



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:36 PM GMT

PDB ID : 1L0O
Title : Crystal Structure of the Bacillus stearothermophilus Anti-Sigma Factor SpoI-IAB with the Sporulation Sigma Factor SigmaF
Authors : Campbell, E.A.; Masuda, S.; Sun, J.L.; Muzzin, O.; Olson, C.A.; Wang, S.; Darst, S.A.
Deposited on : 2002-02-12
Resolution : 2.90 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

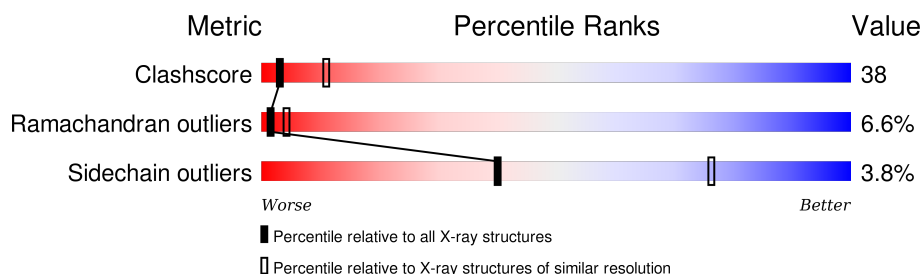
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	150	
1	B	150	
2	C	243	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2736 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 Anti-sigma F factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1097	688	184	219	6			
1	B	141	Total	C	N	O	S	0	0	0
			1072	672	179	215	6			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	MET	THR	SEE REMARK 999	UNP O32727
A	137	HIS	ALA	SEE REMARK 999	UNP O32727
A	138	ILE	TYR	SEE REMARK 999	UNP O32727
A	139	VAL	CYS	SEE REMARK 999	UNP O32727
A	140	LYS	GLU	SEE REMARK 999	UNP O32727
A	141	SER	LYS	SEE REMARK 999	UNP O32727
A	142	LYS	GLN	SEE REMARK 999	UNP O32727
A	143	ARG	-	cloning artifact	UNP O32727
A	144	TYR	-	cloning artifact	UNP O32727
A	145	LEU	-	cloning artifact	UNP O32727
A	146	GLU	-	cloning artifact	UNP O32727
A	147	GLY	-	cloning artifact	UNP O32727
A	148	SER	-	cloning artifact	UNP O32727
A	149	SER	-	cloning artifact	UNP O32727
A	150	PHE	-	cloning artifact	UNP O32727
B	34	MET	THR	SEE REMARK 999	UNP O32727
B	137	HIS	ALA	SEE REMARK 999	UNP O32727
B	138	ILE	TYR	SEE REMARK 999	UNP O32727
B	139	VAL	CYS	SEE REMARK 999	UNP O32727
B	140	LYS	GLU	SEE REMARK 999	UNP O32727
B	141	SER	LYS	SEE REMARK 999	UNP O32727
B	142	LYS	GLN	SEE REMARK 999	UNP O32727
B	143	ARG	-	cloning artifact	UNP O32727
B	144	TYR	-	cloning artifact	UNP O32727
B	145	LEU	-	cloning artifact	UNP O32727

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Chain	Residue	Modelled	Actual	Comment	Reference
B	146	GLU	-	cloning artifact	UNP O32727
B	147	GLY	-	cloning artifact	UNP O32727
B	148	SER	-	cloning artifact	UNP O32727
B	149	SER	-	cloning artifact	UNP O32727
B	150	PHE	-	cloning artifact	UNP O32727

- Molecule 2 is a protein called sigma factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	57	Total	C	N	O	S	0	0	0
			428	262	82	83	1			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	GLY	-	cloning artifact	UNP O32728
C	4	SER	-	cloning artifact	UNP O32728
C	5	HIS	-	cloning artifact	UNP O32728
C	6	MET	-	cloning artifact	UNP O32728
C	132	ALA	SER	SEE REMARK 999	UNP O32728
C	135	VAL	ILE	SEE REMARK 999	UNP O32728
C	215	LYS	ARG	SEE REMARK 999	UNP O32728
C	217	GLN	ARG	SEE REMARK 999	UNP O32728
C	233	MET	VAL	engineered	UNP O32728

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

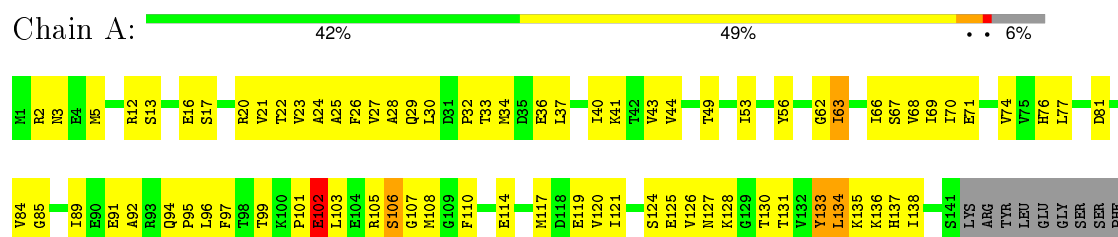
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	41	Total	O	0	0
			41	41		
5	B	31	Total	O	0	0
			31	31		
5	C	11	Total	O	0	0
			11	11		

3 Residue-property plots

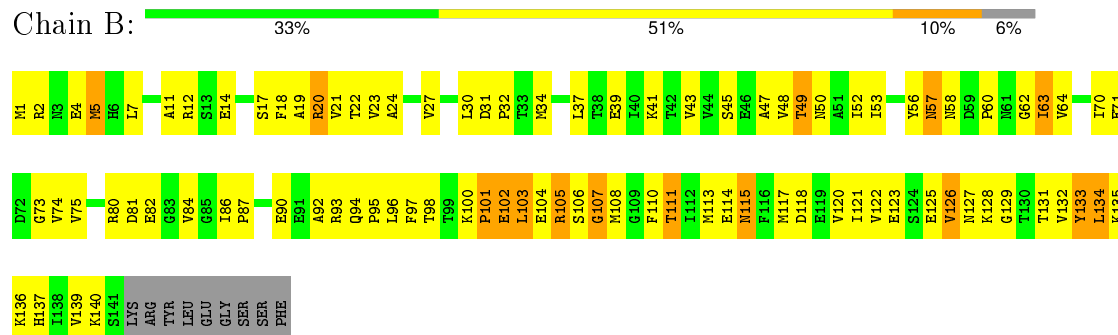
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

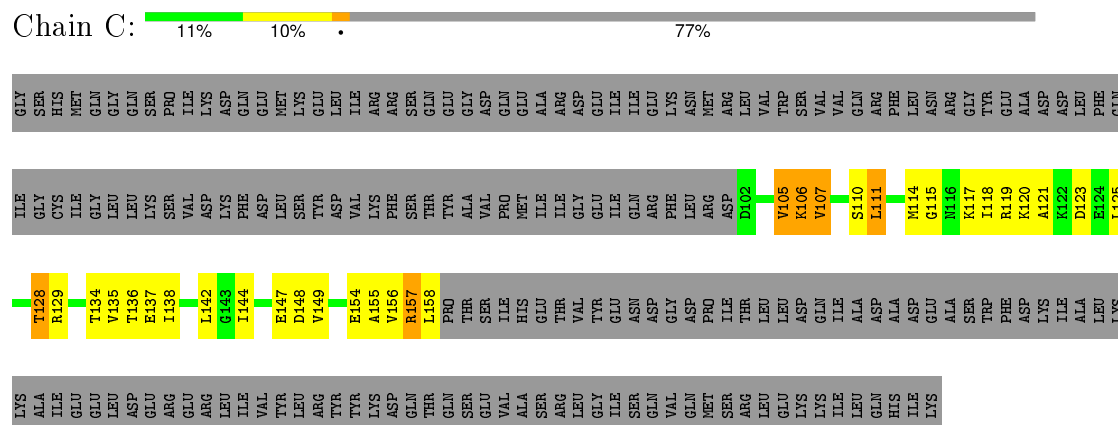
- Molecule 1: Anti-sigma F factor



- Molecule 1: Anti-sigma F factor



- Molecule 2: sigma factor



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	97.31Å 97.31Å 262.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (35.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2736	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

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: MG, ADP

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	0.44	0/1113	0.66	0/1508
1	B	0.38	0/1088	0.65	1/1479 (0.1%)
2	C	0.41	0/430	0.57	0/576
All	All	0.41	0/2631	0.64	1/3563 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	GLY	N-CA-C	-6.08	97.91	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1097	0	1087	73	1
1	B	1072	0	1038	102	0
2	C	428	0	448	43	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	41	0	0	4	1
5	B	31	0	0	1	0
5	C	11	0	0	2	0
All	All	2736	0	2597	200	2

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 38.

All (200) 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:21:VAL:HG21	2:C:147:GLU:HB3	1.40	1.02
1:A:3:ASN:HD22	1:A:29:GLN:HE22	1.13	0.90
1:B:92:ALA:HA	1:B:97:PHE:CD2	2.13	0.83
2:C:111:LEU:HD23	2:C:155:ALA:HB2	1.62	0.80
2:C:118:ILE:HD13	2:C:149:VAL:HG13	1.64	0.78
1:A:20:ARG:HB2	1:A:41:LYS:HG3	1.66	0.78
1:B:98:THR:HG21	1:B:101:PRO:HB3	1.67	0.77
1:B:20:ARG:HH12	1:B:41:LYS:HE2	1.49	0.76
1:B:19:ALA:O	1:B:23:VAL:HG23	1.86	0.75
1:B:45:SER:O	1:B:49:THR:HB	1.88	0.73
1:A:43:VAL:HG21	1:A:117:MET:HG2	1.71	0.73
1:A:33:THR:OG1	1:A:36:GLU:HG3	1.89	0.73
1:B:139:VAL:HG12	1:B:140:LYS:H	1.53	0.72
1:A:34:MET:HA	2:C:107:VAL:HG22	1.71	0.72
1:B:20:ARG:NH1	1:B:41:LYS:HE2	2.05	0.70
1:A:77:LEU:O	1:A:133:TYR:O	2.10	0.69
1:A:3:ASN:HD22	1:A:29:GLN:NE2	1.90	0.68
1:A:40:ILE:HD11	1:A:136:LYS:HG2	1.75	0.68
1:A:2:ARG:H	1:B:12:ARG:HH22	1.42	0.67
1:B:20:ARG:NH1	1:B:41:LYS:HB3	2.10	0.66
2:C:144:ILE:HG23	2:C:148:ASP:HB2	1.77	0.66
1:A:17:SER:HA	1:A:20:ARG:HE	1.60	0.66
1:B:43:VAL:HG21	1:B:117:MET:SD	2.36	0.66
1:B:20:ARG:HB3	1:B:20:ARG:HH11	1.61	0.65
1:B:100:LYS:C	1:B:102:GLU:H	2.00	0.65
1:B:92:ALA:HA	1:B:97:PHE:CE2	2.31	0.65
1:A:21:VAL:HG21	2:C:147:GLU:CB	2.21	0.65
2:C:134:THR:HG22	2:C:136:THR:N	2.11	0.65
1:B:43:VAL:CG1	1:B:134:LEU:HD13	2.26	0.65
2:C:121:ALA:O	2:C:125:LEU:HG	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:CD1	1:A:138:ILE:HD12	2.27	0.64
1:A:91:GLU:O	1:A:94:GLN:HG2	1.97	0.63
1:B:71:GLU:O	1:B:74:VAL:HG22	1.97	0.63
2:C:134:THR:HB	2:C:137:GLU:HG3	1.80	0.63
1:B:101:PRO:C	1:B:103:LEU:H	2.02	0.63
1:B:17:SER:O	1:B:21:VAL:HG23	1.99	0.62
1:B:125:GLU:HB3	1:B:128:LYS:HD2	1.82	0.62
1:B:27:VAL:HA	1:B:70:ILE:HD11	1.81	0.62
1:A:69:ILE:HB	1:A:76:HIS:HB2	1.82	0.62
1:B:101:PRO:O	1:B:103:LEU:N	2.25	0.62
1:B:14:GLU:CD	1:B:14:GLU:H	2.03	0.61
2:C:114:MET:HE3	2:C:117:LYS:HB2	1.83	0.60
1:B:104:GLU:O	1:B:105:ARG:CB	2.51	0.59
1:B:48:VAL:O	1:B:52:ILE:HG12	2.02	0.59
2:C:105:VAL:CG1	2:C:110:SER:HB2	2.31	0.59
1:A:30:LEU:HD12	1:A:138:ILE:HD12	1.84	0.59
1:A:26:PHE:HB2	1:B:18:PHE:CE1	2.37	0.58
1:A:96:LEU:HA	1:A:107:GLY:HA3	1.85	0.58
1:B:56:TYR:CZ	1:B:81:ASP:HB2	2.39	0.57
1:B:49:THR:O	1:B:53:ILE:HG12	2.05	0.57
1:B:98:THR:CG2	1:B:101:PRO:HB3	2.33	0.57
2:C:114:MET:CE	2:C:142:LEU:HD22	2.35	0.57
1:A:114:GLU:HA	1:A:120:VAL:HG21	1.87	0.56
1:B:53:ILE:HG22	1:B:58:ASN:OD1	2.05	0.56
1:B:139:VAL:HG12	1:B:140:LYS:N	2.20	0.56
1:B:32:PRO:O	2:C:135:VAL:HG23	2.05	0.56
1:A:119:GLU:OE2	1:A:121:ILE:HD11	2.06	0.56
2:C:114:MET:HE1	2:C:142:LEU:HD13	1.88	0.56
2:C:114:MET:HE1	2:C:142:LEU:HD22	1.87	0.56
1:B:131:THR:HG22	1:B:131:THR:O	2.04	0.56
1:B:95:PRO:O	1:B:96:LEU:HB2	2.05	0.56
2:C:105:VAL:O	2:C:105:VAL:HG12	2.05	0.56
1:A:133:TYR:O	1:A:134:LEU:HB2	2.06	0.55
2:C:134:THR:HG22	2:C:136:THR:H	1.71	0.55
1:B:120:VAL:HG22	1:B:134:LEU:HD23	1.89	0.55
2:C:107:VAL:O	2:C:111:LEU:HB2	2.07	0.55
1:B:100:LYS:O	1:B:102:GLU:N	2.39	0.55
1:A:30:LEU:HD11	1:A:70:ILE:HG23	1.88	0.55
1:A:102:GLU:OE1	1:A:103:LEU:HG	2.07	0.55
1:B:31:ASP:OD1	2:C:134:THR:HG21	2.07	0.55
1:B:23:VAL:O	1:B:27:VAL:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:VAL:HG12	2:C:110:SER:HB2	1.89	0.54
1:A:20:ARG:HB2	1:A:41:LYS:CG	2.36	0.54
1:A:21:VAL:CG2	2:C:147:GLU:HB3	2.28	0.54
1:B:24:ALA:HA	1:B:27:VAL:HG12	1.90	0.54
1:A:2:ARG:HG3	1:A:2:ARG:O	2.07	0.54
1:A:110:PHE:O	1:A:114:GLU:HG3	2.07	0.54
2:C:128:THR:HG22	2:C:129:ARG:HG2	1.89	0.54
1:B:98:THR:HG21	1:B:101:PRO:CB	2.37	0.53
1:B:74:VAL:O	1:B:74:VAL:HG23	2.09	0.53
1:A:5:MET:HG3	1:B:18:PHE:CZ	2.43	0.53
1:B:32:PRO:HG3	1:B:37:LEU:HD21	1.89	0.53
1:B:20:ARG:CB	1:B:20:ARG:HH11	2.21	0.53
1:B:56:TYR:OH	1:B:82:GLU:N	2.39	0.53
2:C:134:THR:HG22	2:C:137:GLU:H	1.74	0.52
1:B:117:MET:HE3	1:B:135:LYS:C	2.30	0.52
2:C:106:LYS:O	2:C:107:VAL:HB	2.10	0.52
1:B:122:VAL:HG12	1:B:123:GLU:N	2.24	0.52
1:A:95:PRO:HD3	5:A:566:HOH:O	2.08	0.52
1:B:27:VAL:HG23	1:B:75:VAL:CG2	2.40	0.51
1:A:91:GLU:HG3	1:A:94:GLN:NE2	2.25	0.51
1:A:89:ILE:HD11	1:A:124:SER:HB3	1.91	0.51
2:C:134:THR:CG2	2:C:136:THR:HB	2.41	0.51
1:A:43:VAL:HG11	1:A:134:LEU:HD22	1.93	0.51
1:A:125:GLU:HB3	1:A:128:LYS:HB3	1.93	0.51
1:B:53:ILE:O	1:B:57:ASN:HA	2.11	0.51
1:B:34:MET:CG	2:C:138:ILE:HD12	2.41	0.50
1:B:5:MET:HE2	1:B:7:LEU:HB2	1.93	0.50
1:A:32:PRO:HB3	1:A:138:ILE:HD13	1.93	0.50
1:A:106:SER:O	1:A:107:GLY:C	2.49	0.50
1:B:56:TYR:O	1:B:57:ASN:C	2.49	0.50
1:B:43:VAL:HG21	1:B:117:MET:HG2	1.95	0.49
2:C:134:THR:CG2	2:C:136:THR:H	2.25	0.49
1:A:34:MET:HE1	5:A:540:HOH:O	2.12	0.49
1:B:101:PRO:C	1:B:103:LEU:N	2.62	0.48
1:B:90:GLU:O	1:B:94:GLN:HG2	2.13	0.48
1:B:37:LEU:HD11	2:C:135:VAL:HG21	1.95	0.48
1:B:133:TYR:O	1:B:134:LEU:HB2	2.13	0.48
1:B:43:VAL:HG12	1:B:134:LEU:HD13	1.95	0.48
1:B:24:ALA:HA	1:B:27:VAL:CG1	2.43	0.48
1:A:68:VAL:HA	1:A:76:HIS:O	2.14	0.48
2:C:115:GLY:HA3	2:C:156:VAL:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:SER:HA	1:B:20:ARG:HD3	1.96	0.48
1:B:120:VAL:HG13	1:B:134:LEU:HD23	1.96	0.48
1:B:5:MET:CE	1:B:7:LEU:HB2	2.44	0.48
1:B:27:VAL:CG2	1:B:75:VAL:HG21	2.44	0.48
1:B:100:LYS:C	1:B:102:GLU:N	2.67	0.48
1:A:44:VAL:HG22	1:A:77:LEU:HD21	1.96	0.47
1:A:99:THR:HG21	5:A:522:HOH:O	2.14	0.47
1:B:110:PHE:O	1:B:114:GLU:HB2	2.14	0.47
1:A:133:TYR:O	1:A:134:LEU:CB	2.63	0.47
1:A:130:THR:HG22	1:A:131:THR:N	2.28	0.47
1:B:20:ARG:HD3	2:C:154:GLU:OE2	2.14	0.47
1:A:77:LEU:HD23	1:A:134:LEU:HD13	1.96	0.47
1:A:37:LEU:O	1:A:41:LYS:HB2	2.15	0.47
1:A:117:MET:HG3	1:A:134:LEU:HD22	1.96	0.47
1:A:2:ARG:HD3	1:A:71:GLU:OE2	2.14	0.47
1:B:63:ILE:O	1:B:63:ILE:HG22	2.13	0.47
1:B:56:TYR:CD1	1:B:62:GLY:HA3	2.49	0.47
1:B:39:GLU:OE1	1:B:136:LYS:NZ	2.44	0.47
2:C:154:GLU:O	2:C:157:ARG:HG3	2.14	0.46
1:A:25:ALA:O	1:A:28:ALA:HB3	2.15	0.46
1:B:108:MET:HG3	1:B:111:THR:OG1	2.15	0.46
1:A:5:MET:HG3	1:B:18:PHE:HZ	1.80	0.46
1:A:96:LEU:H	1:A:108:MET:HE2	1.80	0.46
1:A:30:LEU:HD13	1:A:138:ILE:HD12	1.96	0.46
1:B:27:VAL:HG23	1:B:75:VAL:HG21	1.97	0.45
1:B:74:VAL:HG12	1:B:137:HIS:CD2	2.51	0.45
1:A:119:GLU:O	1:A:134:LEU:HA	2.16	0.45
1:B:121:ILE:H	1:B:133:TYR:HB3	1.81	0.45
1:B:20:ARG:HB3	1:B:20:ARG:NH1	2.30	0.45
1:B:47:ALA:N	1:B:113:MET:HE2	2.31	0.45
1:A:22:THR:HG23	1:B:22:THR:OG1	2.16	0.45
1:B:14:GLU:CD	1:B:14:GLU:N	2.70	0.45
1:B:50:ASN:HB3	4:B:701:ADP:N7	2.32	0.45
1:A:34:MET:N	2:C:107:VAL:HG23	2.32	0.44
1:A:12:ARG:NH1	1:B:1:MET:HE2	2.32	0.44
2:C:114:MET:SD	2:C:144:ILE:HD12	2.57	0.44
1:B:37:LEU:O	1:B:41:LYS:HG3	2.17	0.44
1:B:132:VAL:HG12	1:B:134:LEU:HG	1.99	0.44
2:C:134:THR:HB	2:C:137:GLU:CG	2.45	0.44
1:A:66:ILE:HG22	1:A:67:SER:N	2.32	0.44
1:B:43:VAL:HG21	1:B:117:MET:CG	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:VAL:HG13	1:A:137:HIS:HD2	1.83	0.44
1:A:34:MET:HA	2:C:107:VAL:CG2	2.43	0.44
1:A:105:ARG:O	1:A:107:GLY:N	2.50	0.44
1:A:126:VAL:HG12	1:A:127:ASN:ND2	2.33	0.44
1:A:34:MET:HG2	5:C:524:HOH:O	2.18	0.43
1:A:56:TYR:CE1	1:A:81:ASP:HB2	2.52	0.43
1:B:98:THR:HG23	1:B:101:PRO:HD3	1.99	0.43
1:B:115:ASN:HA	1:B:115:ASN:HD22	1.64	0.43
1:B:31:ASP:OD1	2:C:134:THR:CG2	2.67	0.43
1:A:40:ILE:HD11	1:A:136:LYS:CG	2.46	0.43
1:A:95:PRO:O	1:A:96:LEU:HB2	2.18	0.43
1:B:133:TYR:O	1:B:134:LEU:CB	2.66	0.42
2:C:134:THR:HG21	2:C:136:THR:HB	2.01	0.42
2:C:120:LYS:HE2	2:C:120:LYS:HB3	1.77	0.42
1:A:102:GLU:O	1:A:103:LEU:HD23	2.19	0.42
2:C:120:LYS:O	2:C:123:ASP:OD1	2.37	0.42
1:A:135:LYS:HD3	5:A:548:HOH:O	2.19	0.42
1:A:92:ALA:HA	1:A:97:PHE:CD2	2.54	0.42
1:A:84:VAL:HG12	1:A:85:GLY:O	2.20	0.42
1:B:52:ILE:HD11	1:B:64:VAL:HG21	2.01	0.42
2:C:119:ARG:HG3	5:C:534:HOH:O	2.19	0.42
1:B:1:MET:HG3	1:B:2:ARG:N	2.34	0.42
1:A:30:LEU:HD21	1:A:70:ILE:CG2	2.49	0.42
1:B:118:ASP:OD2	1:B:136:LYS:HA	2.20	0.42
1:B:52:ILE:CD1	1:B:64:VAL:HG21	2.50	0.41
2:C:111:LEU:HD23	2:C:155:ALA:CB	2.42	0.41
1:B:7:LEU:HD22	1:B:22:THR:HG21	2.02	0.41
1:B:30:LEU:HA	1:B:30:LEU:HD23	1.93	0.41
1:B:93:ARG:HG3	1:B:110:PHE:CD2	2.55	0.41
2:C:157:ARG:NH1	2:C:158:LEU:CB	2.84	0.41
1:B:81:ASP:O	1:B:129:GLY:HA3	2.20	0.41
1:B:126:VAL:HG12	1:B:127:ASN:ND2	2.36	0.41
1:A:101:PRO:C	1:A:103:LEU:H	2.23	0.41
1:B:110:PHE:CE1	4:B:701:ADP:H8	2.38	0.41
1:B:108:MET:HA	5:B:519:HOH:O	2.21	0.41
1:A:49:THR:O	1:A:53:ILE:HG12	2.19	0.41
1:B:120:VAL:HG22	1:B:134:LEU:CD2	2.49	0.41
1:B:125:GLU:O	1:B:126:VAL:C	2.59	0.41
1:B:11:ALA:HA	1:B:52:ILE:CD1	2.50	0.41
1:B:111:THR:O	1:B:115:ASN:HB2	2.21	0.41
1:A:13:SER:O	1:A:16:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:VAL:O	2:C:107:VAL:N	2.51	0.40
1:A:23:VAL:O	1:A:27:VAL:HG12	2.21	0.40
1:B:86:ILE:HG12	4:B:701:ADP:N3	2.37	0.40
1:B:30:LEU:HD22	1:B:73:GLY:HA2	2.02	0.40
1:A:62:GLY:O	1:A:63:ILE:HB	2.21	0.40
1:A:24:ALA:HA	1:A:27:VAL:HG12	2.03	0.40

All (2) 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:106:SER:OG	1:A:106:SER:OG[11_555]	1.63	0.57
5:A:501:HOH:O	5:A:501:HOH:O[11_555]	1.92	0.28

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	139/150 (93%)	121 (87%)	13 (9%)	5 (4%)	4	18
1	B	139/150 (93%)	102 (73%)	23 (16%)	14 (10%)	1	2
2	C	55/243 (23%)	50 (91%)	2 (4%)	3 (6%)	2	7
All	All	333/543 (61%)	273 (82%)	38 (11%)	22 (7%)	1	4

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	105	ARG
1	B	126	VAL
1	A	102	GLU
1	B	133	TYR
2	C	106	LYS

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Mol	Chain	Res	Type
1	B	102	GLU
1	B	106	SER
1	B	107	GLY
1	A	106	SER
1	A	133	TYR
1	A	134	LEU
1	B	57	ASN
1	B	63	ILE
1	B	101	PRO
1	B	87	PRO
1	B	103	LEU
1	B	134	LEU
1	A	63	ILE
1	B	60	PRO
2	C	105	VAL
2	C	107	VAL
1	B	84	VAL

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	124/133 (93%)	123 (99%)	1 (1%)	86	96
1	B	118/133 (89%)	111 (94%)	7 (6%)	24	58
2	C	46/216 (21%)	43 (94%)	3 (6%)	21	52
All	All	288/482 (60%)	277 (96%)	11 (4%)	40	76

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	GLU
1	B	4	GLU
1	B	5	MET
1	B	20	ARG
1	B	49	THR

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Mol	Chain	Res	Type
1	B	80	ARG
1	B	111	THR
1	B	115	ASN
2	C	111	LEU
2	C	128	THR
2	C	157	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	94	GLN
1	A	127	ASN
1	A	137	HIS
1	B	29	GLN
1	B	115	ASN
1	B	127	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	ADP	A	601	3	22,29,29	1.39	4 (18%)	27,45,45	1.19	2 (7%)
4	ADP	B	701	3	22,29,29	1.93	5 (22%)	27,45,45	1.24	2 (7%)

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	ADP	A	601	3	-	0/12/32/32	0/3/3/3
4	ADP	B	701	3	-	0/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	ADP	C8-N7	-3.23	1.28	1.34
4	B	701	ADP	C8-N7	-2.96	1.28	1.34
4	A	601	ADP	PB-O2B	-2.48	1.45	1.54
4	A	601	ADP	C2-N3	2.05	1.35	1.32
4	A	601	ADP	O4'-C1'	2.40	1.44	1.41
4	B	701	ADP	C4-N3	2.47	1.39	1.35
4	B	701	ADP	O4'-C4'	2.58	1.51	1.45
4	B	701	ADP	C2-N3	2.85	1.37	1.32
4	B	701	ADP	O4'-C1'	5.56	1.48	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	ADP	N3-C2-N1	-3.20	126.44	128.89
4	B	701	ADP	N3-C2-N1	-3.19	126.45	128.89
4	B	701	ADP	C2'-C1'-N9	-3.16	109.47	114.29
4	A	601	ADP	C4'-O4'-C1'	2.22	112.16	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	701	ADP	3	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.