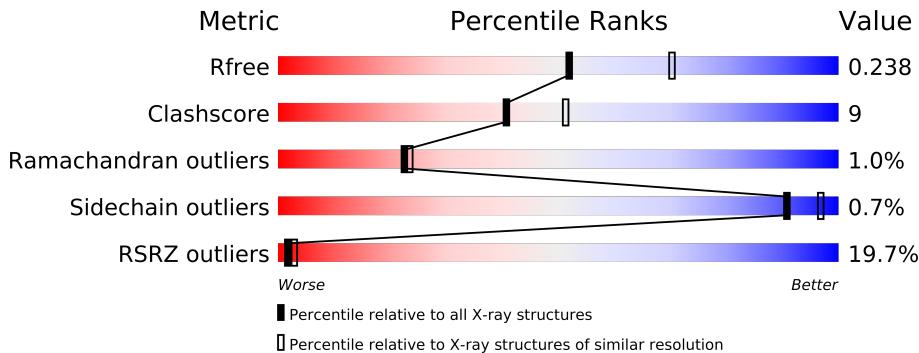
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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 >=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	443	
1	B	443	

2 Entry composition ⓘ

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

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

Chain A:
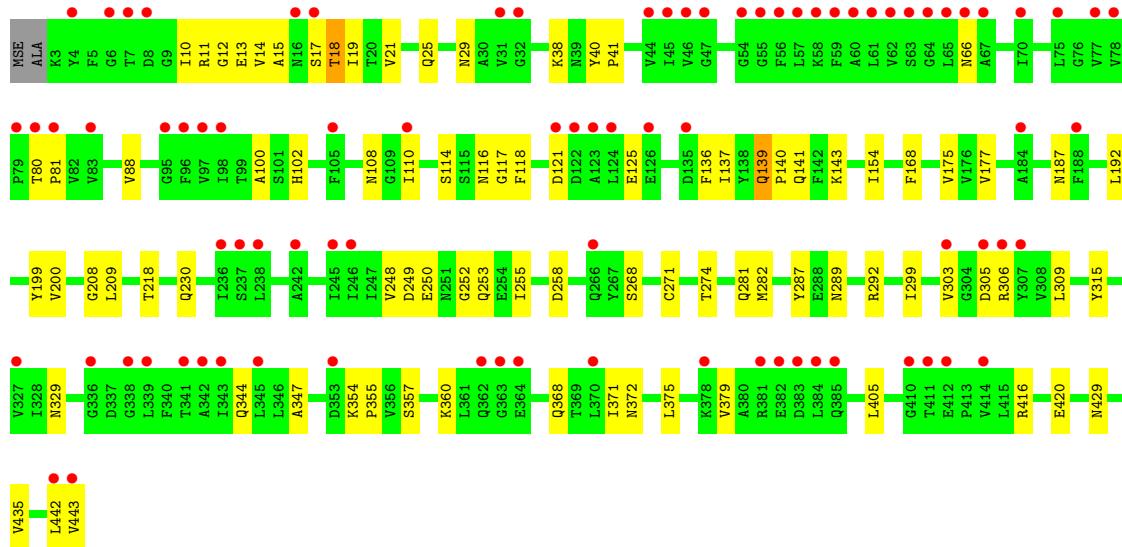
• Molecule 1: Phosphoglucosamine mutase

Chain B:
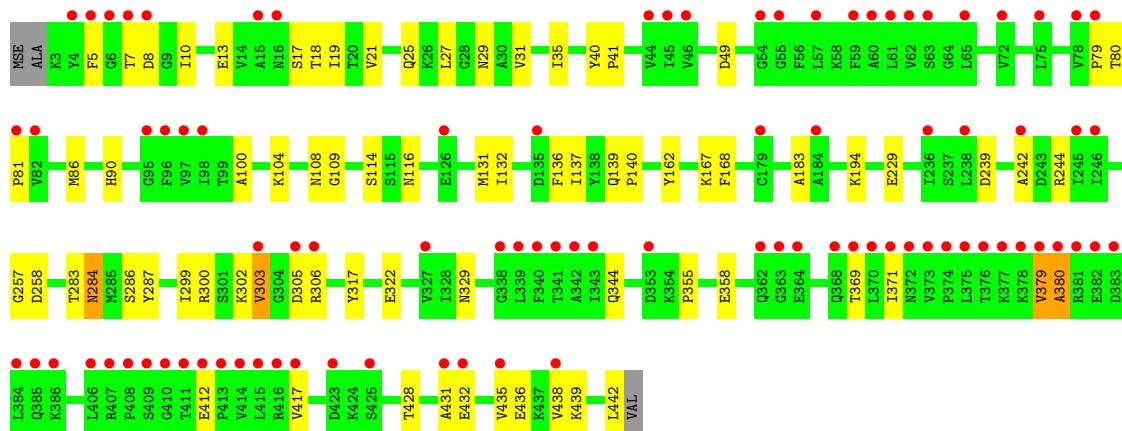
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	104.43Å 206.68Å 44.76Å 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
$< I/\sigma(I) >$ [1]	4.34 (at 2.31Å)	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^2)	36.9	Xtriage
Anisotropy	1.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 33.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Outliers	1 of 43865 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7026	wwPDB-VP
Average B, all atoms (Å^2)	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.*

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[1]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: 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 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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7026	0	6757	125	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 9.

All (125) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:258:ASP:HB3	1:A:287:TYR:CE2	2.50	0.46
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	Distance(Å)	Clash(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

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	438/443 (99%)	416 (95%)	19 (4%)	3 (1%)	30	34
1	B	437/443 (99%)	410 (94%)	21 (5%)	6 (1%)	16	15
All	All	875/886 (99%)	826 (94%)	40 (5%)	9 (1%)	22	23

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%)	84	93
1	B	363/358 (101%)	362 (100%)	1 (0%)	96	99
All	All	727/716 (102%)	722 (99%)	5 (1%)	91	97

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
1	B	230	GLN
1	B	262	ASN
1	B	275	ASN
1	B	281	GLN
1	B	284	ASN

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Mol	Chain	Res	Type
1	B	290	HIS
1	B	331	ASN
1	B	344	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	9,9,10	6.36	3 (33%)	10,12,14	1.41	2 (20%)
1	SEP	B	101	1,2	9,9,10	6.04	3 (33%)	10,12,14	1.45	2 (20%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	SEP	O-C	18.35	1.24	1.11
1	B	101	SEP	O-C	17.22	1.23	1.11
1	B	101	SEP	CA-C	3.54	1.55	1.48
1	B	101	SEP	P-O1P	3.30	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	SEP	CA-C	3.10	1.54	1.48
1	A	101	SEP	P-O1P	3.04	1.61	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	101	SEP	P-OG-CB	-2.77	110.18	118.19
1	A	101	SEP	OG-CB-CA	2.66	112.45	108.69
1	A	101	SEP	P-OG-CB	-2.65	110.52	118.19
1	B	101	SEP	OG-CB-CA	2.60	112.37	108.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

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, 95th 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^2)	Q<0.9
1	A	441/443 (99%)	0.90	84 (19%)	2	3	30, 40, 45, 69	0
1	B	440/443 (99%)	1.11	89 (20%)	2	3	32, 41, 46, 78	0
All	All	881/886 (99%)	1.01	173 (19%)	2	3	30, 40, 46, 78	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	THR	9.2
1	B	413	PRO	9.1
1	B	414	VAL	6.4
1	B	411	THR	6.4
1	A	443	VAL	6.3
1	B	381	ARG	6.0
1	B	382	GLU	6.0
1	A	62	VAL	5.9
1	A	411	THR	5.4
1	B	380	ALA	5.3
1	B	245	ILE	5.3
1	A	410	GLY	5.3
1	A	305	ASP	5.3
1	A	98	ILE	5.2
1	B	378	LYS	5.2
1	A	353	ASP	5.1
1	B	4	TYR	5.1
1	B	362	GLN	5.0
1	A	60	ALA	5.0
1	A	61	LEU	5.0
1	B	375	LEU	4.8
1	B	305	ASP	4.7
1	B	6	GLY	4.7
1	A	363	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	306	ARG	4.6
1	A	7	THR	4.5
1	A	63	SER	4.4
1	B	61	LEU	4.4
1	A	59	PHE	4.2
1	B	15	ALA	4.2
1	A	362	GLN	4.2
1	B	384	LEU	4.2
1	A	65	LEU	4.1
1	A	306	ARG	4.1
1	B	379	VAL	4.1
1	B	65	LEU	4.1
1	B	242	ALA	4.0
1	B	370	LEU	4.0
1	B	236	ILE	4.0
1	B	363	GLY	3.9
1	B	416	ARG	3.9
1	B	412	GLU	3.9
1	B	98	ILE	3.8
1	B	409	SER	3.8
1	B	383	ASP	3.8
1	A	381	ARG	3.7
1	A	303	VAL	3.7
1	A	342	ALA	3.7
1	A	55	GLY	3.6
1	B	340	PHE	3.6
1	B	408	PRO	3.6
1	B	16	ASN	3.6
1	B	338	GLY	3.5
1	A	16	ASN	3.5
1	B	238	LEU	3.5
1	B	59	PHE	3.5
1	A	47	GLY	3.5
1	B	410	GLY	3.5
1	A	46	VAL	3.5
1	B	341	THR	3.5
1	A	97	VAL	3.5
1	B	386	LYS	3.5
1	B	423	ASP	3.5
1	A	339	LEU	3.5
1	A	57	LEU	3.5
1	A	122	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	245	ILE	3.4
1	B	372	ASN	3.4
1	A	238	LEU	3.4
1	A	6	GLY	3.4
1	A	56	PHE	3.3
1	B	376	THR	3.3
1	B	385	GLN	3.3
1	B	126	GLU	3.3
1	A	341	THR	3.2
1	B	63	SER	3.2
1	A	8	ASP	3.2
1	B	353	ASP	3.2
1	B	62	VAL	3.2
1	B	374	PRO	3.2
1	A	126	GLU	3.2
1	B	44	VAL	3.1
1	A	124	LEU	3.1
1	A	96	PHE	3.1
1	B	8	ASP	3.1
1	B	415	LEU	3.1
1	B	97	VAL	3.1
1	A	75	LEU	3.0
1	B	368	GLN	3.0
1	A	414	VAL	2.9
1	B	438	VAL	2.9
1	A	364	GLU	2.9
1	A	385	GLN	2.8
1	A	44	VAL	2.8
1	A	266	GLN	2.8
1	A	78	VAL	2.8
1	A	384	LEU	2.8
1	B	54	GLY	2.8
1	B	407	ARG	2.8
1	B	79	PRO	2.7
1	A	188	PHE	2.7
1	A	242	ALA	2.7
1	B	55	GLY	2.7
1	B	96	PHE	2.7
1	A	58	LYS	2.7
1	B	417	VAL	2.7
1	A	307	TYR	2.7
1	A	121	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	81	PRO	2.7
1	B	246	ILE	2.7
1	A	70	ILE	2.6
1	A	135	ASP	2.6
1	B	81	PRO	2.6
1	B	342	ALA	2.6
1	A	382	GLU	2.6
1	A	31	VAL	2.6
1	A	45	ILE	2.6
1	A	442	LEU	2.6
1	B	327	VAL	2.6
1	B	364	GLU	2.5
1	A	327	VAL	2.5
1	A	66	ASN	2.5
1	A	236	ILE	2.5
1	A	246	ILE	2.5
1	B	435	VAL	2.5
1	B	5	PHE	2.5
1	B	339	LEU	2.5
1	B	184	ALA	2.4
1	B	377	LYS	2.4
1	B	95	GLY	2.4
1	B	135	ASP	2.4
1	B	57	LEU	2.4
1	B	425	SER	2.4
1	A	123	ALA	2.3
1	B	60	ALA	2.3
1	B	179	CYS	2.3
1	B	78	VAL	2.3
1	A	237	SER	2.3
1	A	412	GLU	2.3
1	A	4	TYR	2.3
1	B	46	VAL	2.3
1	A	336	GLY	2.3
1	B	431	ALA	2.3
1	B	45	ILE	2.2
1	A	378	LYS	2.2
1	B	369	THR	2.2
1	B	303	VAL	2.2
1	A	338	GLY	2.2
1	A	64	GLY	2.2
1	A	184	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	75	LEU	2.2
1	A	83	VAL	2.2
1	B	72	VAL	2.2
1	B	82	VAL	2.2
1	B	406	LEU	2.1
1	A	77	VAL	2.1
1	A	95	GLY	2.1
1	A	110	ILE	2.1
1	A	32	GLY	2.1
1	A	54	GLY	2.1
1	A	383	ASP	2.1
1	A	80	THR	2.1
1	A	343	ILE	2.1
1	B	343	ILE	2.1
1	A	105	PHE	2.1
1	B	373	VAL	2.1
1	A	370	LEU	2.0
1	A	17	SER	2.0
1	B	371	ILE	2.0
1	A	67	ALA	2.0
1	A	345	LEU	2.0
1	A	79	PRO	2.0
1	B	432	GLU	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, 95th 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^2)	Q<0.9
1	SEP	A	101	10/11	0.10	-1.49	40,42,44,45	0
1	SEP	B	101	10/11	0.10	-2.16	37,41,42,42	0

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, 95th 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(Å²)	Q<0.9
2	ZN	A	900	1/1	0.23	0.25	68,68,68,68	1
2	ZN	B	900	1/1	0.08	-2.67	57,57,57,57	1

6.5 Other polymers ⓘ

There are no such residues in this entry.