



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:18 AM GMT

PDB ID : 3LM6
Title : Crystal Structure of Stage V sporulation protein AD (spoVAD) from *Bacillus subtilis*, Northeast Structural Genomics Consortium Target SR525
Authors : Forouhar, F.; Su, M.; Seetharaman, J.; Fang, F.; Xiao, R.; Cunningham, K.; Ma, L.; Wang, D.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2010-01-29
Resolution : 2.50 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

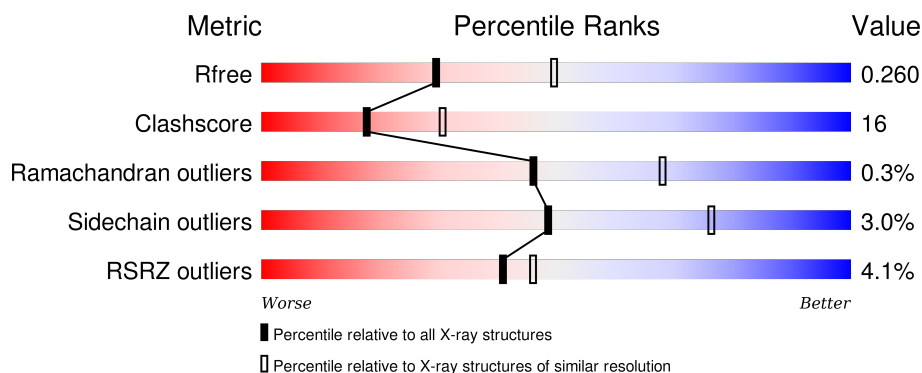
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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.

Mol	Chain	Length	Quality of chain
1	A	346	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>29%</div> <div>• •</div> </div> </div>
1	B	346	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>27%</div> <div>7%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5021 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	Se	0	0	0
			2505	1572	425	493	6	9			
1	B	322	Total	C	N	O	S	Se	0	0	0
			2401	1505	407	474	6	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	LEU	-	expression tag	UNP P40869
A	340	GLU	-	expression tag	UNP P40869
A	341	HIS	-	expression tag	UNP P40869
A	342	HIS	-	expression tag	UNP P40869
A	343	HIS	-	expression tag	UNP P40869
A	344	HIS	-	expression tag	UNP P40869
A	345	HIS	-	expression tag	UNP P40869
A	346	HIS	-	expression tag	UNP P40869
B	339	LEU	-	expression tag	UNP P40869
B	340	GLU	-	expression tag	UNP P40869
B	341	HIS	-	expression tag	UNP P40869
B	342	HIS	-	expression tag	UNP P40869
B	343	HIS	-	expression tag	UNP P40869
B	344	HIS	-	expression tag	UNP P40869
B	345	HIS	-	expression tag	UNP P40869
B	346	HIS	-	expression tag	UNP P40869

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	72	Total	O	0	0
			72	72		
2	B	43	Total	O	0	0
			43	43		

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 ($\text{RSRZ} > 2$). 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.

Chain A:

3% 66% 29%

M1 K2 L3 Q7 V17 G21 T22 A23 K39 E43 M44 H45 C46 N47 Q48 M53 L58 M59 E60 D61 A62 V63 M64 V65 N70 N71 L72 T73 D76 I77 L80 L81 D84 L85 L86 N87 Q88 N89 N93 Y94 V95 K100 I101 G105 M106 F107 S111 T112 S113 M114 E115 V119 A120 G126 G127 F128 R131 A132 L133 A134 A135 A136 S137 S138 R145 Q146 F147 R148 Y149 P150 T151 E152 Y153 P158 D159 T160 A161 T162 V171 Q175 T186 K189 V190 S191 M205 A206 P207 A208 K214 Q215 F216 K218 D225 D234 V238 G239 S240 P241 I242 V243 I246 L247 R248 E249 G255 T256 K257 T267 P268 D269 Q270 Q271 C279 A280 Y287 S288 H289 L290 F291 K292 Q293 L299 M300 R301 A306 T307 L310 L311 S312 P313 T314 M315 I316 Q317 Q318 K319 T322

Chain B:

5% 66% 27% 7%

Chain B items (100 total):

- S111, E115, V119, A120, G126, G127, F128, R131, A132, L133, A134, A135, T136, S137, S138, A143, E144, R145, G146, P147, A148, T149, G150, L151, T152, P153, A154, R155, G156, L157, T158, P159, A160, R161, G162, L163, T164, P165, A166, R167, G168, L169, T170, P171, Q181, T186, K189, V190, L193, T196, F199, D200, M205, A206, P207, A208, H216, D225, D226, Y227, T230, D234, S240, P241, L242, V243, T246, L247, K257, T267, P268, D269, Q270, Q271, A280, Y287, S288, H289, T290, F291, K292, Q293, L299, N300, R301, A306, T307, L310, L311, S312, P313, T314, K315, T316, Q317, Q318, R319, E320, T322, T323, T324

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.97Å 87.66Å 130.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.50 29.23 – 2.49	Depositor EDS
% Data completeness (in resolution range)	82.1 (19.92-2.50) 95.9 (29.23-2.49)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.188 , 0.241 0.211 , 0.260	Depositor DCC
R_{free} test set	1814 reflections (10.64%)	DCC
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 37869 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5021	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.39	0/2543	0.60	0/3438
1	B	0.38	0/2434	0.60	0/3289
All	All	0.39	0/4977	0.60	0/6727

There are no bond length outliers.

There are no bond angle outliers.

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	2505	0	2480	94	0
1	B	2401	0	2385	75	0
2	A	72	0	0	9	0
2	B	43	0	0	2	0
All	All	5021	0	4865	154	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 16.

All (154) 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:289:HIS:O	1:A:293:GLN:HG2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ALA:HB2	1:B:324:THR:HG23	1.64	0.78
1:A:115:GLU:O	1:A:119:VAL:HG12	1.84	0.78
1:A:208:ALA:HB2	1:A:324:THR:HG23	1.64	0.78
1:A:216:HIS:HE1	1:A:227:TYR:OH	1.66	0.78
1:B:289:HIS:O	1:B:293:GLN:HG2	1.84	0.77
1:B:216:HIS:HE1	1:B:227:TYR:OH	1.68	0.75
1:A:59:MSE:HE2	1:A:95:VAL:HG11	1.66	0.74
1:B:115:GLU:O	1:B:119:VAL:HG12	1.87	0.74
1:B:59:MSE:HE2	1:B:95:VAL:HG11	1.68	0.74
1:B:63:VAL:HG13	1:B:133:LEU:HD21	1.71	0.73
1:A:126:GLY:O	1:B:2:LYS:HE2	1.89	0.71
1:A:86:LEU:HA	1:A:146:GLN:HE22	1.54	0.71
1:A:63:VAL:HG13	1:A:133:LEU:HD21	1.72	0.70
1:B:290:ILE:HD13	1:B:293:GLN:HG3	1.73	0.69
1:A:190:VAL:O	1:B:100:LYS:HE2	1.92	0.69
1:B:186:THR:OG1	1:B:216:HIS:HD2	1.75	0.68
1:A:310:LEU:HD13	1:B:93:ASN:OD1	1.94	0.67
1:B:158:PRO:HG2	1:B:160:THR:HG22	1.76	0.67
1:B:61:ASP:O	1:B:65:VAL:HG12	1.94	0.67
1:A:2:LYS:HE2	1:B:126:GLY:O	1.95	0.66
1:A:311:LEU:HG	1:A:322:ILE:HG12	1.77	0.66
1:A:128:PHE:CZ	1:B:2:LYS:HD2	2.32	0.65
1:A:107:PHE:O	1:B:105:CYS:HB3	1.97	0.65
1:A:21:GLY:HA3	1:A:65:VAL:HG13	1.79	0.65
1:B:181:GLN:HB2	1:B:334:ALA:HB2	1.78	0.64
1:A:186:THR:OG1	1:A:216:HIS:HD2	1.78	0.64
1:A:86:LEU:CA	1:A:146:GLN:HE22	2.10	0.64
1:B:21:GLY:HA3	1:B:65:VAL:HG13	1.78	0.64
1:A:61:ASP:O	1:A:65:VAL:HG12	1.98	0.63
1:A:191:SER:HB2	2:A:352:HOH:O	1.99	0.63
1:B:84:ASP:OD1	1:B:89:ASN:HA	2.00	0.62
1:A:84:ASP:OD1	1:A:89:ASN:HA	1.99	0.62
1:A:93:ASN:OD1	1:B:310:LEU:HD13	2.01	0.60
1:A:158:PRO:HB2	1:A:160:THR:HG22	1.82	0.60
1:A:225:ASP:HA	1:A:257:LYS:NZ	2.17	0.59
1:A:70:ASN:HD22	1:A:72:LEU:HD22	1.67	0.59
1:A:86:LEU:CB	1:A:146:GLN:HE22	2.15	0.59
1:B:206:ALA:HB3	1:B:207:PRO:HD3	1.84	0.58
1:B:225:ASP:HA	1:B:257:LYS:NZ	2.19	0.58
1:B:70:ASN:HD22	1:B:72:LEU:HD22	1.69	0.58
1:B:81:LEU:N	1:B:81:LEU:HD12	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD12	1:A:81:LEU:N	2.18	0.58
1:A:73:THR:HG22	1:A:76:ASP:OD2	2.04	0.57
1:A:311:LEU:HB3	2:A:363:HOH:O	2.02	0.57
1:B:311:LEU:HG	1:B:322:ILE:HG12	1.84	0.57
1:B:77:ILE:HB	1:B:101:ILE:HD13	1.86	0.57
1:A:100:LYS:HE2	1:B:190:VAL:O	2.04	0.57
1:A:133:LEU:HD12	1:A:171:VAL:O	2.04	0.56
1:B:133:LEU:HD12	1:B:171:VAL:O	2.05	0.56
1:A:206:ALA:HB3	1:A:207:PRO:HD3	1.86	0.56
1:A:230:ILE:N	1:A:230:ILE:HD12	2.20	0.56
1:A:53:MSE:HE3	2:A:397:HOH:O	2.05	0.56
1:A:311:LEU:HB2	1:A:322:ILE:HG23	1.86	0.56
1:A:81:LEU:HD22	1:A:120:ALA:HB2	1.87	0.55
1:A:175:GLN:HB2	2:A:375:HOH:O	2.07	0.54
1:B:311:LEU:HB2	1:B:322:ILE:HG23	1.88	0.54
1:B:81:LEU:HD22	1:B:120:ALA:HB2	1.89	0.54
1:B:313:PRO:O	1:B:316:ILE:HG22	2.07	0.53
1:A:86:LEU:HD12	1:A:86:LEU:O	2.09	0.53
1:A:313:PRO:O	1:A:316:ILE:HG22	2.08	0.53
1:B:81:LEU:HD23	1:B:106:MSE:HE1	1.91	0.52
1:A:77:ILE:HB	1:A:101:ILE:HD13	1.91	0.52
1:A:81:LEU:HB3	1:A:106:MSE:CE	2.40	0.52
1:B:230:ILE:HD12	1:B:230:ILE:N	2.24	0.52
1:B:17:VAL:HG13	1:B:171:VAL:CG2	2.39	0.52
1:B:73:THR:HG22	1:B:76:ASP:OD2	2.10	0.51
1:B:267:THR:O	1:B:269:ASP:N	2.42	0.51
1:B:186:THR:OG1	1:B:216:HIS:CD2	2.61	0.51
1:B:43:GLU:OE2	1:B:45:HIS:HD2	1.93	0.51
1:B:271:GLN:HB2	2:B:374:HOH:O	2.11	0.51
1:B:43:GLU:HG3	1:B:45:HIS:HB2	1.93	0.51
1:A:271:GLN:HG3	1:A:271:GLN:O	2.10	0.51
1:A:43:GLU:HG3	1:A:45:HIS:H	1.76	0.50
1:A:43:GLU:OE2	1:A:45:HIS:HD2	1.93	0.50
1:A:267:THR:O	1:A:269:ASP:N	2.44	0.50
1:B:70:ASN:O	1:B:72:LEU:HD13	2.12	0.50
1:A:43:GLU:HG3	1:A:45:HIS:HB2	1.94	0.50
1:A:70:ASN:O	1:A:72:LEU:HD13	2.12	0.50
1:A:105:CYS:HB3	1:B:107:PHE:O	2.12	0.50
1:B:86:LEU:HD12	1:B:86:LEU:O	2.11	0.50
1:A:311:LEU:C	1:B:88:GLN:HE22	2.15	0.50
1:B:271:GLN:O	1:B:271:GLN:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLY:HA3	2:A:407:HOH:O	2.12	0.49
1:A:138:SER:HB2	1:A:280:ALA:H	1.77	0.49
1:B:81:LEU:HB3	1:B:106:MSE:CE	2.41	0.49
1:A:17:VAL:HG13	1:A:171:VAL:CG2	2.43	0.49
1:A:43:GLU:OE2	1:A:45:HIS:CD2	2.66	0.49
1:B:17:VAL:HG13	1:B:171:VAL:HG23	1.94	0.48
1:A:2:LYS:HD2	1:B:128:PHE:CZ	2.48	0.48
1:B:43:GLU:OE2	1:B:45:HIS:CD2	2.67	0.48
1:A:150:PRO:HB2	1:A:153:TYR:CE2	2.48	0.48
1:A:111:SER:HA	1:A:306:ALA:HB1	1.96	0.48
1:A:88:GLN:HE22	1:B:311:LEU:C	2.17	0.48
1:A:186:THR:OG1	1:A:216:HIS:CD2	2.65	0.47
1:A:81:LEU:HD23	1:A:106:MSE:HE1	1.97	0.47
1:A:81:LEU:HD23	1:A:119:VAL:HG13	1.97	0.47
1:B:81:LEU:HD23	1:B:119:VAL:HG13	1.97	0.47
1:A:317:GLN:HG2	2:A:368:HOH:O	2.15	0.47
1:A:17:VAL:HG13	1:A:171:VAL:HG23	1.98	0.46
1:B:307:THR:HG22	1:B:326:ALA:HB2	1.98	0.46
1:A:43:GLU:CG	1:A:45:HIS:HB2	2.46	0.46
1:A:314:THR:HG21	2:B:376:HOH:O	2.16	0.46
1:A:7:GLN:OE1	1:A:189:LYS:HE3	2.16	0.46
1:B:43:GLU:HG3	1:B:45:HIS:H	1.80	0.45
1:A:315:MSE:SE	1:B:90:VAL:HG11	2.66	0.45
1:B:7:GLN:OE1	1:B:189:LYS:HE3	2.17	0.45
1:B:43:GLU:CG	1:B:45:HIS:HB2	2.47	0.45
1:B:111:SER:HA	1:B:306:ALA:HB1	1.99	0.45
1:B:293:GLN:HB2	1:B:299:LEU:HD12	1.98	0.45
1:B:81:LEU:O	1:B:134:ALA:HA	2.17	0.45
1:B:81:LEU:HD23	1:B:106:MSE:CE	2.47	0.44
1:A:113:SER:HB2	2:A:356:HOH:O	2.17	0.44
1:A:293:GLN:HB2	1:A:299:LEU:HD12	1.99	0.44
1:B:226:ASP:O	1:B:301:ARG:HD2	2.17	0.44
1:A:240:SER:O	1:A:243:VAL:HG12	2.17	0.44
1:A:238:VAL:HB	2:A:418:HOH:O	2.18	0.43
1:B:240:SER:O	1:B:243:VAL:HG12	2.17	0.43
1:A:70:ASN:HD22	1:A:72:LEU:CD2	2.31	0.43
1:A:267:THR:HG23	1:A:268:PRO:HD2	2.00	0.43
1:A:23:ALA:HA	1:A:39:LYS:O	2.19	0.43
1:A:216:HIS:CE1	1:A:227:TYR:OH	2.58	0.43
1:B:205:MSE:HE1	1:B:234:ASP:OD1	2.19	0.43
1:A:226:ASP:O	1:A:301:ARG:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASP:HA	1:A:257:LYS:HZ3	1.82	0.42
1:B:23:ALA:HA	1:B:39:LYS:O	2.19	0.42
1:B:138:SER:HB2	1:B:280:ALA:H	1.83	0.42
1:B:317:GLN:HG3	1:B:317:GLN:O	2.18	0.42
1:A:46:CYS:O	1:A:48:GLN:HG2	2.19	0.42
1:B:46:CYS:O	1:B:48:GLN:HG2	2.19	0.42
1:B:158:PRO:HB2	1:B:159:ASP:H	1.71	0.42
1:A:287:TYR:HA	1:A:291:PHE:CD2	2.55	0.42
1:A:214:LYS:O	1:A:218:LYS:HG3	2.19	0.42
1:A:93:ASN:CG	1:B:310:LEU:HD13	2.40	0.41
1:B:267:THR:HG23	1:B:268:PRO:HD2	2.01	0.41
1:A:310:LEU:HD13	1:B:93:ASN:CG	2.40	0.41
1:A:247:LEU:HD13	1:A:247:LEU:HA	1.93	0.41
1:A:80:LEU:C	1:A:81:LEU:HD12	2.40	0.41
1:A:311:LEU:HD13	1:A:311:LEU:C	2.41	0.41
1:A:88:GLN:HB3	1:A:88:GLN:HE21	1.75	0.41
1:A:81:LEU:HD23	1:A:106:MSE:CE	2.50	0.41
1:A:81:LEU:O	1:A:134:ALA:HA	2.20	0.41
1:B:320:GLU:HG3	1:B:321:THR:N	2.36	0.41
1:A:43:GLU:HB3	2:A:383:HOH:O	2.21	0.40
1:A:315:MSE:HA	1:A:315:MSE:HE2	2.03	0.40
1:B:242:ILE:O	1:B:246:ILE:HG13	2.21	0.40
1:A:317:GLN:O	1:A:317:GLN:HG3	2.21	0.40
1:A:242:ILE:O	1:A:246:ILE:HG13	2.22	0.40
1:A:138:SER:HB3	1:A:280:ALA:HB3	2.02	0.40
1:A:307:THR:HG22	1:A:326:ALA:HB2	2.04	0.40
1:A:136:THR:CG2	1:A:279:CYS:HB3	2.52	0.40
1:B:315:MSE:HE2	1:B:315:MSE:HA	2.03	0.40
1:A:205:MSE:HE1	1:A:234:ASP:OD1	2.21	0.40
1:B:287:TYR:HA	1:B:291:PHE:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/346 (96%)	314 (95%)	17 (5%)	1 (0%)	46	68
1	B	318/346 (92%)	301 (95%)	16 (5%)	1 (0%)	46	68
All	All	650/692 (94%)	615 (95%)	33 (5%)	2 (0%)	46	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	ASP
1	B	269	ASP

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	270/270 (100%)	261 (97%)	9 (3%)	45	73
1	B	260/270 (96%)	253 (97%)	7 (3%)	52	79
All	All	530/540 (98%)	514 (97%)	16 (3%)	48	76

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	58	LEU
1	A	100	LYS
1	A	131	ARG
1	A	136	THR
1	A	148	ARG
1	A	152	GLU
1	A	247	LEU
1	A	269	ASP
1	B	3	LEU
1	B	58	LEU

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Mol	Chain	Res	Type
1	B	100	LYS
1	B	131	ARG
1	B	136	THR
1	B	247	LEU
1	B	269	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	57	GLN
1	A	70	ASN
1	A	88	GLN
1	A	146	GLN
1	A	156	GLN
1	A	181	GLN
1	A	216	HIS
1	A	221	ASN
1	A	271	GLN
1	B	45	HIS
1	B	57	GLN
1	B	70	ASN
1	B	88	GLN
1	B	181	GLN
1	B	216	HIS
1	B	221	ASN
1	B	271	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	325/346 (93%)	0.08	9 (2%) 56 61	7, 24, 47, 65	0
1	B	313/346 (90%)	0.32	17 (5%) 29 33	4, 26, 51, 69	0
All	All	638/692 (92%)	0.20	26 (4%) 41 46	4, 25, 49, 69	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	LEU	6.1
1	B	199	PHE	4.4
1	B	311	LEU	4.3
1	A	310	LEU	4.3
1	B	145	ARG	3.8
1	B	85	LEU	3.5
1	B	143	ALA	3.2
1	B	159	ASP	3.1
1	B	319	LYS	3.1
1	A	145	ARG	2.8
1	B	313	PRO	2.8
1	A	271	GLN	2.7
1	B	271	GLN	2.7
1	B	196	THR	2.6
1	B	193	LEU	2.5
1	B	158	PRO	2.4
1	A	319	LYS	2.3
1	B	160	THR	2.3
1	A	269	ASP	2.3
1	B	200	ASP	2.2
1	A	162	THR	2.1
1	A	317	GLN	2.1
1	B	42	ASP	2.1
1	B	310	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	249	GLU	2.0
1	B	162	THR	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.