Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 04:18 am BST

PDB ID	:	4AQ1
Title	:	Structure of the SbsB S-layer protein of Geobacillus stearothermophilus PV72p2 in complex with nanobody KB6
Authors	:	Baranova, E.; Remaut, H.
Deposited on	:	2012-04-12
Resolution	:	2.42 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

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 2.42 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.
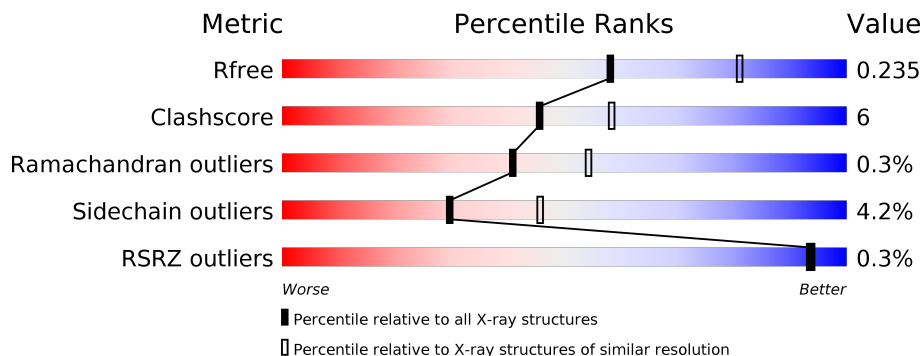
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 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	892	68% 11% · 19%
2	B	130	% 77% 17% · 5%
2	D	130	85% 10% · 5%
3	C	892	63% 7% · 30%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12335 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 SBSB PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	721	Total	C	N	O	S	82	0	0
			5363	3356	881	1124	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	expression tag	UNP Q45664
A	86	GLY	ASP	conflict	UNP Q45664
A	139	ALA	ARG	conflict	UNP Q45664
A	140	HIS	TYR	conflict	UNP Q45664
A	500	GLU	ASP	conflict	UNP Q45664
A	812	GLU	LYS	conflict	UNP Q45664
A	921	GLY	-	expression tag	UNP Q45664
A	922	SER	-	expression tag	UNP Q45664

- Molecule 2 is a protein called NBKB6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	124	Total	C	N	O	S	2	0	0
			924	572	163	184	5			
2	D	124	Total	C	N	O	S	7	0	0
			924	572	163	184	5			

- Molecule 3 is a protein called SBSB PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	627	Total	C	N	O	S	26	0	0
			4641	2899	761	979	2			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	31	MET	-	expression tag	UNP Q45664
C	86	GLY	ASP	conflict	UNP Q45664
C	139	ALA	ARG	conflict	UNP Q45664
C	140	HIS	TYR	conflict	UNP Q45664
C	402	THR	SER	conflict	UNP Q45664
C	500	GLU	ASP	conflict	UNP Q45664
C	812	GLU	LYS	conflict	UNP Q45664
C	921	GLY	-	expression tag	UNP Q45664
C	922	SER	-	expression tag	UNP Q45664

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total 4	Ca 4	0	0
4	C	4	Total 4	Ca 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	253	Total 253	O 253	0	0
5	B	21	Total 21	O 21	0	0
5	C	173	Total 173	O 173	0	0
5	D	28	Total 28	O 28	0	0

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 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: SBSB PROTEIN

• Molecule 2: NBKB6

• Molecule 2: NBKB6

• Molecule 3: SBSB PROTEIN

Chain C:

63%   7%   •   30%
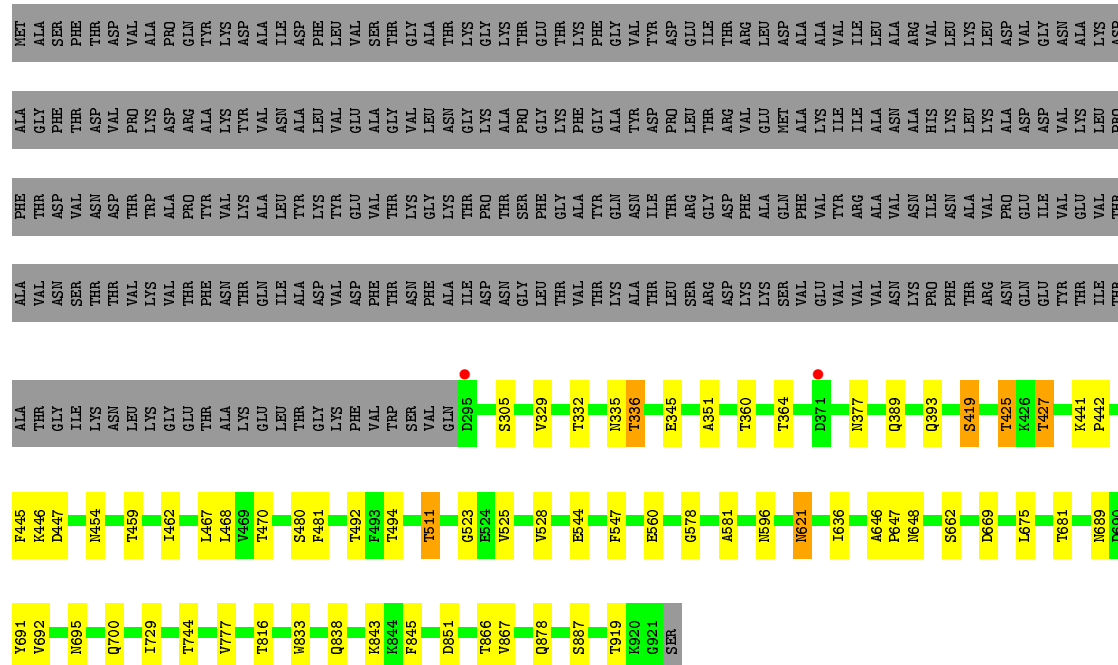
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	68.50Å 88.50Å 95.20Å 112.50° 101.60° 84.70°	Depositor
Resolution (Å)	43.81 – 2.42 43.81 – 2.42	Depositor EDS
% Data completeness (in resolution range)	97.0 (43.81-2.42) 97.1 (43.81-2.42)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.183 , 0.236 0.186 , 0.235	Depositor DCC
R_{free} test set	3729 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.3	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	0.95	EDS
Total number of atoms	12335	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.67	3/5430 (0.1%)	0.77	1/7406 (0.0%)
2	B	0.70	1/943 (0.1%)	0.71	0/1271
2	D	0.70	0/943	0.76	0/1271
3	C	0.63	1/4698 (0.0%)	0.74	1/6409 (0.0%)
All	All	0.66	5/12014 (0.0%)	0.75	2/16357 (0.0%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	GLU	CA-CB	-10.73	1.30	1.53
1	A	275	LYS	CG-CD	-6.83	1.29	1.52
2	B	36	TRP	CD2-CE2	5.83	1.48	1.41
1	A	278	LYS	CD-CE	5.11	1.64	1.51
3	C	833	TRP	CD2-CE2	5.09	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	592	ASP	CB-CG-OD1	5.21	122.99	118.30
3	C	523	GLY	N-CA-C	-5.11	100.34	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	548	GLY	Peptide

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	5363	0	5396	87	0
2	B	924	0	872	15	0
2	D	924	0	872	12	0
3	C	4641	0	4657	39	0
4	A	4	0	0	0	0
4	C	4	0	0	0	0
5	A	253	0	0	9	0
5	B	21	0	0	0	0
5	C	173	0	0	4	0
5	D	28	0	0	1	0
All	All	12335	0	11797	149	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 6.

All (149) 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:440:THR:HG21	5:A:2087:HOH:O	1.46	1.15
1:A:275:LYS:HG3	1:A:281:THR:HG22	1.34	1.04
1:A:271:ALA:HB1	1:A:274:ILE:HD11	1.44	0.98
1:A:293:VAL:HG22	1:A:296:ALA:HB2	1.47	0.96
1:A:838:GLN:HE22	1:A:845:PHE:H	1.15	0.89
1:A:202:ALA:HB1	1:A:223:THR:HG21	1.55	0.88
1:A:275:LYS:HG3	1:A:281:THR:CG2	2.05	0.86
1:A:393:GLN:HE22	1:A:494:THR:H	1.22	0.85
1:A:648:ASN:HD21	1:A:843:LYS:H	1.23	0.84
1:A:689:ASN:ND2	1:A:691:TYR:H	1.76	0.83
3:C:425:THR:HG23	5:C:2033:HOH:O	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:648:ASN:HD21	3:C:843:LYS:H	1.27	0.83
1:A:689:ASN:HD22	1:A:692:VAL:H	1.27	0.81
3:C:838:GLN:HE22	3:C:845:PHE:H	1.29	0.81
2:D:83:MET:HB3	2:D:86:LEU:HD21	1.63	0.79
3:C:425:THR:HG22	3:C:470:THR:HG23	1.67	0.77
3:C:393:GLN:HE22	3:C:494:THR:H	1.32	0.75
1:A:511:THR:HG22	5:A:2024:HOH:O	1.85	0.75
1:A:596:ASN:HD22	1:A:621:ASN:HA	1.50	0.73
1:A:212:VAL:CG1	1:A:632:VAL:HG12	2.20	0.72
3:C:669:ASP:HB3	3:C:675:LEU:HD21	1.71	0.71
1:A:511:THR:CG2	5:A:2024:HOH:O	2.38	0.71
3:C:454:ASN:HD22	3:C:480:SER:H	1.38	0.70
1:A:332:THR:HG22	5:A:2026:HOH:O	1.90	0.70
3:C:441:LYS:HB2	3:C:442:PRO:HD2	1.76	0.68
3:C:560:GLU:HG2	2:D:93:VAL:HG23	1.75	0.68
3:C:336:THR:HB	3:C:511:THR:HG21	1.76	0.67
3:C:544:GLU:HG2	3:C:581:ALA:HB1	1.76	0.67
3:C:689:ASN:HD22	3:C:692:VAL:H	1.43	0.66
1:A:689:ASN:ND2	1:A:692:VAL:H	1.95	0.65
1:A:425:THR:HG22	1:A:470:THR:HG23	1.78	0.65
3:C:866:THR:HG23	3:C:878:GLN:NE2	2.12	0.65
2:B:12:VAL:HG21	2:B:86:LEU:HD12	1.80	0.64
2:B:88:PRO:HA	2:B:122:VAL:HG13	1.78	0.63
3:C:445:PHE:HB3	3:C:462:ILE:HD13	1.80	0.62
1:A:204:PRO:HD3	1:A:276:ASN:HB2	1.83	0.61
1:A:293:VAL:O	1:A:293:VAL:HG13	2.00	0.61
2:D:1:GLN:HG2	2:D:2:VAL:N	2.17	0.60
1:A:276:ASN:O	1:A:277:LEU:C	2.39	0.60
1:A:202:ALA:HB1	1:A:223:THR:CG2	2.30	0.60
1:A:228:VAL:HG11	1:A:233:PHE:HE1	1.66	0.60
1:A:229:ASP:H	1:A:232:ASN:HD22	1.47	0.60
1:A:879:LEU:HD11	1:A:918:VAL:HG12	1.83	0.60
1:A:212:VAL:HG11	1:A:632:VAL:HG12	1.85	0.59
1:A:295:ASP:OD1	1:A:295:ASP:N	2.36	0.58
1:A:652:THR:HG23	5:A:2156:HOH:O	2.03	0.58
1:A:695:ASN:HD22	1:A:700:GLN:HE21	1.52	0.58
1:A:335:ASN:HA	1:A:511:THR:HB	1.85	0.58
1:A:271:ALA:HB1	1:A:274:ILE:CD1	2.27	0.57
1:A:547:PHE:O	1:A:578:GLY:O	2.22	0.56
2:D:72:ARG:HG3	2:D:79:VAL:HG22	1.86	0.56
2:B:20:LEU:HG	2:B:83:MET:CE	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:THR:CG2	1:A:470:THR:HG23	2.36	0.56
3:C:454:ASN:ND2	3:C:480:SER:H	2.05	0.55
2:B:76:LYS:O	2:B:78:THR:HG23	2.06	0.54
3:C:689:ASN:ND2	3:C:691:TYR:H	2.05	0.54
2:D:51:ILE:HG13	2:D:58:THR:HG22	1.90	0.54
3:C:596:ASN:HD22	3:C:621:ASN:HA	1.73	0.54
3:C:646:ALA:HB3	3:C:647:PRO:HD3	1.89	0.54
3:C:648:ASN:ND2	3:C:843:LYS:H	2.02	0.53
1:A:202:ALA:HB2	5:A:2002:HOH:O	2.07	0.53
1:A:567:VAL:HG23	1:A:573:ILE:HG23	1.91	0.53
1:A:778:LYS:HE3	1:A:780:GLU:OE2	2.09	0.53
1:A:393:GLN:HE22	1:A:494:THR:N	2.02	0.52
1:A:228:VAL:CG1	1:A:233:PHE:HE1	2.22	0.52
3:C:393:GLN:HE22	3:C:494:THR:N	2.06	0.52
3:C:468:LEU:HD12	3:C:468:LEU:N	2.25	0.52
1:A:695:ASN:HD22	1:A:700:GLN:NE2	2.08	0.51
1:A:377:ASN:HD21	1:A:636:ILE:H	1.57	0.51
1:A:202:ALA:CB	1:A:223:THR:HG21	2.34	0.51
1:A:228:VAL:HG11	1:A:233:PHE:CE1	2.45	0.51
2:D:1:GLN:CG	2:D:2:VAL:N	2.75	0.50
2:B:92:ALA:HB3	2:B:94:TYR:CE1	2.46	0.49
1:A:611:THR:HG23	1:A:612:PRO:HD2	1.93	0.49
1:A:226:ALA:O	1:A:228:VAL:HG23	2.12	0.49
1:A:204:PRO:HD3	1:A:276:ASN:CB	2.42	0.49
1:A:704:ASN:ND2	3:C:345:GLU:H	2.10	0.49
3:C:481:PHE:O	3:C:492:THR:HA	2.13	0.49
2:B:45:ARG:NH2	2:B:108:HIS:HB3	2.28	0.48
1:A:425:THR:HG22	1:A:470:THR:CG2	2.44	0.48
2:B:45:ARG:HH21	2:B:108:HIS:HB3	1.78	0.48
1:A:275:LYS:CG	1:A:281:THR:CG2	2.88	0.47
1:A:400:ASN:HD21	1:A:402:SER:HB2	1.79	0.47
1:A:235:ILE:HD12	1:A:257:VAL:CG1	2.43	0.47
3:C:389:GLN:HA	5:C:2018:HOH:O	2.13	0.47
1:A:330:GLU:OE1	1:A:366:LYS:HD3	2.14	0.47
3:C:695:ASN:HD22	3:C:700:GLN:NE2	2.13	0.47
1:A:362:ASP:OD1	1:A:380:LYS:NZ	2.44	0.47
1:A:454:ASN:HD22	1:A:480:SER:H	1.62	0.47
3:C:329:VAL:HG11	3:C:351:ALA:HB2	1.96	0.47
1:A:744:THR:HG22	5:A:2104:HOH:O	2.15	0.47
3:C:335:ASN:HA	3:C:511:THR:HB	1.97	0.46
1:A:425:THR:HG22	1:A:470:THR:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:VAL:HG12	2:B:3:GLN:N	2.30	0.46
3:C:525:VAL:HG22	3:C:528:VAL:HB	1.97	0.46
1:A:425:THR:HG22	1:A:470:THR:HA	1.98	0.46
1:A:212:VAL:HG13	1:A:632:VAL:HG12	1.95	0.45
1:A:759:ASN:ND2	1:A:920:LYS:NZ	2.64	0.45
2:D:116:GLN:HG2	5:D:2003:HOH:O	2.15	0.45
1:A:669:ASP:HB3	1:A:675:LEU:HD21	1.98	0.45
3:C:446:LYS:O	3:C:447:ASP:HB2	2.17	0.45
1:A:611:THR:HG22	1:A:612:PRO:O	2.16	0.45
1:A:648:ASN:HD21	1:A:843:LYS:N	2.01	0.45
3:C:377:ASN:HD21	3:C:636:ILE:H	1.64	0.45
1:A:271:ALA:CB	1:A:274:ILE:HD11	2.31	0.45
3:C:467:LEU:C	3:C:468:LEU:HD12	2.37	0.45
1:A:691:TYR:CD1	1:A:710:LEU:HD13	2.52	0.44
2:B:2:VAL:CG2	2:B:32:TYR:CE1	3.00	0.44
3:C:547:PHE:O	3:C:578:GLY:O	2.35	0.44
1:A:293:VAL:CG2	1:A:296:ALA:HB2	2.33	0.44
2:B:20:LEU:HG	2:B:83:MET:HE2	1.98	0.44
1:A:838:GLN:HE22	1:A:845:PHE:N	1.97	0.44
2:B:2:VAL:HG21	2:B:32:TYR:CE1	2.53	0.44
1:A:646:ALA:HB3	1:A:647:PRO:HD3	2.00	0.44
1:A:243:LYS:HB3	1:A:256:VAL:HG13	1.99	0.43
1:A:315:THR:HG21	1:A:317:LYS:HE2	2.00	0.43
1:A:454:ASN:ND2	1:A:480:SER:H	2.16	0.43
1:A:315:THR:CG2	1:A:317:LYS:HE2	2.47	0.43
3:C:441:LYS:HB2	3:C:442:PRO:CD	2.48	0.43
2:D:49:ALA:HB2	2:D:60:TYR:CD2	2.53	0.43
2:D:51:ILE:HD13	2:D:72:ARG:HB2	2.01	0.43
1:A:249:ASP:O	1:A:251:LYS:N	2.51	0.42
1:A:377:ASN:HD22	1:A:727:LYS:NZ	2.17	0.42
3:C:427:THR:HG21	5:C:2024:HOH:O	2.18	0.42
1:A:642:ILE:HG21	1:A:642:ILE:HD13	1.89	0.42
1:A:648:ASN:ND2	1:A:843:LYS:H	2.03	0.42
1:A:881:ASN:HD22	1:A:881:ASN:N	2.17	0.42
1:A:649:THR:OG1	1:A:654:ASP:OD2	2.37	0.42
1:A:729:ILE:CD1	5:A:2148:HOH:O	2.67	0.42
3:C:332:THR:HG23	3:C:364:THR:HB	2.02	0.42
1:A:832:ILE:HG23	1:A:832:ILE:O	2.19	0.42
2:B:29:SER:HA	2:B:32:TYR:HD1	1.84	0.42
2:B:49:ALA:HB2	2:B:60:TYR:CD2	2.55	0.41
1:A:593:LYS:HE2	2:B:95:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASP:H	1:A:232:ASN:ND2	2.15	0.41
1:A:276:ASN:O	1:A:278:LYS:N	2.54	0.41
1:A:838:GLN:HB3	1:A:841:LEU:HD22	2.02	0.41
3:C:393:GLN:NE2	3:C:494:THR:H	2.09	0.41
3:C:525:VAL:CG2	3:C:528:VAL:HB	2.51	0.41
3:C:689:ASN:HD22	3:C:692:VAL:N	2.14	0.41
1:A:689:ASN:HD22	1:A:691:TYR:H	1.62	0.41
3:C:419:SER:HB3	5:C:2031:HOH:O	2.20	0.41
2:D:83:MET:HE2	2:D:86:LEU:HD11	2.02	0.41
1:A:209:VAL:HG12	1:A:289:PHE:HB3	2.03	0.41
1:A:440:THR:CG2	5:A:2087:HOH:O	2.28	0.41
2:D:83:MET:CB	2:D:86:LEU:HD21	2.43	0.41
1:A:560:GLU:OE2	2:B:95:TYR:OH	2.35	0.40
1:A:401:LEU:HA	1:A:401:LEU:HD12	1.86	0.40
2:D:76:LYS:O	2:D:78:THR:HG23	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	719/892 (81%)	692 (96%)	23 (3%)	4 (1%)	25	35
2	B	122/130 (94%)	114 (93%)	8 (7%)	0	100	100
2	D	122/130 (94%)	119 (98%)	3 (2%)	0	100	100
3	C	625/892 (70%)	608 (97%)	16 (3%)	1 (0%)	47	61
All	All	1588/2044 (78%)	1533 (96%)	50 (3%)	5 (0%)	41	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	LYS
1	A	277	LEU
1	A	204	PRO
3	C	867	VAL
1	A	279	GLY

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	617/753 (82%)	586 (95%)	31 (5%)	24	38
2	B	92/98 (94%)	86 (94%)	6 (6%)	17	26
2	D	92/98 (94%)	91 (99%)	1 (1%)	73	86
3	C	534/753 (71%)	516 (97%)	18 (3%)	37	54
All	All	1335/1702 (78%)	1279 (96%)	56 (4%)	30	46

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	VAL
1	A	242	THR
1	A	256	VAL
1	A	276	ASN
1	A	277	LEU
1	A	278	LYS
1	A	280	GLU
1	A	283	LYS
1	A	305	SER
1	A	342	SER
1	A	343	SER
1	A	360	THR
1	A	400	ASN
1	A	440	THR
1	A	459	THR
1	A	509	ASP
1	A	511	THR

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Mol	Chain	Res	Type
1	A	514	LYS
1	A	549	THR
1	A	567	VAL
1	A	595	VAL
1	A	663	VAL
1	A	681	THR
1	A	708	THR
1	A	716	VAL
1	A	729	ILE
1	A	744	THR
1	A	812	GLU
1	A	864	SER
1	A	873	LEU
1	A	887	SER
2	B	12	VAL
2	B	17	SER
2	B	25	SER
2	B	28	THR
2	B	77	ASN
2	B	83	MET
3	C	305	SER
3	C	336	THR
3	C	360	THR
3	C	419	SER
3	C	425	THR
3	C	427	THR
3	C	459	THR
3	C	511	THR
3	C	621	ASN
3	C	662	SER
3	C	681	THR
3	C	729	ILE
3	C	744	THR
3	C	777	VAL
3	C	816	THR
3	C	851	ASP
3	C	887	SER
3	C	919	THR
2	D	78	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	ASN
1	A	302	ASN
1	A	319	GLN
1	A	377	ASN
1	A	393	GLN
1	A	400	ASN
1	A	454	ASN
1	A	472	ASN
1	A	596	ASN
1	A	648	ASN
1	A	689	ASN
1	A	700	GLN
1	A	704	ASN
1	A	759	ASN
1	A	838	GLN
1	A	858	ASN
1	A	881	ASN
1	A	915	ASN
2	B	82	GLN
2	B	84	ASN
2	B	119	GLN
3	C	302	ASN
3	C	377	ASN
3	C	393	GLN
3	C	400	ASN
3	C	454	ASN
3	C	472	ASN
3	C	596	ASN
3	C	621	ASN
3	C	648	ASN
3	C	689	ASN
3	C	697	ASN
3	C	700	GLN
3	C	704	ASN
3	C	755	ASN
3	C	759	ASN
3	C	825	HIS
3	C	838	GLN
3	C	878	GLN
3	C	915	ASN
2	D	5	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	721/892 (80%)	-0.46	1 (0%)	95	95	16, 34, 70, 109	26 (3%)
2	B	124/130 (95%)	-0.19	1 (0%)	86	84	20, 45, 95, 127	1 (0%)
2	D	124/130 (95%)	-0.27	0	100	100	19, 36, 68, 86	3 (2%)
3	C	627/892 (70%)	-0.44	2 (0%)	94	93	18, 37, 65, 91	8 (1%)
All	All	1596/2044 (78%)	-0.42	4 (0%)	94	93	16, 36, 71, 127	38 (2%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	371	ASP	2.3
3	C	295	ASP	2.2
2	B	122	VAL	2.2
1	A	277	LEU	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 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. 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($Å^2$)	Q<0.9
4	CA	C	1925	1/1	0.98	0.09	33,33,33,33	0
4	CA	C	1924	1/1	0.99	0.06	24,24,24,24	0
4	CA	A	1923	1/1	0.99	0.05	25,25,25,25	0
4	CA	C	1923	1/1	0.99	0.04	29,29,29,29	0
4	CA	C	1922	1/1	0.99	0.09	28,28,28,28	0
4	CA	A	1925	1/1	0.99	0.04	22,22,22,22	0
4	CA	A	1926	1/1	0.99	0.07	27,27,27,27	0
4	CA	A	1924	1/1	0.99	0.04	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.