Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 04:55 am BST

PDB ID	:	3LMA
Title	:	Crystal structure of the stage V sporulation protein AD (SpoVAD) from Bacillus licheniformis. Northeast Structural Genomics Consortium Target BiR6.
Authors	:	Vorobiev, S.; Ashok, S.; Seetharaman, J.; Belote, R.L.; Ciccosanti, C.; Patel, D.J.; Janjua, H.; Acton, T.B.; Xiao, R.; Everett, J.K.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2010-01-29
Resolution	:	1.99 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

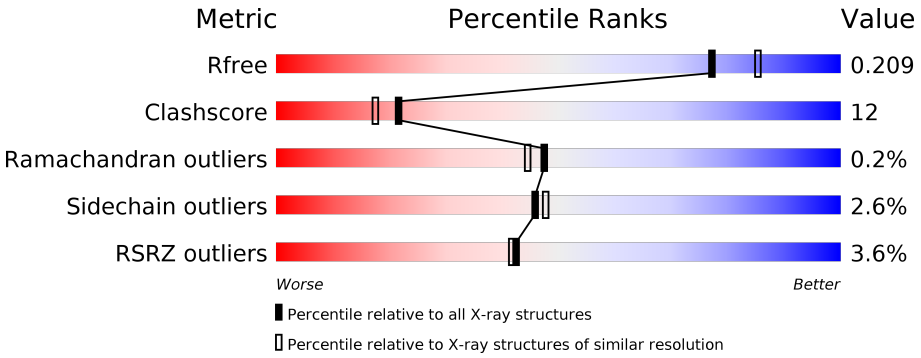
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	347	4% 70% 18% • 11%
1	B	347	4% 75% 14% • 10%
1	C	347	2% 73% 20% • 6%
1	D	347	2% 71% 17% • 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9962 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 V sporulation protein AD (SpoVAD).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	Se	0	0	0
			2298	1441	394	448	7	8			
1	B	311	Total	C	N	O	S	Se	0	0	0
			2316	1457	394	450	7	8			
1	C	327	Total	C	N	O	S	Se	0	0	0
			2445	1532	420	478	7	8			
1	D	311	Total	C	N	O	S	Se	0	0	0
			2316	1456	398	447	7	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	340	LEU	-	expression tag	UNP Q65HU8
A	341	GLU	-	expression tag	UNP Q65HU8
A	342	HIS	-	expression tag	UNP Q65HU8
A	343	HIS	-	expression tag	UNP Q65HU8
A	344	HIS	-	expression tag	UNP Q65HU8
A	345	HIS	-	expression tag	UNP Q65HU8
A	346	HIS	-	expression tag	UNP Q65HU8
A	347	HIS	-	expression tag	UNP Q65HU8
B	340	LEU	-	expression tag	UNP Q65HU8
B	341	GLU	-	expression tag	UNP Q65HU8
B	342	HIS	-	expression tag	UNP Q65HU8
B	343	HIS	-	expression tag	UNP Q65HU8
B	344	HIS	-	expression tag	UNP Q65HU8
B	345	HIS	-	expression tag	UNP Q65HU8
B	346	HIS	-	expression tag	UNP Q65HU8
B	347	HIS	-	expression tag	UNP Q65HU8
C	340	LEU	-	expression tag	UNP Q65HU8
C	341	GLU	-	expression tag	UNP Q65HU8
C	342	HIS	-	expression tag	UNP Q65HU8
C	343	HIS	-	expression tag	UNP Q65HU8
C	344	HIS	-	expression tag	UNP Q65HU8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	345	HIS	-	expression tag	UNP Q65HU8
C	346	HIS	-	expression tag	UNP Q65HU8
C	347	HIS	-	expression tag	UNP Q65HU8
D	340	LEU	-	expression tag	UNP Q65HU8
D	341	GLU	-	expression tag	UNP Q65HU8
D	342	HIS	-	expression tag	UNP Q65HU8
D	343	HIS	-	expression tag	UNP Q65HU8
D	344	HIS	-	expression tag	UNP Q65HU8
D	345	HIS	-	expression tag	UNP Q65HU8
D	346	HIS	-	expression tag	UNP Q65HU8
D	347	HIS	-	expression tag	UNP Q65HU8

- Molecule 2 is water.

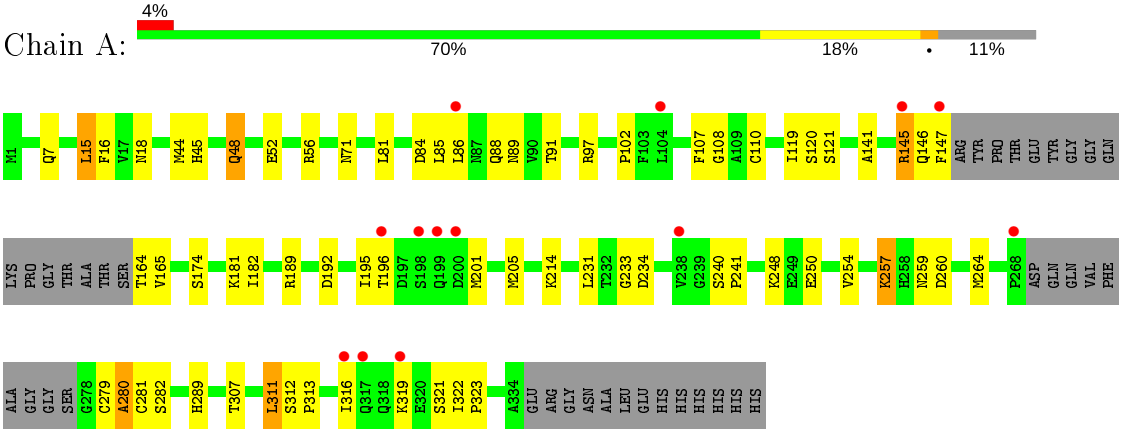
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	155	Total O 155 155	0	0
2	B	118	Total O 118 118	0	0
2	C	168	Total O 168 168	0	0
2	D	146	Total O 146 146	0	0

3 Residue-property plots (i)

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.

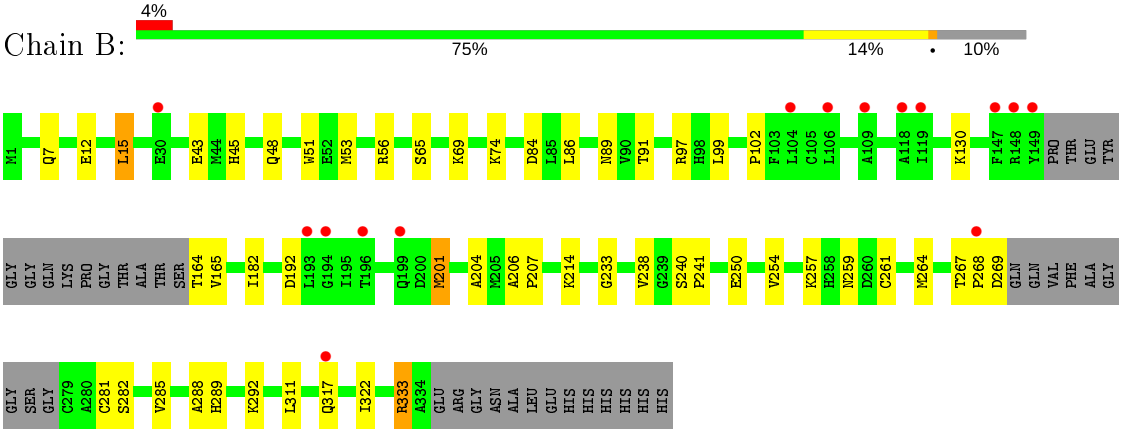
- Molecule 1: Stage V sporulation protein AD (SpoVAD)

Chain A:



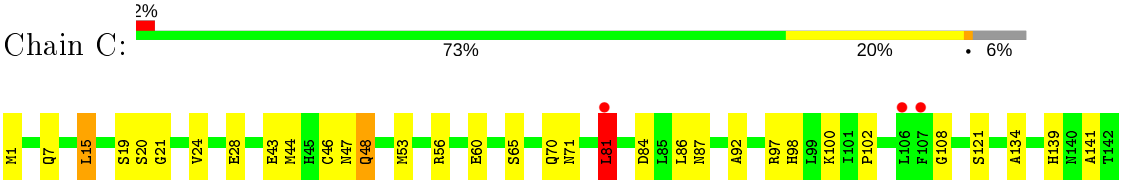
- Molecule 1: Stage V sporulation protein AD (SpoVAD)

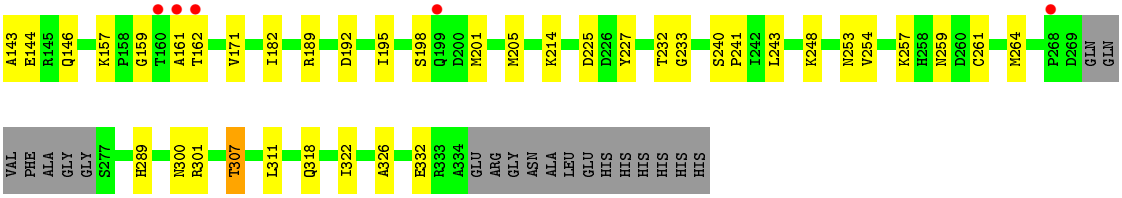
Chain B:



- Molecule 1: Stage V sporulation protein AD (SpoVAD)

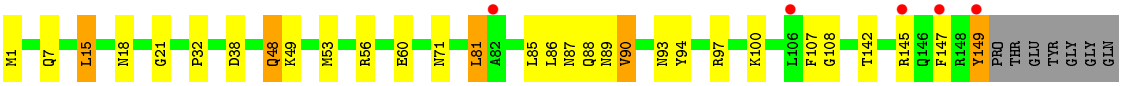
Chain C:

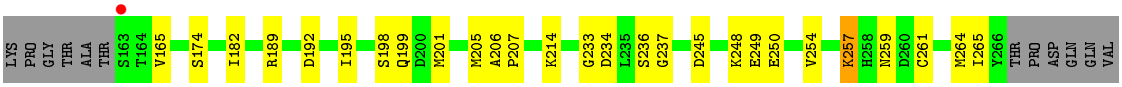




• Molecule 1: Stage V sporulation protein AD (SpoVAD)

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.96Å 83.06Å 103.66Å 90.00° 101.01° 90.00°	Depositor
Resolution (Å)	38.94 – 1.99 38.94 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.94-1.99) 99.0 (38.94-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.51 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2), CNS	Depositor
R, R_{free}	0.168 , 0.211 0.165 , 0.209	Depositor DCC
R_{free} test set	3684 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	21.8	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.2	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	0.96	EDS
Total number of atoms	9962	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.2994e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.42	0/2325	0.66	0/3132
1	B	0.39	0/2345	0.62	0/3161
1	C	0.41	0/2478	0.65	1/3340 (0.0%)
1	D	0.40	0/2344	0.66	1/3156 (0.0%)
All	All	0.41	0/9492	0.65	2/12789 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	81	LEU	CA-CB-CG	-5.86	101.82	115.30
1	C	81	LEU	CA-CB-CG	-5.24	103.25	115.30

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	2298	0	2298	73	0
1	B	2316	0	2308	46	0
1	C	2445	0	2440	56	0
1	D	2316	0	2315	72	0
2	A	155	0	0	6	0
2	B	118	0	0	8	0
2	C	168	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	146	0	0	13	0
All	All	9962	0	9361	223	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 12.

All (223) 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:333:ARG:HH11	1:B:333:ARG:HG3	1.24	1.00
1:B:261:CYS:HB2	2:B:903:HOH:O	1.60	1.00
1:D:87:ASN:HD21	1:D:108:GLY:H	1.10	0.94
1:A:85:LEU:HD13	1:A:280:ALA:HB1	1.51	0.90
1:C:87:ASN:HD21	1:C:108:GLY:N	1.71	0.89
1:C:87:ASN:ND2	1:C:108:GLY:H	1.71	0.89
1:A:201:MSE:HE2	1:A:201:MSE:HA	1.55	0.86
1:A:231:LEU:CD1	1:A:264:MSE:HE1	2.08	0.84
1:A:195:ILE:H	1:A:195:ILE:HD12	1.39	0.83
1:B:201:MSE:HE1	1:B:322:ILE:HD12	1.61	0.83
1:A:97:ARG:HD2	1:D:192:ASP:HB3	1.61	0.80
1:A:84:ASP:O	1:A:108:GLY:HA3	1.86	0.76
1:A:86:LEU:HD21	1:A:164:THR:HG21	1.66	0.75
1:B:288:ALA:O	1:B:292:LYS:HE2	1.86	0.75
1:A:84:ASP:O	1:A:108:GLY:CA	2.36	0.74
1:C:44:MSE:HE3	1:C:139:HIS:HE1	1.52	0.74
1:A:192:ASP:HB3	1:D:97:ARG:HD3	1.71	0.72
1:C:307:THR:HG23	1:C:326:ALA:HB2	1.70	0.72
1:C:44:MSE:HE3	1:C:139:HIS:CE1	2.25	0.71
1:C:201:MSE:HE1	1:C:322:ILE:HD13	1.73	0.71
1:A:196:THR:HG22	1:A:321:SER:HA	1.74	0.70
1:A:107:PHE:CE2	1:D:89:ASN:OD1	2.45	0.69
1:A:231:LEU:HD11	1:A:264:MSE:HE1	1.74	0.69
1:A:192:ASP:HB3	1:D:97:ARG:CD	2.22	0.69
1:D:88:GLN:HB2	1:D:90:VAL:HG22	1.75	0.68
1:B:281:CYS:SG	2:B:903:HOH:O	2.51	0.68
1:C:225:ASP:HB3	2:C:894:HOH:O	1.94	0.67
1:A:165:VAL:HG21	1:A:281:CYS:HB3	1.75	0.67
1:A:311:LEU:O	1:D:89:ASN:ND2	2.28	0.67
1:A:15:LEU:HD13	1:A:182:ILE:HB	1.75	0.66
1:C:198:SER:HA	1:C:201:MSE:HE3	1.77	0.66
1:D:87:ASN:HA	2:D:487:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:ARG:NH1	1:B:333:ARG:HG3	2.01	0.65
1:D:86:LEU:HD11	1:D:142:THR:HB	1.78	0.65
1:C:44:MSE:HE1	1:C:141:ALA:HB2	1.79	0.64
1:D:259:ASN:HB3	1:D:264:MSE:CE	2.28	0.64
1:D:201:MSE:HG2	1:D:205:MSE:HE2	1.80	0.63
1:D:48:GLN:HG3	1:D:53:MSE:HB3	1.79	0.63
1:B:15:LEU:HD13	1:B:182:ILE:HB	1.79	0.63
1:C:214:LYS:HE3	2:C:819:HOH:O	1.99	0.63
1:A:254:VAL:O	1:A:257:LYS:HB2	1.99	0.62
1:B:261:CYS:HB3	1:B:285:VAL:HG21	1.81	0.62
1:C:144:GLU:OE1	1:C:161:ALA:HB1	1.98	0.62
1:B:84:ASP:H	1:B:89:ASN:ND2	1.97	0.62
1:B:201:MSE:HA	1:B:201:MSE:HE3	1.82	0.62
1:A:110:CYS:HB3	1:A:234:ASP:OD2	2.00	0.61
1:C:97:ARG:NH2	1:C:98:HIS:CE1	2.68	0.61
1:B:86:LEU:HD11	1:B:164:THR:HG21	1.81	0.61
1:B:233:GLY:HA3	1:B:282:SER:OG	2.01	0.61
1:D:189:ARG:CZ	2:D:888:HOH:O	2.48	0.61
1:B:192:ASP:HB3	1:C:97:ARG:HD2	1.83	0.61
1:A:165:VAL:HG21	1:A:281:CYS:CB	2.30	0.61
1:C:195:ILE:HD12	1:C:195:ILE:H	1.66	0.61
1:B:238:VAL:O	1:B:241:PRO:HD2	2.01	0.60
1:D:87:ASN:HD21	1:D:108:GLY:N	1.90	0.60
1:A:86:LEU:HD21	1:A:164:THR:CG2	2.32	0.60
1:C:46:CYS:O	1:C:47:ASN:HB2	2.02	0.59
1:D:145:ARG:HG2	1:D:149:TYR:CE1	2.37	0.59
1:B:43:GLU:OE1	1:B:45:HIS:HB2	2.02	0.59
1:C:15:LEU:HD11	1:C:121:SER:HB3	1.82	0.59
1:A:7:GLN:HE22	1:A:189:ARG:HH11	1.51	0.59
1:C:15:LEU:HD13	1:C:182:ILE:HB	1.85	0.58
1:B:268:PRO:O	1:B:269:ASP:CB	2.52	0.58
1:A:102:PRO:HG3	1:D:7:GLN:HG2	1.85	0.58
1:A:195:ILE:H	1:A:195:ILE:CD1	2.16	0.58
1:A:165:VAL:CG2	1:A:281:CYS:HB3	2.33	0.57
1:B:201:MSE:HE1	1:B:322:ILE:CD1	2.34	0.57
1:A:86:LEU:CD2	1:A:164:THR:HG21	2.34	0.57
1:B:233:GLY:CA	2:B:903:HOH:O	2.53	0.56
1:A:56:ARG:HA	1:A:91:THR:HG23	1.87	0.56
1:A:192:ASP:CB	1:D:97:ARG:HD3	2.34	0.56
1:D:48:GLN:CG	1:D:53:MSE:HB3	2.35	0.56
1:A:214:LYS:HE2	2:A:974:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:SER:HB2	1:A:241:PRO:HD3	1.87	0.56
1:C:56:ARG:O	1:C:60:GLU:HG3	2.06	0.55
1:C:19:SER:HB3	1:C:70:GLN:HG2	1.87	0.55
1:B:192:ASP:HB3	1:C:97:ARG:CD	2.35	0.55
1:C:195:ILE:N	1:C:195:ILE:HD12	2.21	0.55
1:A:84:ASP:H	1:A:89:ASN:ND2	2.05	0.55
1:B:53:MSE:HE3	2:B:953:HOH:O	2.07	0.55
1:D:145:ARG:HG2	1:D:149:TYR:HE1	1.71	0.54
1:B:267:THR:HB	1:B:268:PRO:HD2	1.89	0.54
1:C:189:ARG:CZ	2:C:575:HOH:O	2.55	0.54
1:A:260:ASP:O	1:A:264:MSE:HE3	2.07	0.54
1:A:164:THR:HA	1:A:279:CYS:HA	1.90	0.54
1:B:7:GLN:HG2	1:C:102:PRO:HG3	1.90	0.54
1:A:201:MSE:CE	1:A:201:MSE:HA	2.33	0.53
1:B:254:VAL:O	1:B:257:LYS:HB2	2.08	0.53
1:D:234:ASP:OD1	1:D:279:CYS:HB3	2.09	0.53
1:D:248:LYS:HE3	2:D:700:HOH:O	2.07	0.53
1:D:205:MSE:HB3	1:D:307:THR:HG21	1.89	0.53
1:D:56:ARG:O	1:D:60:GLU:HG3	2.09	0.53
1:D:147:PHE:CD1	1:D:198:SER:OG	2.62	0.52
1:D:53:MSE:HE3	2:D:897:HOH:O	2.08	0.52
1:D:198:SER:O	1:D:201:MSE:HE3	2.10	0.52
1:D:233:GLY:HA3	2:D:519:HOH:O	2.08	0.52
1:A:145:ARG:C	1:A:146:GLN:HG2	2.29	0.52
1:A:260:ASP:C	1:A:264:MSE:HE3	2.30	0.51
1:D:254:VAL:O	1:D:257:LYS:HB2	2.10	0.51
1:A:84:ASP:O	1:A:108:GLY:HA2	2.09	0.51
1:A:52:GLU:HG2	2:D:882:HOH:O	2.11	0.51
1:A:233:GLY:HA3	1:A:282:SER:HB3	1.92	0.51
1:A:259:ASN:HB2	2:A:844:HOH:O	2.11	0.51
1:C:7:GLN:HE22	1:C:189:ARG:HH11	1.59	0.51
2:A:965:HOH:O	1:D:100:LYS:HA	2.10	0.50
1:A:97:ARG:CD	1:D:192:ASP:HB3	2.37	0.50
1:D:147:PHE:HD1	1:D:198:SER:HG	1.58	0.50
1:D:49:LYS:HD3	2:D:612:HOH:O	2.11	0.50
1:B:201:MSE:HA	1:B:201:MSE:CE	2.42	0.50
1:D:7:GLN:HE22	1:D:189:ARG:HH11	1.61	0.49
1:C:44:MSE:CE	1:C:141:ALA:HB2	2.43	0.49
1:C:254:VAL:O	1:C:257:LYS:HB2	2.12	0.49
1:C:289:HIS:HD2	2:C:626:HOH:O	1.95	0.49
1:D:15:LEU:HD13	1:D:182:ILE:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:GLU:HG3	2:B:666:HOH:O	2.11	0.49
1:B:259:ASN:ND2	1:B:264:MSE:HE3	2.28	0.49
1:D:245:ASP:O	1:D:249:GLU:HG3	2.12	0.49
1:B:56:ARG:HA	1:B:91:THR:HG23	1.94	0.48
1:A:7:GLN:HE22	1:A:189:ARG:NH1	2.11	0.48
1:A:312:SER:HB2	1:A:313:PRO:HD2	1.95	0.48
1:B:165:VAL:HG21	1:B:281:CYS:HB3	1.95	0.48
1:A:205:MSE:HB3	1:A:307:THR:HG21	1.96	0.47
1:A:88:GLN:O	1:D:107:PHE:CE1	2.67	0.47
1:A:44:MSE:HE3	1:A:141:ALA:HB2	1.96	0.47
1:D:201:MSE:CE	1:D:311:LEU:HD21	2.45	0.47
1:A:196:THR:HG22	1:A:321:SER:CA	2.42	0.47
1:D:206:ALA:HB3	1:D:207:PRO:HD3	1.95	0.47
1:A:311:LEU:HD22	1:A:316:ILE:HD11	1.95	0.47
1:D:90:VAL:HG22	2:D:884:HOH:O	2.13	0.47
1:C:97:ARG:NH2	1:C:98:HIS:HE1	2.08	0.47
1:A:319:LYS:HE3	2:A:999:HOH:O	2.15	0.47
1:A:102:PRO:CG	1:D:7:GLN:HG2	2.44	0.47
1:A:107:PHE:HZ	1:D:89:ASN:ND2	2.13	0.47
1:A:18:ASN:ND2	1:A:174:SER:OG	2.42	0.47
1:C:43:GLU:HB3	2:C:998:HOH:O	2.15	0.47
1:D:147:PHE:HE1	1:D:201:MSE:HE1	1.80	0.47
1:D:233:GLY:O	1:D:261:CYS:HB2	2.15	0.47
1:B:233:GLY:HA2	2:B:903:HOH:O	2.13	0.46
1:D:214:LYS:HE3	1:D:250:GLU:OE1	2.16	0.46
1:D:86:LEU:HD11	1:D:142:THR:CB	2.43	0.46
1:B:206:ALA:HB3	1:B:207:PRO:HD3	1.97	0.46
1:D:199:GLN:C	1:D:201:MSE:H	2.17	0.46
1:A:195:ILE:HD12	1:A:195:ILE:N	2.20	0.46
1:A:289:HIS:HD2	2:A:424:HOH:O	1.99	0.46
1:B:97:ARG:HD2	1:C:192:ASP:HB3	1.97	0.46
1:C:233:GLY:O	1:C:261:CYS:HB2	2.15	0.46
1:A:107:PHE:HZ	1:D:89:ASN:HD21	1.64	0.46
1:D:236:SER:HB3	1:D:237:GLY:H	1.64	0.46
1:D:89:ASN:OD1	1:D:93:ASN:ND2	2.48	0.46
1:A:192:ASP:HB3	1:D:97:ARG:HD2	1.95	0.45
1:D:147:PHE:HD1	1:D:198:SER:OG	1.98	0.45
1:B:86:LEU:HD11	1:B:164:THR:CG2	2.46	0.45
1:D:18:ASN:ND2	1:D:174:SER:OG	2.41	0.45
1:D:32:PRO:HD2	1:D:265:ILE:O	2.16	0.45
1:D:56:ARG:HD3	1:D:94:TYR:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:VAL:CG2	2:D:884:HOH:O	2.64	0.45
1:C:300:ASN:O	1:C:332:GLU:HA	2.17	0.45
1:A:231:LEU:HD13	1:A:264:MSE:HE1	1.94	0.45
1:B:86:LEU:CD1	1:B:164:THR:HG21	2.46	0.45
1:A:201:MSE:HB3	1:A:205:MSE:HE2	1.99	0.45
1:C:143:ALA:O	1:C:146:GLN:HG3	2.16	0.44
1:B:333:ARG:NH1	1:B:333:ARG:CG	2.70	0.44
1:C:20:SER:HB3	1:C:171:VAL:HG12	1.99	0.44
1:C:189:ARG:NE	2:C:575:HOH:O	2.49	0.44
1:C:232:THR:HG21	1:C:243:LEU:HD22	1.98	0.44
1:C:84:ASP:CG	1:C:92:ALA:H	2.21	0.44
1:A:259:ASN:CG	1:A:264:MSE:HE2	2.38	0.44
1:B:201:MSE:HE2	1:B:204:ALA:CB	2.48	0.44
1:C:240:SER:HB2	1:C:241:PRO:HD3	1.99	0.44
1:B:201:MSE:HE2	1:B:204:ALA:HB3	1.99	0.44
1:C:15:LEU:HD11	1:C:121:SER:CB	2.48	0.44
1:A:322:ILE:HA	1:A:323:PRO:HD3	1.90	0.44
1:B:204:ALA:O	1:B:207:PRO:HD2	2.18	0.44
1:A:81:LEU:HD21	1:A:119:ILE:HG22	2.00	0.43
1:A:145:ARG:O	1:A:146:GLN:HG2	2.17	0.43
1:A:146:GLN:O	1:A:147:PHE:CB	2.66	0.43
1:C:227:TYR:CE2	1:C:301:ARG:HD3	2.52	0.43
1:B:102:PRO:HG3	1:C:7:GLN:HG2	2.00	0.43
1:A:81:LEU:HD22	1:A:120:SER:OG	2.18	0.43
2:B:869:HOH:O	1:C:100:LYS:HA	2.17	0.43
1:A:312:SER:OG	1:D:88:GLN:O	2.35	0.43
1:C:24:VAL:HB	1:C:28:GLU:HB2	2.01	0.43
1:D:195:ILE:HD12	1:D:195:ILE:N	2.33	0.43
1:D:90:VAL:HG23	2:D:761:HOH:O	2.19	0.43
1:D:89:ASN:HA	1:D:93:ASN:ND2	2.33	0.43
1:C:311:LEU:C	1:C:311:LEU:HD12	2.38	0.43
1:A:16:PHE:CE1	1:A:181:LYS:HG2	2.54	0.42
1:B:289:HIS:HD2	2:B:433:HOH:O	2.02	0.42
1:C:201:MSE:HB3	1:C:205:MSE:HE2	2.01	0.42
1:D:56:ARG:HD3	1:D:94:TYR:CD1	2.54	0.42
1:C:21:GLY:HA3	1:C:65:SER:HB3	2.00	0.42
1:D:85:LEU:HA	2:D:883:HOH:O	2.18	0.42
1:C:259:ASN:CG	1:C:264:MSE:HE3	2.40	0.42
1:D:205:MSE:HB3	1:D:307:THR:CG2	2.49	0.42
1:A:107:PHE:CZ	1:D:89:ASN:OD1	2.71	0.42
1:A:52:GLU:CD	1:D:318:GLN:HE22	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:ASP:OD1	1:D:280:ALA:N	2.53	0.42
1:B:65:SER:O	1:B:69:LYS:HG3	2.20	0.42
1:C:48:GLN:HG2	1:C:53:MSE:HB3	2.02	0.42
1:D:165:VAL:HG21	1:D:281:CYS:HB3	2.01	0.42
1:B:74:LYS:HD2	1:B:99:LEU:O	2.20	0.41
1:C:257:LYS:HD2	2:C:690:HOH:O	2.20	0.41
1:D:48:GLN:HG3	2:D:609:HOH:O	2.20	0.41
1:B:130:LYS:HA	1:C:1:MSE:HE1	2.03	0.41
1:D:21:GLY:HA2	1:D:38:ASP:OD2	2.21	0.41
1:C:248:LYS:HE2	1:C:253:ASN:HD21	1.85	0.41
1:B:214:LYS:HD2	1:B:250:GLU:HG3	2.01	0.41
1:B:102:PRO:CG	1:C:7:GLN:HG2	2.51	0.41
1:D:86:LEU:HD21	1:D:142:THR:O	2.21	0.41
1:A:214:LYS:HD2	1:A:250:GLU:HG3	2.02	0.41
1:B:240:SER:HB2	1:B:241:PRO:HD3	2.02	0.41
1:D:49:LYS:HG2	2:D:609:HOH:O	2.21	0.41
1:A:312:SER:HB2	1:A:313:PRO:CD	2.50	0.41
1:C:318:GLN:HA	1:D:1:MSE:HE2	2.02	0.41
1:A:15:LEU:HD11	1:A:121:SER:HB3	2.03	0.40
1:D:259:ASN:CG	1:D:264:MSE:HE2	2.41	0.40
1:A:97:ARG:NE	2:A:835:HOH:O	2.53	0.40
1:C:81:LEU:O	1:C:134:ALA:HA	2.21	0.40
1:C:157:LYS:HG2	1:C:159:GLY:H	1.86	0.40
1:C:195:ILE:HD13	2:C:439:HOH:O	2.22	0.40
1:A:248:LYS:NZ	1:A:248:LYS:HB3	2.36	0.40
1:A:45:HIS:O	1:A:48:GLN:HB2	2.21	0.40
1:B:45:HIS:CE1	1:B:51:TRP:CH2	3.10	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	303/347 (87%)	294 (97%)	7 (2%)	2 (1%)	22 16
1	B	305/347 (88%)	298 (98%)	7 (2%)	0	100 100
1	C	323/347 (93%)	318 (98%)	5 (2%)	0	100 100
1	D	305/347 (88%)	299 (98%)	6 (2%)	0	100 100
All	All	1236/1388 (89%)	1209 (98%)	25 (2%)	2 (0%)	47 44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	ALA
1	A	145	ARG

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	247/272 (91%)	242 (98%)	5 (2%)	55 58
1	B	248/272 (91%)	242 (98%)	6 (2%)	49 51
1	C	263/272 (97%)	256 (97%)	7 (3%)	44 46
1	D	247/272 (91%)	239 (97%)	8 (3%)	39 38
All	All	1005/1088 (92%)	979 (97%)	26 (3%)	46 48

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	48	GLN
1	A	71	ASN
1	A	257	LYS
1	A	311	LEU
1	B	15	LEU
1	B	48	GLN
1	B	201	MSE
1	B	311	LEU

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Mol	Chain	Res	Type
1	B	317	GLN
1	B	333	ARG
1	C	15	LEU
1	C	48	GLN
1	C	71	ASN
1	C	81	LEU
1	C	86	LEU
1	C	162	THR
1	C	307	THR
1	D	15	LEU
1	D	48	GLN
1	D	71	ASN
1	D	81	LEU
1	D	90	VAL
1	D	149	TYR
1	D	257	LYS
1	D	282	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	18	ASN
1	A	71	ASN
1	A	87	ASN
1	A	89	ASN
1	A	289	HIS
1	A	318	GLN
1	B	7	GLN
1	B	18	ASN
1	B	70	GLN
1	B	87	ASN
1	B	89	ASN
1	B	93	ASN
1	B	289	HIS
1	B	318	GLN
1	C	7	GLN
1	C	18	ASN
1	C	48	GLN
1	C	70	GLN
1	C	87	ASN
1	C	98	HIS

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Mol	Chain	Res	Type
1	C	253	ASN
1	C	289	HIS
1	D	7	GLN
1	D	18	ASN
1	D	64	GLN
1	D	87	ASN
1	D	89	ASN
1	D	93	ASN
1	D	318	GLN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	301/347 (86%)	0.01	13 (4%)	35	34	10, 21, 58, 85	0
1	B	303/347 (87%)	0.09	15 (4%)	28	28	12, 24, 56, 73	0
1	C	319/347 (91%)	-0.06	8 (2%)	57	56	11, 22, 48, 72	0
1	D	303/347 (87%)	0.08	8 (2%)	56	54	10, 24, 47, 72	0
All	All	1226/1388 (88%)	0.03	44 (3%)	42	42	10, 23, 52, 85	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	149	TYR	6.4
1	C	199	GLN	5.0
1	A	199	GLN	4.6
1	D	147	PHE	4.4
1	B	147	PHE	4.2
1	A	196	THR	3.8
1	A	316	ILE	3.8
1	B	106	LEU	3.5
1	C	268	PRO	3.4
1	B	317	GLN	3.4
1	B	194	GLY	3.2
1	A	147	PHE	3.0
1	D	106	LEU	3.0
1	C	160	THR	2.9
1	C	106	LEU	2.9
1	B	193	LEU	2.9
1	A	317	GLN	2.9
1	B	196	THR	2.8
1	A	268	PRO	2.7
1	A	198	SER	2.7
1	A	319	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	104	LEU	2.6
1	B	104	LEU	2.6
1	B	199	GLN	2.6
1	B	30	GLU	2.5
1	B	109	ALA	2.5
1	B	268	PRO	2.5
1	C	161	ALA	2.5
1	C	107	PHE	2.4
1	B	119	ILE	2.4
1	C	81	LEU	2.3
1	C	162	THR	2.3
1	D	163	SER	2.3
1	B	148	ARG	2.3
1	B	149	TYR	2.2
1	A	145	ARG	2.2
1	A	86	LEU	2.2
1	D	145	ARG	2.1
1	B	118	ALA	2.1
1	D	318	GLN	2.1
1	A	238	VAL	2.0
1	D	82	ALA	2.0
1	D	316	ILE	2.0
1	A	200	ASP	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.