Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:47 AM GMT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

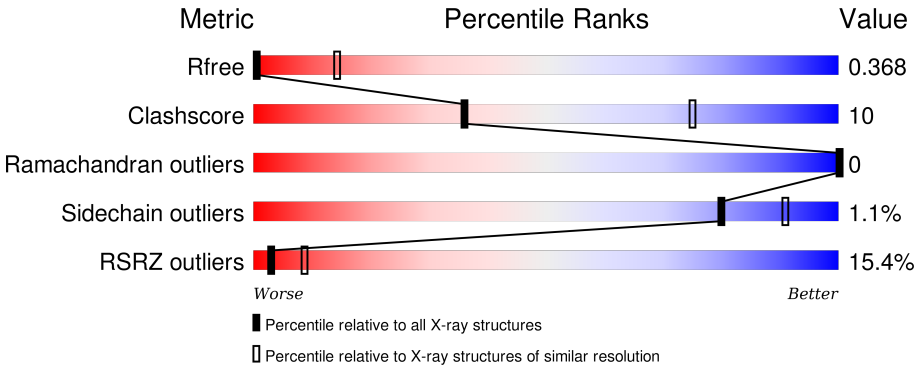
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (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.



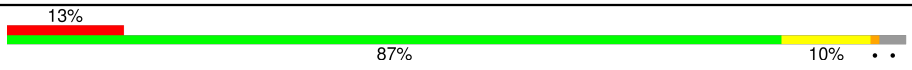
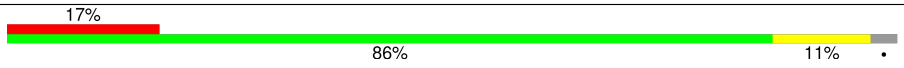
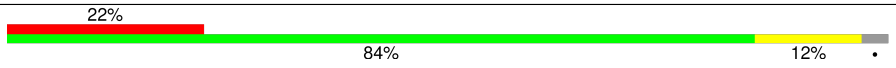
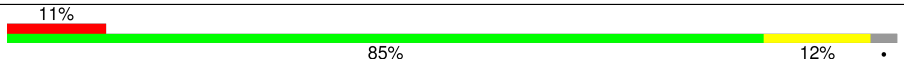
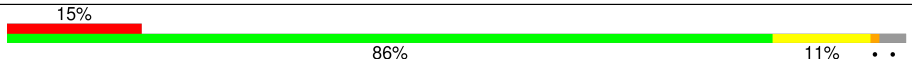
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	305	12% 88% 9% •
1	B	305	12% 85% 12% •
1	C	305	11% 85% 12% •
1	D	305	17% 87% 10% • •
1	E	305	18% 84% 13% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	305	
1	G	305	
1	H	305	
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

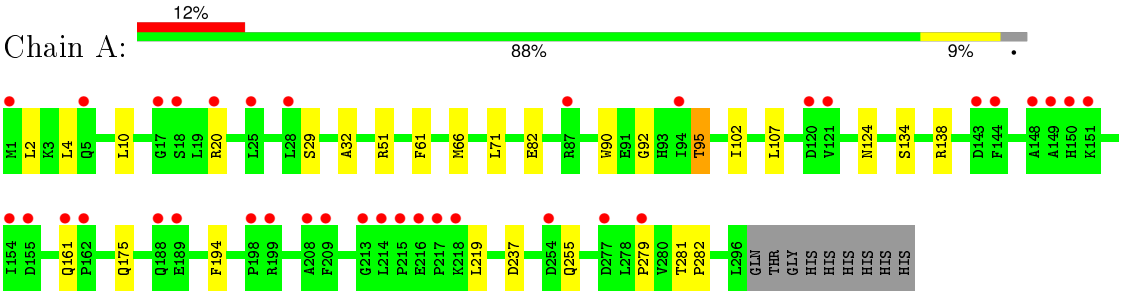
Chain	Residue	Modelled	Actual	Comment	Reference
H	301	HIS	-	EXPRESSION TAG	UNP P94678
H	302	HIS	-	EXPRESSION TAG	UNP P94678
H	303	HIS	-	EXPRESSION TAG	UNP P94678
H	304	HIS	-	EXPRESSION TAG	UNP P94678
H	305	HIS	-	EXPRESSION TAG	UNP P94678
I	2	LEU	-	SEE REMARK 999	UNP P94678
I	300	HIS	-	EXPRESSION TAG	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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

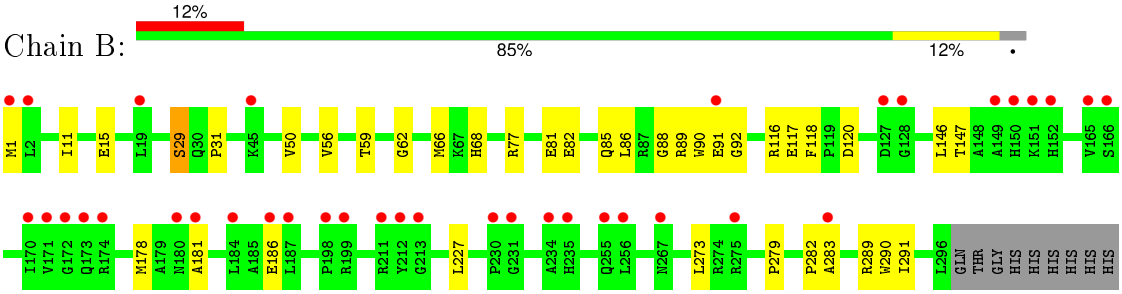
- Molecule 1: LysR type regulator of tsaMBCD

Chain A:



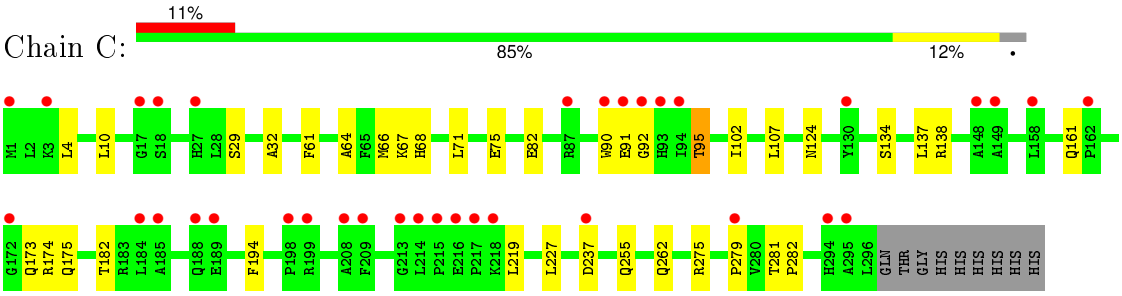
- Molecule 1: LysR type regulator of tsaMBCD

Chain B:



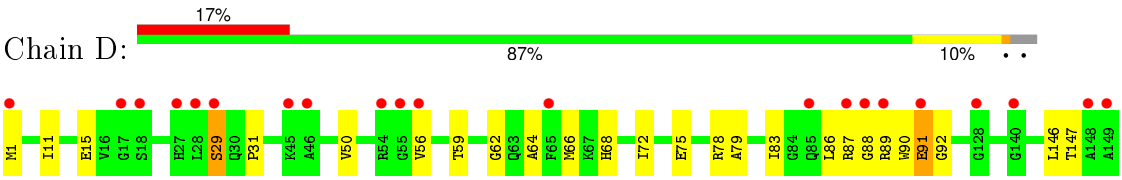
- Molecule 1: LysR type regulator of tsaMBCD

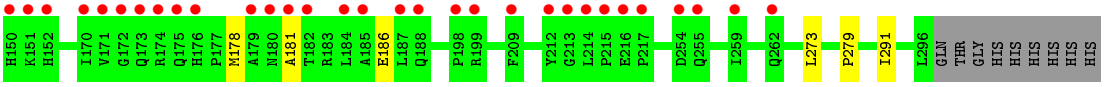
Chain C:



- Molecule 1: LysR type regulator of tsaMBCD

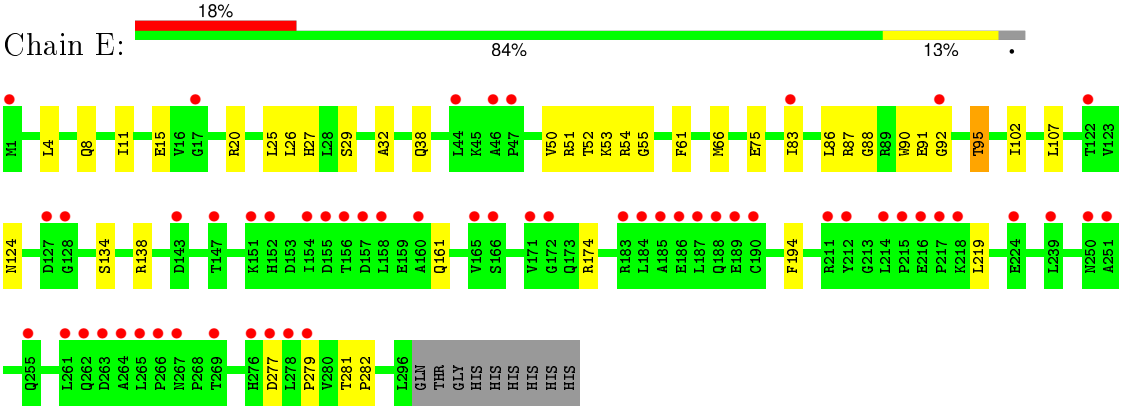
Chain D:





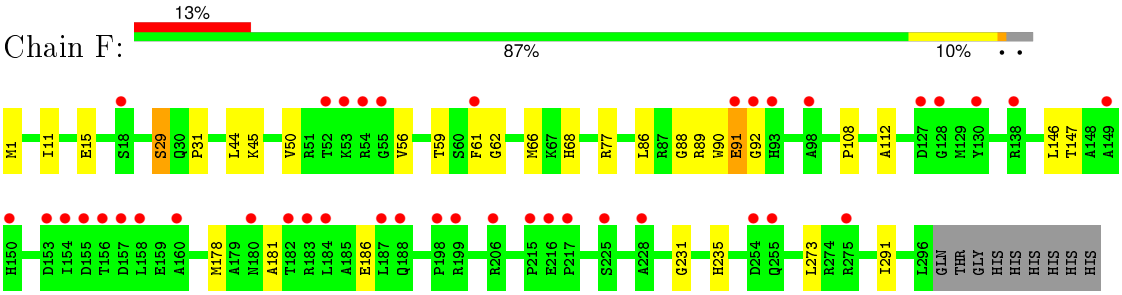
• Molecule 1: LysR type regulator of tsaMBCD

Chain E:



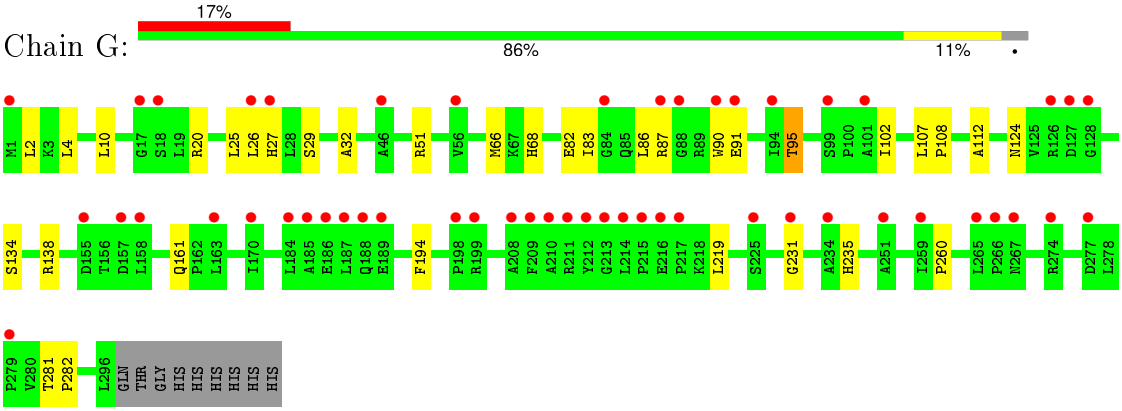
• Molecule 1: LysR type regulator of tsaMBCD

Chain F:



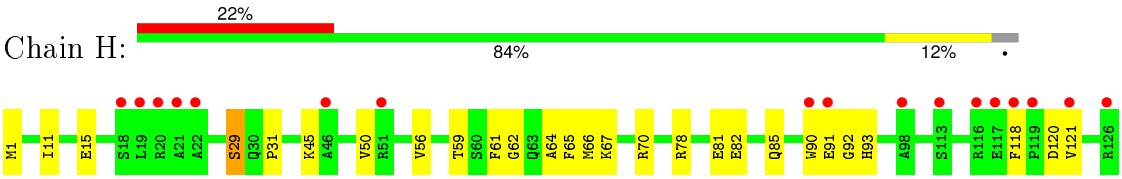
• Molecule 1: LysR type regulator of tsaMBCD

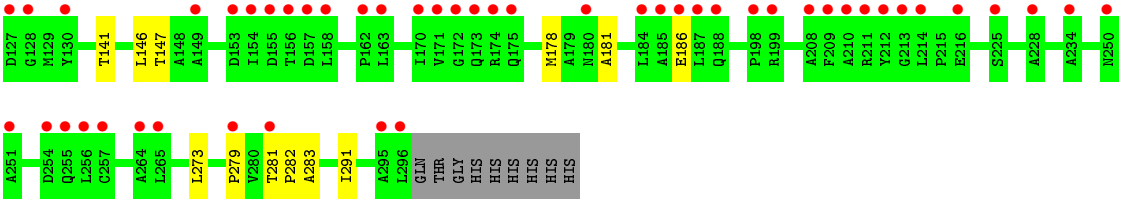
Chain G:



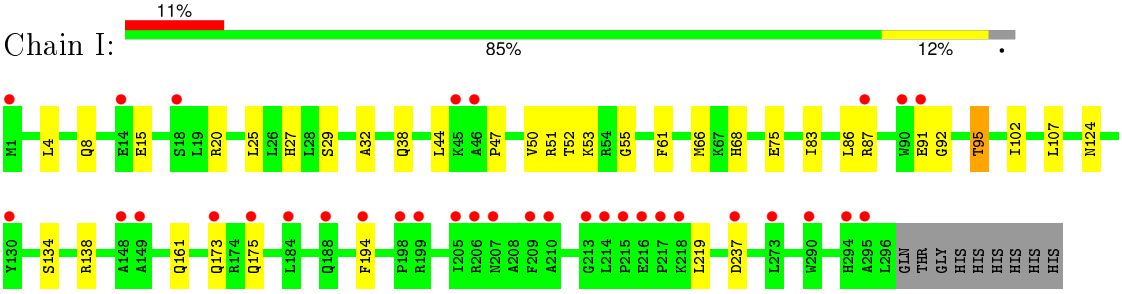
• Molecule 1: LysR type regulator of tsaMBCD

Chain H:

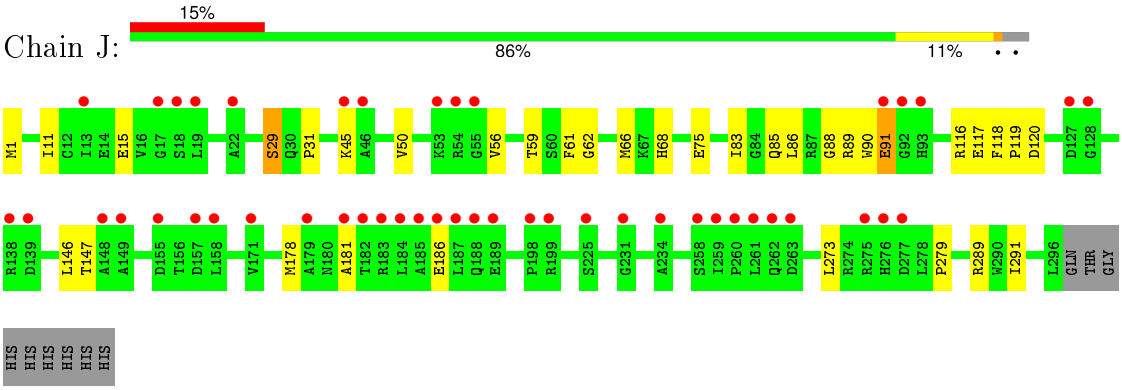




• Molecule 1: LysR type regulator of tsaMBCD



• Molecule 1: LysR type regulator of tsaMBCD



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) 0.374 , 0.368	Depositor DCC
R_{free} test set	535 reflections (5.00%)	DCC
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 , 130.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 11235 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.60	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

All (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

Continued on next page...

Continued from previous page...

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
1	B	91	GLU	CA-C-N	10.63	137.46	116.20
1	B	91	GLU	C-N-CA	9.99	143.27	122.30
1	F	91	GLU	CA-C-N	5.45	127.09	116.20
1	H	273	LEU	CB-CG-CD1	-5.17	102.21	111.00
1	D	273	LEU	CB-CG-CD1	-5.17	102.22	111.00
1	F	273	LEU	CB-CG-CD1	-5.15	102.25	111.00
1	B	273	LEU	CB-CG-CD1	-5.14	102.26	111.00
1	J	273	LEU	CB-CG-CD1	-5.14	102.27	111.00
1	F	77	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	77	ARG	NE-CZ-NH2	-5.03	117.79	120.30

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.

All (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:E:53:LYS:O	1:J:89:ARG:HA	1.20	1.30
1:D:91:GLU:C	1:D:92:GLY:N	1.85	1.30
1:C:237:ASP:OD2	1:E:27:HIS:CE1	1.88	1.27
1:C:90:TRP:NE1	1:C:281:THR:CG2	2.01	1.24
1:C:90:TRP:O	1:C:92:GLY:N	1.71	1.23
1:B:86:LEU:O	1:I:20:ARG:HD3	1.39	1.19
1:B:88:GLY:O	1:I:52:THR:O	1.59	1.19
1:A:61:PHE:CE1	1:I:20:ARG:NH2	2.12	1.17
1:C:175:GLN:HB2	1:E:26:LEU:HD21	1.21	1.17
1:G:68:HIS:CE1	1:H:279:PRO:HG2	1.81	1.16
1:C:90:TRP:CZ2	1:C:281:THR:HA	1.79	1.15
1:C:68:HIS:CG	1:D:79:ALA:HB2	1.82	1.13
1:E:90:TRP:NE1	1:E:281:THR:HG22	1.62	1.13
1:G:86:LEU:C	1:H:61:PHE:HE1	1.51	1.13
1:C:175:GLN:CB	1:E:26:LEU:HD21	1.78	1.12
1:E:55:GLY:HA2	1:J:88:GLY:HA3	1.23	1.11
1:E:55:GLY:HA2	1:J:88:GLY:CA	1.80	1.10
1:E:53:LYS:O	1:J:89:ARG:CA	1.99	1.10
1:H:90:TRP:HB3	1:H:118:PHE:HD1	1.08	1.09
1:G:90:TRP:O	1:G:281:THR:CG2	2.02	1.08
1:C:175:GLN:HB2	1:E:26:LEU:CD2	1.82	1.08
1:C:90:TRP:CE2	1:C:281:THR:HG22	1.89	1.06
1:E:90:TRP:CE2	1:E:281:THR:HG22	1.90	1.06
1:C:90:TRP:CH2	1:C:282:PRO:HD3	1.91	1.05
1:C:68:HIS:NE2	1:D:79:ALA:HA	1.71	1.05
1:C:175:GLN:CB	1:E:26:LEU:CD2	2.35	1.04
1:B:88:GLY:CA	1:I:55:GLY:HA2	1.87	1.04
1:C:68:HIS:CD2	1:D:79:ALA:CA	2.41	1.03
1:C:90:TRP:HE1	1:C:281:THR:CG2	1.65	1.02
1:B:88:GLY:HA3	1:I:55:GLY:HA2	1.04	1.01
1:H:85:GLN:OE1	1:H:283:ALA:N	1.93	1.01
1:C:255:GLN:HG2	1:E:15:GLU:OE2	1.60	1.01
1:H:85:GLN:NE2	1:H:283:ALA:HB2	1.74	1.01
1:C:175:GLN:NE2	1:E:8:GLN:HB3	1.76	1.00
1:A:90:TRP:NE1	1:A:281:THR:HG22	1.76	1.00
1:C:67:LYS:HD3	1:D:279:PRO:HB3	1.42	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:TRP:CE3	1:H:118:PHE:CE1	2.50	0.99
1:C:237:ASP:CG	1:E:27:HIS:CE1	2.36	0.99
1:H:90:TRP:CD2	1:H:118:PHE:HE1	1.81	0.98
1:C:67:LYS:HB3	1:D:279:PRO:HG3	1.41	0.98
1:E:20:ARG:NH2	1:I:61:PHE:HE1	1.32	0.98
1:C:68:HIS:CB	1:D:79:ALA:HB2	1.93	0.97
1:E:91:GLU:C	1:E:92:GLY:N	2.17	0.97
1:I:87:ARG:HD3	1:J:45:LYS:O	1.64	0.97
1:B:88:GLY:HA3	1:I:55:GLY:CA	1.95	0.97
1:G:90:TRP:O	1:G:281:THR:HG21	1.65	0.96
1:G:86:LEU:C	1:H:61:PHE:CE1	2.39	0.95
1:B:117:GLU:HA	1:I:50:VAL:HG23	1.45	0.95
1:H:90:TRP:HB3	1:H:118:PHE:CD1	2.01	0.95
1:C:90:TRP:HZ2	1:C:281:THR:HA	1.25	0.94
1:I:75:GLU:OE2	1:J:68:HIS:ND1	2.00	0.94
1:E:90:TRP:CZ2	1:E:281:THR:HA	2.04	0.92
1:B:117:GLU:CA	1:I:50:VAL:HG23	2.01	0.91
1:H:82:GLU:HA	1:H:282:PRO:HD2	1.51	0.91
1:A:71:LEU:HD11	1:B:279:PRO:HD3	1.53	0.90
1:E:86:LEU:HB3	1:F:61:PHE:CE1	2.05	0.90
1:C:68:HIS:CG	1:D:79:ALA:CB	2.56	0.89
1:H:90:TRP:CD2	1:H:118:PHE:CE1	2.60	0.89
1:G:90:TRP:O	1:G:281:THR:HG22	1.72	0.89
1:H:85:GLN:NE2	1:H:283:ALA:CB	2.36	0.88
1:I:87:ARG:CD	1:J:45:LYS:O	2.22	0.88
1:B:86:LEU:HB3	1:I:20:ARG:NH1	1.89	0.88
1:F:178:MET:HE3	1:F:181:ALA:HB2	1.52	0.88
1:B:89:ARG:HA	1:I:53:LYS:HA	1.54	0.87
1:C:90:TRP:CD1	1:C:281:THR:HG22	2.10	0.87
1:C:255:GLN:HG2	1:E:15:GLU:CD	1.95	0.87
1:C:67:LYS:CB	1:D:279:PRO:HG3	2.04	0.87
1:B:178:MET:HE3	1:B:181:ALA:HB2	1.56	0.86
1:C:237:ASP:OD2	1:E:27:HIS:NE2	2.09	0.85
1:H:90:TRP:CB	1:H:118:PHE:HD1	1.88	0.85
1:E:86:LEU:HB3	1:F:61:PHE:HE1	1.40	0.85
1:C:90:TRP:CH2	1:C:282:PRO:CD	2.58	0.84
1:B:117:GLU:C	1:I:50:VAL:HG23	1.96	0.84
1:C:175:GLN:NE2	1:E:8:GLN:CB	2.40	0.84
1:C:175:GLN:HB3	1:E:26:LEU:CD2	2.09	0.83
1:A:82:GLU:OE1	1:B:68:HIS:NE2	2.12	0.83
1:H:91:GLU:C	1:H:92:GLY:N	2.32	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:178:MET:HE3	1:H:181:ALA:HB2	1.58	0.83
1:E:53:LYS:C	1:J:89:ARG:HA	1.99	0.82
1:J:90:TRP:O	1:J:120:ASP:HB2	1.78	0.82
1:H:90:TRP:CE3	1:H:118:PHE:HE1	1.95	0.82
1:E:55:GLY:CA	1:J:88:GLY:HA3	2.06	0.82
1:C:61:PHE:CE1	1:D:87:ARG:HG2	2.14	0.82
1:E:279:PRO:HD3	1:F:50:VAL:CG1	2.09	0.82
1:H:85:GLN:CB	1:H:282:PRO:HB2	2.09	0.81
1:C:61:PHE:HE1	1:D:87:ARG:HG2	1.44	0.81
1:C:68:HIS:CD2	1:D:79:ALA:CB	2.63	0.81
1:B:86:LEU:HB3	1:I:20:ARG:HH11	1.45	0.81
1:D:178:MET:HE3	1:D:181:ALA:HB2	1.61	0.81
1:E:95:THR:HB	1:E:124:ASN:HB3	1.63	0.81
1:J:178:MET:HE3	1:J:181:ALA:HB2	1.62	0.81
1:A:95:THR:HB	1:A:124:ASN:HB3	1.63	0.80
1:B:117:GLU:O	1:I:50:VAL:HG23	1.82	0.80
1:C:255:GLN:CG	1:E:15:GLU:OE2	2.30	0.80
1:G:95:THR:HB	1:G:124:ASN:HB3	1.63	0.79
1:C:175:GLN:HB3	1:E:26:LEU:HD22	1.63	0.79
1:E:90:TRP:NE1	1:E:281:THR:CG2	2.44	0.79
1:C:95:THR:HB	1:C:124:ASN:HB3	1.63	0.78
1:I:95:THR:HB	1:I:124:ASN:HB3	1.63	0.78
1:I:86:LEU:HB3	1:J:61:PHE:CE1	2.19	0.78
1:E:279:PRO:HD3	1:F:50:VAL:HG11	1.66	0.77
1:I:91:GLU:C	1:I:92:GLY:N	2.38	0.77
1:G:86:LEU:CB	1:H:61:PHE:CD1	2.69	0.76
1:I:68:HIS:ND1	1:J:75:GLU:OE2	2.17	0.76
1:E:52:THR:O	1:J:90:TRP:HD1	1.68	0.75
1:C:90:TRP:HE1	1:C:281:THR:HG22	0.93	0.75
1:B:89:ARG:HA	1:I:53:LYS:CA	2.16	0.74
1:E:55:GLY:N	1:J:88:GLY:O	2.19	0.74
1:H:91:GLU:C	1:H:121:VAL:HG22	2.07	0.74
1:G:86:LEU:HB3	1:H:61:PHE:CD1	2.22	0.74
1:C:67:LYS:CD	1:D:279:PRO:HB3	2.16	0.74
1:C:75:GLU:HG2	1:D:72:ILE:HG13	1.70	0.74
1:H:85:GLN:OE1	1:H:282:PRO:HB2	1.88	0.73
1:C:75:GLU:OE2	1:D:68:HIS:HA	1.88	0.73
1:H:85:GLN:HB3	1:H:282:PRO:HB2	1.71	0.73
1:G:82:GLU:CD	1:H:64:ALA:HB1	2.08	0.72
1:E:50:VAL:HG23	1:J:116:ARG:O	1.89	0.72
1:G:86:LEU:HB2	1:H:61:PHE:HD1	1.53	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LEU:O	1:I:20:ARG:CD	2.28	0.71
1:G:68:HIS:CE1	1:H:279:PRO:CG	2.70	0.71
1:G:87:ARG:HD3	1:H:45:LYS:O	1.90	0.71
1:G:87:ARG:CD	1:H:45:LYS:O	2.38	0.71
1:C:90:TRP:C	1:C:92:GLY:N	2.45	0.71
1:A:71:LEU:HD11	1:B:279:PRO:CD	2.20	0.70
1:C:71:LEU:HD12	1:D:75:GLU:OE2	1.90	0.70
1:C:175:GLN:NE2	1:E:8:GLN:CA	2.55	0.70
1:E:20:ARG:HD3	1:J:86:LEU:O	1.92	0.70
1:G:86:LEU:HB3	1:H:61:PHE:CE1	2.26	0.70
1:F:91:GLU:O	1:F:92:GLY:N	2.25	0.69
1:E:50:VAL:CG2	1:J:116:ARG:O	2.40	0.69
1:H:70:ARG:HD3	1:H:141:THR:HG21	1.75	0.69
1:J:178:MET:CE	1:J:181:ALA:HB2	2.23	0.68
1:A:90:TRP:CZ2	1:A:281:THR:HA	2.28	0.68
1:F:178:MET:CE	1:F:181:ALA:HB2	2.23	0.68
1:C:61:PHE:CE1	1:D:87:ARG:CG	2.76	0.68
1:C:68:HIS:NE2	1:D:79:ALA:CA	2.53	0.68
1:C:68:HIS:CE1	1:D:79:ALA:N	2.61	0.68
1:E:20:ARG:HH22	1:I:61:PHE:HE1	0.83	0.68
1:G:86:LEU:O	1:H:61:PHE:HE1	1.75	0.68
1:D:178:MET:CE	1:D:181:ALA:HB2	2.23	0.68
1:I:86:LEU:CB	1:J:61:PHE:CE1	2.76	0.68
1:E:279:PRO:HG3	1:F:50:VAL:HG12	1.75	0.68
1:H:178:MET:CE	1:H:181:ALA:HB2	2.23	0.67
1:H:85:GLN:CD	1:H:283:ALA:H	1.97	0.67
1:E:279:PRO:CD	1:F:50:VAL:CG1	2.72	0.67
1:E:52:THR:O	1:J:90:TRP:CD1	2.48	0.67
1:E:90:TRP:O	1:E:92:GLY:N	2.28	0.67
1:E:75:GLU:OE2	1:F:68:HIS:ND1	2.19	0.67
1:B:178:MET:CE	1:B:181:ALA:HB2	2.23	0.66
1:E:279:PRO:CG	1:F:50:VAL:CG1	2.74	0.66
1:I:44:LEU:O	1:J:83:ILE:HG21	1.96	0.66
1:I:86:LEU:CB	1:J:61:PHE:HE1	2.09	0.66
1:C:90:TRP:HH2	1:C:282:PRO:HD3	1.54	0.66
1:B:116:ARG:O	1:I:50:VAL:HG21	1.94	0.66
1:G:86:LEU:CB	1:H:61:PHE:HD1	2.09	0.66
1:C:237:ASP:CG	1:E:27:HIS:HE1	1.98	0.66
1:G:87:ARG:N	1:H:61:PHE:CE1	2.63	0.66
1:B:90:TRP:CE3	1:B:118:PHE:CD1	2.84	0.66
1:B:86:LEU:CB	1:I:20:ARG:HH11	2.09	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:GLN:HE22	1:E:8:GLN:CB	2.07	0.65
1:B:89:ARG:HA	1:I:53:LYS:O	1.96	0.65
1:B:289[B]:ARG:CD	1:I:38:GLN:OE1	2.44	0.65
1:A:71:LEU:CD1	1:B:279:PRO:CD	2.74	0.65
1:I:86:LEU:HB3	1:J:61:PHE:HE1	1.59	0.65
1:B:82:GLU:HG3	1:B:282:PRO:CD	2.27	0.65
1:B:289[B]:ARG:HD2	1:I:38:GLN:HE22	1.61	0.65
1:C:237:ASP:CB	1:E:27:HIS:HE1	2.10	0.65
1:E:279:PRO:HD3	1:F:50:VAL:HG12	1.79	0.65
1:I:44:LEU:O	1:J:83:ILE:CG2	2.45	0.65
1:A:4:LEU:HB3	1:B:1:MET:SD	2.37	0.65
1:H:82:GLU:HG3	1:H:282:PRO:HD3	1.79	0.65
1:B:86:LEU:CB	1:I:20:ARG:NH1	2.60	0.64
1:G:86:LEU:HB2	1:H:61:PHE:CD1	2.30	0.64
1:E:279:PRO:CG	1:F:50:VAL:HG12	2.28	0.64
1:J:178:MET:HE1	1:J:186:GLU:HB3	1.80	0.64
1:B:90:TRP:O	1:B:120:ASP:HB2	1.97	0.64
1:B:117:GLU:O	1:I:50:VAL:CG2	2.45	0.64
1:C:175:GLN:HE22	1:E:8:GLN:CA	2.11	0.63
1:D:178:MET:HE1	1:D:186:GLU:HB3	1.80	0.63
1:H:82:GLU:HG3	1:H:282:PRO:CD	2.28	0.63
1:C:91:GLU:C	1:C:92:GLY:N	2.52	0.63
1:E:83:ILE:HG21	1:F:44:LEU:HB3	1.81	0.63
1:G:86:LEU:CB	1:H:61:PHE:CE1	2.81	0.62
1:F:108:PRO:HB3	1:G:231:GLY:O	1.98	0.62
1:E:4:LEU:HB3	1:F:1:MET:SD	2.38	0.62
1:E:279:PRO:CD	1:F:50:VAL:HG11	2.30	0.62
1:H:81:GLU:OE2	1:H:92:GLY:HA2	2.00	0.62
1:I:86:LEU:C	1:J:61:PHE:HE1	2.04	0.62
1:B:289[B]:ARG:HD3	1:I:38:GLN:OE1	1.99	0.61
1:B:90:TRP:NE1	1:I:51:ARG:CB	2.29	0.61
1:H:91:GLU:HG2	1:H:120:ASP:CB	2.30	0.61
1:B:82:GLU:OE2	1:B:282:PRO:HD3	2.00	0.61
1:F:112:ALA:HB2	1:G:235:HIS:O	2.01	0.61
1:E:53:LYS:HA	1:J:90:TRP:H	1.67	0.60
1:B:89:ARG:HA	1:I:53:LYS:C	2.22	0.60
1:A:90:TRP:HE1	1:A:281:THR:HG22	1.66	0.60
1:C:75:GLU:HB3	1:D:72:ILE:CG1	2.32	0.59
1:B:117:GLU:HA	1:I:50:VAL:CG2	2.27	0.59
1:C:173:GLN:NE2	1:E:25:LEU:HD23	2.17	0.59
1:A:90:TRP:CH2	1:A:282:PRO:HD3	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:178:MET:HE1	1:H:186:GLU:HB3	1.84	0.59
1:H:82:GLU:CG	1:H:282:PRO:HD3	2.33	0.59
1:C:237:ASP:CB	1:E:27:HIS:CE1	2.86	0.58
1:C:68:HIS:CG	1:D:79:ALA:CA	2.84	0.58
1:C:90:TRP:CZ2	1:C:281:THR:CA	2.72	0.58
1:C:173:GLN:HE22	1:E:26:LEU:HD23	1.68	0.58
1:E:54:ARG:C	1:J:88:GLY:O	2.42	0.58
1:C:75:GLU:CG	1:D:72:ILE:HG13	2.32	0.58
1:B:90:TRP:HB2	1:I:51:ARG:HG3	1.81	0.58
1:G:86:LEU:O	1:H:61:PHE:CE1	2.54	0.58
1:G:82:GLU:OE2	1:H:64:ALA:HB1	2.04	0.58
1:E:86:LEU:CB	1:F:61:PHE:CE1	2.84	0.58
1:E:51:ARG:O	1:J:119:PRO:HD2	2.03	0.57
1:C:175:GLN:HE22	1:E:8:GLN:HA	1.70	0.57
1:E:38:GLN:OE1	1:J:289[B]:ARG:CD	2.53	0.57
1:G:90:TRP:HB2	1:H:61:PHE:HZ	1.70	0.57
1:H:85:GLN:CD	1:H:283:ALA:HB2	2.23	0.57
1:B:89:ARG:CA	1:I:53:LYS:O	2.53	0.57
1:E:90:TRP:CD1	1:E:281:THR:HG22	2.37	0.57
1:B:178:MET:HE1	1:B:186:GLU:HB3	1.87	0.57
1:C:71:LEU:CD1	1:D:75:GLU:OE2	2.52	0.57
1:C:255:GLN:CD	1:E:15:GLU:OE2	2.43	0.56
1:A:279:PRO:HG3	1:B:50:VAL:CG1	2.35	0.56
1:G:91:GLU:HG2	1:G:282:PRO:CD	2.34	0.56
1:C:175:GLN:HE21	1:E:8:GLN:C	2.08	0.56
1:E:90:TRP:CH2	1:E:282:PRO:HD3	2.40	0.56
1:I:83:ILE:HD12	1:J:61:PHE:HB3	1.85	0.56
1:I:75:GLU:CD	1:J:68:HIS:HD1	2.05	0.56
1:C:174:ARG:NH1	1:E:11:ILE:HG21	2.21	0.56
1:B:90:TRP:CZ3	1:B:118:PHE:CE1	2.93	0.56
1:E:86:LEU:HB3	1:F:61:PHE:CD1	2.40	0.56
1:C:4:LEU:HB3	1:D:1:MET:SD	2.45	0.56
1:G:2:LEU:HB3	1:H:1:MET:SD	2.46	0.56
1:H:91:GLU:HG2	1:H:120:ASP:HB3	1.88	0.56
1:E:20:ARG:CZ	1:I:61:PHE:HE1	2.12	0.55
1:A:61:PHE:CE1	1:I:20:ARG:CZ	2.88	0.55
1:E:53:LYS:O	1:J:88:GLY:O	2.24	0.55
1:H:85:GLN:HE22	1:H:283:ALA:HB3	1.70	0.55
1:A:71:LEU:CD1	1:B:279:PRO:HD2	2.35	0.55
1:E:51:ARG:N	1:J:117:GLU:O	2.31	0.55
1:J:90:TRP:O	1:J:120:ASP:CB	2.51	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ARG:O	1:I:50:VAL:CG2	2.55	0.55
1:I:87:ARG:HD2	1:J:45:LYS:O	2.05	0.54
1:I:66:MET:HE2	1:I:66:MET:HA	1.90	0.54
1:H:85:GLN:OE1	1:H:282:PRO:CB	2.54	0.54
1:H:81:GLU:OE2	1:H:92:GLY:CA	2.56	0.54
1:H:85:GLN:HE22	1:H:283:ALA:CB	2.18	0.53
1:H:81:GLU:CD	1:H:92:GLY:CA	2.77	0.53
1:E:87:ARG:HD3	1:F:45:LYS:O	2.08	0.53
1:E:134:SER:OG	1:E:138:ARG:NH1	2.42	0.53
1:H:82:GLU:HA	1:H:282:PRO:CD	2.33	0.53
1:H:81:GLU:CD	1:H:92:GLY:HA3	2.29	0.53
1:E:279:PRO:CD	1:F:50:VAL:HG12	2.36	0.53
1:E:66:MET:HA	1:E:66:MET:HE2	1.90	0.53
1:F:235:HIS:O	1:G:112:ALA:HB2	2.09	0.52
1:A:90:TRP:CD1	1:A:281:THR:HG22	2.43	0.52
1:A:134:SER:OG	1:A:138:ARG:NH1	2.42	0.52
1:B:90:TRP:CE3	1:B:118:PHE:HD1	2.26	0.52
1:B:90:TRP:CD1	1:I:51:ARG:CA	2.57	0.52
1:B:290:TRP:CZ2	1:I:47:PRO:HG3	2.44	0.52
1:H:85:GLN:HB2	1:H:282:PRO:HB2	1.88	0.52
1:B:289[B]:ARG:HD2	1:I:38:GLN:NE2	2.22	0.52
1:C:255:GLN:HG2	1:E:15:GLU:OE1	2.10	0.52
1:C:134:SER:OG	1:C:138:ARG:NH1	2.42	0.52
1:G:134:SER:OG	1:G:138:ARG:NH1	2.42	0.52
1:I:134:SER:OG	1:I:138:ARG:NH1	2.42	0.52
1:G:90:TRP:CB	1:H:61:PHE:HZ	2.22	0.52
1:B:89:ARG:HB2	1:I:53:LYS:O	2.10	0.52
1:E:53:LYS:C	1:J:88:GLY:O	2.49	0.51
1:C:90:TRP:CZ2	1:C:282:PRO:HD3	2.42	0.51
1:H:82:GLU:HG3	1:H:282:PRO:CG	2.41	0.51
1:H:91:GLU:HG2	1:H:120:ASP:HB2	1.91	0.51
1:H:85:GLN:CD	1:H:283:ALA:N	2.61	0.51
1:H:90:TRP:CG	1:H:118:PHE:CD1	2.98	0.51
1:F:178:MET:HE1	1:F:186:GLU:HB3	1.92	0.51
1:E:50:VAL:HG21	1:J:116:ARG:O	2.11	0.51
1:A:279:PRO:HD3	1:B:50:VAL:HG11	1.93	0.51
1:C:68:HIS:CE1	1:D:78:ARG:C	2.85	0.51
1:C:175:GLN:NE2	1:E:8:GLN:O	2.44	0.50
1:G:91:GLU:HA	1:G:282:PRO:HD2	1.93	0.50
1:G:87:ARG:HD2	1:H:45:LYS:O	2.11	0.50
1:I:68:HIS:CE1	1:J:279:PRO:HG2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:ARG:CD	1:F:45:LYS:HB2	2.42	0.49
1:H:91:GLU:CA	1:H:121:VAL:HG22	2.42	0.49
1:B:86:LEU:C	1:I:20:ARG:HH11	2.16	0.49
1:A:90:TRP:CE2	1:A:281:THR:HG22	2.46	0.49
1:C:71:LEU:HD13	1:D:75:GLU:CD	2.32	0.49
1:H:62:GLY:O	1:H:66:MET:HG2	2.13	0.49
1:F:62:GLY:O	1:F:66:MET:HG2	2.13	0.49
1:C:90:TRP:CH2	1:C:282:PRO:HD2	2.43	0.49
1:B:85:GLN:CD	1:B:283:ALA:HB2	2.33	0.49
1:C:175:GLN:CG	1:E:26:LEU:HD21	2.40	0.49
1:H:82:GLU:CA	1:H:282:PRO:HD2	2.32	0.49
1:E:279:PRO:HG3	1:F:50:VAL:CG1	2.41	0.49
1:E:51:ARG:HB3	1:J:118:PHE:HA	1.94	0.48
1:G:91:GLU:HG2	1:G:282:PRO:HD2	1.95	0.48
1:D:29:SER:OG	1:D:31:PRO:HD2	2.13	0.48
1:B:29:SER:OG	1:B:31:PRO:HD2	2.13	0.48
1:I:4:LEU:HB3	1:J:1:MET:SD	2.53	0.48
1:B:90:TRP:HD1	1:I:52:THR:N	2.11	0.48
1:J:29:SER:OG	1:J:31:PRO:HD2	2.13	0.48
1:C:90:TRP:CD1	1:C:281:THR:CG2	2.82	0.48
1:G:83:ILE:HD11	1:H:65:PHE:HB2	1.94	0.48
1:E:50:VAL:HG23	1:J:117:GLU:HA	1.95	0.48
1:B:88:GLY:C	1:I:55:GLY:HA2	2.34	0.48
1:I:194:PHE:CD2	1:I:219:LEU:HD13	2.49	0.48
1:B:62:GLY:O	1:B:66:MET:HG2	2.13	0.48
1:B:227:LEU:HA	1:C:227:LEU:HD13	1.96	0.48
1:A:194:PHE:CD2	1:A:219:LEU:HD13	2.49	0.48
1:H:29:SER:OG	1:H:31:PRO:HD2	2.13	0.48
1:E:194:PHE:CD2	1:E:219:LEU:HD13	2.49	0.48
1:B:81:GLU:CD	1:B:92:GLY:HA2	2.35	0.48
1:J:62:GLY:O	1:J:66:MET:HG2	2.13	0.48
1:D:62:GLY:O	1:D:66:MET:HG2	2.13	0.48
1:E:20:ARG:NH2	1:I:61:PHE:CZ	2.72	0.47
1:B:90:TRP:NE1	1:I:51:ARG:HB2	2.20	0.47
1:C:279:PRO:HD3	1:D:50:VAL:HG11	1.95	0.47
1:E:53:LYS:HA	1:J:90:TRP:N	2.30	0.47
1:F:29:SER:OG	1:F:31:PRO:HD2	2.13	0.47
1:G:194:PHE:CD2	1:G:219:LEU:HD13	2.49	0.47
1:C:255:GLN:OE1	1:E:15:GLU:OE2	2.33	0.47
1:A:66:MET:HE2	1:A:66:MET:HA	1.96	0.47
1:C:262:GLN:OE1	1:E:88:GLY:HA3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:HIS:HB3	1:D:79:ALA:HB2	1.89	0.47
1:E:51:ARG:NH2	1:J:85:GLN:O	2.48	0.47
1:B:90:TRP:CB	1:I:51:ARG:HG3	1.89	0.47
1:G:87:ARG:HA	1:H:61:PHE:CZ	2.50	0.47
1:C:194:PHE:CD2	1:C:219:LEU:HD13	2.49	0.47
1:E:86:LEU:CB	1:F:61:PHE:HE1	2.19	0.47
1:C:182:THR:HG21	1:E:87:ARG:NH2	2.29	0.47
1:C:68:HIS:HE1	1:D:78:ARG:HB3	1.80	0.47
1:H:91:GLU:CG	1:H:120:ASP:HB2	2.45	0.47
1:I:86:LEU:C	1:J:61:PHE:CE1	2.87	0.47
1:E:53:LYS:CA	1:J:89:ARG:HA	2.45	0.46
1:E:55:GLY:O	1:J:90:TRP:CD1	2.67	0.46
1:I:86:LEU:HB2	1:J:61:PHE:CD1	2.49	0.46
1:H:178:MET:CE	1:H:186:GLU:HB3	2.46	0.46
1:C:90:TRP:CE2	1:C:281:THR:CG2	2.79	0.46
1:I:87:ARG:HD3	1:J:45:LYS:C	2.33	0.46
1:E:90:TRP:CZ2	1:E:281:THR:CA	2.90	0.46
1:F:178:MET:CE	1:F:186:GLU:HB3	2.46	0.46
1:G:2:LEU:HD13	1:H:1:MET:HB3	1.98	0.46
1:B:89:ARG:CB	1:I:53:LYS:O	2.64	0.46
1:C:64:ALA:HB2	1:D:86:LEU:HD11	1.98	0.46
1:I:86:LEU:CB	1:J:61:PHE:CD1	2.98	0.46
1:G:4:LEU:HB3	1:H:1:MET:SD	2.55	0.46
1:C:61:PHE:HE1	1:D:87:ARG:CG	2.17	0.46
1:C:64:ALA:HB3	1:D:83:ILE:CD1	2.46	0.46
1:B:117:GLU:O	1:I:51:ARG:N	2.47	0.46
1:C:61:PHE:O	1:D:83:ILE:HD11	2.16	0.45
1:C:66:MET:HA	1:C:66:MET:HE2	1.97	0.45
1:C:61:PHE:CZ	1:D:87:ARG:HD2	2.52	0.45
1:G:10:LEU:HB3	1:G:66:MET:HE1	1.99	0.45
1:C:90:TRP:CZ2	1:C:282:PRO:CD	2.98	0.45
1:C:175:GLN:NE2	1:E:8:GLN:C	2.69	0.45
1:B:90:TRP:CG	1:I:51:ARG:HB3	2.33	0.45
1:B:82:GLU:HG3	1:B:282:PRO:CG	2.47	0.45
1:C:10:LEU:HB3	1:C:66:MET:HE1	1.99	0.45
1:E:90:TRP:CH2	1:E:281:THR:HA	2.49	0.45
1:B:178:MET:CE	1:B:186:GLU:HB3	2.46	0.45
1:B:11:ILE:O	1:B:15:GLU:HG2	2.17	0.45
1:C:67:LYS:CD	1:D:279:PRO:CB	2.92	0.45
1:D:11:ILE:O	1:D:15:GLU:HG2	2.17	0.45
1:G:82:GLU:OE2	1:H:67:LYS:NZ	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:TRP:CE3	1:H:118:PHE:CD1	3.03	0.45
1:D:178:MET:CE	1:D:186:GLU:HB3	2.46	0.45
1:B:88:GLY:O	1:I:55:GLY:N	2.49	0.45
1:C:67:LYS:HB2	1:D:279:PRO:HG3	1.94	0.45
1:H:70:ARG:HD3	1:H:141:THR:CG2	2.46	0.45
1:F:50:VAL:HG13	1:F:59:THR:HG22	1.99	0.44
1:C:68:HIS:CE1	1:D:79:ALA:CA	3.00	0.44
1:D:50:VAL:HG13	1:D:59:THR:HG22	2.00	0.44
1:H:11:ILE:O	1:H:15:GLU:HG2	2.17	0.44
1:A:90:TRP:O	1:A:92:GLY:N	2.50	0.44
1:G:66:MET:HA	1:G:66:MET:HE2	1.98	0.44
1:H:50:VAL:HG13	1:H:59:THR:HG22	1.99	0.44
1:J:11:ILE:O	1:J:15:GLU:HG2	2.17	0.44
1:B:85:GLN:O	1:I:51:ARG:CZ	2.66	0.44
1:E:86:LEU:CB	1:F:61:PHE:CD1	3.00	0.44
1:A:10:LEU:HB3	1:A:66:MET:HE1	2.00	0.44
1:J:50:VAL:HG13	1:J:59:THR:HG22	2.00	0.44
1:C:67:LYS:HD3	1:D:279:PRO:CB	2.31	0.44
1:F:11:ILE:O	1:F:15:GLU:HG2	2.17	0.44
1:B:117:GLU:HG3	1:I:50:VAL:HA	1.99	0.43
1:E:55:GLY:CA	1:J:88:GLY:O	2.66	0.43
1:E:277:ASP:O	1:F:50:VAL:HB	2.17	0.43
1:H:90:TRP:CG	1:H:118:PHE:CE1	3.05	0.43
1:H:85:GLN:HB3	1:H:282:PRO:CB	2.43	0.43
1:B:90:TRP:CH2	1:B:118:PHE:HE1	2.35	0.43
1:C:82:GLU:OE2	1:D:64:ALA:HB1	2.18	0.43
1:H:78:ARG:HG2	1:H:281:THR:HG21	1.99	0.43
1:E:53:LYS:O	1:J:89:ARG:N	2.50	0.43
1:I:29:SER:HB3	1:I:32:ALA:HB3	2.00	0.43
1:E:29:SER:HB3	1:E:32:ALA:HB3	2.00	0.43
1:B:50:VAL:HG13	1:B:59:THR:HG22	1.99	0.43
1:G:86:LEU:HD11	1:H:64:ALA:CB	2.49	0.43
1:B:89:ARG:CA	1:I:53:LYS:HA	2.37	0.43
1:E:87:ARG:CD	1:F:45:LYS:O	2.67	0.43
1:C:29:SER:HB3	1:C:32:ALA:HB3	2.00	0.43
1:A:29:SER:HB3	1:A:32:ALA:HB3	2.00	0.43
1:G:102:ILE:HG22	1:G:107:LEU:HG	2.01	0.42
1:A:61:PHE:HE1	1:I:20:ARG:CZ	2.31	0.42
1:F:231:GLY:O	1:G:108:PRO:HB3	2.19	0.42
1:A:102:ILE:HG22	1:A:107:LEU:HG	2.01	0.42
1:I:102:ILE:HG22	1:I:107:LEU:HG	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:146:LEU:HD11	1:H:291:ILE:HD13	2.02	0.42
1:J:178:MET:CE	1:J:186:GLU:HB3	2.46	0.42
1:G:29:SER:HB3	1:G:32:ALA:HB3	2.00	0.42
1:C:75:GLU:OE2	1:D:68:HIS:ND1	2.48	0.42
1:C:102:ILE:HG22	1:C:107:LEU:HG	2.01	0.42
1:F:112:ALA:CB	1:G:235:HIS:O	2.66	0.42
1:B:90:TRP:CD2	1:B:118:PHE:HD1	2.38	0.42
1:I:44:LEU:O	1:J:83:ILE:HG22	2.19	0.42
1:D:146:LEU:HD11	1:D:291:ILE:HD13	2.02	0.41
1:B:146:LEU:HD11	1:B:291:ILE:HD13	2.02	0.41
1:J:146:LEU:HD11	1:J:291:ILE:HD13	2.02	0.41
1:H:90:TRP:CD2	1:H:118:PHE:CD1	3.07	0.41
1:G:2:LEU:CB	1:H:1:MET:SD	3.08	0.41
1:E:102:ILE:HG22	1:E:107:LEU:HG	2.01	0.41
1:F:146:LEU:HD11	1:F:291:ILE:HD13	2.02	0.41
1:B:289[B]:ARG:HD3	1:I:38:GLN:CD	2.40	0.41
1:B:82:GLU:CG	1:B:282:PRO:CD	2.97	0.41
1:C:237:ASP:HB3	1:E:27:HIS:HE1	1.81	0.41
1:B:227:LEU:HD13	1:C:227:LEU:HA	2.03	0.41
1:C:68:HIS:HB2	1:D:79:ALA:HB2	1.89	0.40
1:H:81:GLU:CD	1:H:93:HIS:H	2.24	0.40
1:A:2:LEU:HD13	1:B:1:MET:HB3	2.02	0.40
1:C:61:PHE:O	1:D:83:ILE:CD1	2.70	0.40
1:H:90:TRP:CB	1:H:118:PHE:CD1	2.78	0.40
1:H:82:GLU:CG	1:H:282:PRO:CD	2.97	0.40
1:C:137:LEU:O	1:C:275:ARG:HD2	2.22	0.40

All (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
1:A:51:ARG:NE	1:D:88:GLY:O[6_544]	1.25	0.95
1:F:90:TRP:NE1	1:G:51:ARG:CD[5_545]	1.26	0.94
1:F:90:TRP:CD1	1:G:51:ARG:CG[5_545]	1.32	0.88
1:F:88:GLY:C	1:G:51:ARG:CZ[5_545]	1.33	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ARG:CD	1:D:90:TRP:CD1[6_544]	1.33	0.87
1:A:51:ARG:NH2	1:D:88:GLY:C[6_544]	1.35	0.85
1:F:88:GLY:O	1:G:51:ARG:NH2[5_545]	1.36	0.84
1:F:88:GLY:CA	1:G:51:ARG:NH2[5_545]	1.36	0.84
1:F:86:LEU:O	1:G:20:ARG:CD[5_545]	1.37	0.83
1:F:89:ARG:N	1:G:51:ARG:NH2[5_545]	1.39	0.81
1:A:20:ARG:NH1	1:D:87:ARG:CG[6_544]	1.39	0.81
1:A:51:ARG:NH1	1:D:88:GLY:O[6_544]	1.41	0.79
1:G:27:HIS:NE2	1:I:237:ASP:CB[3_445]	1.44	0.76
1:A:255:GLN:OE1	1:I:15:GLU:OE2[6_444]	1.46	0.74
1:F:90:TRP:CG	1:G:51:ARG:CG[5_545]	1.46	0.74
1:F:88:GLY:CA	1:G:51:ARG:CZ[5_545]	1.48	0.72
1:F:90:TRP:CD1	1:G:51:ARG:NE[5_545]	1.53	0.67
1:A:51:ARG:NH1	1:D:88:GLY:C[6_544]	1.53	0.67
1:A:51:ARG:NH1	1:D:88:GLY:CA[6_544]	1.53	0.67
1:E:174:ARG:NH2	1:G:260:PRO:CG[4_554]	1.55	0.65
1:A:51:ARG:NH2	1:D:89:ARG:N[6_544]	1.55	0.65
1:A:51:ARG:NH2	1:D:88:GLY:O[6_544]	1.55	0.65
1:F:88:GLY:CA	1:G:51:ARG:NH1[5_545]	1.55	0.65
1:G:27:HIS:CE1	1:I:237:ASP:CG[3_445]	1.55	0.65
1:F:88:GLY:O	1:G:51:ARG:CZ[5_545]	1.61	0.59
1:G:27:HIS:CD2	1:I:237:ASP:OD2[3_445]	1.63	0.57
1:A:175:GLN:NE2	1:I:8:GLN:CB[6_444]	1.65	0.55
1:A:51:ARG:NE	1:D:88:GLY:C[6_544]	1.70	0.50
1:F:90:TRP:CG	1:G:51:ARG:CD[5_545]	1.70	0.50
1:E:61:PHE:CZ	1:G:20:ARG:NH2[5_545]	1.71	0.49
1:A:20:ARG:NH2	1:C:61:PHE:CZ[6_544]	1.78	0.42
1:A:255:GLN:CD	1:I:15:GLU:OE2[6_444]	1.80	0.40
1:A:51:ARG:CG	1:D:90:TRP:CB[6_544]	1.80	0.40
1:G:25:LEU:O	1:I:237:ASP:OD1[3_445]	1.81	0.39
1:G:27:HIS:NE2	1:I:237:ASP:OD2[3_445]	1.82	0.38
1:G:27:HIS:NE2	1:I:237:ASP:CG[3_445]	1.86	0.34
1:A:20:ARG:NH1	1:D:87:ARG:CD[6_544]	1.86	0.34
1:A:175:GLN:NE2	1:I:8:GLN:CA[6_444]	1.86	0.34
1:A:51:ARG:CZ	1:D:89:ARG:N[6_544]	1.87	0.33
1:E:61:PHE:CE1	1:G:20:ARG:NH2[5_545]	1.87	0.33
1:A:51:ARG:CG	1:D:90:TRP:CD1[6_544]	1.89	0.31
1:A:237:ASP:OD2	1:I:27:HIS:CE1[6_444]	1.94	0.26
1:G:27:HIS:CG	1:I:237:ASP:OD2[3_445]	1.94	0.26
1:G:27:HIS:ND1	1:I:237:ASP:CG[3_445]	1.95	0.25
1:A:51:ARG:CG	1:D:90:TRP:CG[6_544]	1.97	0.23

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ASP:OD1	1:I:25:LEU:O[6_444]	1.97	0.23
1:F:90:TRP:CB	1:G:51:ARG:CG[5_545]	1.99	0.21
1:A:51:ARG:CZ	1:D:88:GLY:CA[6_544]	2.02	0.18
1:A:237:ASP:OD2	1:I:27:HIS:NE2[6_444]	2.07	0.13
1:G:26:LEU:CD2	1:I:175:GLN:CB[3_445]	2.08	0.12
1:A:237:ASP:CG	1:I:27:HIS:CE1[6_444]	2.08	0.12
1:F:88:GLY:O	1:G:51:ARG:NE[5_545]	2.10	0.10
1:G:25:LEU:CD2	1:I:173:GLN:OE1[3_445]	2.11	0.09
1:A:20:ARG:NH1	1:D:87:ARG:CB[6_544]	2.12	0.08
1:G:26:LEU:CD2	1:I:175:GLN:O[3_445]	2.12	0.08
1:A:51:ARG:NH2	1:D:89:ARG:CA[6_544]	2.15	0.05
1:A:255:GLN:CG	1:I:15:GLU:OE2[6_444]	2.16	0.04
1:A:237:ASP:CB	1:I:27:HIS:CE1[6_444]	2.16	0.04
1:G:27:HIS:CE1	1:I:237:ASP:OD2[3_445]	2.19	0.01

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%)	86	94
1	B	229/248 (92%)	226 (99%)	3 (1%)	76	89
1	C	237/248 (96%)	235 (99%)	2 (1%)	86	94
1	D	229/248 (92%)	226 (99%)	3 (1%)	76	89
1	E	237/248 (96%)	235 (99%)	2 (1%)	86	94
1	F	229/248 (92%)	226 (99%)	3 (1%)	76	89
1	G	237/248 (96%)	235 (99%)	2 (1%)	86	94
1	H	229/248 (92%)	226 (99%)	3 (1%)	76	89
1	I	237/248 (96%)	235 (99%)	2 (1%)	86	94
1	J	229/248 (92%)	226 (99%)	3 (1%)	76	89
All	All	2330/2480 (94%)	2305 (99%)	25 (1%)	80	91

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	THR
1	A	161	GLN
1	B	29	SER
1	B	56	VAL
1	B	147	THR
1	C	95	THR
1	C	161	GLN
1	D	29	SER
1	D	56	VAL
1	D	147	THR
1	E	95	THR
1	E	161	GLN
1	F	29	SER
1	F	56	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	147	THR
1	G	95	THR
1	G	161	GLN
1	H	29	SER
1	H	56	VAL
1	H	147	THR
1	I	95	THR
1	I	161	GLN
1	J	29	SER
1	J	56	VAL
1	J	147	THR

Some 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 (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

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	296/305 (97%)	0.93	36 (12%) 5 11	8, 15, 27, 35	14 (4%)
1	B	296/305 (97%)	0.96	37 (12%) 5 11	5, 14, 26, 30	8 (2%)
1	C	296/305 (97%)	0.93	35 (11%) 6 12	8, 15, 27, 35	14 (4%)
1	D	296/305 (97%)	1.04	52 (17%) 2 8	5, 14, 26, 30	8 (2%)
1	E	296/305 (97%)	1.06	56 (18%) 2 7	8, 15, 27, 35	14 (4%)
1	F	296/305 (97%)	0.85	40 (13%) 4 10	5, 14, 26, 30	8 (2%)
1	G	296/305 (97%)	1.02	52 (17%) 2 8	8, 15, 27, 35	14 (4%)
1	H	296/305 (97%)	1.25	66 (22%) 1 6	5, 14, 26, 30	8 (2%)
1	I	296/305 (97%)	0.93	34 (11%) 6 12	8, 15, 27, 35	14 (4%)
1	J	296/305 (97%)	0.99	47 (15%) 3 8	5, 14, 26, 30	8 (2%)
All	All	2960/3050 (97%)	1.00	455 (15%) 3 9	5, 14, 26, 35	110 (3%)

All (455) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	215	PRO	8.3
1	E	46	ALA	7.7
1	D	215	PRO	6.9
1	C	215	PRO	6.5
1	I	217	PRO	6.3
1	G	213	GLY	6.2
1	I	216	GLU	6.0
1	B	234	ALA	6.0
1	A	188	GLN	6.0
1	I	214	LEU	5.8
1	D	214	LEU	5.6
1	C	216	GLU	5.3
1	H	213	GLY	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	149	ALA	5.1
1	A	149	ALA	5.1
1	B	149	ALA	5.0
1	D	216	GLU	4.9
1	F	91	GLU	4.8
1	E	156	THR	4.8
1	H	214	LEU	4.8
1	G	214	LEU	4.7
1	A	216	GLU	4.7
1	I	1	MET	4.6
1	H	155	ASP	4.6
1	A	215	PRO	4.5
1	I	209	PHE	4.5
1	A	214	LEU	4.5
1	D	87	ARG	4.5
1	D	149	ALA	4.5
1	J	18	SER	4.4
1	H	212	TYR	4.4
1	H	156	THR	4.4
1	G	87	ARG	4.4
1	C	149	ALA	4.4
1	D	27	HIS	4.4
1	H	198	PRO	4.3
1	E	188	GLN	4.3
1	D	175	GLN	4.3
1	D	217	PRO	4.3
1	E	216	GLU	4.3
1	J	54	ARG	4.3
1	E	185	ALA	4.2
1	H	254	ASP	4.2
1	E	184	LEU	4.2
1	C	214	LEU	4.2
1	F	199	ARG	4.2
1	G	212	TYR	4.2
1	D	28	LEU	4.1
1	A	154	ILE	4.1
1	H	184	LEU	4.0
1	I	213	GLY	4.0
1	G	184	LEU	4.0
1	D	150	HIS	4.0
1	H	211	ARG	4.0
1	F	150	HIS	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	188	GLN	3.9
1	E	155	ASP	3.9
1	J	149	ALA	3.9
1	A	189	GLU	3.9
1	E	189	GLU	3.8
1	C	91	GLU	3.8
1	B	1	MET	3.8
1	H	199	ARG	3.8
1	H	117	GLU	3.8
1	I	205	ILE	3.8
1	G	17	GLY	3.7
1	J	189	GLU	3.7
1	E	165	VAL	3.7
1	D	188	GLN	3.7
1	E	127	ASP	3.7
1	A	20	ARG	3.6
1	A	217	PRO	3.6
1	E	215	PRO	3.6
1	I	198	PRO	3.6
1	A	1	MET	3.6
1	D	184	LEU	3.6
1	F	198	PRO	3.6
1	E	277	ASP	3.6
1	I	210	ALA	3.5
1	D	209	PHE	3.5
1	G	187	LEU	3.5
1	E	239	LEU	3.5
1	H	172	GLY	3.5
1	C	90	TRP	3.5
1	E	263	ASP	3.5
1	C	198	PRO	3.5
1	G	208	ALA	3.5
1	H	185	ALA	3.5
1	J	184	LEU	3.5
1	E	279	PRO	3.4
1	E	166	SER	3.4
1	D	174	ARG	3.4
1	B	150	HIS	3.4
1	C	217	PRO	3.4
1	E	218	LYS	3.4
1	G	266	PRO	3.4
1	E	217	PRO	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	1	MET	3.4
1	G	1	MET	3.4
1	H	187	LEU	3.4
1	G	211	ARG	3.3
1	E	250	ASN	3.3
1	H	225	SER	3.3
1	J	260	PRO	3.3
1	A	143	ASP	3.3
1	B	199	ARG	3.3
1	H	19	LEU	3.3
1	H	255	GLN	3.3
1	C	87	ARG	3.3
1	B	151	LYS	3.3
1	J	187	LEU	3.3
1	G	188	GLN	3.3
1	H	157	ASP	3.3
1	H	154	ILE	3.3
1	G	88	GLY	3.2
1	J	93	HIS	3.2
1	F	225	SER	3.2
1	H	163	LEU	3.2
1	E	157	ASP	3.2
1	I	206	ARG	3.2
1	J	19	LEU	3.2
1	G	189	GLU	3.2
1	H	162	PRO	3.2
1	G	209	PHE	3.2
1	G	91	GLU	3.2
1	I	91	GLU	3.2
1	E	151	LYS	3.1
1	B	173	GLN	3.1
1	F	155	ASP	3.1
1	H	295	ALA	3.1
1	A	209	PHE	3.1
1	H	170	ILE	3.1
1	D	88	GLY	3.1
1	F	216	GLU	3.1
1	D	213	GLY	3.1
1	I	199	ARG	3.1
1	B	172	GLY	3.1
1	H	228	ALA	3.1
1	E	265	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	152	HIS	3.0
1	E	183	ARG	3.0
1	H	18	SER	3.0
1	E	154	ILE	3.0
1	H	264	ALA	3.0
1	D	173	GLN	3.0
1	B	184	LEU	3.0
1	H	173	GLN	3.0
1	G	127	ASP	3.0
1	F	92	GLY	3.0
1	B	198	PRO	3.0
1	D	198	PRO	3.0
1	D	91	GLU	3.0
1	B	187	LEU	3.0
1	E	267	ASN	3.0
1	G	155	ASP	3.0
1	D	1	MET	3.0
1	D	255	GLN	3.0
1	C	199	ARG	3.0
1	J	92	GLY	3.0
1	H	174	ARG	3.0
1	F	182	THR	3.0
1	A	277	ASP	3.0
1	I	90	TRP	2.9
1	J	158	LEU	2.9
1	H	118	PHE	2.9
1	J	234	ALA	2.9
1	C	92	GLY	2.9
1	J	259	ILE	2.9
1	J	157	ASP	2.9
1	G	215	PRO	2.9
1	C	1	MET	2.9
1	D	17	GLY	2.9
1	J	46	ALA	2.9
1	C	93	HIS	2.9
1	F	61	PHE	2.9
1	E	186	GLU	2.9
1	I	87	ARG	2.9
1	J	148	ALA	2.9
1	C	94	ILE	2.9
1	H	234	ALA	2.9
1	A	87	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	151	LYS	2.8
1	G	18	SER	2.8
1	G	185	ALA	2.8
1	A	17	GLY	2.8
1	D	148	ALA	2.8
1	G	234	ALA	2.8
1	H	209	PHE	2.8
1	B	255	GLN	2.8
1	F	154	ILE	2.8
1	C	18	SER	2.8
1	D	187	LEU	2.8
1	A	144	PHE	2.8
1	B	2	LEU	2.8
1	J	17	GLY	2.8
1	I	46	ALA	2.8
1	E	212	TYR	2.8
1	A	18	SER	2.8
1	J	138	ARG	2.8
1	B	235	HIS	2.8
1	D	179	ALA	2.8
1	H	128	GLY	2.8
1	G	216	GLU	2.8
1	G	225	SER	2.8
1	G	56	VAL	2.8
1	E	266	PRO	2.8
1	H	279	PRO	2.8
1	F	138	ARG	2.8
1	B	45	LYS	2.7
1	B	91	GLU	2.7
1	C	17	GLY	2.7
1	H	127	ASP	2.7
1	A	121	VAL	2.7
1	A	150	HIS	2.7
1	B	127	ASP	2.7
1	A	198	PRO	2.7
1	B	152	HIS	2.7
1	C	3	LYS	2.7
1	D	56	VAL	2.7
1	D	172	GLY	2.7
1	E	128	GLY	2.7
1	G	186	GLU	2.7
1	J	53	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	185	ALA	2.7
1	D	212	TYR	2.7
1	D	18	SER	2.7
1	E	122	THR	2.7
1	I	45	LYS	2.7
1	H	208	ALA	2.7
1	F	130	TYR	2.7
1	G	279	PRO	2.7
1	H	188	GLN	2.7
1	H	119	PRO	2.6
1	I	294	HIS	2.6
1	J	181	ALA	2.6
1	H	153	ASP	2.6
1	E	224	GLU	2.6
1	D	46	ALA	2.6
1	D	45	LYS	2.6
1	J	261	LEU	2.6
1	D	65	PHE	2.6
1	D	199	ARG	2.6
1	E	269	THR	2.6
1	H	171	VAL	2.6
1	A	161	GLN	2.6
1	B	213	GLY	2.6
1	C	209	PHE	2.6
1	H	158	LEU	2.6
1	F	149	ALA	2.6
1	A	279	PRO	2.6
1	A	162	PRO	2.6
1	F	158	LEU	2.6
1	H	113	SER	2.6
1	I	18	SER	2.6
1	J	275	ARG	2.6
1	A	155	ASP	2.6
1	F	54	ARG	2.6
1	A	120	ASP	2.6
1	G	277	ASP	2.6
1	F	156	THR	2.6
1	H	130	TYR	2.6
1	J	258	SER	2.6
1	J	262	GLN	2.6
1	D	254	ASP	2.6
1	G	267	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	256	LEU	2.5
1	G	217	PRO	2.5
1	J	277	ASP	2.5
1	B	186	GLU	2.5
1	J	13	ILE	2.5
1	H	91	GLU	2.5
1	B	211	ARG	2.5
1	E	264	ALA	2.5
1	G	84	GLY	2.5
1	H	256	LEU	2.5
1	J	225	SER	2.5
1	F	206	ARG	2.5
1	H	216	GLU	2.5
1	D	181	ALA	2.5
1	A	254	ASP	2.5
1	C	189	GLU	2.5
1	H	116	ARG	2.5
1	B	165	VAL	2.5
1	E	83	ILE	2.5
1	E	147	THR	2.5
1	A	151	LYS	2.5
1	I	295	ALA	2.5
1	F	127	ASP	2.5
1	H	90	TRP	2.5
1	H	265	LEU	2.4
1	F	254	ASP	2.4
1	J	188	GLN	2.4
1	C	130	TYR	2.4
1	E	160	ALA	2.4
1	F	160	ALA	2.4
1	B	19	LEU	2.4
1	B	231	GLY	2.4
1	F	157	ASP	2.4
1	F	188	GLN	2.4
1	I	173	GLN	2.4
1	J	22	ALA	2.4
1	F	187	LEU	2.4
1	H	149	ALA	2.4
1	H	186	GLU	2.4
1	A	28	LEU	2.4
1	H	296	LEU	2.4
1	D	259	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	210	ALA	2.4
1	B	170	ILE	2.4
1	G	101	ALA	2.4
1	B	267	ASN	2.4
1	C	184	LEU	2.4
1	D	171	VAL	2.4
1	F	184	LEU	2.4
1	F	53	LYS	2.4
1	J	186	GLU	2.4
1	C	279	PRO	2.4
1	I	148	ALA	2.4
1	E	187	LEU	2.4
1	A	199	ARG	2.4
1	G	231	GLY	2.4
1	F	98	ALA	2.4
1	F	55	GLY	2.3
1	D	29	SER	2.3
1	G	157	ASP	2.3
1	F	153	ASP	2.3
1	G	274	ARG	2.3
1	C	294	HIS	2.3
1	E	278	LEU	2.3
1	G	128	GLY	2.3
1	E	211	ARG	2.3
1	D	170	ILE	2.3
1	I	175	GLN	2.3
1	J	276	HIS	2.3
1	F	180	ASN	2.3
1	I	130	TYR	2.3
1	J	55	GLY	2.3
1	I	273	LEU	2.3
1	D	55	GLY	2.3
1	E	172	GLY	2.3
1	E	251	ALA	2.3
1	J	179	ALA	2.3
1	G	99	SER	2.3
1	H	20	ARG	2.3
1	D	140	GLY	2.3
1	G	158	LEU	2.2
1	J	91	GLU	2.2
1	J	199	ARG	2.2
1	B	171	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	182	THR	2.2
1	J	183	ARG	2.2
1	H	210	ALA	2.2
1	I	207	ASN	2.2
1	E	171	VAL	2.2
1	G	259	ILE	2.2
1	H	250	ASN	2.2
1	A	148	ALA	2.2
1	J	128	GLY	2.2
1	J	185	ALA	2.2
1	J	171	VAL	2.2
1	B	174	ARG	2.2
1	J	155	ASP	2.2
1	J	231	GLY	2.2
1	D	152	HIS	2.2
1	G	90	TRP	2.2
1	D	54	ARG	2.2
1	E	158	LEU	2.2
1	H	180	ASN	2.2
1	I	218	LYS	2.2
1	H	251	ALA	2.2
1	H	175	GLN	2.2
1	A	25	LEU	2.2
1	C	213	GLY	2.2
1	G	199	ARG	2.2
1	B	212	TYR	2.2
1	I	188	GLN	2.2
1	I	14	GLU	2.2
1	J	263	ASP	2.2
1	D	128	GLY	2.2
1	F	255	GLN	2.2
1	F	52	THR	2.1
1	G	163	LEU	2.1
1	E	276	HIS	2.1
1	B	230	PRO	2.1
1	H	98	ALA	2.1
1	E	190	CYS	2.1
1	I	237	ASP	2.1
1	E	214	LEU	2.1
1	B	166	SER	2.1
1	B	128	GLY	2.1
1	B	283	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	172	GLY	2.1
1	E	262	GLN	2.1
1	C	185	ALA	2.1
1	F	228	ALA	2.1
1	J	139	ASP	2.1
1	F	183	ARG	2.1
1	H	51	ARG	2.1
1	F	217	PRO	2.1
1	D	180	ASN	2.1
1	C	162	PRO	2.1
1	C	237	ASP	2.1
1	F	18	SER	2.1
1	A	213	GLY	2.1
1	I	290	TRP	2.1
1	C	208	ALA	2.1
1	D	85	GLN	2.1
1	F	93	HIS	2.1
1	G	27	HIS	2.1
1	D	89	ARG	2.1
1	H	21	ALA	2.1
1	H	22	ALA	2.1
1	H	121	VAL	2.1
1	J	45	LYS	2.1
1	C	27	HIS	2.1
1	G	46	ALA	2.1
1	G	265	LEU	2.1
1	B	180	ASN	2.1
1	B	181	ALA	2.1
1	G	126	ARG	2.1
1	J	127	ASP	2.1
1	D	176	HIS	2.1
1	A	94	ILE	2.1
1	E	255	GLN	2.1
1	F	128	GLY	2.1
1	C	148	ALA	2.1
1	F	215	PRO	2.1
1	C	295	ALA	2.1
1	A	218	LYS	2.0
1	E	143	ASP	2.0
1	E	92	GLY	2.0
1	G	251	ALA	2.0
1	F	275	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	218	LYS	2.0
1	E	44	LEU	2.0
1	I	184	LEU	2.0
1	H	46	ALA	2.0
1	D	262	GLN	2.0
1	E	261	LEU	2.0
1	A	208	ALA	2.0
1	H	126	ARG	2.0
1	E	47	PRO	2.0
1	G	170	ILE	2.0
1	G	198	PRO	2.0
1	J	198	PRO	2.0
1	E	17	GLY	2.0
1	G	94	ILE	2.0
1	H	257[A]	CYS	2.0
1	H	281	THR	2.0
1	B	275	ARG	2.0
1	C	158	LEU	2.0
1	A	5	GLN	2.0
1	I	194	PHE	2.0
1	D	182	THR	2.0
1	G	26	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.