Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 05:07 PM EST

PDB ID	:	3T91
Title	:	Structure of the Phosphatase Domain of the Cell Fate Determinant SpoIIE from Bacillus subtilis
Authors	:	Levdikov, V.M.; Blagova, E.V.; Wilkinson, A.J.
Deposited on	:	2011-08-02
Resolution	:	2.64 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:

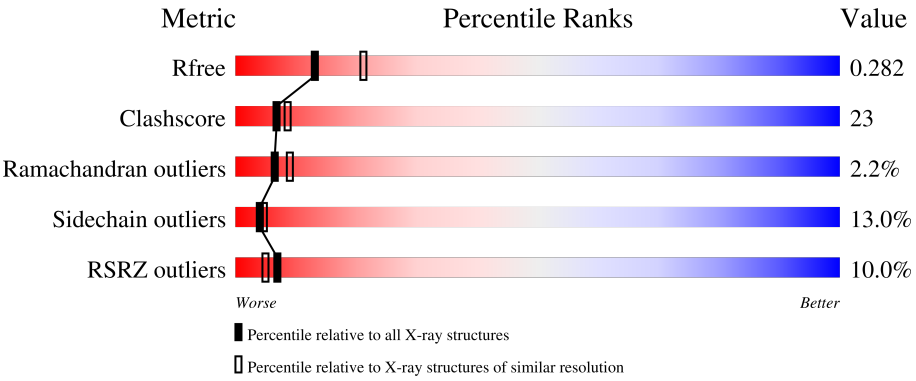
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 <=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	6% 60% 21% 5% 13%
1	B	242	12% 58% 26% 5% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3586 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	210	Total	C	N	O	S	0	7	0
			1677	1051	288	326	12			
1	B	219	Total	C	N	O	S	0	5	0
			1723	1081	293	338	11			

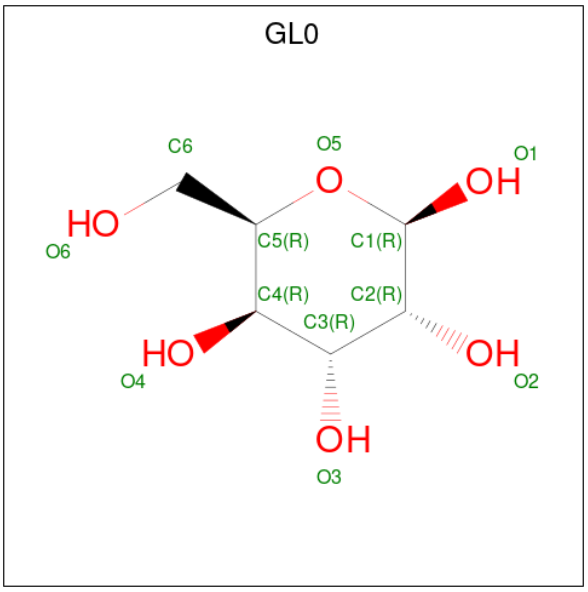
There are 8 discrepancies between the modelled and reference sequences:

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 (three-letter code: MN) (formula: Mn).

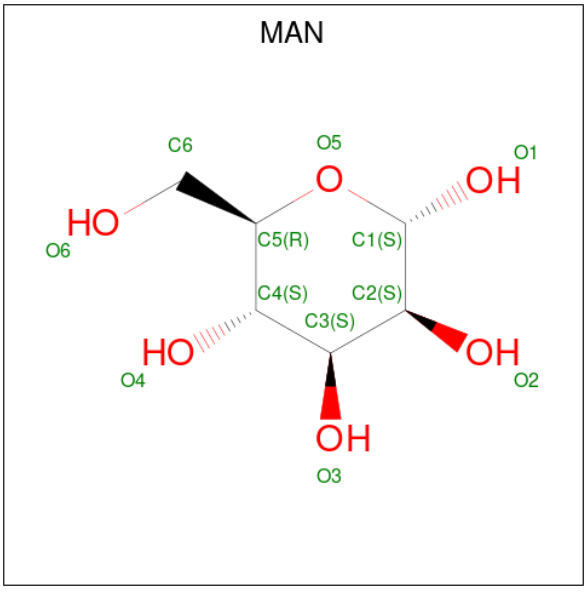
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

- Molecule 3 is beta-D-gulopyranose (three-letter code: GL0) (formula: $C_6H_{12}O_6$).



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

- Molecule 4 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 12 6 6	0	1

- Molecule 5 is water.

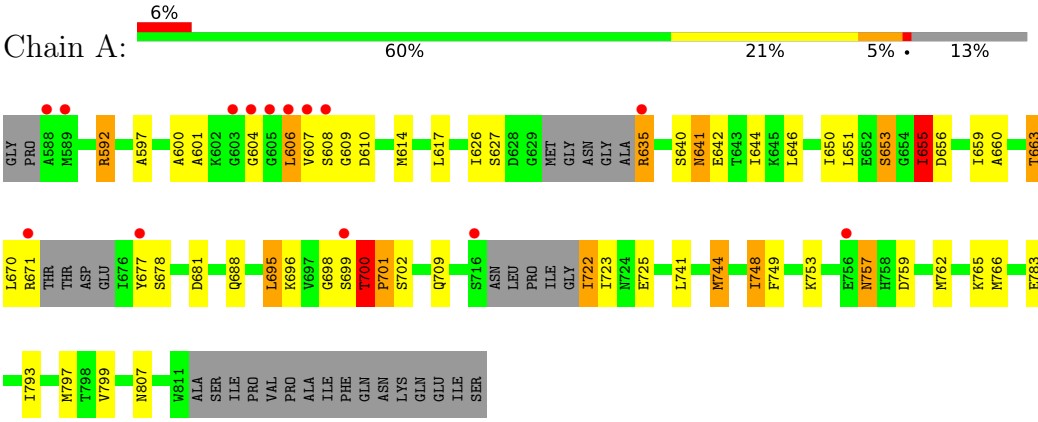
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	91	Total O 91 91	0	0
5	B	69	Total O 69 69	0	0

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.

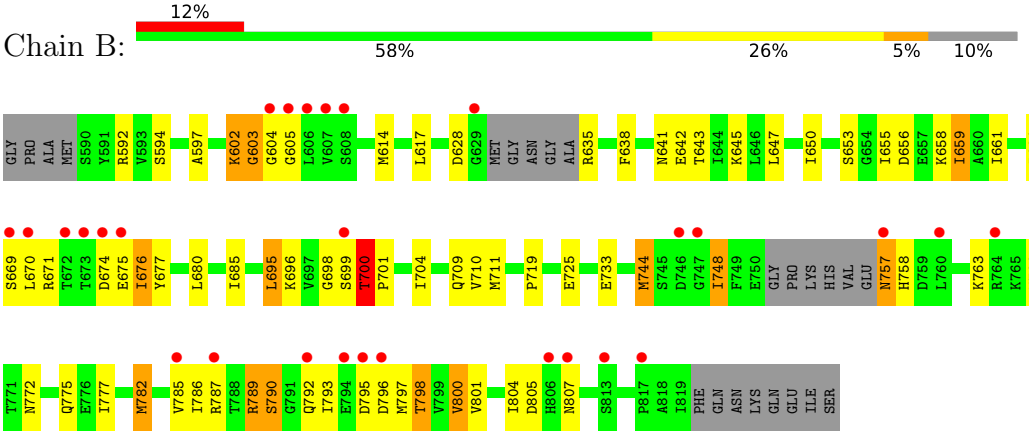
• Molecule 1: Stage II sporulation protein E

Chain A:



• Molecule 1: Stage II sporulation protein E

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	87.62Å 87.62Å 321.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.64 10.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-2.64) 99.7 (10.00-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.279 0.222 , 0.282	Depositor DCC
R_{free} test set	1185 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	65.3	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 62.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3586	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MAN, MN, GL0

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	0.41	0/1699	0.64	0/2279
1	B	0.42	0/1744	0.60	0/2348
All	All	0.42	0/3443	0.62	0/4627

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	700[B]	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1677	0	1704	97	1
1	B	1723	0	1747	80	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	12	0	12	1	0
4	B	12	0	12	0	0
5	A	91	0	0	2	0
5	B	69	0	0	2	0
All	All	3586	0	3475	161	1

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 23.

All (161) 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:B:659:ILE:H	1:B:659:ILE:CD1	1.44	1.25
1:B:659:ILE:HD12	1:B:659:ILE:N	1.49	1.19
1:A:655:ILE:HD11	1:A:659:ILE:HG13	1.17	1.13
1:A:653:SER:OG	1:A:655:ILE:HG22	1.47	1.11
1:B:744:MET:HE2	1:B:748:ILE:HD11	1.16	1.09
1:A:700[A]:THR:HB	1:A:701[A]:PRO:CA	1.84	1.06
1:A:700[A]:THR:CB	1:A:701[A]:PRO:HA	1.86	1.06
1:A:655:ILE:CD1	1:A:659:ILE:HG13	1.85	1.05
1:A:668:LEU:HD22	1:A:671:ARG:NH1	1.71	1.05
1:A:635:ARG:HH11	1:A:635:ARG:CG	1.69	1.03
1:A:659:ILE:O	1:A:663:THR:HG22	1.59	1.03
1:B:700:THR:HG23	1:B:701:PRO:HA	1.03	1.02
1:A:700[A]:THR:HB	1:A:701[A]:PRO:HA	1.39	1.01
1:B:696:LYS:HZ2	1:B:700:THR:HG21	1.26	0.99
1:B:700:THR:CG2	1:B:701:PRO:HA	1.94	0.97
1:B:744:MET:CE	1:B:748:ILE:HD11	1.94	0.97
1:A:635:ARG:HH11	1:A:635:ARG:HG3	1.29	0.95
1:A:635:ARG:HH11	1:A:635:ARG:CB	1.81	0.93
1:B:696:LYS:NZ	1:B:700:THR:HG21	1.83	0.93
1:A:681:ASP:CG	1:A:700[A]:THR:HG21	1.88	0.92
1:B:700:THR:HG23	1:B:701:PRO:CA	1.98	0.92
1:A:655:ILE:HD11	1:A:659:ILE:CG1	1.99	0.91
1:A:655:ILE:CD1	1:A:659:ILE:CG1	2.51	0.89
1:A:700[B]:THR:O	1:A:700[B]:THR:OG1	1.82	0.87
1:B:744:MET:HE2	1:B:748:ILE:CD1	2.03	0.86
1:A:681:ASP:CG	1:A:700[A]:THR:CG2	2.45	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700[A]:THR:CB	1:A:701[A]:PRO:CA	2.51	0.83
1:A:635:ARG:HG3	1:A:635:ARG:NH1	1.90	0.83
1:A:744:MET:HE2	1:A:748:ILE:HG21	1.60	0.82
1:B:659:ILE:H	1:B:659:ILE:HD12	0.65	0.81
1:B:748:ILE:HG22	1:B:797:MET:HB3	1.65	0.79
1:B:676:ILE:O	1:B:676:ILE:HD13	1.83	0.78
1:A:700[A]:THR:OG1	1:A:701[A]:PRO:HA	1.82	0.78
1:A:681:ASP:OD2	1:A:700[A]:THR:CG2	2.33	0.77
1:A:635:ARG:HH11	1:A:635:ARG:HB2	1.50	0.76
1:B:696:LYS:HZ2	1:B:700:THR:CG2	1.97	0.76
1:A:653:SER:HG	1:A:655:ILE:HG22	1.51	0.75
1:A:641:ASN:C	1:A:641:ASN:HD22	1.90	0.74
1:A:659:ILE:O	1:A:663:THR:CG2	2.34	0.74
1:B:656:ASP:HB3	1:B:659:ILE:HD11	1.69	0.73
1:A:651:LEU:HD11	1:A:695:LEU:HB2	1.69	0.73
1:A:671:ARG:NH1	1:A:677:TYR:HB3	2.04	0.72
1:A:655:ILE:HG13	1:A:659:ILE:HG12	1.72	0.71
1:B:769:LEU:HD13	1:B:777:ILE:HD13	1.72	0.70
1:B:782:MET:O	1:B:785:VAL:HG22	1.91	0.70
1:B:650:ILE:HD11	1:B:667:ILE:HD12	1.73	0.69
1:B:763:LYS:O	1:B:767:LYS:HG3	1.93	0.69
1:A:698:GLY:O	1:A:700[B]:THR:HG22	1.93	0.68
1:A:635:ARG:CB	1:A:635:ARG:NH1	2.57	0.68
1:A:608:SER:OG	1:B:796:ASP:CG	2.32	0.67
1:A:783:GLU:OE2	1:A:787:ARG:NH1	2.28	0.67
1:B:656:ASP:HB3	1:B:659:ILE:CD1	2.24	0.67
1:A:600:ALA:HB3	1:B:782:MET:HE3	1.76	0.66
1:A:681:ASP:OD2	1:A:700[A]:THR:HG22	1.94	0.66
1:B:671:ARG:NH2	1:B:676:ILE:O	2.23	0.66
1:B:695:LEU:HD12	1:B:696:LYS:N	2.10	0.65
1:A:681:ASP:OD2	1:A:700[A]:THR:HG21	1.94	0.64
1:B:659:ILE:CD1	1:B:659:ILE:N	2.25	0.63
1:A:671:ARG:HD2	1:A:677:TYR:HB2	1.81	0.62
1:A:757:ASN:HD21	1:A:759:ASP:HB2	1.65	0.62
1:A:597:ALA:H	1:B:775:GLN:HE22	1.47	0.62
1:A:608:SER:HG	1:B:796:ASP:CG	2.02	0.61
1:A:655:ILE:HG13	1:A:659:ILE:CG1	2.30	0.61
1:A:696:LYS:HZ1	1:A:700[A]:THR:HG21	1.65	0.61
1:B:789:ARG:HD3	1:B:789:ARG:C	2.21	0.60
1:A:660:ALA:HA	1:A:663:THR:HG23	1.83	0.60
1:B:671:ARG:NE	1:B:677:TYR:HB3	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:650:ILE:HD11	1:B:667:ILE:CD1	2.32	0.59
1:A:592:ARG:NH2	1:B:597:ALA:O	2.36	0.59
1:A:606:LEU:CD1	1:A:607:VAL:HG22	2.33	0.59
1:A:700[A]:THR:HB	1:A:701[A]:PRO:C	2.23	0.59
1:A:700[A]:THR:HG1	1:A:701[A]:PRO:HA	1.68	0.59
1:A:744:MET:CE	1:A:748:ILE:HG21	2.32	0.59
1:B:671:ARG:CZ	1:B:677:TYR:HB3	2.33	0.59
1:B:710:VAL:HG13	1:B:766:MET:HE1	1.85	0.59
1:A:677:TYR:O	1:A:678:SER:OG	2.13	0.58
1:A:600:ALA:CB	1:B:782:MET:HE3	2.34	0.58
1:A:655:ILE:CG1	1:A:659:ILE:CG1	2.81	0.57
1:A:655:ILE:CG1	1:A:659:ILE:HG12	2.35	0.57
1:B:653:SER:OG	1:B:655:ILE:HD12	2.05	0.57
1:A:669:SER:O	1:A:670:LEU:HD23	2.05	0.57
1:A:748:ILE:HG22	1:A:749:PHE:N	2.20	0.57
1:A:668:LEU:HD22	1:A:671:ARG:HH11	1.63	0.57
1:B:704:ILE:HD12	1:B:711[B]:MET:HE2	1.85	0.57
1:A:681:ASP:OD1	1:A:700[A]:THR:HG21	2.04	0.56
1:A:671:ARG:CD	1:A:677:TYR:HB2	2.36	0.56
1:B:698[A]:GLY:O	1:B:699:SER:O	2.24	0.56
1:B:748:ILE:C	1:B:748:ILE:HD12	2.26	0.55
1:B:748:ILE:HG22	1:B:797:MET:CB	2.35	0.54
1:B:685:ILE:HD13	1:B:804:ILE:HD11	1.90	0.54
1:B:671:ARG:NE	1:B:677:TYR:CB	2.71	0.53
1:B:603:GLY:O	1:B:605:GLY:N	2.42	0.53
1:A:635:ARG:NH1	1:A:635:ARG:HB2	2.20	0.53
1:B:647:LEU:HD22	1:B:664:ILE:HG23	1.89	0.53
1:A:765:LYS:NZ	1:A:784:GLU:OE2	2.26	0.53
1:B:787:ARG:NH2	5:B:16:HOH:O	2.41	0.53
1:B:793:ILE:HG22	1:B:795:ASP:H	1.74	0.53
1:A:606:LEU:HD13	1:A:607:VAL:HG22	1.91	0.53
1:A:748:ILE:HD13	1:A:799:VAL:HB	1.91	0.53
1:A:641:ASN:ND2	1:A:644:ILE:H	2.07	0.52
1:A:601:ALA:HB3	1:A:604:GLY:CA	2.40	0.52
1:A:793:ILE:HG22	1:B:602:LYS:HA	1.92	0.52
1:B:733:GLU:OE2	1:B:733:GLU:HA	2.11	0.51
1:A:655:ILE:CG1	1:A:656:ASP:N	2.72	0.51
1:B:748:ILE:CD1	1:B:785:VAL:HG11	2.41	0.51
1:A:700[A]:THR:HG22	5:A:96:HOH:O	2.10	0.51
1:A:696:LYS:NZ	1:A:700[A]:THR:HG21	2.26	0.51
1:B:748:ILE:HD12	1:B:748:ILE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:ILE:HD12	1:B:719:PRO:HG2	1.93	0.50
1:A:650:ILE:HD11	1:A:667:ILE:CD1	2.41	0.50
1:A:641:ASN:HD21	1:A:644:ILE:H	1.59	0.50
1:A:698:GLY:C	1:A:700[B]:THR:HG22	2.32	0.50
1:A:626:ILE:HD11	1:B:800:VAL:HG13	1.92	0.50
1:A:678:SER:HB2	1:B:628:ASP:O	2.11	0.50
1:B:782:MET:O	1:B:785:VAL:CG2	2.60	0.49
1:A:641:ASN:C	1:A:641:ASN:ND2	2.63	0.49
1:B:650:ILE:CD1	1:B:667:ILE:HD12	2.42	0.49
1:A:601:ALA:HB3	1:A:604:GLY:HA2	1.94	0.49
1:B:748:ILE:HD13	1:B:785:VAL:HG11	1.94	0.49
1:A:671:ARG:NH1	1:A:677:TYR:CB	2.75	0.48
1:A:762:MET:HG3	1:A:766:MET:CE	2.43	0.48
1:B:666:SER:O	1:B:669:SER:HB2	2.13	0.48
1:B:792:GLN:N	5:B:63:HOH:O	2.46	0.48
1:A:655:ILE:HD11	1:A:660:ALA:N	2.28	0.47
1:A:614:MET:HB2	3:B:900[A]:GL0:H2	1.97	0.47
1:A:610:ASP:HB3	1:B:798:THR:HG21	1.97	0.47
1:A:653:SER:CB	1:A:655:ILE:HG22	2.41	0.47
1:B:656:ASP:C	1:B:659:ILE:HD13	2.35	0.46
1:A:722:ILE:HG23	1:A:723:ILE:N	2.30	0.46
1:A:744:MET:CE	1:A:748:ILE:CG2	2.93	0.46
1:A:786:ILE:HG12	1:A:797:MET:HE1	1.98	0.46
1:B:695:LEU:HD12	1:B:695:LEU:C	2.35	0.45
1:B:789:ARG:O	1:B:790:SER:HB3	2.16	0.45
1:B:674:ASP:HA	1:B:675:GLU:HA	1.69	0.45
1:B:661:ILE:CD1	1:B:719:PRO:HG2	2.47	0.45
1:B:665:ASN:O	1:B:669:SER:N	2.46	0.44
1:B:757:ASN:HD22	1:B:758:HIS:N	2.15	0.44
1:B:769:LEU:CD1	1:B:777:ILE:HG23	2.47	0.44
1:A:610:ASP:HB3	1:B:798:THR:CG2	2.47	0.44
1:A:609:GLY:N	1:B:796:ASP:OD2	2.50	0.44
1:A:725:GLU:HG3	5:A:80:HOH:O	2.17	0.43
1:B:782:MET:O	1:B:786:ILE:HG13	2.18	0.43
1:A:807:ASN:HB2	1:B:592:ARG:HG2	1.99	0.43
1:A:701[A]:PRO:HD2	1:A:749:PHE:CD2	2.54	0.43
1:A:793:ILE:HG12	1:A:797:MET:HE1	2.01	0.42
1:B:744:MET:HE3	1:B:744:MET:HB3	1.86	0.42
1:A:641:ASN:HD21	1:A:644:ILE:HG13	1.85	0.42
1:A:601:ALA:HB3	1:A:604:GLY:HA3	2.02	0.42
1:B:789:ARG:O	1:B:790:SER:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:789:ARG:HD3	1:B:789:ARG:O	2.20	0.42
1:A:744:MET:HE2	1:A:748:ILE:CG2	2.39	0.41
1:B:710:VAL:CG1	1:B:766:MET:HE1	2.49	0.41
1:A:597:ALA:HB3	1:B:592:ARG:HH22	1.85	0.41
1:A:677:TYR:O	1:A:677:TYR:CD1	2.74	0.41
1:B:656:ASP:O	1:B:659:ILE:HD13	2.21	0.41
1:B:793:ILE:HG22	1:B:795:ASP:N	2.34	0.41
1:A:600:ALA:CB	1:B:782:MET:CE	2.98	0.41
1:A:655:ILE:CD1	1:A:659:ILE:CD1	2.99	0.41
1:A:650:ILE:CD1	1:A:667:ILE:CD1	2.98	0.41
1:B:696:LYS:NZ	1:B:700:THR:CG2	2.66	0.40
1:A:640:SER:HA	1:B:638:PHE:HD1	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:GLU:OE2	1:B:645:LYS:NZ[10_444]	2.17	0.03

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	209/242 (86%)	191 (91%)	11 (5%)	7 (3%)	4	4
1	B	218/242 (90%)	203 (93%)	10 (5%)	5 (2%)	6	8
All	All	427/484 (88%)	394 (92%)	21 (5%)	12 (3%)	6	6

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	604	GLY

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Mol	Chain	Res	Type
1	B	641	ASN
1	A	699[A]	SER
1	A	699[B]	SER
1	B	603	GLY
1	B	790	SER
1	B	700	THR
1	A	701[A]	PRO
1	A	701[B]	PRO
1	A	700[A]	THR
1	A	700[B]	THR
1	A	655	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	187/205 (91%)	165 (88%)	22 (12%)	5 6
1	B	192/205 (94%)	164 (85%)	28 (15%)	3 3
All	All	379/410 (92%)	329 (87%)	50 (13%)	4 4

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	592	ARG
1	A	606	LEU
1	A	617	LEU
1	A	627	SER
1	A	635	ARG
1	A	641	ASN
1	A	646	LEU
1	A	653	SER
1	A	655	ILE
1	A	663	THR
1	A	688	GLN
1	A	695	LEU

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Mol	Chain	Res	Type
1	A	700[A]	THR
1	A	700[B]	THR
1	A	702	SER
1	A	709	GLN
1	A	722	ILE
1	A	741	LEU
1	A	744	MET
1	A	748	ILE
1	A	753	LYS
1	A	757	ASN
1	B	594	SER
1	B	602	LYS
1	B	614	MET
1	B	617	LEU
1	B	635	ARG
1	B	642	GLU
1	B	643	THR
1	B	658	LYS
1	B	659	ILE
1	B	670	LEU
1	B	676	ILE
1	B	680	LEU
1	B	695	LEU
1	B	700	THR
1	B	709	GLN
1	B	725	GLU
1	B	744	MET
1	B	748	ILE
1	B	757	ASN
1	B	772	ASN
1	B	782	MET
1	B	789	ARG
1	B	798	THR
1	B	800	VAL
1	B	801	VAL
1	B	805	ASP
1	B	807[A]	ASN
1	B	807[B]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	637	HIS
1	A	641	ASN
1	A	734	GLN
1	A	757	ASN
1	B	637	HIS
1	B	641	ASN
1	B	734	GLN
1	B	757	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	MAN	B	901[B]	-	12,12,12	0.61	0	17,17,17	1.02	0
3	GL0	B	900[A]	-	12,12,12	0.83	0	17,17,17	1.93	5 (29%)

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
4	MAN	B	901[B]	-	-	2/2/22/22	0/1/1/1
3	GL0	B	900[A]	-	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	900[A]	GL0	C3-C4-C5	4.49	118.24	110.24
3	B	900[A]	GL0	C1-O5-C5	-3.06	107.89	113.66
3	B	900[A]	GL0	C4-C3-C2	2.49	115.17	110.82
3	B	900[A]	GL0	O4-C4-C3	-2.08	105.54	110.35
3	B	900[A]	GL0	O5-C5-C6	2.04	111.52	106.44

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	900[A]	GL0	O5-C5-C6-O6
4	B	901[B]	MAN	O5-C5-C6-O6
3	B	900[A]	GL0	C4-C5-C6-O6
4	B	901[B]	MAN	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	900[A]	GL0	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	210/242 (86%)	-0.03	14 (6%) 17 15	28, 54, 110, 135	1 (0%)
1	B	219/242 (90%)	0.38	29 (13%) 3 2	30, 63, 123, 136	2 (0%)
All	All	429/484 (88%)	0.18	43 (10%) 7 5	28, 58, 117, 136	3 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	604	GLY	9.4
1	A	606	LEU	7.9
1	A	588	ALA	7.0
1	A	605	GLY	6.8
1	B	674	ASP	5.8
1	B	629	GLY	5.1
1	B	673	THR	5.1
1	B	670	LEU	4.8
1	B	606	LEU	4.7
1	B	792	GLN	4.6
1	B	672	THR	4.4
1	B	607	VAL	4.4
1	B	807[A]	ASN	4.0
1	A	607	VAL	4.0
1	B	795	ASP	3.7
1	B	794	GLU	3.5
1	B	699	SER	3.4
1	A	756	GLU	3.3
1	B	757	ASN	2.9
1	A	608	SER	2.9
1	A	699[A]	SER	2.9
1	B	764	ARG	2.8
1	B	675	GLU	2.8
1	B	746	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	760	LEU	2.8
1	B	669	SER	2.7
1	B	787	ARG	2.6
1	B	747	GLY	2.6
1	B	605	GLY	2.6
1	B	817	PRO	2.5
1	A	603	GLY	2.5
1	B	813	SER	2.3
1	A	716	SER	2.3
1	B	806[A]	HIS	2.3
1	A	671	ARG	2.3
1	B	604	GLY	2.2
1	B	796	ASP	2.2
1	A	589	MET	2.2
1	A	635	ARG	2.1
1	B	770	LYS	2.1
1	B	608	SER	2.1
1	A	677	TYR	2.1
1	B	785	VAL	2.0

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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MN	B	3	1/1	0.93	0.44	113,113,113,113	0
4	MAN	B	901[B]	12/12	0.95	0.14	44,51,60,63	12
3	GL0	B	900[A]	12/12	0.96	0.15	20,36,44,44	12
2	MN	A	1	1/1	0.98	0.14	89,89,89,89	0

6.5 Other polymers (i)

There are no such residues in this entry.