WORLDWIDE
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 08:58 am BST

PDB ID	:	3H7X
Title	:	A transition from strong right-handed to canonical left-handed supercoiling in a conserved coiled coil segment of trimeric autotransporter adhesins - the wildtype structure
Authors	:	Zeth, K.; Hernandez-Alvarez, B.; Lupas, A.N.
Deposited on	:	2009-04-28
Resolution	:	2.00 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 (i)) were used in the production of this report:

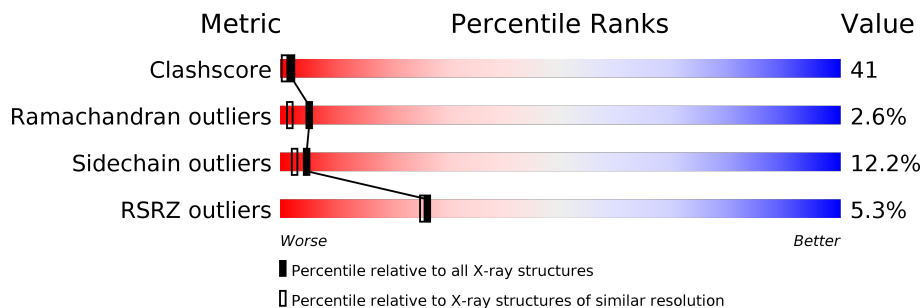|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.00 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	Percentile Ranks	Value
Clashscore		41
Ramachandran outliers		2.6%
Sidechain outliers		12.2%
RSRZ outliers		5.3%

Worse   Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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	64	3% 41% 38% 9% • 11%
1	B	64	5% 34% 38% 8% 20%
1	C	64	5% 25% 44% 9% • 20%
1	D	64	8% 30% 47% 8% 16%
1	E	64	5% 27% 53% • 17%
1	F	64	2% 31% 39% 9% • 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2724 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 Adhesin yadA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	57	Total 462	C 280	N 89	O 93	0	3	0
1	B	51	Total 421	C 257	N 79	O 85	0	2	0
1	C	51	Total 430	C 265	N 81	O 84	0	3	0
1	D	54	Total 455	C 281	N 84	O 90	0	4	0
1	E	53	Total 435	C 267	N 82	O 86	0	3	0
1	F	53	Total 420	C 256	N 78	O 86	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	17	Total 17	O 17	0	0
2	B	22	Total 22	O 22	0	0
2	C	17	Total 17	O 17	0	0
2	D	15	Total 15	O 15	0	0
2	E	17	Total 17	O 17	0	0
2	F	13	Total 13	O 13	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.
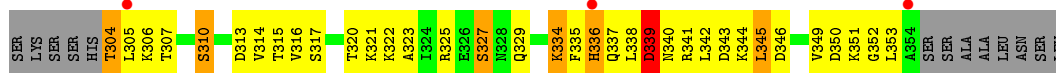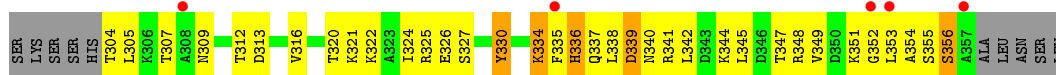
- Molecule 1: Adhesin yadA
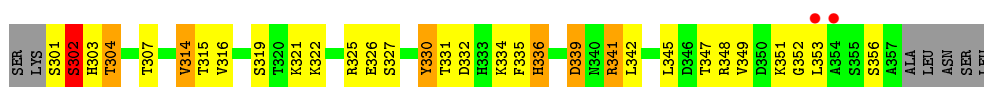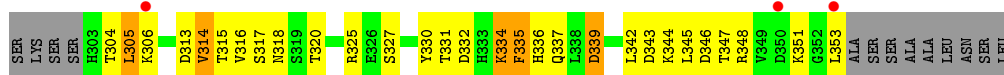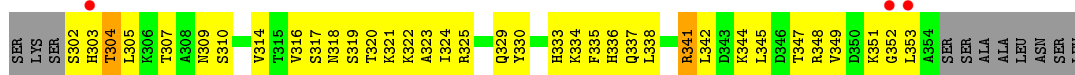

- Molecule 1: Adhesin yadA
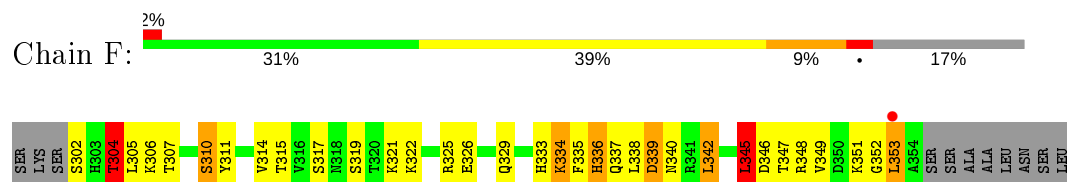

- Molecule 1: Adhesin yadA

- Molecule 1: Adhesin yadA

- Molecule 1: Adhesin yadA

- Molecule 1: Adhesin yadA

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	39.83Å 105.55Å 44.71Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	34.00 – 2.00 34.11 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.2 (34.00-2.00) 90.6 (34.11-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0063	Depositor
R, R_{free}	0.249 , 0.298 0.273 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 44.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.143 for h,-k,-l	Xtriage
Reported twinning fraction	0.523 for H, K, L 0.477 for -h,-k,l	Depositor
Outliers	0 of 22596 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	2724	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.22% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1.36	4/475 (0.8%)	1.26	3/638 (0.5%)
1	B	1.34	3/431 (0.7%)	1.23	1/579 (0.2%)
1	C	1.24	0/443	1.27	3/593 (0.5%)
1	D	1.20	2/472 (0.4%)	1.19	0/633
1	E	1.11	0/447	1.08	1/598 (0.2%)
1	F	1.21	1/424 (0.2%)	1.32	6/571 (1.1%)
All	All	1.25	10/2692 (0.4%)	1.22	14/3612 (0.4%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	SER	C-N	-10.46	1.09	1.34
1	A	302	SER	C-O	7.98	1.38	1.23
1	D	327	SER	CB-OG	7.15	1.51	1.42
1	B	314	VAL	CB-CG1	-6.78	1.38	1.52
1	A	326	GLU	CB-CG	5.58	1.62	1.52
1	F	334	LYS	CG-CD	5.48	1.71	1.52
1	D	330	TYR	CD2-CE2	-5.46	1.31	1.39
1	B	335	PHE	CD1-CE1	-5.32	1.28	1.39
1	A	330	TYR	CD1-CE1	-5.31	1.31	1.39
1	B	332	ASP	CB-CG	-5.18	1.40	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	339	ASP	CB-CG-OD1	7.69	125.22	118.30
1	C	313	ASP	CB-CG-OD1	7.46	125.01	118.30
1	B	334	LYS	CD-CE-NZ	-6.78	96.10	111.70
1	F	339	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	342	LEU	CB-CG-CD1	-6.11	100.62	111.00
1	C	334	LYS	CA-CB-CG	5.89	126.37	113.40
1	E	341	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	C	339	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	302	SER	CA-C-O	-5.27	109.03	120.10
1	A	303	HIS	CA-C-N	5.22	128.69	117.20
1	F	342	LEU	CB-CG-CD1	-5.18	102.19	111.00
1	F	345	LEU	CA-CB-CG	5.12	127.09	115.30
1	F	346	ASP	CB-CG-OD2	5.08	122.88	118.30
1	F	304	THR	N-CA-C	5.05	124.63	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	302	SER	Mainchain

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	462	0	463	36	5
1	B	421	0	422	47	3
1	C	430	0	446	54	8
1	D	455	0	465	54	7
1	E	435	0	436	52	1
1	F	420	0	411	45	4
2	A	17	0	0	8	0
2	B	22	0	0	7	2
2	C	17	0	0	7	0
2	D	15	0	0	9	1
2	E	17	0	0	14	2
2	F	13	0	0	10	1
All	All	2724	0	2643	215	17

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 41.

All (215) 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:D:316:VAL:HB	2:D:112:HOH:O	1.17	1.32
1:F:315:THR:HG22	2:F:113:HOH:O	1.22	1.30
1:B:325:ARG:HB2	2:B:93:HOH:O	1.46	1.15
1:F:315:THR:CG2	2:F:113:HOH:O	1.80	1.07
1:A:341[B]:ARG:NH2	1:C:346:ASP:OD2	1.86	1.06
1:E:302:SER:N	1:E:305:LEU:HD12	1.76	0.99
1:E:337:GLN:NE2	2:E:62:HOH:O	1.94	0.97
1:D:339:ASP:OD1	1:E:341:ARG:NH1	1.97	0.97
1:A:321:LYS:O	1:A:325[B]:ARG:HG2	1.64	0.97
1:A:330:TYR:HB2	2:A:14:HOH:O	1.65	0.93
1:D:342:LEU:CD2	1:F:342:LEU:HD21	1.99	0.92
1:D:326:GLU:OE1	2:D:73:HOH:O	1.87	0.91
1:E:341:ARG:HB2	2:E:104:HOH:O	1.68	0.91
1:F:307:THR:HG22	2:F:106:HOH:O	1.71	0.91
1:D:326:GLU:CD	2:D:73:HOH:O	2.09	0.88
1:E:333:HIS:CD2	1:E:334[B]:LYS:HE2	2.10	0.87
1:E:338:LEU:HA	2:E:104:HOH:O	1.76	0.85
1:A:322:LYS:HE3	1:C:320:THR:HG21	1.58	0.85
1:E:338:LEU:O	2:E:104:HOH:O	1.95	0.84
1:E:309:ASN:OD1	2:E:81:HOH:O	1.97	0.82
1:B:342:LEU:HD21	2:C:114:HOH:O	1.82	0.79
1:A:307:THR:HB	1:C:305:LEU:HD21	1.63	0.79
1:F:307:THR:O	2:F:106:HOH:O	1.99	0.79
1:C:321[A]:LYS:HB3	1:C:325[A]:ARG:NH2	1.99	0.78
1:E:342:LEU:HD21	1:F:342:LEU:HD23	1.63	0.78
1:F:322:LYS:HG2	2:F:98:HOH:O	1.84	0.78
1:C:334:LYS:HE3	1:C:337:GLN:NE2	1.98	0.78
1:A:351:LYS:C	1:A:353:LEU:H	1.86	0.77
1:E:316:VAL:HG21	2:F:113:HOH:O	1.83	0.77
1:C:334:LYS:HE3	1:C:337:GLN:HE21	1.48	0.77
1:B:342:LEU:HB3	1:C:341:ARG:NH2	1.98	0.77
1:A:307:THR:O	2:A:80:HOH:O	2.02	0.77
1:C:342:LEU:HA	2:C:114:HOH:O	1.84	0.77
1:A:301:SER:O	1:A:302:SER:OG	2.03	0.76
1:A:325[B]:ARG:NH1	2:A:28:HOH:O	2.21	0.74
1:B:342:LEU:CD2	2:C:114:HOH:O	2.36	0.73
1:A:351:LYS:O	1:A:353:LEU:N	2.23	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:LYS:C	1:D:353:LEU:H	1.93	0.72
1:B:320:THR:HG21	1:C:322:LYS:HE3	1.70	0.72
1:A:341[A]:ARG:HD3	1:C:342:LEU:HD13	1.70	0.71
1:C:317:SER:OG	2:C:75:HOH:O	2.06	0.71
1:E:341:ARG:CB	2:E:104:HOH:O	2.32	0.71
1:A:334:LYS:HE3	1:C:335:PHE:CG	2.26	0.71
1:E:322:LYS:HG2	2:E:44:HOH:O	1.91	0.70
1:B:335:PHE:CG	1:C:334:LYS:HE2	2.26	0.70
1:D:338:LEU:HD11	1:F:335:PHE:CD1	2.26	0.70
1:A:307:THR:HB	1:C:305:LEU:CD2	2.21	0.70
1:E:333:HIS:CD2	1:E:334[B]:LYS:CE	2.74	0.70
1:A:334:LYS:HE3	1:C:335:PHE:CD1	2.27	0.70
1:D:339:ASP:CG	1:E:341:ARG:HH12	1.94	0.69
1:C:304:THR:HG23	1:C:304:THR:O	1.92	0.69
1:D:342:LEU:HD23	1:F:342:LEU:HD21	1.73	0.69
1:A:341[A]:ARG:NH2	1:C:343:ASP:OD1	2.17	0.69
1:D:335[A]:PHE:CZ	2:E:62:HOH:O	2.45	0.69
1:B:318:ASN:OD1	2:B:78:HOH:O	2.11	0.68
1:A:335:PHE:CD1	1:B:334:LYS:HE3	2.29	0.68
1:B:305:LEU:CD2	1:C:307:THR:CG2	2.72	0.67
1:E:333:HIS:HD2	1:E:334[B]:LYS:CE	2.08	0.67
1:B:330:TYR:CZ	1:B:334:LYS:HD3	2.30	0.66
1:F:351:LYS:C	1:F:353:LEU:H	2.00	0.65
1:A:345:LEU:HD11	1:C:345:LEU:HD22	1.77	0.65
1:F:307:THR:CG2	2:F:106:HOH:O	2.33	0.65
1:B:305:LEU:HD21	1:C:307:THR:HB	1.79	0.64
1:B:330:TYR:O	1:B:334:LYS:HG2	1.97	0.64
1:E:351:LYS:C	1:E:353:LEU:H	2.02	0.63
1:C:321[A]:LYS:CB	1:C:325[A]:ARG:NH2	2.62	0.63
1:B:305:LEU:CD2	1:C:307:THR:HG22	2.29	0.62
1:D:344:LYS:O	1:D:347:THR:HG22	1.99	0.62
1:D:351:LYS:O	1:D:353:LEU:N	2.33	0.62
1:D:354:ALA:C	1:D:356:SER:H	2.02	0.62
1:D:321[B]:LYS:CE	2:D:110:HOH:O	2.48	0.61
1:F:302:SER:HA	1:F:305:LEU:HD12	1.81	0.61
1:E:342:LEU:HD21	1:F:342:LEU:CD2	2.31	0.61
1:B:335:PHE:CE1	1:C:338:LEU:HG	2.35	0.60
1:B:339:ASP:OD1	1:C:341:ARG:NH1	2.34	0.60
1:D:326:GLU:CG	2:D:73:HOH:O	2.48	0.60
1:A:307:THR:CG2	1:C:305:LEU:HD22	2.31	0.60
1:C:351:LYS:C	1:C:353:LEU:H	2.05	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:ASN:O	1:C:344[B]:LYS:HD2	2.01	0.60
1:E:320:THR:O	1:E:324:ILE:HG13	2.02	0.59
1:D:342:LEU:HD21	1:F:342:LEU:HD21	1.81	0.58
1:B:325:ARG:CZ	2:B:93:HOH:O	2.51	0.58
1:D:320:THR:HG1	1:E:319:SER:HG	1.50	0.58
1:F:333:HIS:O	1:F:336:HIS:HB2	2.03	0.58
1:B:351:LYS:C	1:B:353:LEU:H	2.07	0.58
1:B:335:PHE:CD1	1:C:334:LYS:HE2	2.39	0.57
2:A:24:HOH:O	1:B:331:THR:OG1	2.17	0.57
1:D:304:THR:OG1	1:D:307:THR:HB	2.04	0.57
1:D:351:LYS:C	1:D:353:LEU:N	2.56	0.56
1:A:334:LYS:HE3	1:C:335:PHE:CD2	2.41	0.56
1:F:322:LYS:CG	2:F:98:HOH:O	2.46	0.56
1:E:344:LYS:O	1:E:347:THR:HG22	2.05	0.56
1:B:305:LEU:HD22	1:C:307:THR:CG2	2.37	0.55
1:F:347:THR:HG23	1:F:348:ARG:N	2.22	0.55
1:E:302:SER:O	1:E:303:HIS:C	2.45	0.55
1:F:347:THR:CG2	1:F:348:ARG:N	2.70	0.54
2:E:81:HOH:O	1:F:311:TYR:HD2	1.90	0.54
1:B:344:LYS:O	1:B:347:THR:HG22	2.07	0.54
1:E:351:LYS:C	1:E:353:LEU:N	2.60	0.54
1:C:321[A]:LYS:NZ	2:C:84:HOH:O	2.41	0.53
1:C:351:LYS:C	1:C:353:LEU:N	2.62	0.53
1:C:323:ALA:O	1:C:327:SER:OG	2.27	0.53
1:A:307:THR:HG22	1:C:305:LEU:HD22	1.90	0.53
1:E:305:LEU:HD21	1:F:304:THR:HG23	1.89	0.53
1:E:321:LYS:HB3	1:E:325[A]:ARG:NH2	2.24	0.53
1:D:338:LEU:HG	1:F:335:PHE:CE1	2.44	0.52
1:A:345:LEU:HD22	1:B:345:LEU:HD11	1.92	0.52
1:E:333:HIS:O	1:E:337:GLN:HG3	2.10	0.52
1:F:347:THR:CG2	1:F:348:ARG:H	2.23	0.52
1:D:349:VAL:CG2	1:F:349:VAL:HG21	2.40	0.52
1:D:305:LEU:HD21	1:E:304:THR:O	2.09	0.51
1:A:332:ASP:OD1	1:B:330:TYR:OH	2.25	0.51
1:D:353:LEU:O	1:D:356:SER:HB2	2.11	0.51
1:E:330:TYR:O	1:E:334[A]:LYS:HG2	2.10	0.51
1:B:316:VAL:HG11	1:C:315:THR:HG22	1.93	0.51
1:E:345:LEU:HD22	1:F:345:LEU:HD21	1.92	0.51
1:D:324:ILE:HD11	2:E:44:HOH:O	2.11	0.51
1:A:348:ARG:HD3	1:C:349:VAL:HG11	1.93	0.51
1:F:351:LYS:C	1:F:353:LEU:N	2.61	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:LYS:C	1:A:353:LEU:N	2.52	0.50
1:B:334:LYS:HA	1:B:337:GLN:HE21	1.76	0.50
1:B:305:LEU:HD21	1:C:307:THR:CG2	2.40	0.50
1:D:338:LEU:CD1	1:F:335:PHE:CD1	2.93	0.50
1:F:326:GLU:HG3	2:F:98:HOH:O	2.11	0.50
2:A:15:HOH:O	1:C:335:PHE:CD2	2.55	0.50
1:E:321:LYS:O	1:E:325[B]:ARG:HG3	2.11	0.49
1:A:314:VAL:HG12	1:A:315:THR:N	2.26	0.49
1:B:313:ASP:O	1:B:317[B]:SER:OG	2.31	0.49
1:B:351:LYS:C	1:B:353:LEU:N	2.65	0.49
1:C:304:THR:CG2	1:C:304:THR:O	2.59	0.49
1:D:335[A]:PHE:CD1	1:E:334[A]:LYS:HB3	2.48	0.49
1:D:334:LYS:O	1:F:335:PHE:HE1	1.96	0.48
1:C:336:HIS:HB3	2:C:99:HOH:O	2.13	0.48
1:D:321[A]:LYS:HD2	2:D:110:HOH:O	2.13	0.48
1:F:351:LYS:O	1:F:353:LEU:N	2.45	0.48
1:E:334[B]:LYS:HD3	1:E:337:GLN:HE21	1.78	0.48
1:B:325:ARG:NE	2:B:93:HOH:O	2.47	0.48
1:B:346:ASP:OD2	2:B:49:HOH:O	2.20	0.48
1:D:335[B]:PHE:HD2	1:E:334[B]:LYS:HB3	1.78	0.48
1:D:342:LEU:HD23	1:F:342:LEU:CD2	2.42	0.48
1:D:304:THR:OG1	1:D:307:THR:CB	2.61	0.48
1:E:322:LYS:HE3	2:E:44:HOH:O	2.13	0.47
1:E:322:LYS:HA	1:E:325[B]:ARG:NH1	2.29	0.47
1:D:347:THR:HG23	1:D:348:ARG:N	2.29	0.47
1:D:342:LEU:CG	1:F:342:LEU:HD21	2.45	0.47
1:D:340:ASN:O	1:D:344:LYS:HG3	2.15	0.47
1:B:305:LEU:HD22	1:C:307:THR:HG22	1.96	0.47
1:D:337[B]:GLN:HE21	1:D:341:ARG:HH11	1.62	0.46
1:A:301:SER:C	1:A:302:SER:HG	2.09	0.46
1:F:304:THR:O	1:F:304:THR:HG23	2.15	0.46
1:A:327:SER:HB2	1:B:327:SER:OG	2.15	0.46
1:A:331:THR:HG21	2:A:24:HOH:O	2.15	0.46
1:A:319:SER:HB2	1:C:316:VAL:CG1	2.46	0.45
1:D:321[B]:LYS:NZ	2:D:110:HOH:O	2.35	0.45
1:A:345:LEU:HD21	1:C:345:LEU:HD22	1.99	0.45
2:A:15:HOH:O	1:C:335:PHE:HD2	1.95	0.45
1:B:305:LEU:HD21	1:C:307:THR:CB	2.43	0.45
1:F:334:LYS:NZ	1:F:337:GLN:HE22	2.14	0.45
1:E:334[B]:LYS:HD3	1:E:337:GLN:NE2	2.32	0.45
1:E:353:LEU:O	1:E:353:LEU:HG	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:PHE:CD1	1:F:338:LEU:HD11	2.52	0.45
1:F:306:LYS:O	1:F:310:SER:HB3	2.17	0.45
1:E:347:THR:HG23	1:E:348:ARG:N	2.31	0.45
1:D:309:ASN:O	1:D:312:THR:HB	2.17	0.45
1:E:333:HIS:HD2	1:E:334[B]:LYS:HE3	1.79	0.45
1:E:349:VAL:HG21	1:F:349:VAL:HG23	1.98	0.45
1:A:316:VAL:HG11	1:B:315:THR:HG22	1.98	0.45
1:E:351:LYS:O	1:E:353:LEU:N	2.50	0.45
1:D:349:VAL:O	1:D:353:LEU:HB2	2.17	0.45
1:D:322:LYS:NZ	1:D:326:GLU:OE2	2.48	0.44
1:D:347:THR:CG2	1:D:348:ARG:N	2.81	0.44
1:B:342:LEU:HD13	1:C:341:ARG:CZ	2.48	0.44
1:D:313:ASP:O	2:D:112:HOH:O	2.21	0.44
1:A:302:SER:O	1:A:304:THR:N	2.50	0.44
1:B:330:TYR:CE2	1:B:334:LYS:HD3	2.53	0.44
1:F:321:LYS:O	1:F:325:ARG:HG3	2.17	0.44
1:C:306:LYS:O	1:C:310:SER:HB3	2.18	0.43
1:E:321:LYS:HB3	1:E:325[A]:ARG:HH22	1.83	0.43
1:D:349:VAL:CG2	1:F:349:VAL:CG2	2.96	0.43
1:E:349:VAL:HG21	1:F:349:VAL:CG2	2.48	0.43
1:E:318:ASN:ND2	2:E:35:HOH:O	2.44	0.43
1:A:349:VAL:O	1:A:353:LEU:HB2	2.17	0.43
1:B:343:ASP:HA	2:B:49:HOH:O	2.17	0.43
1:F:317:SER:O	1:F:321:LYS:HG3	2.19	0.43
1:D:304:THR:HG21	1:F:305:LEU:HD11	2.00	0.43
1:B:342:LEU:HB3	1:C:341:ARG:HH22	1.81	0.43
1:E:347:THR:CG2	1:E:348:ARG:H	2.31	0.43
1:B:346:ASP:OD1	1:C:345:LEU:CD1	2.67	0.43
1:D:320:THR:HG23	1:E:323:ALA:HB2	2.00	0.42
1:D:354:ALA:C	1:D:356:SER:N	2.72	0.42
1:A:345:LEU:HD13	1:C:345:LEU:HD13	2.01	0.42
1:C:351:LYS:O	1:C:353:LEU:N	2.51	0.42
1:B:347:THR:CG2	1:B:348:ARG:N	2.83	0.42
1:E:334[B]:LYS:HA	1:E:334[B]:LYS:HD3	1.58	0.41
1:B:345:LEU:HD22	1:C:345:LEU:HD11	2.01	0.41
1:B:342:LEU:HD22	2:C:114:HOH:O	2.15	0.41
1:A:321:LYS:CE	2:A:19:HOH:O	2.68	0.41
1:D:324:ILE:HD11	1:E:323:ALA:HA	2.02	0.41
1:B:325:ARG:NH2	2:B:93:HOH:O	2.53	0.41
1:B:334:LYS:HB3	1:B:334:LYS:HE3	1.79	0.41
1:D:330:TYR:HB2	2:D:7:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:VAL:HG21	1:B:345:LEU:HD21	2.02	0.40
1:D:342:LEU:CD2	1:F:342:LEU:CD2	2.86	0.40
1:E:334[A]:LYS:HA	1:E:337:GLN:HE21	1.86	0.40
1:E:347:THR:CG2	1:E:348:ARG:N	2.83	0.40
1:F:322:LYS:O	2:F:98:HOH:O	2.22	0.40
1:B:305:LEU:HD22	1:C:307:THR:HG21	2.02	0.40
1:E:338:LEU:CA	2:E:104:HOH:O	2.45	0.40
1:B:335:PHE:CD1	1:C:338:LEU:HD11	2.57	0.40
1:D:342:LEU:HG	1:F:342:LEU:HD21	2.03	0.40
1:D:349:VAL:HG23	1:F:349:VAL:HG21	2.02	0.40
1:D:324:ILE:CD1	2:E:44:HOH:O	2.67	0.40
1:D:305:LEU:CD2	1:E:307:THR:HB	2.52	0.40

All (17) 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:B:306:LYS:NZ	2:E:34:HOH:O[2_555]	1.30	0.90
1:C:325[B]:ARG:NH1	1:D:339:ASP:OD2[2_556]	1.44	0.76
1:A:325[A]:ARG:NH2	1:F:340:ASN:OD1[2_656]	1.58	0.62
1:A:325[A]:ARG:CZ	1:F:340:ASN:OD1[2_656]	1.73	0.47
1:C:329:GLN:OE1	1:D:336:HIS:CD2[2_556]	1.75	0.45
1:C:325[B]:ARG:NH1	2:D:70:HOH:O[2_556]	1.82	0.38
1:A:339:ASP:OD1	2:F:55:HOH:O[2_656]	1.83	0.37
1:C:340:ASN:OD1	1:D:325[A]:ARG:NE[2_556]	1.83	0.37
1:A:325[A]:ARG:NE	1:F:340:ASN:OD1[2_656]	1.89	0.31
1:C:339:ASP:OD2	1:D:325[B]:ARG:NH2[2_556]	1.93	0.27
1:A:336:HIS:CD2	1:F:329:GLN:OE1[2_656]	2.01	0.19
1:C:325[B]:ARG:CZ	1:D:339:ASP:OD2[2_556]	2.01	0.19
1:C:350:ASP:CB	2:B:96:HOH:O[1_556]	2.08	0.12
1:B:306:LYS:CE	1:E:329:GLN:NE2[2_555]	2.08	0.12
1:C:339:ASP:OD2	1:D:325[B]:ARG:CZ[2_556]	2.09	0.11
1:B:306:LYS:CE	2:E:34:HOH:O[2_555]	2.15	0.05
1:D:351:LYS:NZ	2:B:100:HOH:O[2_546]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	58/64 (91%)	52 (90%)	4 (7%)	2 (3%)	3	1
1	B	51/64 (80%)	49 (96%)	2 (4%)	0	100	100
1	C	52/64 (81%)	50 (96%)	1 (2%)	1 (2%)	8	3
1	D	56/64 (88%)	53 (95%)	1 (2%)	2 (4%)	3	1
1	E	53/64 (83%)	49 (92%)	2 (4%)	2 (4%)	3	1
1	F	51/64 (80%)	47 (92%)	3 (6%)	1 (2%)	7	3
All	All	321/384 (84%)	300 (94%)	13 (4%)	8 (2%)	5	2

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	352	GLY
1	A	356	SER
1	D	352	GLY
1	D	355	SER
1	E	304	THR
1	F	352	GLY
1	C	352	GLY
1	E	352	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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	53/58 (91%)	46 (87%)	7 (13%)	4	2
1	B	49/58 (84%)	44 (90%)	5 (10%)	7	4
1	C	50/58 (86%)	43 (86%)	7 (14%)	3	2
1	D	53/58 (91%)	48 (91%)	5 (9%)	8	5
1	E	49/58 (84%)	45 (92%)	4 (8%)	11	7
1	F	47/58 (81%)	39 (83%)	8 (17%)	2	1
All	All	301/348 (86%)	265 (88%)	36 (12%)	5	2

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	THR
1	A	314	VAL
1	A	336	HIS
1	A	339	ASP
1	A	341[A]	ARG
1	A	341[B]	ARG
1	A	347	THR
1	B	304	THR
1	B	305	LEU
1	B	314	VAL
1	B	336	HIS
1	B	339	ASP
1	C	304	THR
1	C	310	SER
1	C	314	VAL
1	C	327	SER
1	C	336	HIS
1	C	339	ASP
1	C	345	LEU
1	D	334	LYS
1	D	336	HIS
1	D	339	ASP
1	D	345	LEU
1	D	356	SER
1	E	310	SER
1	E	314	VAL
1	E	317	SER

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type
1	E	336	HIS
1	F	304	THR
1	F	310	SER
1	F	314	VAL
1	F	319	SER
1	F	336	HIS
1	F	339	ASP
1	F	345	LEU
1	F	353	LEU

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	337	GLN
1	B	337	GLN
1	C	336	HIS
1	C	337	GLN
1	E	333	HIS
1	E	337	GLN
1	F	337	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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	353:LEU	C	354:ALA	N	2.99
1	A	302:SER	C	303:HIS	N	1.10

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	57/64 (89%)	0.51	2 (3%)	44	43	17, 31, 59, 63	0
1	B	51/64 (79%)	0.39	3 (5%)	22	21	21, 31, 48, 63	0
1	C	51/64 (79%)	0.51	3 (5%)	22	21	21, 30, 54, 63	0
1	D	54/64 (84%)	0.58	5 (9%)	8	8	22, 32, 62, 64	0
1	E	53/64 (82%)	0.49	3 (5%)	23	23	21, 31, 54, 63	0
1	F	53/64 (82%)	0.29	1 (1%)	66	65	22, 31, 54, 63	0
All	All	319/384 (83%)	0.46	17 (5%)	26	25	17, 31, 59, 64	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	357	ALA	6.2
1	F	353	LEU	3.9
1	B	353	LEU	3.6
1	D	335[A]	PHE	3.1
1	A	354	ALA	2.8
1	B	350	ASP	2.7
1	C	336	HIS	2.5
1	E	353	LEU	2.5
1	A	353	LEU	2.3
1	C	305	LEU	2.3
1	B	306	LYS	2.3
1	D	352	GLY	2.3
1	D	353	LEU	2.2
1	C	354	ALA	2.2
1	E	352	GLY	2.2
1	E	303	HIS	2.2
1	D	308	ALA	2.1

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.