Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:02 am BST

PDB ID	:	4YO3
Title	:	Enteroaggregative Escherichia Coli TssA N-terminal fragment
Authors	:	Durand, E.; Zoued, A.; Spinelli, S.; Douzi, B.; Brunet, Y.R.; Bebeacua, C.; Legrand, P.; Journet, L.; Mignot, T.; Cambillau, C.; Cascales, E.
Deposited on	:	2015-03-11
Resolution	:	3.37 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 following versions of software and data (see references ⓘ) were used in the production of this report:

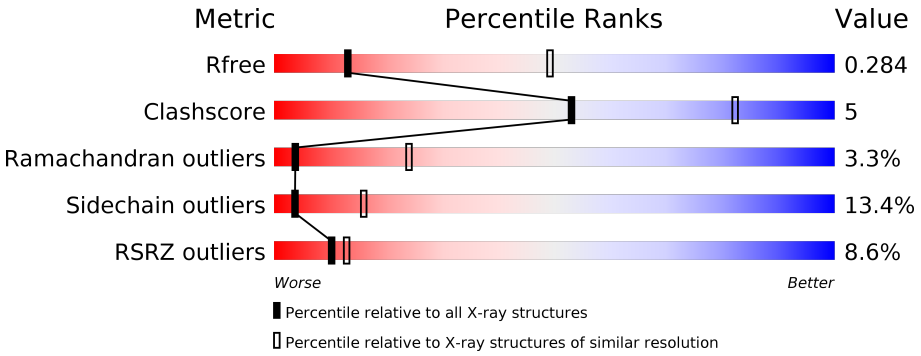
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.37 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	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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	157	3% 75% 22%
1	B	157	4% 74% 23%
1	C	157	4% 74% 23%
1	D	157	4% 77% 21%
1	E	157	% 77% 20%
1	F	157	3% 78% 19%

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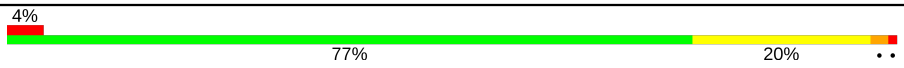
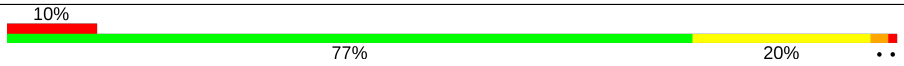
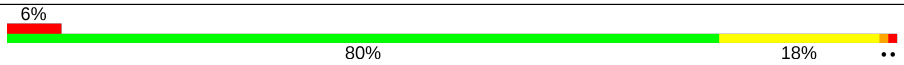
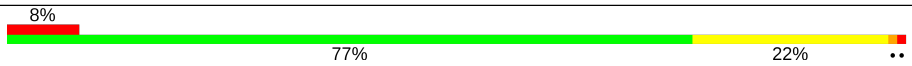
Mol	Chain	Length	Quality of chain
1	G	157	
1	H	157	
1	I	157	
1	J	157	
1	K	157	
1	L	157	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14496 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 TssA.

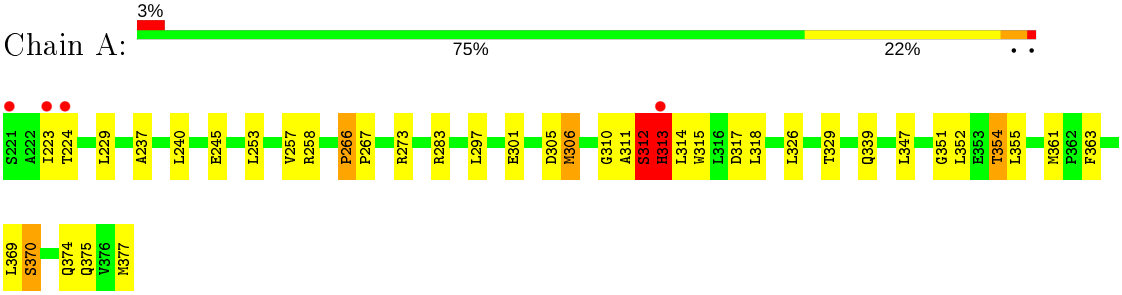
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	B	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	C	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	D	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	E	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	F	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	G	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	H	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	I	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	J	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	K	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			
1	L	157	Total	C	N	O	S	Se	0	0	0
			1208	774	210	219	1	4			

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.

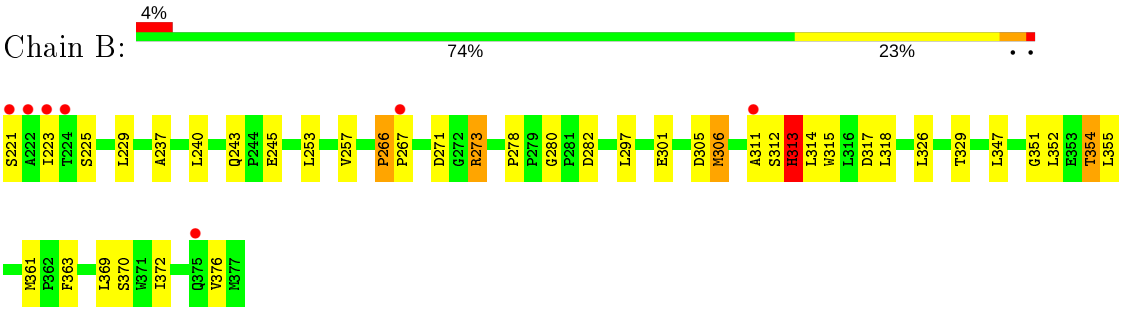
- Molecule 1: TssA

Chain A:



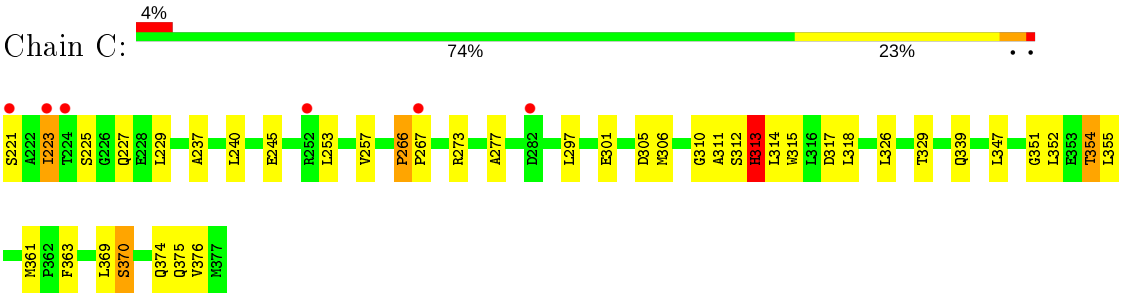
- Molecule 1: TssA

Chain B:



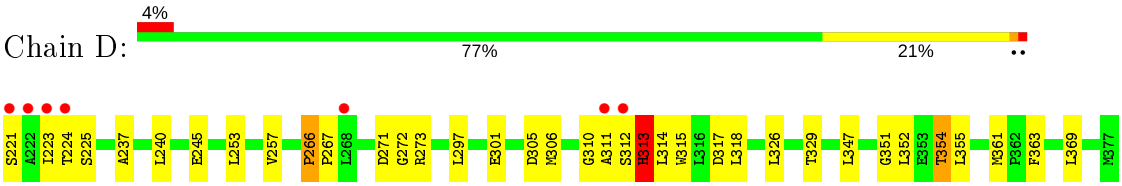
- Molecule 1: TssA

Chain C:



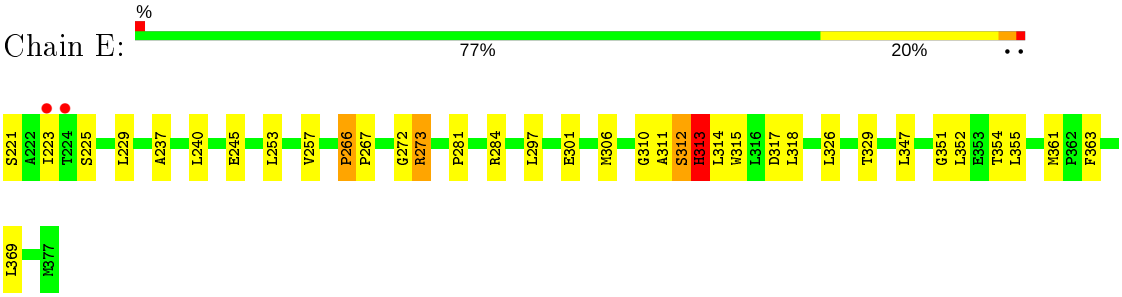
- Molecule 1: TssA

Chain D:



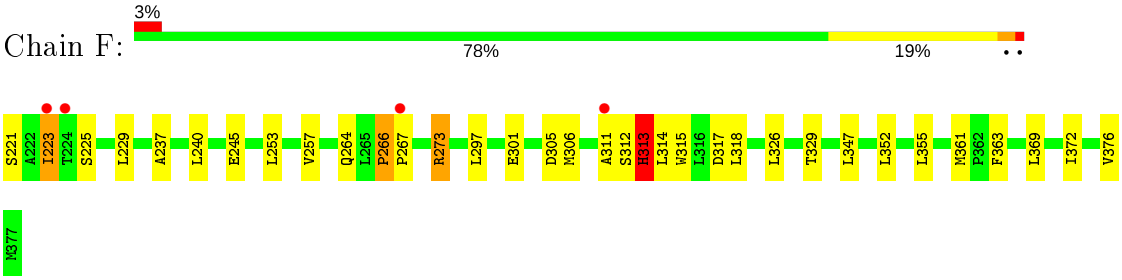
• Molecule 1: TssA

Chain E:



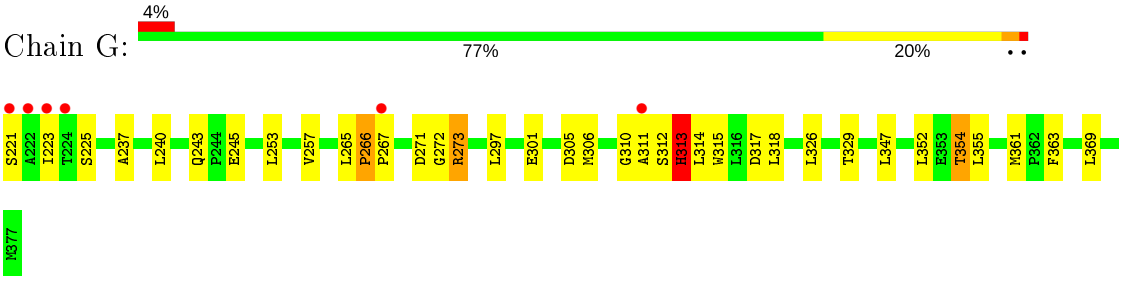
• Molecule 1: TssA

Chain F:



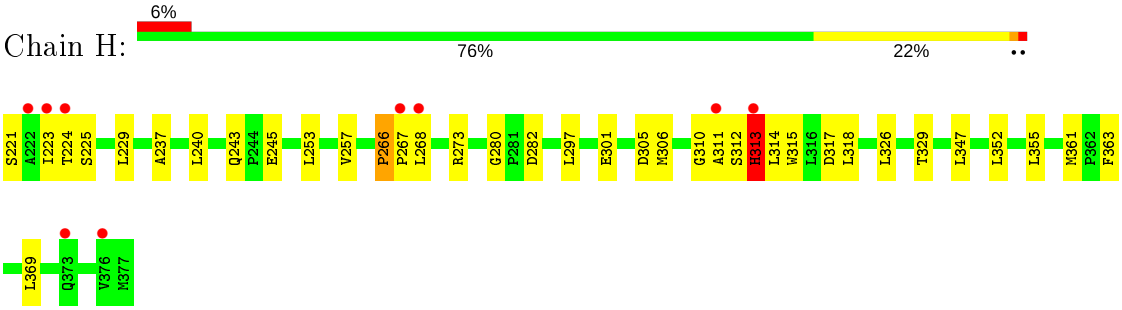
• Molecule 1: TssA

Chain G:



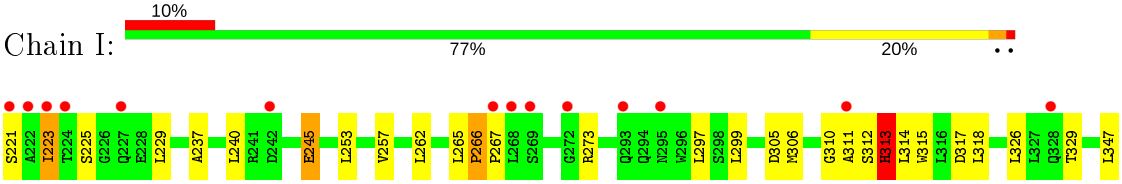
• Molecule 1: TssA

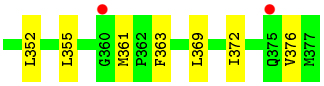
Chain H:



• Molecule 1: TssA

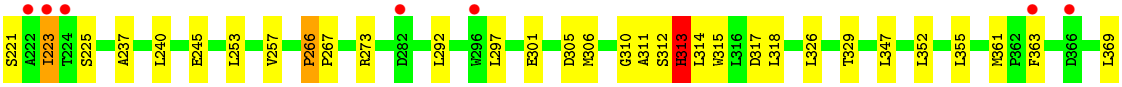
Chain I:





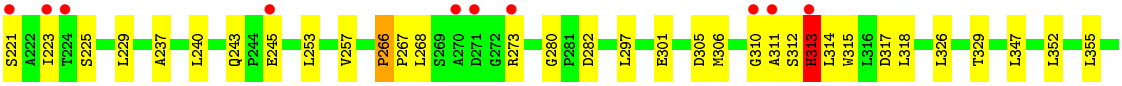
• Molecule 1: TssA

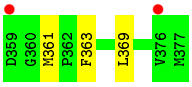
Chain J:



• Molecule 1: TssA

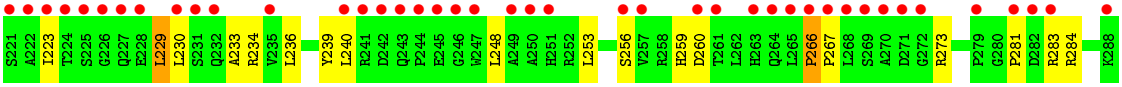
Chain K:

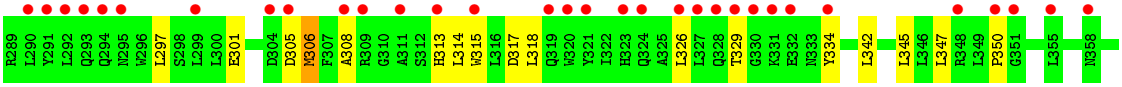


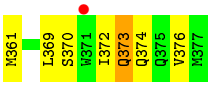


• Molecule 1: TssA

Chain L:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	134.13Å 178.05Å 106.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.39 – 3.37 28.16 – 3.37	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.39-3.37) 100.0 (28.16-3.37)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 3.39Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.250 , 0.261 0.277 , 0.284	Depositor DCC
R_{free} test set	1839 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	94.3	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 69.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	14496	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.48% 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	0.52	0/1232	0.75	1/1673 (0.1%)
1	B	0.52	0/1232	0.72	0/1673
1	C	0.49	0/1232	0.72	0/1673
1	D	0.49	0/1232	0.72	0/1673
1	E	0.48	0/1232	0.70	1/1673 (0.1%)
1	F	0.47	0/1232	0.70	0/1673
1	G	0.50	0/1232	0.72	0/1673
1	H	0.47	0/1232	0.69	0/1673
1	I	0.47	0/1232	0.71	0/1673
1	J	0.47	0/1232	0.69	0/1673
1	K	0.46	0/1232	0.69	0/1673
1	L	0.54	0/1232	0.74	0/1673
All	All	0.49	0/14784	0.71	2/20076 (0.0%)

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
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	2
1	J	0	1
1	K	0	1
1	L	0	1
All	All	0	13

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	A	312	SER	C-N-CA	5.09	134.42	121.70
1	E	312	SER	C-N-CA	5.02	134.24	121.70

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	PRO	Peptide
1	B	266	PRO	Peptide
1	C	266	PRO	Peptide
1	D	266	PRO	Peptide
1	E	266	PRO	Peptide
1	F	266	PRO	Peptide
1	G	266	PRO	Peptide
1	H	266	PRO	Peptide
1	I	265	LEU	Peptide
1	I	266	PRO	Peptide
1	J	266	PRO	Peptide
1	K	266	PRO	Peptide
1	L	266	PRO	Peptide

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	1208	0	1151	14	0
1	B	1208	0	1151	17	0
1	C	1208	0	1151	16	0
1	D	1208	0	1151	13	0
1	E	1208	0	1151	16	0
1	F	1208	0	1151	12	0
1	G	1208	0	1151	13	0
1	H	1208	0	1151	13	0
1	I	1208	0	1151	12	0
1	J	1208	0	1151	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1208	0	1151	12	0
1	L	1208	0	1151	18	0
All	All	14496	0	13812	152	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 5.

All (152) 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:306:MSE:SE	1:B:306:MSE:CE	2.18	1.41
1:L:236:LEU:HD23	1:L:253:LEU:HD11	1.49	0.95
1:L:236:LEU:CD2	1:L:253:LEU:HD11	2.23	0.67
1:C:370:SER:O	1:C:374:GLN:HG2	1.95	0.66
1:G:311:ALA:C	1:G:313:HIS:H	1.99	0.65
1:L:240:LEU:HD22	1:L:253:LEU:HD12	1.78	0.64
1:L:259:HIS:HB3	1:L:345:LEU:HD13	1.80	0.62
1:D:310:GLY:HA3	1:D:313:HIS:CE1	2.35	0.62
1:B:282:ASP:HA	1:E:272:GLY:CA	2.32	0.60
1:D:311:ALA:C	1:D:313:HIS:H	2.05	0.59
1:J:311:ALA:C	1:J:313:HIS:H	2.06	0.59
1:B:282:ASP:HA	1:E:272:GLY:HA3	1.84	0.58
1:D:221:SER:N	1:D:225:SER:HG	2.01	0.58
1:I:311:ALA:C	1:I:313:HIS:H	2.07	0.57
1:F:311:ALA:C	1:F:313:HIS:H	2.07	0.57
1:H:311:ALA:C	1:H:313:HIS:H	2.06	0.57
1:K:311:ALA:C	1:K:313:HIS:H	2.07	0.57
1:E:311:ALA:C	1:E:313:HIS:H	2.09	0.56
1:B:311:ALA:C	1:B:313:HIS:H	2.07	0.55
1:G:310:GLY:HA3	1:G:313:HIS:CE1	2.41	0.55
1:C:311:ALA:C	1:C:313:HIS:H	2.09	0.54
1:A:310:GLY:HA3	1:A:313:HIS:CE1	2.42	0.54
1:A:311:ALA:C	1:A:313:HIS:H	2.11	0.54
1:F:352:LEU:HA	1:F:355:LEU:HD12	1.91	0.53
1:E:352:LEU:HA	1:E:355:LEU:HD12	1.91	0.52
1:J:352:LEU:HA	1:J:355:LEU:HD12	1.92	0.52
1:C:352:LEU:HA	1:C:355:LEU:HD12	1.93	0.51
1:G:221:SER:N	1:G:225:SER:HG	2.07	0.51
1:K:352:LEU:HA	1:K:355:LEU:HD12	1.93	0.51
1:L:248:LEU:HB2	1:L:334:TYR:CE1	2.45	0.51
1:L:342:LEU:HD23	1:L:376:VAL:HG21	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:352:LEU:HA	1:H:355:LEU:HD12	1.91	0.51
1:K:310:GLY:HA3	1:K:313:HIS:CE1	2.45	0.51
1:L:372:ILE:HA	1:L:376:VAL:HG22	1.92	0.51
1:D:272:GLY:CA	1:K:282:ASP:HA	2.40	0.51
1:A:352:LEU:HA	1:A:355:LEU:HD12	1.93	0.50
1:E:221:SER:N	1:E:225:SER:HG	2.09	0.50
1:D:352:LEU:HA	1:D:355:LEU:HD12	1.93	0.50
1:I:352:LEU:HA	1:I:355:LEU:HD12	1.92	0.50
1:H:243:GLN:HE22	1:I:223:ILE:HD12	1.77	0.50
1:L:281:PRO:HA	1:L:284:ARG:HG2	1.94	0.50
1:A:339:GLN:HE22	1:A:375:GLN:HG3	1.76	0.50
1:L:283:ARG:HD3	1:L:306:MSE:HG2	1.92	0.50
1:G:352:LEU:HA	1:G:355:LEU:HD12	1.92	0.50
1:C:221:SER:N	1:C:225:SER:HG	2.10	0.49
1:J:223:ILE:HD12	1:K:243:GLN:HE22	1.77	0.49
1:I:221:SER:N	1:I:225:SER:HG	2.09	0.49
1:C:310:GLY:HA3	1:C:313:HIS:CE1	2.48	0.49
1:D:354:THR:HG23	1:K:280:GLY:HA2	1.94	0.49
1:J:221:SER:N	1:J:225:SER:HG	2.11	0.49
1:B:352:LEU:HA	1:B:355:LEU:HD12	1.94	0.49
1:L:370:SER:O	1:L:374:GLN:HG2	2.13	0.48
1:A:370:SER:O	1:A:374:GLN:HG2	2.13	0.48
1:B:221:SER:N	1:B:225:SER:HG	2.11	0.48
1:H:221:SER:N	1:H:225:SER:HG	2.12	0.47
1:G:354:THR:HG23	1:H:280:GLY:HA2	1.97	0.47
1:D:326:LEU:HA	1:D:329:THR:HG22	1.97	0.47
1:B:326:LEU:HA	1:B:329:THR:HG22	1.96	0.47
1:J:310:GLY:HA3	1:J:313:HIS:CE1	2.48	0.47
1:B:315:TRP:CD1	1:B:318:LEU:HD13	2.50	0.47
1:C:277:ALA:HB2	1:L:373:GLN:CD	2.35	0.47
1:F:221:SER:N	1:F:225:SER:HG	2.12	0.47
1:L:326:LEU:HA	1:L:329:THR:HG22	1.97	0.46
1:C:326:LEU:HA	1:C:329:THR:HG22	1.97	0.46
1:J:315:TRP:CD1	1:J:318:LEU:HD13	2.51	0.46
1:B:355:LEU:HB2	1:B:363:PHE:CE2	2.50	0.46
1:L:315:TRP:O	1:L:318:LEU:HB2	2.15	0.46
1:C:227:GLN:NE2	1:L:350:PRO:HG3	2.31	0.46
1:G:326:LEU:HA	1:G:329:THR:HG22	1.98	0.46
1:F:223:ILE:HD12	1:G:243:GLN:HE22	1.81	0.45
1:F:315:TRP:CD1	1:F:318:LEU:HD13	2.51	0.45
1:F:264:GLN:HE22	1:J:310:GLY:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:LEU:HA	1:F:329:THR:HG22	1.98	0.45
1:G:315:TRP:CD1	1:G:318:LEU:HD13	2.51	0.45
1:K:221:SER:N	1:K:225:SER:HG	2.15	0.45
1:A:326:LEU:HA	1:A:329:THR:HG22	1.99	0.45
1:G:355:LEU:HB2	1:G:363:PHE:CE2	2.52	0.45
1:C:315:TRP:CD1	1:C:318:LEU:HD13	2.52	0.45
1:H:326:LEU:HA	1:H:329:THR:HG22	1.99	0.45
1:A:355:LEU:HB2	1:A:363:PHE:CE2	2.52	0.44
1:H:315:TRP:CD1	1:H:318:LEU:HD13	2.53	0.44
1:K:315:TRP:CD1	1:K:318:LEU:HD13	2.52	0.44
1:B:278:PRO:HG2	1:E:354:THR:HG21	1.99	0.44
1:C:374:GLN:HG3	1:C:375:GLN:N	2.33	0.44
1:D:355:LEU:HB2	1:D:363:PHE:CE2	2.53	0.44
1:E:315:TRP:CD1	1:E:318:LEU:HD13	2.52	0.44
1:B:355:LEU:HB2	1:B:363:PHE:CD2	2.53	0.44
1:D:315:TRP:CD1	1:D:318:LEU:HD13	2.52	0.44
1:E:326:LEU:HA	1:E:329:THR:HG22	2.00	0.44
1:B:280:GLY:HA2	1:E:354:THR:HG23	2.00	0.44
1:F:237:ALA:HA	1:F:240:LEU:HD12	1.99	0.44
1:G:272:GLY:CA	1:H:282:ASP:HA	2.48	0.44
1:B:273:ARG:H	1:B:273:ARG:HG2	1.55	0.43
1:F:273:ARG:HG2	1:F:273:ARG:H	1.61	0.43
1:I:310:GLY:HA3	1:I:313:HIS:CE1	2.53	0.43
1:L:230:LEU:HA	1:L:233:ALA:HB3	2.01	0.43
1:A:315:TRP:CD1	1:A:318:LEU:HD13	2.53	0.43
1:B:243:GLN:HE22	1:C:223:ILE:HD12	1.82	0.43
1:J:326:LEU:HA	1:J:329:THR:HG22	1.99	0.43
1:E:310:GLY:HA3	1:E:313:HIS:CE1	2.54	0.43
1:I:355:LEU:HB2	1:I:363:PHE:CE2	2.54	0.43
1:B:237:ALA:HA	1:B:240:LEU:HD12	2.00	0.43
1:B:351:GLY:O	1:B:354:THR:HG22	2.19	0.43
1:H:237:ALA:HA	1:H:240:LEU:HD12	2.00	0.43
1:A:311:ALA:C	1:A:313:HIS:N	2.72	0.43
1:I:326:LEU:HA	1:I:329:THR:HG22	1.99	0.43
1:J:355:LEU:HB2	1:J:363:PHE:CE2	2.54	0.43
1:B:372:ILE:HA	1:B:376:VAL:HG22	2.01	0.43
1:E:355:LEU:HB2	1:E:363:PHE:CE2	2.54	0.43
1:I:237:ALA:HA	1:I:240:LEU:HD12	2.01	0.43
1:K:326:LEU:HA	1:K:329:THR:HG22	2.00	0.43
1:L:229:LEU:O	1:L:233:ALA:HB2	2.19	0.43
1:D:224:THR:HG22	1:D:225:SER:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:ALA:HA	1:D:240:LEU:HD12	2.00	0.42
1:G:273:ARG:HG2	1:G:273:ARG:H	1.56	0.42
1:K:237:ALA:HA	1:K:240:LEU:HD12	2.01	0.42
1:C:355:LEU:HB2	1:C:363:PHE:CE2	2.54	0.42
1:H:355:LEU:HB2	1:H:363:PHE:CE2	2.55	0.42
1:C:237:ALA:HA	1:C:240:LEU:HD12	2.01	0.42
1:E:237:ALA:HA	1:E:240:LEU:HD12	2.01	0.42
1:E:273:ARG:HG2	1:E:273:ARG:H	1.59	0.42
1:E:351:GLY:O	1:E:354:THR:HG22	2.20	0.42
1:A:237:ALA:HA	1:A:240:LEU:HD12	2.02	0.42
1:I:315:TRP:CD1	1:I:318:LEU:HD13	2.54	0.42
1:K:355:LEU:HB2	1:K:363:PHE:CD2	2.55	0.42
1:H:310:GLY:HA3	1:H:313:HIS:CE1	2.55	0.42
1:K:355:LEU:HB2	1:K:363:PHE:CE2	2.54	0.42
1:F:372:ILE:HA	1:F:376:VAL:HG22	2.02	0.42
1:L:256:SER:HA	1:L:260:ASP:OD2	2.20	0.42
1:E:355:LEU:HB2	1:E:363:PHE:CD2	2.55	0.41
1:G:237:ALA:HA	1:G:240:LEU:HD12	2.02	0.41
1:J:355:LEU:HB2	1:J:363:PHE:CD2	2.55	0.41
1:A:351:GLY:O	1:A:354:THR:HG22	2.20	0.41
1:G:355:LEU:HB2	1:G:363:PHE:CD2	2.55	0.41
1:H:355:LEU:HB2	1:H:363:PHE:CD2	2.55	0.41
1:C:339:GLN:HE21	1:C:376:VAL:HG12	1.85	0.41
1:C:351:GLY:O	1:C:354:THR:HG22	2.21	0.41
1:F:355:LEU:HB2	1:F:363:PHE:CE2	2.56	0.41
1:D:351:GLY:O	1:D:354:THR:HG22	2.21	0.41
1:I:355:LEU:HB2	1:I:363:PHE:CD2	2.56	0.41
1:A:283:ARG:CD	1:A:306:MSE:HE3	2.51	0.40
1:A:355:LEU:HB2	1:A:363:PHE:CD2	2.56	0.40
1:E:281:PRO:HA	1:E:284:ARG:HG2	2.03	0.40
1:F:355:LEU:HB2	1:F:363:PHE:CD2	2.56	0.40
1:L:234:ARG:HD3	1:L:308:ALA:HB1	2.03	0.40
1:A:258:ARG:NH2	1:A:312:SER:H	2.19	0.40
1:C:355:LEU:HB2	1:C:363:PHE:CD2	2.56	0.40
1:D:355:LEU:HB2	1:D:363:PHE:CD2	2.56	0.40
1:H:224:THR:HG22	1:H:225:SER:H	1.87	0.40
1:I:372:ILE:HA	1:I:376:VAL:HG22	2.03	0.40
1:J:237:ALA:HA	1:J:240:LEU:HD12	2.02	0.40
1:I:262:LEU:HA	1:I:262:LEU:HD13	1.98	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	155/157 (99%)	140 (90%)	10 (6%)	5 (3%)	4	24
1	B	155/157 (99%)	141 (91%)	9 (6%)	5 (3%)	4	24
1	C	155/157 (99%)	140 (90%)	10 (6%)	5 (3%)	4	24
1	D	155/157 (99%)	141 (91%)	9 (6%)	5 (3%)	4	24
1	E	155/157 (99%)	142 (92%)	8 (5%)	5 (3%)	4	24
1	F	155/157 (99%)	141 (91%)	9 (6%)	5 (3%)	4	24
1	G	155/157 (99%)	140 (90%)	9 (6%)	6 (4%)	3	20
1	H	155/157 (99%)	141 (91%)	9 (6%)	5 (3%)	4	24
1	I	155/157 (99%)	141 (91%)	8 (5%)	6 (4%)	3	20
1	J	155/157 (99%)	141 (91%)	9 (6%)	5 (3%)	4	24
1	K	155/157 (99%)	141 (91%)	9 (6%)	5 (3%)	4	24
1	L	155/157 (99%)	138 (89%)	13 (8%)	4 (3%)	5	28
All	All	1860/1884 (99%)	1687 (91%)	112 (6%)	61 (3%)	4	24

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	PRO
1	A	267	PRO
1	B	223	ILE
1	B	266	PRO
1	B	267	PRO
1	C	223	ILE
1	C	266	PRO
1	C	267	PRO
1	D	223	ILE
1	D	266	PRO
1	D	267	PRO
1	E	266	PRO

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Mol	Chain	Res	Type
1	E	267	PRO
1	F	266	PRO
1	F	267	PRO
1	G	266	PRO
1	G	267	PRO
1	H	266	PRO
1	H	267	PRO
1	I	245	GLU
1	I	266	PRO
1	I	267	PRO
1	J	223	ILE
1	J	266	PRO
1	J	267	PRO
1	K	266	PRO
1	K	267	PRO
1	L	266	PRO
1	L	267	PRO
1	A	223	ILE
1	A	313	HIS
1	B	313	HIS
1	C	313	HIS
1	D	313	HIS
1	E	223	ILE
1	E	313	HIS
1	F	223	ILE
1	F	313	HIS
1	G	223	ILE
1	G	312	SER
1	G	313	HIS
1	H	223	ILE
1	H	313	HIS
1	I	223	ILE
1	I	313	HIS
1	J	313	HIS
1	K	223	ILE
1	K	313	HIS
1	L	223	ILE
1	A	312	SER
1	D	312	SER
1	E	312	SER
1	F	312	SER
1	H	312	SER

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Mol	Chain	Res	Type
1	J	312	SER
1	K	312	SER
1	L	313	HIS
1	B	312	SER
1	C	312	SER
1	I	312	SER
1	G	265	LEU

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	118/129 (92%)	99 (84%)	19 (16%)	2	10
1	B	118/129 (92%)	100 (85%)	18 (15%)	2	12
1	C	118/129 (92%)	101 (86%)	17 (14%)	3	14
1	D	118/129 (92%)	102 (86%)	16 (14%)	3	16
1	E	118/129 (92%)	104 (88%)	14 (12%)	5	20
1	F	118/129 (92%)	103 (87%)	15 (13%)	4	18
1	G	118/129 (92%)	102 (86%)	16 (14%)	3	16
1	H	118/129 (92%)	102 (86%)	16 (14%)	3	16
1	I	118/129 (92%)	103 (87%)	15 (13%)	4	18
1	J	118/129 (92%)	103 (87%)	15 (13%)	4	18
1	K	118/129 (92%)	102 (86%)	16 (14%)	3	16
1	L	118/129 (92%)	105 (89%)	13 (11%)	6	24
All	All	1416/1548 (92%)	1226 (87%)	190 (13%)	4	16

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	THR
1	A	229	LEU
1	A	245	GLU

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Mol	Chain	Res	Type
1	A	253	LEU
1	A	257	VAL
1	A	273	ARG
1	A	297	LEU
1	A	301	GLU
1	A	305	ASP
1	A	306	MSE
1	A	313	HIS
1	A	314	LEU
1	A	317	ASP
1	A	347	LEU
1	A	354	THR
1	A	361	MSE
1	A	369	LEU
1	A	370	SER
1	A	377	MSE
1	B	229	LEU
1	B	245	GLU
1	B	253	LEU
1	B	257	VAL
1	B	271	ASP
1	B	273	ARG
1	B	297	LEU
1	B	301	GLU
1	B	305	ASP
1	B	306	MSE
1	B	313	HIS
1	B	314	LEU
1	B	317	ASP
1	B	347	LEU
1	B	354	THR
1	B	361	MSE
1	B	369	LEU
1	B	370	SER
1	C	229	LEU
1	C	245	GLU
1	C	253	LEU
1	C	257	VAL
1	C	273	ARG
1	C	297	LEU
1	C	301	GLU
1	C	305	ASP

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Mol	Chain	Res	Type
1	C	306	MSE
1	C	313	HIS
1	C	314	LEU
1	C	317	ASP
1	C	347	LEU
1	C	354	THR
1	C	361	MSE
1	C	369	LEU
1	C	370	SER
1	D	245	GLU
1	D	253	LEU
1	D	257	VAL
1	D	271	ASP
1	D	273	ARG
1	D	297	LEU
1	D	301	GLU
1	D	305	ASP
1	D	306	MSE
1	D	313	HIS
1	D	314	LEU
1	D	317	ASP
1	D	347	LEU
1	D	354	THR
1	D	361	MSE
1	D	369	LEU
1	E	229	LEU
1	E	245	GLU
1	E	253	LEU
1	E	257	VAL
1	E	273	ARG
1	E	297	LEU
1	E	301	GLU
1	E	306	MSE
1	E	313	HIS
1	E	314	LEU
1	E	317	ASP
1	E	347	LEU
1	E	361	MSE
1	E	369	LEU
1	F	229	LEU
1	F	245	GLU
1	F	253	LEU

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Mol	Chain	Res	Type
1	F	257	VAL
1	F	273	ARG
1	F	297	LEU
1	F	301	GLU
1	F	305	ASP
1	F	306	MSE
1	F	313	HIS
1	F	314	LEU
1	F	317	ASP
1	F	347	LEU
1	F	361	MSE
1	F	369	LEU
1	G	245	GLU
1	G	253	LEU
1	G	257	VAL
1	G	271	ASP
1	G	273	ARG
1	G	297	LEU
1	G	301	GLU
1	G	305	ASP
1	G	306	MSE
1	G	313	HIS
1	G	314	LEU
1	G	317	ASP
1	G	347	LEU
1	G	354	THR
1	G	361	MSE
1	G	369	LEU
1	H	229	LEU
1	H	245	GLU
1	H	253	LEU
1	H	257	VAL
1	H	268	LEU
1	H	273	ARG
1	H	297	LEU
1	H	301	GLU
1	H	305	ASP
1	H	306	MSE
1	H	313	HIS
1	H	314	LEU
1	H	317	ASP
1	H	347	LEU

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Mol	Chain	Res	Type
1	H	361	MSE
1	H	369	LEU
1	I	229	LEU
1	I	245	GLU
1	I	253	LEU
1	I	257	VAL
1	I	273	ARG
1	I	297	LEU
1	I	299	LEU
1	I	305	ASP
1	I	306	MSE
1	I	313	HIS
1	I	314	LEU
1	I	317	ASP
1	I	347	LEU
1	I	361	MSE
1	I	369	LEU
1	J	245	GLU
1	J	253	LEU
1	J	257	VAL
1	J	273	ARG
1	J	292	LEU
1	J	297	LEU
1	J	301	GLU
1	J	305	ASP
1	J	306	MSE
1	J	313	HIS
1	J	314	LEU
1	J	317	ASP
1	J	347	LEU
1	J	361	MSE
1	J	369	LEU
1	K	229	LEU
1	K	245	GLU
1	K	253	LEU
1	K	257	VAL
1	K	268	LEU
1	K	273	ARG
1	K	297	LEU
1	K	301	GLU
1	K	305	ASP
1	K	306	MSE

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Mol	Chain	Res	Type
1	K	313	HIS
1	K	314	LEU
1	K	317	ASP
1	K	347	LEU
1	K	361	MSE
1	K	369	LEU
1	L	229	LEU
1	L	239	TYR
1	L	273	ARG
1	L	297	LEU
1	L	301	GLU
1	L	305	ASP
1	L	306	MSE
1	L	314	LEU
1	L	317	ASP
1	L	347	LEU
1	L	361	MSE
1	L	369	LEU
1	L	373	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	HIS
1	A	339	GLN
1	B	243	GLN
1	B	339	GLN
1	B	374	GLN
1	C	227	GLN
1	C	339	GLN
1	D	339	GLN
1	E	339	GLN
1	F	243	GLN
1	F	264	GLN
1	F	339	GLN
1	G	243	GLN
1	G	313	HIS
1	G	339	GLN
1	H	243	GLN
1	H	339	GLN
1	I	339	GLN
1	J	243	GLN

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Mol	Chain	Res	Type
1	J	339	GLN
1	K	243	GLN
1	K	339	GLN
1	L	323	HIS

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	153/157 (97%)	0.04	4 (2%) 56 59	54, 76, 109, 162	0
1	B	153/157 (97%)	0.05	7 (4%) 32 36	57, 81, 116, 175	0
1	C	153/157 (97%)	0.12	6 (3%) 39 43	63, 102, 138, 171	0
1	D	153/157 (97%)	0.16	7 (4%) 32 36	65, 98, 130, 168	0
1	E	153/157 (97%)	0.09	2 (1%) 77 81	57, 95, 135, 170	0
1	F	153/157 (97%)	0.13	4 (2%) 56 59	69, 106, 145, 160	0
1	G	153/157 (97%)	0.08	6 (3%) 39 43	66, 89, 119, 176	0
1	H	153/157 (97%)	0.14	9 (5%) 22 26	74, 109, 149, 167	0
1	I	153/157 (97%)	0.59	16 (10%) 6 8	76, 134, 169, 181	0
1	J	153/157 (97%)	0.36	9 (5%) 22 26	93, 125, 159, 178	0
1	K	153/157 (97%)	0.41	12 (7%) 13 16	92, 122, 157, 178	0
1	L	153/157 (97%)	2.90	75 (49%) 0 0	121, 184, 211, 221	0
All	All	1836/1884 (97%)	0.42	157 (8%) 10 13	54, 106, 182, 221	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	221	SER	13.7
1	L	264	GLN	13.3
1	L	266	PRO	12.5
1	L	291	TYR	11.0
1	L	222	ALA	10.5
1	L	267	PRO	9.9
1	L	328	GLN	9.8
1	L	223	ILE	9.5
1	L	244	PRO	9.5
1	L	246	GLY	9.1
1	L	225	SER	8.6

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Mol	Chain	Res	Type	RSRZ
1	L	323	HIS	8.6
1	L	265	LEU	8.2
1	L	293	GLN	7.8
1	E	223	ILE	7.7
1	L	249	ALA	7.3
1	G	223	ILE	7.1
1	L	231	SER	6.9
1	L	327	LEU	6.9
1	L	245	GLU	6.8
1	L	235	VAL	6.7
1	L	330	GLY	6.7
1	L	292	LEU	6.7
1	B	223	ILE	6.4
1	L	243	GLN	6.3
1	K	223	ILE	6.2
1	K	311	ALA	6.1
1	I	224	THR	5.8
1	L	224	THR	5.7
1	E	224	THR	5.6
1	L	305	ASP	5.5
1	J	223	ILE	5.5
1	L	294	GLN	5.2
1	F	223	ILE	5.2
1	L	263	HIS	5.0
1	D	223	ILE	4.9
1	L	251	HIS	4.9
1	L	269	SER	4.8
1	I	223	ILE	4.8
1	L	250	ALA	4.7
1	G	222	ALA	4.6
1	L	279	PRO	4.6
1	L	242	ASP	4.6
1	L	321	TYR	4.5
1	C	223	ILE	4.5
1	I	311	ALA	4.5
1	D	222	ALA	4.3
1	D	224	THR	4.3
1	I	328	GLN	4.2
1	H	223	ILE	4.2
1	L	282	ASP	4.2
1	L	309	ARG	4.2
1	L	329	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	L	308	ALA	4.0
1	L	247	TRP	3.9
1	C	224	THR	3.9
1	L	331	LYS	3.9
1	K	221	SER	3.8
1	L	261	THR	3.7
1	L	295	ASN	3.6
1	L	313	HIS	3.6
1	C	282	ASP	3.6
1	K	224	THR	3.5
1	L	228	GLU	3.5
1	L	271	ASP	3.5
1	L	351	GLY	3.4
1	L	350	PRO	3.4
1	L	311	ALA	3.3
1	L	281	PRO	3.3
1	G	224	THR	3.3
1	D	311	ALA	3.3
1	L	232	GLN	3.3
1	L	283	ARG	3.2
1	L	358	ASN	3.2
1	B	222	ALA	3.2
1	K	270	ALA	3.2
1	K	359	ASP	3.2
1	L	227	GLN	3.2
1	L	288	LYS	3.2
1	K	271	ASP	3.1
1	L	272	GLY	3.1
1	L	268	LEU	3.1
1	L	256	SER	3.1
1	F	311	ALA	3.0
1	L	270	ALA	3.0
1	K	310	GLY	3.0
1	D	221	SER	2.9
1	I	222	ALA	2.9
1	L	319	GLN	2.9
1	L	334	TYR	2.9
1	B	224	THR	2.9
1	L	240	LEU	2.8
1	I	293	GLN	2.8
1	I	375	GLN	2.8
1	L	304	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	371	TRP	2.7
1	H	373	GLN	2.7
1	L	326	LEU	2.7
1	J	282	ASP	2.7
1	I	267	PRO	2.7
1	I	272	GLY	2.7
1	H	224	THR	2.6
1	H	376	VAL	2.6
1	L	260	ASP	2.6
1	L	226	GLY	2.6
1	B	375	GLN	2.6
1	L	320	TRP	2.6
1	H	222	ALA	2.6
1	B	221	SER	2.5
1	A	223	ILE	2.5
1	K	245	GLU	2.5
1	I	269	SER	2.5
1	K	313	HIS	2.5
1	A	224	THR	2.4
1	I	360	GLY	2.4
1	C	221	SER	2.4
1	I	227	GLN	2.4
1	I	268	LEU	2.4
1	B	267	PRO	2.4
1	G	267	PRO	2.3
1	J	224	THR	2.3
1	L	315	TRP	2.3
1	K	273	ARG	2.3
1	I	242	ASP	2.3
1	L	348	ARG	2.3
1	L	257	VAL	2.3
1	C	252	ARG	2.3
1	L	230	LEU	2.3
1	J	222	ALA	2.2
1	L	324	GLN	2.2
1	J	363	PHE	2.2
1	H	268	LEU	2.2
1	L	332	GLU	2.2
1	A	313	HIS	2.2
1	G	221	SER	2.2
1	L	355	LEU	2.2
1	D	312	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	221	SER	2.1
1	L	290	LEU	2.1
1	A	221	SER	2.1
1	B	311	ALA	2.1
1	F	224	THR	2.1
1	J	374	GLN	2.1
1	J	373	GLN	2.1
1	J	296	TRP	2.1
1	D	268	LEU	2.1
1	F	267	PRO	2.1
1	H	267	PRO	2.1
1	G	311	ALA	2.1
1	L	241	ARG	2.1
1	C	267	PRO	2.1
1	J	366	ASP	2.1
1	H	311	ALA	2.0
1	K	376	VAL	2.0
1	L	299	LEU	2.0
1	H	313	HIS	2.0
1	I	295	ASN	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.