



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:35 PM UTC

PDB ID : 3H7X / pdb_00003h7x
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

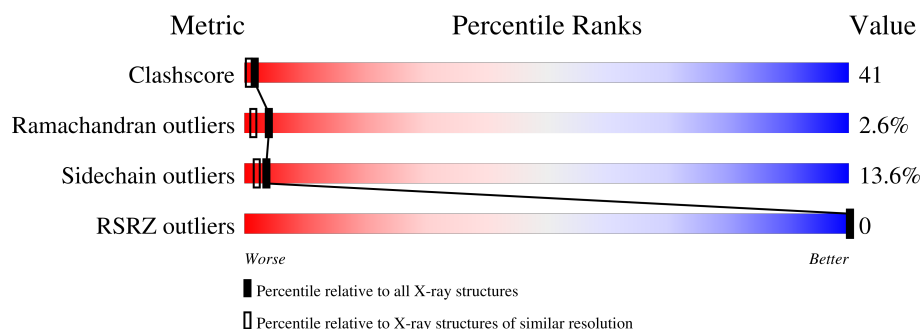
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of 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 $\leq 5\%$. 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	64	
1	B	64	
1	C	64	
1	D	64	
1	E	64	
1	F	64	

2 Entry composition

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

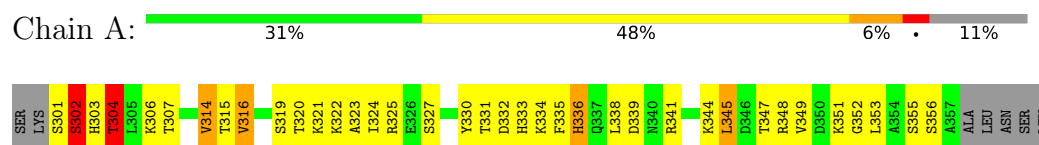
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	17	Total	O	0	0
			17	17		
2	B	22	Total	O	0	0
			22	22		
2	C	17	Total	O	0	0
			17	17		
2	D	15	Total	O	0	0
			15	15		
2	E	17	Total	O	0	0
			17	17		
2	F	13	Total	O	0	0
			13	13		

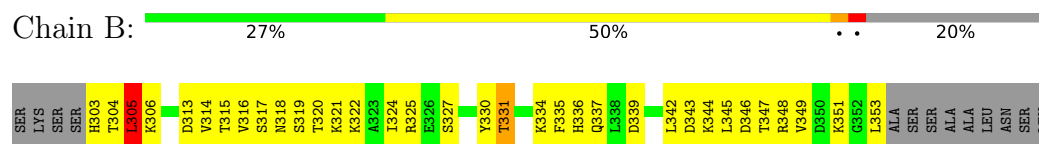
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

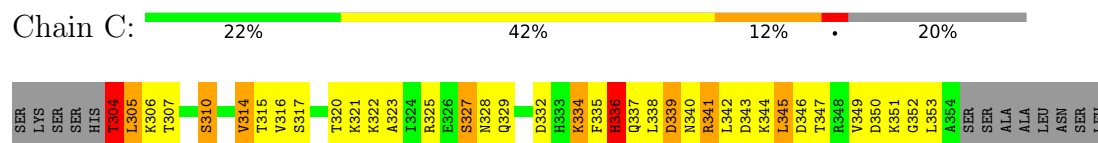
• Molecule 1: Adhesin yadA



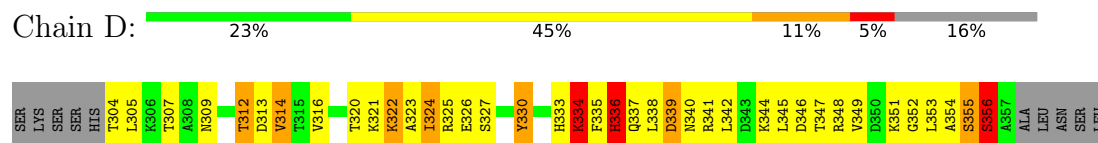
• Molecule 1: Adhesin yadA



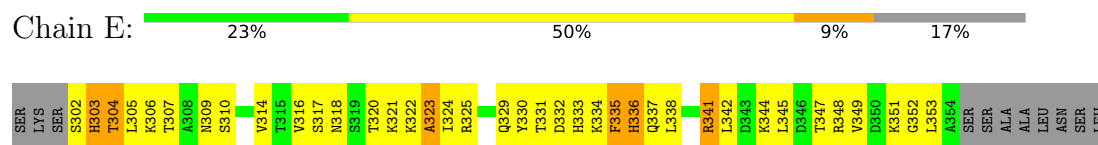
• Molecule 1: Adhesin yadA



• Molecule 1: Adhesin yadA



• Molecule 1: Adhesin yadA



• Molecule 1: Adhesin yadA



SER	LYS	SER	S302	H303	T304	L305	K306	T307	S310	Y311	T312	D313	V314	T315	V316	S317	N318	S319	T320	K321	K322	R325	E326	S327	N328	Q329	H333	K334	F335	H336	Q337	L338	D339	N340	R341	L342	L345	D346	T347	R348	V349	D350	K351	G352	L353	K354	SER	SER	ALA	ALA	ALA	LEU	ASN	SER	LEU
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4 Data and refinement statistics

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 34.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.2 (34.00-2.00) 90.6 (34.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0063	Depositor
R, R_{free}	0.249 , 0.298 0.272 , (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)	0.38 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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	0.89	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	1.84	3/475 (0.6%)	1.78	12/638 (1.9%)
1	B	1.71	5/431 (1.2%)	1.63	2/579 (0.3%)
1	C	1.51	4/443 (0.9%)	1.71	9/593 (1.5%)
1	D	1.47	4/472 (0.8%)	1.59	10/633 (1.6%)
1	E	1.42	3/447 (0.7%)	1.51	4/598 (0.7%)
1	F	1.56	5/424 (1.2%)	1.77	7/571 (1.2%)
All	All	1.59	24/2692 (0.9%)	1.67	44/3612 (1.2%)

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 (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	SER	C-N	-17.98	1.09	1.33
1	A	302	SER	C-O	13.90	1.38	1.24
1	B	321	LYS	CA-C	-7.41	1.43	1.52
1	D	333	HIS	N-CA	-7.10	1.38	1.46
1	D	324	ILE	CA-C	7.04	1.61	1.52
1	B	303	HIS	C-N	6.81	1.43	1.33
1	C	328	ASN	CA-C	6.30	1.61	1.52
1	F	334	LYS	CG-CD	6.21	1.71	1.52
1	E	303	HIS	C-N	6.16	1.42	1.33
1	E	336	HIS	CA-C	-5.98	1.45	1.52
1	F	327	SER	N-CA	-5.94	1.39	1.46
1	C	336	HIS	CA-CB	-5.92	1.44	1.53
1	D	327	SER	CA-C	5.68	1.60	1.52
1	B	322	LYS	N-CA	-5.57	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	HIS	N-CA	-5.54	1.39	1.46
1	B	324	ILE	CA-C	-5.49	1.46	1.52
1	C	336	HIS	N-CA	-5.40	1.39	1.46
1	D	323	ALA	CA-CB	5.32	1.61	1.53
1	E	335	PHE	N-CA	-5.26	1.40	1.46
1	C	341	ARG	N-CA	5.24	1.52	1.46
1	F	333	HIS	N-CA	-5.17	1.40	1.46
1	F	333	HIS	C-O	-5.03	1.18	1.24
1	B	331	THR	CA-C	5.01	1.59	1.52
1	F	336	HIS	CA-CB	-5.01	1.45	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	304	THR	N-CA-C	12.05	124.63	110.41
1	F	336	HIS	N-CA-C	8.40	121.19	111.11
1	A	355	SER	N-CA-C	7.74	121.82	112.38
1	A	323	ALA	N-CA-C	-7.66	102.94	111.82
1	F	328	ASN	N-CA-C	7.33	123.46	111.37
1	E	306	LYS	N-CA-C	7.01	119.53	111.11
1	A	304	THR	CB-CA-C	6.89	124.13	110.42
1	C	314	VAL	N-CA-C	-6.49	103.93	111.00
1	D	322	LYS	CA-C-N	6.43	129.23	120.54
1	D	322	LYS	C-N-CA	6.43	129.23	120.54
1	D	330	TYR	N-CA-C	-6.40	104.38	111.36
1	A	320	THR	N-CA-C	-6.26	104.00	111.69
1	C	334	LYS	CA-CB-CG	6.13	126.37	114.10
1	A	302	SER	CA-C-O	-6.12	109.03	119.13
1	F	320	THR	N-CA-C	6.02	117.51	111.07
1	B	305	LEU	N-CA-C	-5.98	104.76	111.28
1	F	336	HIS	CB-CA-C	-5.75	101.61	110.81
1	A	303	HIS	CA-C-O	-5.71	111.91	119.10
1	D	336	HIS	CB-CA-C	-5.70	101.89	110.90
1	A	302	SER	CB-CA-C	-5.62	110.11	116.63
1	D	314	VAL	N-CA-C	-5.62	105.05	110.72
1	E	336	HIS	CB-CA-C	-5.56	101.40	110.85
1	D	356	SER	N-CA-C	5.53	117.31	111.28
1	A	344	LYS	N-CA-C	-5.49	106.42	113.23
1	F	313	ASP	CA-C-N	5.47	127.45	120.56
1	F	313	ASP	C-N-CA	5.47	127.45	120.56
1	A	306	LYS	N-CA-C	5.39	117.15	111.28
1	D	346	ASP	N-CA-C	5.38	117.56	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	304	THR	CA-C-N	5.36	127.46	120.28
1	C	304	THR	C-N-CA	5.36	127.46	120.28
1	E	332	ASP	N-CA-C	5.35	117.81	111.33
1	D	355	SER	CA-C-N	5.35	127.45	120.28
1	D	355	SER	C-N-CA	5.35	127.45	120.28
1	D	334	LYS	N-CA-C	-5.31	105.16	111.69
1	C	336	HIS	CB-CA-C	-5.29	102.00	110.79
1	C	341	ARG	N-CA-C	5.29	117.04	111.28
1	A	316	VAL	N-CA-C	-5.28	105.39	110.72
1	A	338	LEU	N-CA-C	5.28	117.03	111.28
1	B	319	SER	N-CA-C	5.27	117.44	111.11
1	C	332	ASP	N-CA-C	5.08	117.48	111.33
1	A	324	ILE	N-CA-C	-5.03	105.52	111.00
1	C	305	LEU	N-CA-C	-5.03	105.80	111.28
1	E	323	ALA	N-CA-C	5.03	117.14	111.11
1	C	347	THR	N-CA-C	-5.00	105.74	111.14

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	47	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	17	0	0	15	2
2	F	13	0	0	10	1
All	All	2724	0	2643	217	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 (217) 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:326:GLU:CD	2:D:73:HOH:O	2.09	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: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:A:351:LYS:C	1:A:353:LEU:H	1.86	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:LYS:C	1:D:353:LEU:H	1.93	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:D:339:ASP:CG	1:E:341:ARG:HH12	1.94	0.74
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
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:F:351:LYS:C	1:F:353:LEU:H	2.00	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:C:304:THR:O	1:C:304:THR:HG23	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:E:351:LYS:C	1:E:353:LEU:H	2.02	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:D:354:ALA:C	1:D:356:SER:H	2.02	0.66
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:C:351:LYS:C	1:C:353:LEU:H	2.05	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:B:351:LYS:C	1:B:353:LEU:H	2.07	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:C	1:D:353:LEU:N	2.56	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:LYS:O	1:D:353:LEU:N	2.33	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:A:307:THR:CG2	1:C:305:LEU:HD22	2.31	0.60
1:C:340:ASN:O	1:C:344[B]:LYS:HD2	2.01	0.60
1:E:302:SER:O	1:E:303:HIS:C	2.45	0.59
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:A:301:SER:C	1:A:302:SER:HG	2.09	0.58
1:F:333:HIS:O	1:F:336:HIS:HB2	2.03	0.58
1:E:351:LYS:C	1:E:353:LEU:N	2.60	0.58
1:C:351:LYS:C	1:C:353:LEU:N	2.62	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: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: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:F:351:LYS:C	1:F:353:LEU:N	2.61	0.54
1:B:344:LYS:O	1:B:347:THR:HG22	2.07	0.54
1:B:351:LYS:C	1:B:353:LEU:N	2.65	0.54
1:C:321[A]:LYS:NZ	2:C:84:HOH:O	2.41	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:F:334:LYS:HZ3	1:F:337:GLN:HE22	1.57	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:D:349:VAL:CG2	1:F:349:VAL:HG21	2.40	0.52
1:F:347:THR:CG2	1:F:348:ARG:H	2.23	0.52
1:D:305:LEU:HD21	1:E:304:THR:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:326:GLU:CG	2:D:73:HOH:O	2.48	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: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:C:304:THR:O	1:C:304:THR:CG2	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:342:LEU:CG	1:F:342:LEU:HD21	2.45	0.47
1:D:347:THR:HG23	1:D:348:ARG:N	2.29	0.47
1:D:340:ASN:O	1:D:344:LYS:HG3	2.15	0.47
1:E:337:GLN:CD	2:E:62:HOH:O	2.47	0.47
1:D:354:ALA:C	1:D:356:SER:N	2.72	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:351:LYS:C	1:A:353:LEU:N	2.52	0.46
1:F:304:THR:HG23	1:F:304:THR:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:F:334:LYS:NZ	1:F:337:GLN:HE22	2.14	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:D:349:VAL:CG2	1:F:349:VAL:CG2	2.96	0.43
1:E:321:LYS:HB3	1:E:325[A]:ARG:HH22	1.83	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: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:D:337[B]:GLN:CD	1:F:335:PHE:HZ	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:334[B]:LYS:HD3	1:E:334[B]:LYS:HA	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:HE3	1:B:334:LYS:HB3	1.79	0.41
1:D:330:TYR:HB2	2:D:7:HOH:O	2.20	0.41
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:305:LEU:CD2	1:E:307:THR:HB	2.52	0.40
1:D:324:ILE:CD1	2:E:44:HOH:O	2.67	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:B:306:LYS:CE	1:E:329:GLN:NE2[2_555]	2.08	0.12
1:C:350:ASP:CB	2:B:96:HOH:O[1_556]	2.08	0.12
1:C:339:ASP:OD2	1:D:325[B]:ARG:CZ[2_556]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	6	3
1	D	56/64 (88%)	53 (95%)	1 (2%)	2 (4%)	2	1
1	E	53/64 (83%)	49 (92%)	2 (4%)	2 (4%)	2	1
1	F	51/64 (80%)	47 (92%)	3 (6%)	1 (2%)	6	2
All	All	321/384 (84%)	300 (94%)	13 (4%)	8 (2%)	4	1

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 ⓘ

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	53/58 (91%)	48 (91%)	5 (9%)	8	5
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%)	46 (87%)	7 (13%)	4	2
1	E	49/58 (84%)	43 (88%)	6 (12%)	5	3
1	F	47/58 (81%)	38 (81%)	9 (19%)	1	1
All	All	301/348 (86%)	262 (87%)	39 (13%)	3	2

All (39) 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	345	LEU
1	A	347	THR
1	B	304	THR
1	B	305	LEU
1	B	314	VAL
1	B	336	HIS
1	B	349	VAL
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	312	THR
1	D	314	VAL
1	D	334	LYS
1	D	336	HIS
1	D	339	ASP

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Mol	Chain	Res	Type
1	D	345	LEU
1	D	356	SER
1	E	310	SER
1	E	314	VAL
1	E	317	SER
1	E	331	THR
1	E	336	HIS
1	E	341	ARG
1	F	304	THR
1	F	310	SER
1	F	314	VAL
1	F	319	SER
1	F	334	LYS
1	F	336	HIS
1	F	339	ASP
1	F	345	LEU
1	F	353	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	ASN
1	B	337	GLN
1	C	328	ASN
1	C	337	GLN
1	D	333	HIS
1	E	333	HIS
1	E	337	GLN
1	F	337	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 [i](#)

There are no oligosaccharides 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	E	1
1	A	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%)	-0.64	0 100 100	10, 31, 59, 63	3 (5%)
1	B	51/64 (79%)	-0.77	0 100 100	14, 30, 48, 63	2 (3%)
1	C	51/64 (79%)	-0.70	0 100 100	12, 30, 54, 63	3 (5%)
1	D	54/64 (84%)	-0.72	0 100 100	14, 32, 62, 64	4 (7%)
1	E	53/64 (82%)	-0.83	0 100 100	12, 31, 54, 63	3 (5%)
1	F	53/64 (82%)	-0.82	0 100 100	22, 31, 54, 63	0
All	All	319/384 (83%)	-0.75	0 100 100	10, 31, 59, 64	15 (4%)

There are no RSRZ outliers to report.

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 oligosaccharides 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.