



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:42 PM UTC

PDB ID : 3T9Q / pdb_00003t9q
Title : Structure of the Phosphatase Domain of the Cell Fate Determinant SpoIIE from *Bacillus subtilis* (Mn presoaked)
Authors : Levnikov, V.M.; Blagova, E.V.; Wilkinson, A.J.
Deposited on : 2011-08-03
Resolution : 2.76 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

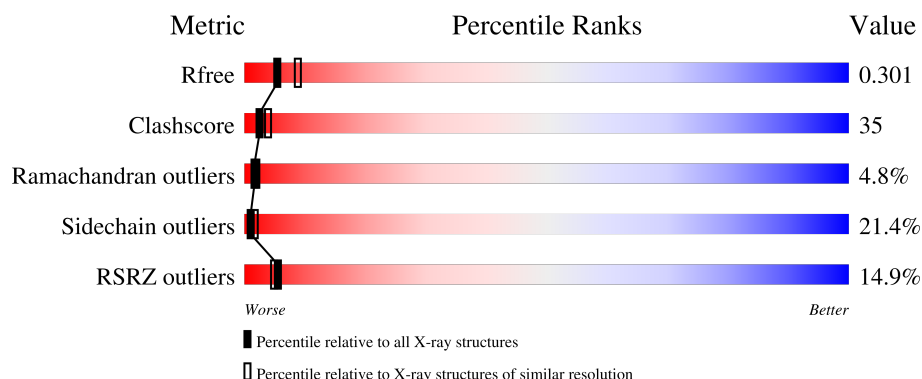
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	242	13% 49% 29% 10% 11%
1	B	242	14% 43% 38% 12% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3460 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 Stage II sporulation protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1666	1043	284	328	11			
1	B	227	Total	C	N	O	S	0	0	0
			1745	1097	296	341	11			

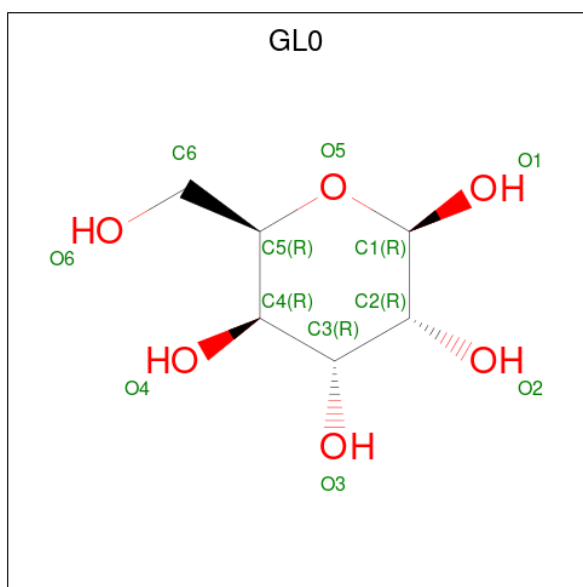
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	586	GLY	-	expression tag	UNP P37475
A	587	PRO	-	expression tag	UNP P37475
A	588	ALA	-	expression tag	UNP P37475
A	589	MET	-	expression tag	UNP P37475
B	586	GLY	-	expression tag	UNP P37475
B	587	PRO	-	expression tag	UNP P37475
B	588	ALA	-	expression tag	UNP P37475
B	589	MET	-	expression tag	UNP P37475

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 3 is beta-D-gulopyranose (CCD ID: GL0) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		

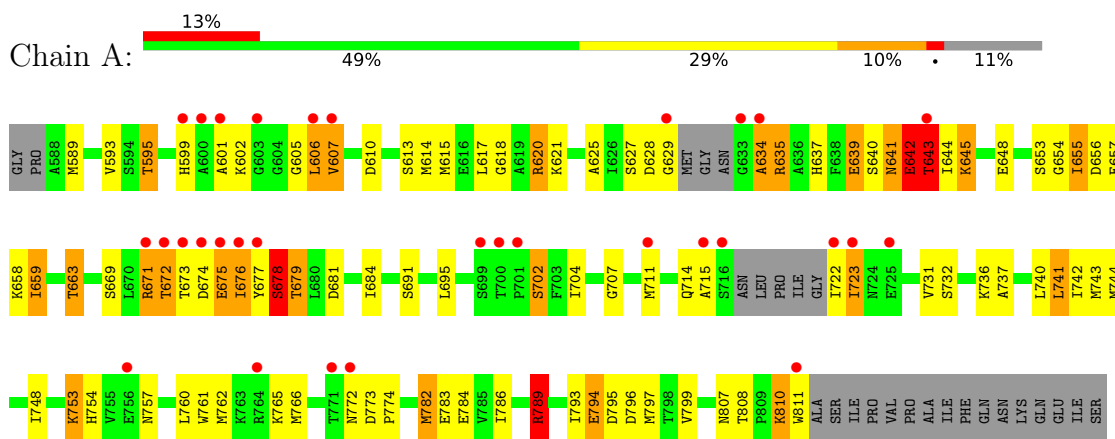
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	B	14	Total	O	0	0
			14	14		

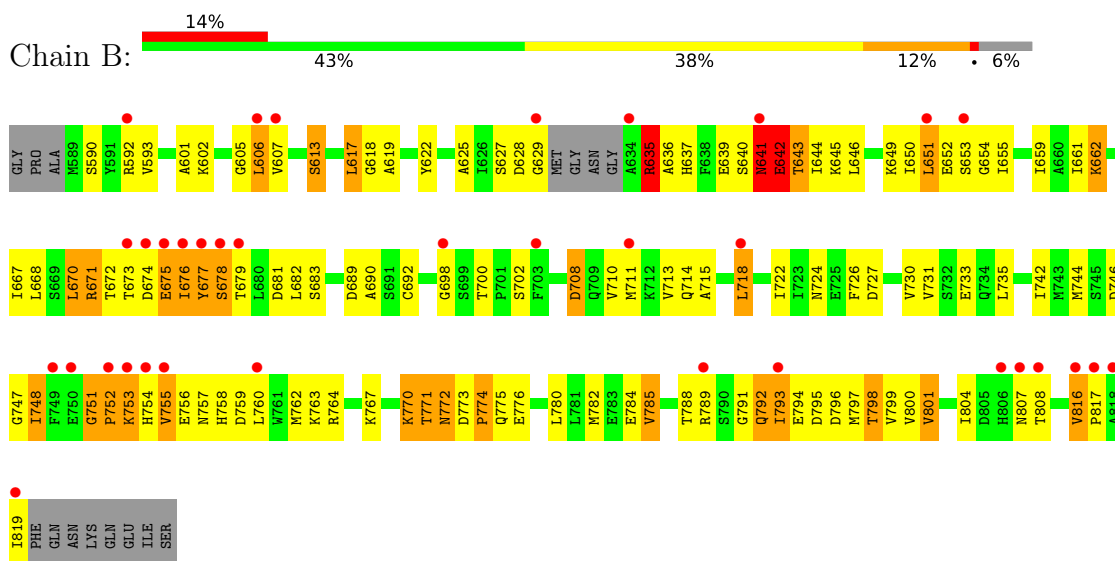
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Stage II sporulation protein E



• Molecule 1: Stage II sporulation protein E



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	86.01 Å 86.01 Å 322.47 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.58 – 2.76 43.58 – 2.76	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.58-2.76) 99.3 (43.58-2.76)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.90 (at 2.77 Å)	Xtriage
Refinement program	REFMAC 5.6.0086	Depositor
R, R_{free}	0.224 , 0.300 0.231 , 0.301	Depositor DCC
R_{free} test set	979 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3460	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GL0, MN

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	1.19	2/1685 (0.1%)	1.22	4/2262 (0.2%)
1	B	1.08	2/1768 (0.1%)	1.20	7/2381 (0.3%)
All	All	1.13	4/3453 (0.1%)	1.21	11/4643 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	620	ARG	CA-C	6.27	1.59	1.53
1	A	799	VAL	CA-CB	6.15	1.63	1.54
1	B	636	ALA	CA-CB	-5.12	1.45	1.53
1	B	682	LEU	N-CA	-5.05	1.40	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	789	ARG	N-CA-C	-9.34	97.05	110.59
1	B	642	GLU	CA-C-N	-8.55	108.15	120.29
1	B	642	GLU	C-N-CA	-8.55	108.15	120.29
1	A	782	MET	N-CA-C	-7.73	102.79	111.14
1	A	679	THR	N-CA-C	-6.04	100.79	110.14
1	B	804	ILE	CB-CA-C	-5.76	103.76	110.91
1	B	771	THR	N-CA-C	5.74	117.47	110.41
1	B	641	ASN	N-CA-C	5.66	122.86	110.80
1	B	635	ARG	N-CA-C	5.30	118.19	109.76
1	B	662	LYS	N-CA-C	-5.12	105.59	111.07
1	A	595	THR	N-CA-C	5.04	117.04	109.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1666	0	1686	144	0
1	B	1745	0	1777	129	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	12	0	12	2	0
4	A	21	0	0	3	0
4	B	14	0	0	0	0
All	All	3460	0	3475	240	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 35.

All (240) 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:675:GLU:HG2	1:A:676:ILE:CA	1.61	1.30
1:A:675:GLU:HG2	1:A:677:TYR:CA	1.68	1.21
1:B:635:ARG:HG2	1:B:635:ARG:HH11	1.13	1.13
1:A:675:GLU:CG	1:A:677:TYR:CA	2.30	1.10
1:A:675:GLU:CG	1:A:677:TYR:HA	1.81	1.10
1:B:671:ARG:HG2	1:B:676:ILE:HG12	1.29	1.10
1:A:675:GLU:CG	1:A:676:ILE:CA	2.30	1.09
1:A:675:GLU:CG	1:A:676:ILE:HA	1.82	1.09
1:A:676:ILE:N	1:A:677:TYR:HA	1.63	1.08
1:A:629:GLY:HA2	1:B:678:SER:HB3	1.30	1.06
1:A:675:GLU:HG2	1:A:677:TYR:HA	1.12	1.04
1:A:675:GLU:HG3	1:A:677:TYR:HB2	1.39	1.03
1:B:641:ASN:O	1:B:642:GLU:HB2	1.49	1.03
1:A:675:GLU:HG2	1:A:676:ILE:C	1.85	1.01
1:B:671:ARG:CB	1:B:676:ILE:HG13	1.91	1.00
1:A:659:ILE:O	1:A:663:THR:HG22	1.61	0.98
1:A:675:GLU:HG3	1:A:677:TYR:CB	1.95	0.96
1:A:675:GLU:CD	1:A:676:ILE:C	2.34	0.95
1:A:762:MET:HG3	1:A:766:MET:CE	1.95	0.95
1:A:762:MET:HG3	1:A:766:MET:HE3	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:ILE:N	1:A:677:TYR:CA	2.30	0.94
1:B:641:ASN:HD22	1:B:644:ILE:HG13	1.32	0.92
1:A:675:GLU:HG2	1:A:677:TYR:N	1.84	0.92
1:A:675:GLU:C	1:A:677:TYR:HA	1.95	0.92
1:A:656:ASP:HB2	1:A:659:ILE:HG22	1.51	0.91
1:A:675:GLU:CG	1:A:676:ILE:C	2.44	0.89
1:A:676:ILE:H	1:A:678:SER:N	1.70	0.89
1:B:710:VAL:HG12	1:B:710:VAL:O	1.75	0.87
1:A:641:ASN:HD22	1:A:641:ASN:C	1.83	0.86
1:B:671:ARG:CG	1:B:676:ILE:HG12	2.06	0.86
1:B:671:ARG:HB2	1:B:676:ILE:HG13	1.58	0.86
1:B:718:LEU:HD23	1:B:718:LEU:H	1.40	0.85
1:A:675:GLU:HG2	1:A:676:ILE:N	1.77	0.85
1:B:672:THR:O	1:B:674:ASP:HA	1.77	0.85
1:B:671:ARG:CB	1:B:676:ILE:CG1	2.54	0.84
1:A:677:TYR:HD2	1:A:677:TYR:O	1.59	0.84
1:A:675:GLU:CG	1:A:677:TYR:N	2.41	0.83
1:A:676:ILE:H	1:A:678:SER:H	1.28	0.80
4:A:21:HOH:O	1:B:592:ARG:HD2	1.82	0.80
1:A:635:ARG:HH21	1:B:643:THR:HG23	1.47	0.79
1:A:676:ILE:O	1:A:676:ILE:CG1	2.30	0.79
1:A:678:SER:CB	1:B:628:ASP:O	2.30	0.79
1:A:675:GLU:CD	1:A:676:ILE:HA	2.07	0.79
1:A:675:GLU:HG3	1:A:677:TYR:CA	2.12	0.78
1:A:671:ARG:HG3	1:A:677:TYR:HD1	1.48	0.78
1:A:677:TYR:O	1:A:677:TYR:CD2	2.37	0.78
1:B:635:ARG:HG2	1:B:635:ARG:NH1	1.91	0.77
1:B:671:ARG:HB3	1:B:676:ILE:HG13	1.65	0.77
1:A:589:MET:HE2	1:B:807:ASN:O	1.84	0.77
1:A:789:ARG:CG	1:A:789:ARG:HH11	1.99	0.76
1:A:757:ASN:OD1	1:A:760:LEU:HB2	1.86	0.75
1:A:628:ASP:O	1:B:678:SER:CB	2.35	0.75
1:A:678:SER:HB3	1:B:628:ASP:O	1.86	0.74
1:A:641:ASN:HD21	1:A:643:THR:HG23	1.52	0.74
1:A:676:ILE:O	1:A:676:ILE:HG12	1.85	0.74
1:B:774:PRO:HA	1:B:801:VAL:CG2	2.17	0.74
1:A:675:GLU:OE1	1:A:676:ILE:HA	1.88	0.73
1:A:629:GLY:HA2	1:B:678:SER:CB	2.14	0.73
1:B:671:ARG:HG2	1:B:676:ILE:CG1	2.15	0.72
1:A:676:ILE:O	1:A:676:ILE:HD13	1.88	0.72
1:A:635:ARG:NH2	1:B:643:THR:H	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:THR:HG22	1:B:635:ARG:HH21	1.55	0.71
1:B:755:VAL:HG12	1:B:756:GLU:H	1.54	0.70
1:B:708:ASP:O	1:B:710:VAL:HG23	1.90	0.70
1:B:702:SER:O	1:B:713:VAL:HG23	1.91	0.70
1:A:671:ARG:HB2	1:A:675:GLU:OE2	1.92	0.69
1:A:678:SER:HB3	1:B:629:GLY:HA3	1.75	0.69
1:A:675:GLU:CD	1:A:676:ILE:CA	2.62	0.69
1:B:757:ASN:HD21	1:B:759:ASP:HB2	1.58	0.68
1:A:789:ARG:HH11	1:A:789:ARG:HG2	1.57	0.68
1:B:671:ARG:CG	1:B:676:ILE:CG1	2.70	0.68
1:A:642:GLU:O	1:A:643:THR:C	2.35	0.68
1:A:676:ILE:O	1:A:676:ILE:CD1	2.40	0.68
1:B:672:THR:O	1:B:674:ASP:CA	2.41	0.67
1:B:671:ARG:HB2	1:B:676:ILE:CG1	2.21	0.67
1:B:770:LYS:HE2	1:B:770:LYS:H	1.58	0.67
1:B:816:VAL:HG23	1:B:817:PRO:HD2	1.76	0.67
1:A:675:GLU:CB	1:A:676:ILE:HA	2.18	0.67
1:A:782:MET:SD	1:A:797:MET:HE3	2.35	0.67
1:A:635:ARG:NH2	1:B:643:THR:CG2	2.59	0.66
1:A:641:ASN:ND2	1:A:643:THR:HG23	2.10	0.66
1:A:671:ARG:HA	1:A:671:ARG:NE	2.10	0.65
1:A:595:THR:HG23	3:A:5:GL0:O4	1.96	0.65
1:A:635:ARG:NH2	1:B:643:THR:HG23	2.11	0.65
1:A:678:SER:HB2	1:B:628:ASP:O	1.96	0.65
1:A:635:ARG:HH22	1:B:643:THR:H	1.44	0.65
1:A:715:ALA:HB2	1:A:731:VAL:HG22	1.79	0.65
1:B:605:GLY:O	1:B:606:LEU:HB2	1.97	0.64
1:B:641:ASN:ND2	1:B:644:ILE:HG13	2.10	0.64
1:B:718:LEU:H	1:B:718:LEU:CD2	2.11	0.64
1:A:675:GLU:H	1:A:676:ILE:HB	1.62	0.63
1:B:757:ASN:ND2	1:B:759:ASP:HB2	2.13	0.63
1:B:613:SER:OG	1:B:637:HIS:HD2	1.81	0.63
1:A:811:TRP:CE2	1:B:782:MET:HG2	2.34	0.63
1:A:789:ARG:HH11	1:A:789:ARG:CB	2.12	0.63
1:A:671:ARG:CG	1:A:677:TYR:HD1	2.12	0.62
1:B:744:MET:HE2	1:B:762:MET:HE3	1.81	0.62
1:A:643:THR:HG22	1:B:635:ARG:NH2	2.14	0.61
1:A:671:ARG:HB3	1:A:675:GLU:CD	2.25	0.61
1:A:589:MET:HG3	1:B:808:THR:HG23	1.82	0.61
1:B:774:PRO:HA	1:B:801:VAL:HG21	1.83	0.61
1:A:628:ASP:O	1:B:678:SER:HB3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:GLU:N	1:A:676:ILE:HA	2.17	0.60
1:B:775:GLN:HG3	1:B:775:GLN:O	2.01	0.60
1:A:628:ASP:O	1:B:678:SER:HB2	2.00	0.60
1:A:656:ASP:HB2	1:A:659:ILE:CG2	2.31	0.60
1:B:668:LEU:HD22	1:B:676:ILE:HD12	1.84	0.60
1:A:671:ARG:CB	1:A:675:GLU:OE2	2.49	0.60
1:A:675:GLU:OE1	1:A:676:ILE:CA	2.51	0.59
1:B:690:ALA:O	1:B:735:LEU:HB2	2.03	0.58
1:A:672:THR:O	1:A:673:THR:C	2.47	0.57
1:A:675:GLU:H	1:A:676:ILE:CA	2.18	0.57
1:A:795:ASP:OD1	1:A:796:ASP:N	2.34	0.57
1:B:742:ILE:HD12	1:B:742:ILE:N	2.20	0.57
1:A:610:ASP:OD2	1:B:798:THR:HG23	2.05	0.56
1:B:770:LYS:H	1:B:770:LYS:CE	2.18	0.56
1:B:771:THR:OG1	1:B:772:ASN:N	2.38	0.56
1:A:641:ASN:C	1:A:641:ASN:ND2	2.55	0.56
1:B:715:ALA:HB2	1:B:731:VAL:HG22	1.88	0.55
1:A:677:TYR:O	1:A:678:SER:C	2.49	0.55
1:B:641:ASN:CB	1:B:644:ILE:H	2.20	0.55
1:B:760:LEU:HA	1:B:763:LYS:HD3	1.89	0.55
1:B:773:ASP:HB3	1:B:776:GLU:HB2	1.89	0.55
1:B:774:PRO:HA	1:B:801:VAL:HG22	1.87	0.55
1:B:744:MET:HG3	1:B:748:ILE:HG13	1.88	0.55
1:A:635:ARG:HH22	1:B:642:GLU:HB3	1.73	0.54
1:B:667:ILE:O	1:B:670:LEU:HB2	2.07	0.54
1:A:757:ASN:OD1	1:A:760:LEU:CB	2.56	0.53
1:B:639:GLU:CD	1:B:645:LYS:HZ1	2.15	0.53
1:A:793:ILE:HG22	1:A:795:ASP:O	2.08	0.53
1:B:613:SER:OG	1:B:637:HIS:CD2	2.60	0.53
1:A:613:SER:OG	1:A:637:HIS:HD2	1.92	0.53
1:A:794:GLU:O	1:B:602:LYS:HE2	2.08	0.53
1:A:753:LYS:HG2	1:A:754:HIS:CD2	2.44	0.53
1:A:810:LYS:O	1:A:811:TRP:HB3	2.09	0.53
1:A:789:ARG:HG2	1:A:789:ARG:NH1	2.24	0.53
1:B:747:GLY:HA3	1:B:796:ASP:O	2.09	0.52
1:B:689:ASP:OD1	1:B:689:ASP:C	2.50	0.52
1:B:601:ALA:HB3	1:B:605:GLY:HA2	1.92	0.52
1:B:710:VAL:O	1:B:710:VAL:CG1	2.46	0.52
1:B:816:VAL:HG23	1:B:817:PRO:CD	2.39	0.52
1:A:675:GLU:H	1:A:676:ILE:CB	2.22	0.52
1:B:791:GLY:O	1:B:792:GLN:O	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:LEU:O	1:B:618:GLY:C	2.53	0.51
1:B:649:LYS:O	1:B:652:GLU:HB2	2.10	0.51
1:B:793:ILE:HD13	1:B:795:ASP:H	1.74	0.51
1:A:642:GLU:O	1:A:645:LYS:N	2.44	0.51
1:A:786:ILE:O	1:A:789:ARG:O	2.29	0.51
1:A:635:ARG:NH2	1:B:643:THR:HG22	2.25	0.51
1:A:753:LYS:O	1:A:754:HIS:C	2.54	0.51
1:B:671:ARG:NE	1:B:671:ARG:HA	2.25	0.51
1:A:673:THR:O	1:A:676:ILE:HG13	2.11	0.50
1:A:676:ILE:H	1:A:677:TYR:C	2.17	0.50
1:B:789:ARG:O	1:B:789:ARG:HG3	2.10	0.50
1:A:640:SER:HB3	1:A:644:ILE:CG2	2.41	0.50
1:A:761:TRP:CE2	1:A:765:LYS:HE3	2.47	0.50
1:A:599:HIS:ND1	1:B:798:THR:HG22	2.26	0.50
1:A:629:GLY:CA	1:B:678:SER:HB3	2.22	0.50
1:B:789:ARG:HD2	1:B:793:ILE:HA	1.94	0.50
1:A:676:ILE:N	1:A:677:TYR:C	2.69	0.50
1:A:610:ASP:HB3	1:B:798:THR:CG2	2.43	0.49
1:B:793:ILE:HD13	1:B:794:GLU:N	2.27	0.49
1:B:793:ILE:HG13	1:B:797:MET:SD	2.53	0.49
1:A:613:SER:OG	1:A:637:HIS:CD2	2.65	0.49
1:A:675:GLU:N	1:A:676:ILE:CA	2.75	0.49
1:A:627:SER:HA	1:B:679:THR:O	2.12	0.49
1:B:650:ILE:O	1:B:652:GLU:N	2.46	0.48
1:A:677:TYR:O	1:A:678:SER:O	2.30	0.48
1:A:807:ASN:HB2	4:A:21:HOH:O	2.13	0.48
1:A:606:LEU:HD12	1:A:607:VAL:H	1.79	0.48
1:B:679:THR:HB	1:B:698:GLY:O	2.13	0.48
1:B:641:ASN:HB2	1:B:644:ILE:H	1.79	0.48
1:A:637:HIS:CD2	1:A:637:HIS:H	2.32	0.48
1:B:733:GLU:OE2	1:B:733:GLU:HA	2.14	0.48
1:A:641:ASN:HD22	1:A:642:GLU:N	2.11	0.47
1:A:741:LEU:HD22	1:A:742:ILE:N	2.30	0.47
1:B:635:ARG:HH11	1:B:635:ARG:CG	2.04	0.47
1:A:676:ILE:N	1:A:678:SER:N	2.51	0.47
1:B:593:VAL:HG21	1:B:622:TYR:CD2	2.49	0.47
1:A:635:ARG:HB2	1:B:675:GLU:OE1	2.14	0.47
1:A:741:LEU:CD2	1:A:742:ILE:N	2.78	0.47
1:A:681:ASP:O	1:B:625:ALA:HA	2.14	0.46
1:B:785:VAL:HG22	1:B:797:MET:HE1	1.96	0.46
1:A:642:GLU:HB3	1:A:643:THR:H	1.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:ALA:HB3	1:A:605:GLY:HA3	1.98	0.46
1:B:730:VAL:C	1:B:731:VAL:CG2	2.89	0.46
1:B:755:VAL:HG13	1:B:758:HIS:CE1	2.50	0.46
1:A:625:ALA:HA	1:B:681:ASP:O	2.16	0.45
1:A:614:MET:HG3	3:A:5:GL0:H2	1.98	0.45
1:B:753:LYS:HD2	1:B:753:LYS:HA	1.76	0.45
1:B:650:ILE:C	1:B:652:GLU:N	2.74	0.45
1:A:796:ASP:OD1	1:B:601:ALA:HA	2.17	0.45
1:B:757:ASN:C	1:B:757:ASN:HD22	2.24	0.45
1:B:676:ILE:HG22	1:B:676:ILE:O	2.16	0.45
1:B:774:PRO:CA	1:B:801:VAL:HG22	2.46	0.45
1:B:671:ARG:HD2	1:B:676:ILE:HD11	1.98	0.45
1:B:692:CYS:HB2	1:B:735:LEU:CD1	2.47	0.45
1:B:746:ASP:OD1	1:B:747:GLY:N	2.51	0.44
1:A:639:GLU:N	1:B:639:GLU:O	2.46	0.44
1:B:788:THR:O	1:B:788:THR:HG22	2.18	0.44
1:A:653:SER:O	1:A:655:ILE:N	2.51	0.44
1:A:641:ASN:O	1:A:642:GLU:O	2.35	0.43
1:B:641:ASN:HB3	1:B:644:ILE:H	1.82	0.43
1:A:704:ILE:HA	1:A:740:LEU:O	2.17	0.43
1:A:618:GLY:O	1:A:620:ARG:HD3	2.18	0.43
1:B:668:LEU:CD2	1:B:676:ILE:HD12	2.48	0.43
1:A:675:GLU:OE1	1:A:676:ILE:HG12	2.18	0.43
1:B:659:ILE:O	1:B:662:LYS:HB3	2.19	0.43
1:B:751:GLY:O	1:B:752:PRO:C	2.61	0.43
1:A:644:ILE:O	1:A:645:LYS:C	2.62	0.43
1:A:722:ILE:HG23	1:A:723:ILE:H	1.83	0.43
1:A:810:LYS:O	1:A:811:TRP:CB	2.67	0.42
1:B:639:GLU:CD	1:B:645:LYS:NZ	2.77	0.42
1:A:634:ALA:HB3	1:B:675:GLU:OE2	2.19	0.42
1:A:671:ARG:O	4:A:33:HOH:O	2.21	0.42
1:B:679:THR:CG2	1:B:698:GLY:O	2.67	0.42
1:A:675:GLU:OE1	1:A:676:ILE:C	2.62	0.42
1:A:642:GLU:O	1:A:644:ILE:N	2.53	0.42
1:A:675:GLU:H	1:A:676:ILE:HA	1.77	0.42
1:A:702:SER:HB3	1:A:743:MET:HA	2.01	0.42
1:B:644:ILE:O	1:B:645:LYS:C	2.61	0.42
1:A:741:LEU:CD2	1:A:741:LEU:C	2.92	0.42
1:B:668:LEU:HD23	1:B:668:LEU:HA	1.80	0.41
1:B:751:GLY:O	1:B:789:ARG:NH2	2.53	0.41
1:A:773:ASP:HA	1:A:774:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:PHE:O	1:B:727:ASP:C	2.63	0.41
1:B:763:LYS:H	1:B:763:LYS:HG3	1.65	0.41
1:A:656:ASP:O	1:A:657:GLU:C	2.63	0.41
1:B:674:ASP:OD2	1:B:677:TYR:CD1	2.74	0.41
1:B:724:ASN:OD1	1:B:727:ASP:N	2.53	0.41
1:A:736:LYS:O	1:A:737:ALA:C	2.63	0.41
1:A:741:LEU:HD22	1:A:741:LEU:C	2.46	0.41
1:B:757:ASN:ND2	1:B:760:LEU:H	2.19	0.41
1:A:643:THR:O	1:A:644:ILE:C	2.64	0.41
1:B:650:ILE:C	1:B:652:GLU:H	2.29	0.40
1:B:816:VAL:HA	1:B:817:PRO:HD3	1.91	0.40
1:A:678:SER:HB2	1:A:679:THR:H	1.63	0.40
1:B:650:ILE:HD11	1:B:667:ILE:HD11	2.03	0.40
1:A:648:GLU:HG2	1:A:684:ILE:HD11	2.03	0.40
1:A:783:GLU:O	1:A:784:GLU:C	2.65	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	210/242 (87%)	175 (83%)	28 (13%)	7 (3%)	3	5
1	B	223/242 (92%)	169 (76%)	40 (18%)	14 (6%)	1	1
All	All	433/484 (90%)	344 (79%)	68 (16%)	21 (5%)	2	2

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	642	GLU
1	A	643	THR
1	A	678	SER

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Mol	Chain	Res	Type
1	B	606	LEU
1	B	641	ASN
1	B	642	GLU
1	B	655	ILE
1	B	755	VAL
1	B	792	GLN
1	A	654	GLY
1	B	619	ALA
1	B	651	LEU
1	B	654	GLY
1	B	673	THR
1	B	751	GLY
1	A	634	ALA
1	A	655	ILE
1	B	752	PRO
1	B	784	GLU
1	B	590	SER
1	A	707	GLY

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	184/205 (90%)	145 (79%)	39 (21%)	1	2
1	B	194/205 (95%)	152 (78%)	42 (22%)	1	1
All	All	378/410 (92%)	297 (79%)	81 (21%)	1	2

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	593	VAL
1	A	602	LYS
1	A	606	LEU
1	A	607	VAL
1	A	615	MET

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Mol	Chain	Res	Type
1	A	617	LEU
1	A	621	LYS
1	A	635	ARG
1	A	639	GLU
1	A	641	ASN
1	A	642	GLU
1	A	643	THR
1	A	645	LYS
1	A	658	LYS
1	A	659	ILE
1	A	663	THR
1	A	669	SER
1	A	671	ARG
1	A	672	THR
1	A	674	ASP
1	A	675	GLU
1	A	676	ILE
1	A	678	SER
1	A	691	SER
1	A	695	LEU
1	A	702	SER
1	A	711	MET
1	A	714	GLN
1	A	723	ILE
1	A	732	SER
1	A	741	LEU
1	A	744	MET
1	A	748	ILE
1	A	753	LYS
1	A	772	ASN
1	A	789	ARG
1	A	794	GLU
1	A	808	THR
1	A	810	LYS
1	B	607	VAL
1	B	613	SER
1	B	617	LEU
1	B	627	SER
1	B	635	ARG
1	B	640	SER
1	B	642	GLU
1	B	643	THR

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Mol	Chain	Res	Type
1	B	646	LEU
1	B	651	LEU
1	B	653	SER
1	B	661	ILE
1	B	670	LEU
1	B	671	ARG
1	B	675	GLU
1	B	676	ILE
1	B	677	TYR
1	B	678	SER
1	B	683	SER
1	B	700	THR
1	B	708	ASP
1	B	711	MET
1	B	714	GLN
1	B	718	LEU
1	B	722	ILE
1	B	748	ILE
1	B	753	LYS
1	B	754	HIS
1	B	764	ARG
1	B	767	LYS
1	B	770	LYS
1	B	772	ASN
1	B	774	PRO
1	B	780	LEU
1	B	785	VAL
1	B	793	ILE
1	B	798	THR
1	B	799	VAL
1	B	800	VAL
1	B	801	VAL
1	B	816	VAL
1	B	819	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	637	HIS
1	A	641	ASN
1	A	714	GLN
1	A	734	GLN

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Mol	Chain	Res	Type
1	A	758	HIS
1	B	599	HIS
1	B	637	HIS
1	B	641	ASN
1	B	734	GLN
1	B	757	ASN
1	B	772	ASN
1	B	775	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
3	GL0	A	5	-	12,12,12	0.84	0	17,17,17	1.94	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GL0	A	5	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5	GL0	C3-C4-C5	5.01	119.31	110.23
3	A	5	GL0	C4-C3-C2	4.19	118.18	110.83
3	A	5	GL0	O5-C5-C6	3.03	113.94	106.44
3	A	5	GL0	O2-C2-C1	2.14	114.19	109.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5	GL0	2	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, 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	216/242 (89%)	0.70	31 (14%) 6 5	9, 54, 107, 124	8 (3%)
1	B	227/242 (93%)	0.77	35 (15%) 5 4	23, 67, 115, 140	7 (3%)
All	All	443/484 (91%)	0.74	66 (14%) 5 5	9, 61, 113, 140	15 (3%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	771	THR	15.7
1	A	672	THR	9.2
1	B	807	ASN	9.2
1	B	711	MET	8.9
1	A	700	THR	8.8
1	B	808	THR	7.9
1	A	701	PRO	7.5
1	A	772	ASN	7.2
1	B	678	SER	6.7
1	B	806	HIS	6.6
1	B	676	ILE	6.2
1	A	676	ILE	6.1
1	B	698	GLY	6.0
1	A	673	THR	5.6
1	A	711	MET	5.4
1	A	699	SER	5.1
1	A	764	ARG	5.0
1	A	643	THR	4.7
1	A	677	TYR	4.6
1	A	671	ARG	4.6
1	B	817	PRO	4.4
1	A	674	ASP	4.1
1	B	818	ALA	4.0
1	A	629	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	629	GLY	3.7
1	A	675	GLU	3.7
1	B	819	ILE	3.6
1	B	677	TYR	3.5
1	B	755	VAL	3.5
1	A	607	VAL	3.5
1	A	633	GLY	3.4
1	B	634	ALA	3.3
1	A	811	TRP	3.3
1	B	749	PHE	3.3
1	B	750	GLU	3.3
1	B	793	ILE	3.3
1	A	634	ALA	3.1
1	B	760	LEU	3.0
1	B	679	THR	3.0
1	A	756	GLU	2.9
1	A	600	ALA	2.9
1	B	816	VAL	2.9
1	A	599	HIS	2.9
1	A	723	ILE	2.9
1	A	725	GLU	2.9
1	B	592	ARG	2.9
1	B	718	LEU	2.8
1	B	607	VAL	2.8
1	B	653	SER	2.6
1	B	703	PHE	2.6
1	A	603	GLY	2.6
1	B	673	THR	2.5
1	B	675	GLU	2.5
1	B	674	ASP	2.4
1	A	606	LEU	2.4
1	A	715	ALA	2.4
1	B	641	ASN	2.3
1	B	606	LEU	2.3
1	B	752	PRO	2.3
1	A	716	SER	2.2
1	B	651	LEU	2.2
1	B	754	HIS	2.2
1	A	601	ALA	2.2
1	A	722	ILE	2.2
1	B	789	ARG	2.1
1	B	753	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GL0	A	5	12/12	0.78	0.20	76,104,110,115	0
2	MN	B	3	1/1	0.99	0.02	66,66,66,66	0
2	MN	A	1	1/1	1.00	0.02	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.