wwPDB X-ray Structure Validation Summary Report (i)

Oct 24, 2023 – 11:32 PM EDT

PDB ID	:	3FZJ
Title	:	TsaR low resolution crystal structure, tetragonal form
Authors	:	Monferrer, D.; Tralau, T.; Kertesz, M.A.; Dix, I.; Kikhney, A.G.; Svergun, D.I.; Uson, I.
Deposited on	:	2009-01-26
Resolution	:	7.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

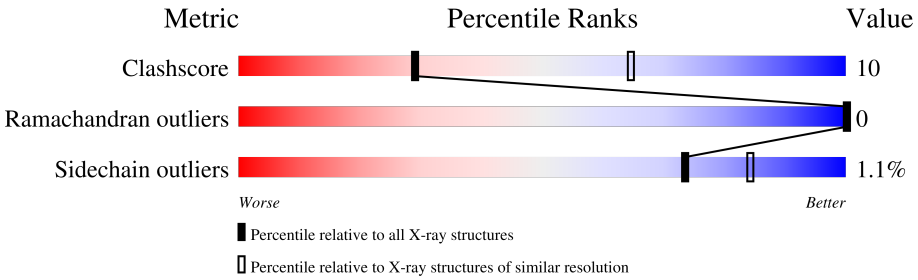
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 7.10 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	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	305	88% 9% •
1	B	305	85% 12% •
1	C	305	85% 12% •
1	D	305	87% 10% • •
1	E	305	84% 13% •
1	F	305	87% 10% • •
1	G	305	86% 11% •
1	H	305	84% 12% •

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Mol	Chain	Length	Quality of chain
1	I	305	
1	J	305	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 22575 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 LysR type regulator of tsaMBCD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	1	0
			2277	1450	409	409	9			
1	B	296	Total	C	N	O	S	0	2	0
			2238	1420	403	406	9			
1	C	296	Total	C	N	O	S	0	1	0
			2277	1450	409	409	9			
1	D	296	Total	C	N	O	S	0	2	0
			2238	1420	403	406	9			
1	E	296	Total	C	N	O	S	0	1	0
			2277	1450	409	409	9			
1	F	296	Total	C	N	O	S	0	2	0
			2238	1420	403	406	9			
1	G	296	Total	C	N	O	S	0	1	0
			2277	1450	409	409	9			
1	H	296	Total	C	N	O	S	0	2	0
			2238	1420	403	406	9			
1	I	296	Total	C	N	O	S	0	1	0
			2277	1450	409	409	9			
1	J	296	Total	C	N	O	S	0	2	0
			2238	1420	403	406	9			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	LEU	-	SEE REMARK 999	UNP P94678
A	300	HIS	-	expression tag	UNP P94678
A	301	HIS	-	expression tag	UNP P94678
A	302	HIS	-	expression tag	UNP P94678
A	303	HIS	-	expression tag	UNP P94678
A	304	HIS	-	expression tag	UNP P94678
A	305	HIS	-	expression tag	UNP P94678
B	2	LEU	-	SEE REMARK 999	UNP P94678
B	300	HIS	-	expression tag	UNP P94678

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Chain	Residue	Modelled	Actual	Comment	Reference
B	301	HIS	-	expression tag	UNP P94678
B	302	HIS	-	expression tag	UNP P94678
B	303	HIS	-	expression tag	UNP P94678
B	304	HIS	-	expression tag	UNP P94678
B	305	HIS	-	expression tag	UNP P94678
C	2	LEU	-	SEE REMARK 999	UNP P94678
C	300	HIS	-	expression tag	UNP P94678
C	301	HIS	-	expression tag	UNP P94678
C	302	HIS	-	expression tag	UNP P94678
C	303	HIS	-	expression tag	UNP P94678
C	304	HIS	-	expression tag	UNP P94678
C	305	HIS	-	expression tag	UNP P94678
D	2	LEU	-	SEE REMARK 999	UNP P94678
D	300	HIS	-	expression tag	UNP P94678
D	301	HIS	-	expression tag	UNP P94678
D	302	HIS	-	expression tag	UNP P94678
D	303	HIS	-	expression tag	UNP P94678
D	304	HIS	-	expression tag	UNP P94678
D	305	HIS	-	expression tag	UNP P94678
E	2	LEU	-	SEE REMARK 999	UNP P94678
E	300	HIS	-	expression tag	UNP P94678
E	301	HIS	-	expression tag	UNP P94678
E	302	HIS	-	expression tag	UNP P94678
E	303	HIS	-	expression tag	UNP P94678
E	304	HIS	-	expression tag	UNP P94678
E	305	HIS	-	expression tag	UNP P94678
F	2	LEU	-	SEE REMARK 999	UNP P94678
F	300	HIS	-	expression tag	UNP P94678
F	301	HIS	-	expression tag	UNP P94678
F	302	HIS	-	expression tag	UNP P94678
F	303	HIS	-	expression tag	UNP P94678
F	304	HIS	-	expression tag	UNP P94678
F	305	HIS	-	expression tag	UNP P94678
G	2	LEU	-	SEE REMARK 999	UNP P94678
G	300	HIS	-	expression tag	UNP P94678
G	301	HIS	-	expression tag	UNP P94678
G	302	HIS	-	expression tag	UNP P94678
G	303	HIS	-	expression tag	UNP P94678
G	304	HIS	-	expression tag	UNP P94678
G	305	HIS	-	expression tag	UNP P94678
H	2	LEU	-	SEE REMARK 999	UNP P94678
H	300	HIS	-	expression tag	UNP P94678

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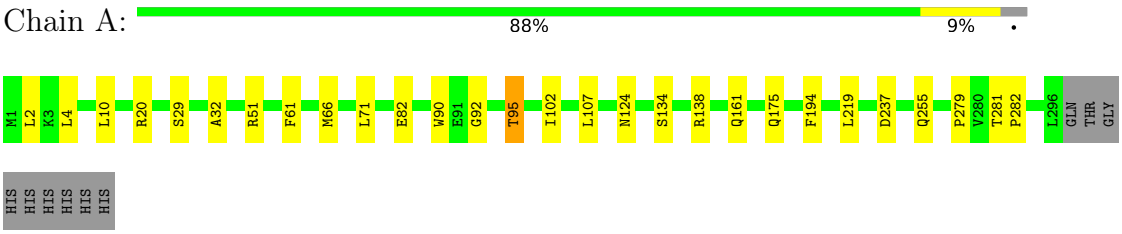
Chain	Residue	Modelled	Actual	Comment	Reference
H	301	HIS	-	expression tag	UNP P94678
H	302	HIS	-	expression tag	UNP P94678
H	303	HIS	-	expression tag	UNP P94678
H	304	HIS	-	expression tag	UNP P94678
H	305	HIS	-	expression tag	UNP P94678
I	2	LEU	-	SEE REMARK 999	UNP P94678
I	300	HIS	-	expression tag	UNP P94678
I	301	HIS	-	expression tag	UNP P94678
I	302	HIS	-	expression tag	UNP P94678
I	303	HIS	-	expression tag	UNP P94678
I	304	HIS	-	expression tag	UNP P94678
I	305	HIS	-	expression tag	UNP P94678
J	2	LEU	-	SEE REMARK 999	UNP P94678
J	300	HIS	-	expression tag	UNP P94678
J	301	HIS	-	expression tag	UNP P94678
J	302	HIS	-	expression tag	UNP P94678
J	303	HIS	-	expression tag	UNP P94678
J	304	HIS	-	expression tag	UNP P94678
J	305	HIS	-	expression tag	UNP P94678

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. 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. 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.

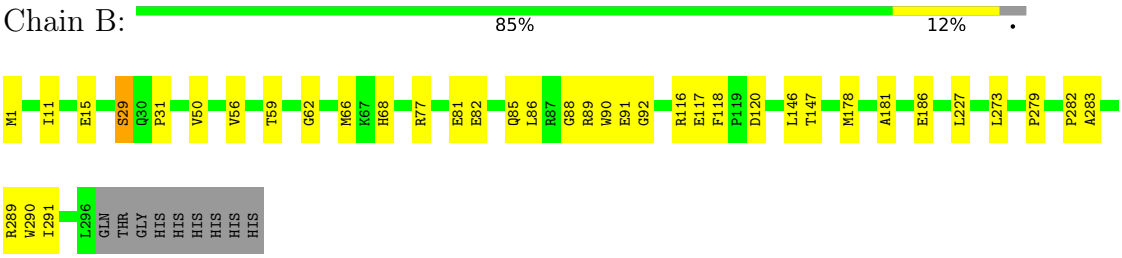
• Molecule 1: LysR type regulator of tsaMBCD

Chain A:



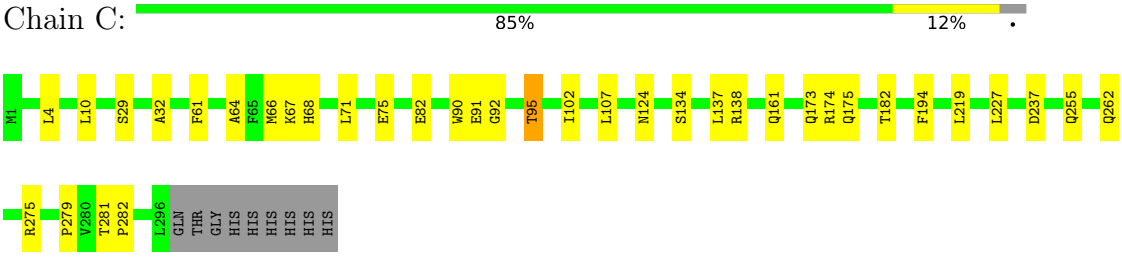
• Molecule 1: LysR type regulator of tsaMBCD

Chain B:



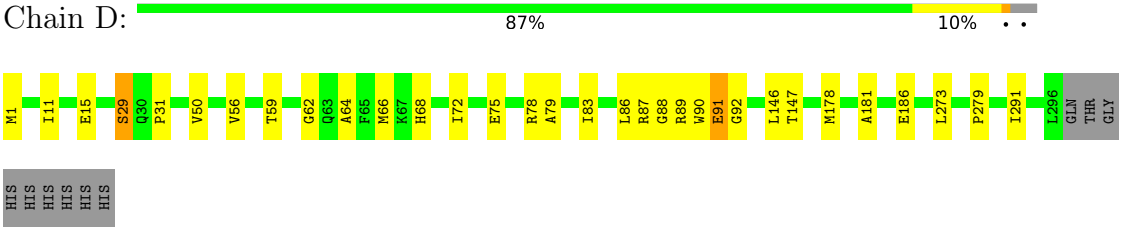
• Molecule 1: LysR type regulator of tsaMBCD

Chain C:



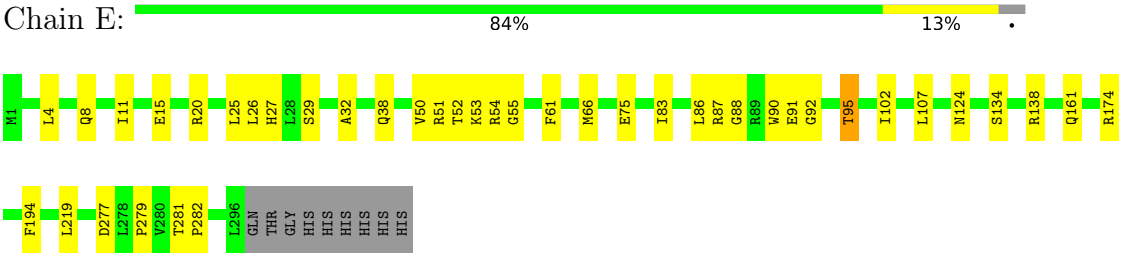
• Molecule 1: LysR type regulator of tsaMBCD

Chain D:



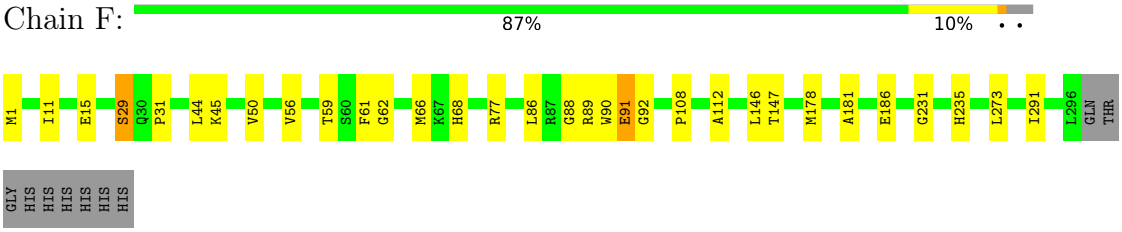
• Molecule 1: LysR type regulator of tsaMBCD

Chain E:



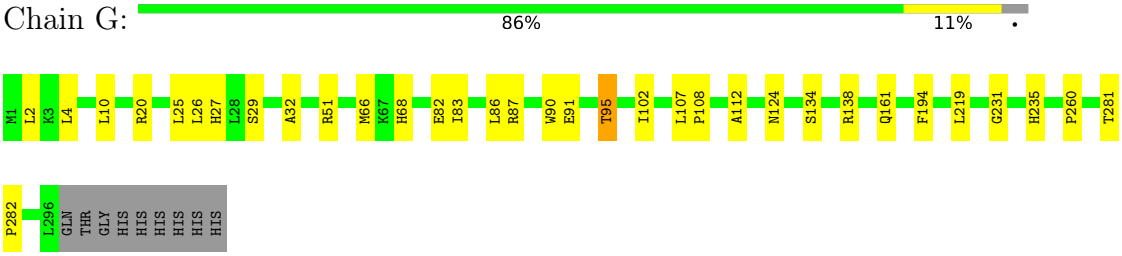
• Molecule 1: LysR type regulator of tsaMBCD

Chain F:



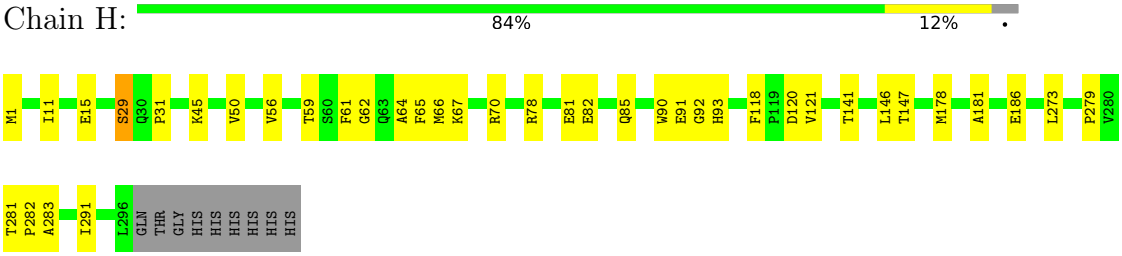
• Molecule 1: LysR type regulator of tsaMBCD

Chain G:



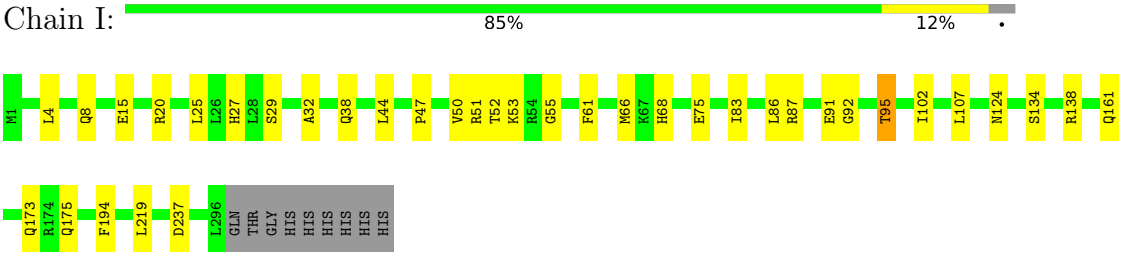
• Molecule 1: LysR type regulator of tsaMBCD

Chain H:



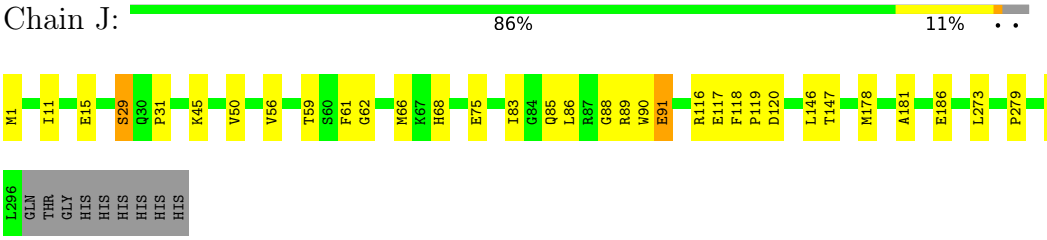
• Molecule 1: LysR type regulator of tsaMBCD

Chain I:



• Molecule 1: LysR type regulator of tsaMBCD

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	204.37Å 204.37Å 336.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.34 – 7.10 42.34 – 7.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.34-7.10) 99.8 (42.34-7.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	4.46 (at 7.34Å)	Xtriage
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	535 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	360.0	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 128.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.71	EDS
Total number of atoms	22575	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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	0.60	0/2326	0.65	0/3168
1	B	0.64	0/2292	0.76	5/3122 (0.2%)
1	C	0.60	0/2326	0.65	0/3168
1	D	0.88	1/2292 (0.0%)	0.67	1/3122 (0.0%)
1	E	0.60	0/2326	0.65	0/3168
1	F	0.82	1/2292 (0.0%)	0.75	4/3122 (0.1%)
1	G	0.60	0/2326	0.65	0/3168
1	H	0.64	0/2291	0.67	1/3119 (0.0%)
1	I	0.60	0/2326	0.65	0/3168
1	J	0.66	1/2292 (0.0%)	0.82	4/3122 (0.1%)
All	All	0.67	3/23089 (0.0%)	0.69	15/31447 (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	J	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	91	GLU	C-N	29.07	1.85	1.33
1	F	91	GLU	C-N	25.23	1.78	1.33
1	J	91	GLU	C-N	-8.99	1.16	1.33

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	91	GLU	O-C-N	-20.20	88.86	123.20
1	F	91	GLU	O-C-N	-17.07	94.19	123.20
1	B	91	GLU	O-C-N	-13.03	101.04	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	91	GLU	CA-C-N	12.41	141.02	116.20
1	J	91	GLU	C-N-CA	11.59	146.63	122.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	91	GLU	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	2277	0	2308	26	31
1	B	2238	0	2234	77	0
1	C	2277	0	2308	106	1
1	D	2238	0	2235	52	20
1	E	2277	0	2305	106	3
1	F	2238	0	2235	39	17
1	G	2277	0	2308	47	33
1	H	2238	0	2235	87	0
1	I	2277	0	2306	81	23
1	J	2238	0	2235	60	0
All	All	22575	0	22709	435	64

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 10.

The worst 5 of 435 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:E:20:ARG:NH2	1:I:61:PHE:CE1	1.87	1.38
1:C:90:TRP:NE1	1:C:281:THR:HG22	1.07	1.36
1:F:91:GLU:C	1:F:92:GLY:N	1.78	1.35
1:C:68:HIS:CD2	1:D:79:ALA:HA	1.65	1.31
1:D:91:GLU:C	1:D:92:GLY:N	1.85	1.30

The worst 5 of 64 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:F:88:GLY:C	1:G:51:ARG:NH2[5_545]	0.17	2.03
1:F:90:TRP:CD1	1:G:51:ARG:CD[5_545]	0.34	1.86
1:A:51:ARG:CZ	1:D:88:GLY:O[6_544]	0.48	1.72
1:A:51:ARG:CZ	1:D:88:GLY:C[6_544]	0.77	1.43
1:G:27:HIS:CE1	1:I:237:ASP:CB[3_445]	0.99	1.21

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	292/305 (96%)	286 (98%)	6 (2%)	0	100	100
1	B	295/305 (97%)	290 (98%)	5 (2%)	0	100	100
1	C	292/305 (96%)	286 (98%)	6 (2%)	0	100	100
1	D	295/305 (97%)	290 (98%)	5 (2%)	0	100	100
1	E	292/305 (96%)	286 (98%)	6 (2%)	0	100	100
1	F	295/305 (97%)	290 (98%)	5 (2%)	0	100	100
1	G	292/305 (96%)	286 (98%)	6 (2%)	0	100	100
1	H	293/305 (96%)	288 (98%)	5 (2%)	0	100	100
1	I	292/305 (96%)	286 (98%)	6 (2%)	0	100	100
1	J	295/305 (97%)	290 (98%)	5 (2%)	0	100	100
All	All	2933/3050 (96%)	2878 (98%)	55 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	237/248 (96%)	235 (99%)	2 (1%)	81	89
1	B	229/248 (92%)	226 (99%)	3 (1%)	69	81
1	C	237/248 (96%)	235 (99%)	2 (1%)	81	89
1	D	229/248 (92%)	226 (99%)	3 (1%)	69	81
1	E	237/248 (96%)	235 (99%)	2 (1%)	81	89
1	F	229/248 (92%)	226 (99%)	3 (1%)	69	81
1	G	237/248 (96%)	235 (99%)	2 (1%)	81	89
1	H	229/248 (92%)	226 (99%)	3 (1%)	69	81
1	I	237/248 (96%)	235 (99%)	2 (1%)	81	89
1	J	229/248 (92%)	226 (99%)	3 (1%)	69	81
All	All	2330/2480 (94%)	2305 (99%)	25 (1%)	73	84

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	147	THR
1	H	29	SER
1	J	147	THR
1	G	161	GLN
1	H	56	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	292	GLN
1	C	68	HIS
1	C	175	GLN
1	E	27	HIS

5.3.3 RNA

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 monosaccharides 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	G	1
1	A	1
1	C	1
1	I	1
1	H	1
1	E	1
1	D	1
1	F	1
1	J	1

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	91:GLU	C	92:GLY	N	3.41
1	A	91:GLU	C	92:GLY	N	3.14
1	C	91:GLU	C	92:GLY	N	2.52
1	I	91:GLU	C	92:GLY	N	2.38
1	H	91:GLU	C	92:GLY	N	2.32

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.