Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 06:27 am GMT

PDB ID	:	3ZTE
Title	:	Crystal Structure of the TRP RNA-Binding Attenuation Protein (TRAP) from Bacillus Licheniformis.
Authors	:	Shevtsov, M.B.; Chen, Y.; Gollnick, P.; Antson, A.A.
Deposited on	:	2011-07-07
Resolution	:	2.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

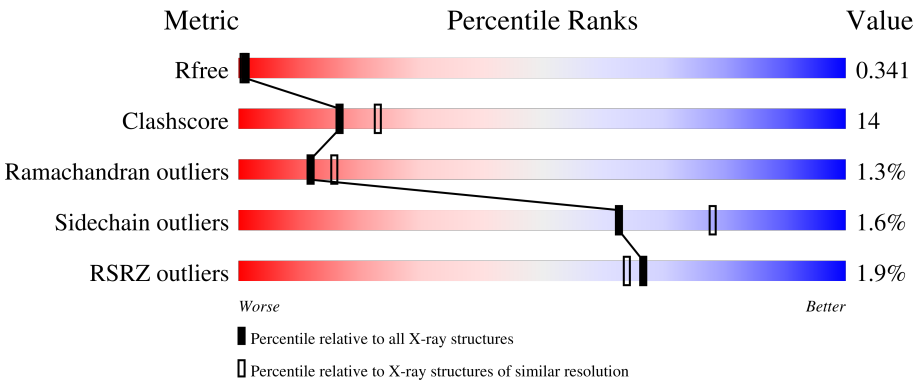
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.41 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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% 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	78	3%, 63%, 24%, •, 12%
1	B	78	74%, 13%, •, 12%
1	C	78	4%, 62%, 26%, •, 12%
1	D	78	3%, 68%, 19%, •, 12%
1	E	78	%, 69%, 17%, •, 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	78	%, 59%, 27%, 12%
1	G	78	3%, 72%, 15%, 12%
1	H	78	3%, 59%, 29%, 12%
1	I	78	5%, 60%, 27%, 12%
1	J	78	%, 71%, 18%, 10%
1	K	78	3%, 67%, 19%, 12%
1	L	78	4%, 62%, 27%, 9%
1	M	78	%, 68%, 17%, 12%
1	N	78	62%, 24%, 12%
1	O	78	3%, 60%, 28%, 12%
1	P	78	%, 55%, 31%, 12%
1	Q	78	%, 60%, 26%, 12%
1	R	78	67%, 19%, 12%
1	S	78	%, 63%, 23%, 12%
1	T	78	68%, 21%, 12%
1	U	78	68%, 21%, 10%
1	V	78	64%, 21%, 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12416 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 TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP).

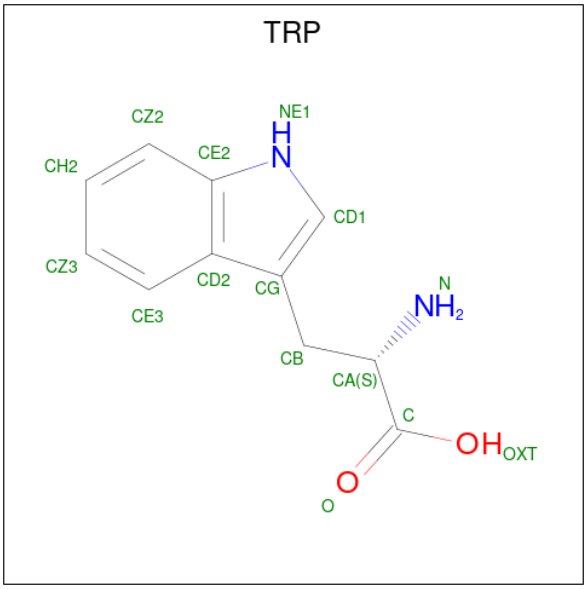
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	69	525	324	94	104	3	0	0	1
1	B	69	531	328	94	106	3	0	1	1
1	C	69	525	324	94	104	3	0	0	1
1	D	69	525	324	94	104	3	0	0	1
1	E	69	525	324	94	104	3	0	0	1
1	F	69	531	328	94	106	3	0	1	1
1	G	69	525	324	94	104	3	0	0	1
1	H	69	525	324	94	104	3	0	0	1
1	I	69	525	324	94	104	3	0	0	1
1	J	70	533	328	96	106	3	0	0	1
1	K	69	525	324	94	104	3	0	0	1
1	L	71	545	335	97	110	3	0	1	1
1	M	69	525	324	94	104	3	0	0	1
1	N	69	525	324	94	104	3	0	0	1
1	O	69	533	332	94	104	3	0	1	1
1	P	69	533	329	97	104	3	0	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	69	525	324	94	104	3	0	0	1
			Total	C	N	O	S			
1	R	69	525	324	94	104	3	0	0	1
			Total	C	N	O	S			
1	S	69	525	324	94	104	3	0	0	1
			Total	C	N	O	S			
1	T	69	525	324	94	104	3	0	0	1
			Total	C	N	O	S			
1	U	70	533	328	96	106	3	0	0	1
			Total	C	N	O	S			
1	V	69	525	324	94	104	3	0	0	1

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	15	11	2	2	0	0
			Total	C	N	O		
2	B	1	15	11	2	2	0	0
			Total	C	N	O		
2	C	1	15	11	2	2	0	0
			Total	C	N	O		
2	D	1	15	11	2	2	0	0
			Total	C	N	O		
2	E	1	15	11	2	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	F	1	15	11	2	2	0	0
2	G	1	15	11	2	2	0	0
2	H	1	15	11	2	2	0	0
2	I	1	15	11	2	2	0	0
2	J	1	15	11	2	2	0	0
2	K	1	15	11	2	2	0	0
2	L	1	15	11	2	2	0	0
2	M	1	15	11	2	2	0	0
2	N	1	15	11	2	2	0	0
2	O	1	15	11	2	2	0	0
2	P	1	15	11	2	2	0	0
2	Q	1	15	11	2	2	0	0
2	R	1	15	11	2	2	0	0
2	S	1	15	11	2	2	0	0
2	T	1	15	11	2	2	0	0
2	U	1	15	11	2	2	0	0
2	V	1	15	11	2	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	32	32	32	0	0
3	B	28	28	28	0	0

Continued on next page...

Continued from previous page...

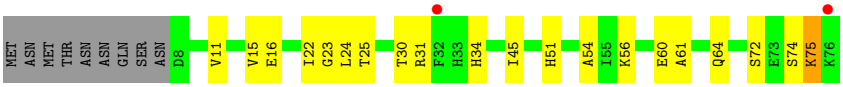
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	16	Total O 16 16	0	0
3	D	32	Total O 32 32	0	0
3	E	30	Total O 30 30	0	0
3	F	22	Total O 22 22	0	0
3	G	20	Total O 20 20	0	0
3	H	15	Total O 15 15	0	0
3	I	23	Total O 23 23	0	0
3	J	21	Total O 21 21	0	0
3	K	10	Total O 10 10	0	0
3	L	26	Total O 26 26	0	0
3	M	18	Total O 18 18	0	0
3	N	19	Total O 19 19	0	0
3	O	25	Total O 25 25	0	0
3	P	20	Total O 20 20	0	0
3	Q	16	Total O 16 16	0	0
3	R	19	Total O 19 19	0	0
3	S	14	Total O 14 14	0	0
3	T	23	Total O 23 23	0	0
3	U	26	Total O 26 26	0	0
3	V	17	Total O 17 17	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

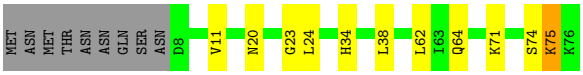
• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain A:



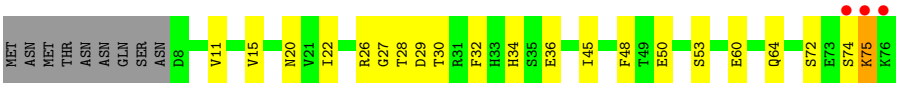
• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain B:



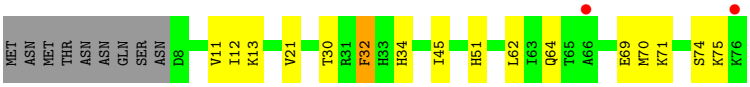
• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain C:



• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain D:



• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain E:

• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain F: %
59% 27% • 12%

MET ASN MET THR ASN ASN GLN SER ASN D8 F9 V10 K13 E16 D17 I22 G27 T30 R31 F32 H33 H34 S35 G41 E42 V43 M44 I45 F48 E60 A61 L62 I63 Q64 T65 E69 M70 K71 S72 K75 K76

• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain G: 3%
72% 15% • 12%

MET ASN MET THR ASN ASN GLN SER ASN D8 V15 E16 L24 T30 R31 F32 I45 H51 A54 I55 K56 Q64 E69 S74 K75 K76

• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain H: 3%
59% 29% 12%

MET ASN MET THR ASN ASN GLN SER ASN D8 V11 V15 N20 V21 I22 G23 L24 D29 T30 R31 F32 H33 H34 S35 E36 K37 L38 M44 F48 T49 A54 I55 K56 E60 A61 L62 I63 Q64 K71 S72 E73 S74 K75 K76

• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain I: 5%
60% 27% • 12%

MET ASN MET THR ASN ASN GLN SER ASN D8 V11 I12 K13 A14 V15 E16 I22 T25 T30 R31 F32 L38 V43 M44 I45 F48 H51 K56 E60 A61 Q64 K71 S74 K75 K76

• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain J: %
71% 18% • 10%

MET ASN MET THR ASN ASN GLN SER N7 K13 E16 N20 V21 I22 T30 R31 F32 H33 H34 S35 V43 M44 I45 K56 E60 Q64 E69 S72 K75 K76

• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain K: 3%
67% 19% • 12%

MET ASN MET THR ASN ASN GLN SER ASN D8 I12 K13 N20 V21 I22 R26 T30 R31 F32 H33 H34 S35 I45 E50 Q64 E69 E73 S74 K75 K76

• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain L: 4%
62% 27% • 9%

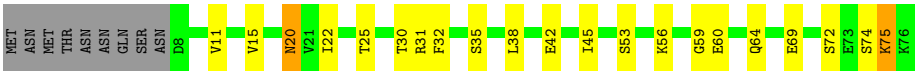
MET ASN MET THR ASN ASN GLN S6 N7 V11 I12 K13 A14 V15 E16 L24 T25 R26 T30 E36 K37 L38 D39 K40 V43 M44 E50 H51 A54 I55 K56 E60 Q64 M70 K71 S72 E73 S74 K75 K76

• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain M:

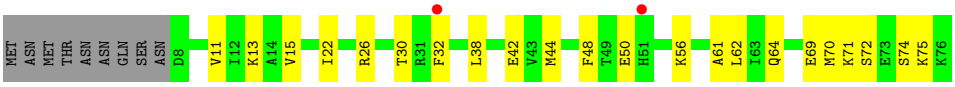
• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain N:



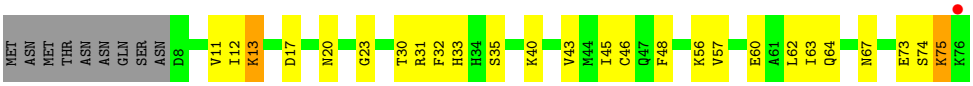
• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain O:



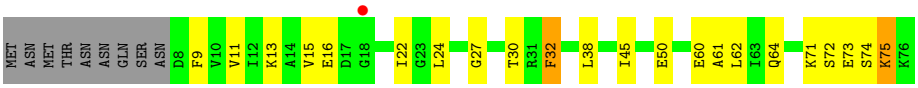
• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain P:



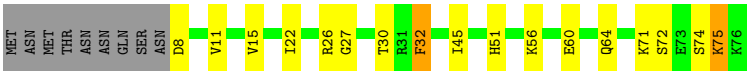
• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain Q:



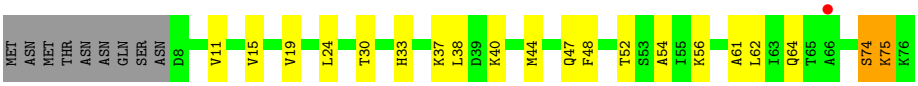
• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain R:



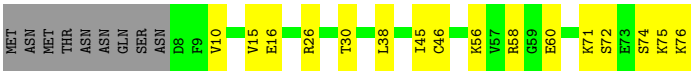
• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain S:



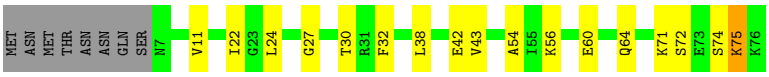
• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain T:



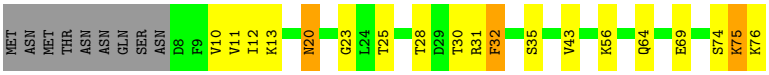
• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain U:



• Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)

Chain V:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	145.43Å 145.43Å 183.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.83 – 2.41 44.83 – 2.41	Depositor EDS
% Data completeness (in resolution range)	96.5 (44.83-2.41) 96.5 (44.83-2.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.47 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.281 , 0.346 0.276 , 0.341	Depositor DCC
R_{free} test set	3709 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12416	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5969e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

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	0.31	0/530	0.42	0/710
1	B	0.31	0/539	0.47	0/722
1	C	0.32	0/530	0.46	0/710
1	D	0.33	0/530	0.46	0/710
1	E	0.33	0/530	0.47	0/710
1	F	0.32	0/539	0.44	0/722
1	G	0.31	0/530	0.44	0/710
1	H	0.32	0/530	0.46	0/710
1	I	0.31	0/530	0.45	0/710
1	J	0.31	0/538	0.43	0/721
1	K	0.32	0/530	0.47	0/710
1	L	0.31	0/553	0.45	0/741
1	M	0.32	0/530	0.46	0/710
1	N	0.33	0/530	0.46	0/710
1	O	0.32	0/542	0.44	0/726
1	P	0.32	0/541	0.46	0/724
1	Q	0.32	0/530	0.43	0/710
1	R	0.32	0/530	0.45	0/710
1	S	0.32	0/530	0.47	0/710
1	T	0.32	0/530	0.45	0/710
1	U	0.32	0/538	0.45	0/721
1	V	0.32	0/530	0.46	0/710
All	All	0.32	0/11740	0.45	0/15727

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	525	0	524	20	0
1	B	531	0	530	13	0
1	C	525	0	524	14	0
1	D	525	0	524	16	0
1	E	525	0	524	12	0
1	F	531	0	530	20	0
1	G	525	0	524	15	0
1	H	525	0	524	27	0
1	I	525	0	524	23	0
1	J	533	0	530	12	0
1	K	525	0	524	13	0
1	L	545	0	541	19	0
1	M	525	0	524	14	0
1	N	525	0	524	17	0
1	O	533	0	533	17	0
1	P	533	0	537	20	0
1	Q	525	0	524	26	0
1	R	525	0	524	21	0
1	S	525	0	524	21	0
1	T	525	0	524	18	0
1	U	533	0	530	15	0
1	V	525	0	524	15	0
2	A	15	0	9	0	0
2	B	15	0	9	1	0
2	C	15	0	9	0	0
2	D	15	0	9	2	0
2	E	15	0	9	1	0
2	F	15	0	9	0	0
2	G	15	0	9	1	0
2	H	15	0	9	2	0
2	I	15	0	9	1	0
2	J	15	0	9	1	0
2	K	15	0	9	1	0
2	L	15	0	9	1	0
2	M	15	0	9	1	0
2	N	15	0	9	1	0
2	O	15	0	9	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	15	0	9	2	0
2	Q	15	0	9	1	0
2	R	15	0	9	2	0
2	S	15	0	9	1	0
2	T	15	0	9	2	0
2	U	15	0	9	1	0
2	V	15	0	9	2	0
3	A	32	0	0	1	0
3	B	28	0	0	4	0
3	C	16	0	0	0	0
3	D	32	0	0	1	0
3	E	30	0	0	2	0
3	F	22	0	0	0	0
3	G	20	0	0	0	0
3	H	15	0	0	1	0
3	I	23	0	0	1	0
3	J	21	0	0	2	0
3	K	10	0	0	0	0
3	L	26	0	0	2	0
3	M	18	0	0	0	0
3	N	19	0	0	0	0
3	O	25	0	0	1	0
3	P	20	0	0	2	0
3	Q	16	0	0	1	0
3	R	19	0	0	1	0
3	S	14	0	0	1	0
3	T	23	0	0	1	0
3	U	26	0	0	0	0
3	V	17	0	0	0	0
All	All	12416	0	11789	337	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 14.

All (337) 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:J:32:PHE:HE2	1:J:35:SER:HG	1.06	0.98
1:M:32:PHE:HD1	1:M:32:PHE:H	1.11	0.93
1:R:56:LYS:HE3	1:S:38:LEU:HD23	1.52	0.90
1:N:74:SER:O	1:N:75:LYS:HB2	1.68	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:74:SER:O	1:M:75:LYS:HB2	1.72	0.88
1:A:74:SER:O	1:A:75:LYS:HB2	1.71	0.87
1:V:74:SER:O	1:V:75:LYS:HB2	1.81	0.80
1:H:30:THR:HG1	2:I:80:TRP:N	1.80	0.79
1:D:11:VAL:HB	1:D:64:GLN:HB2	1.65	0.78
1:C:74:SER:O	1:C:75:LYS:HB2	1.82	0.78
1:N:59:GLY:HA2	1:N:74:SER:HB3	1.67	0.77
3:L:2007:HOH:O	1:V:76:LYS:N	2.18	0.76
1:B:74:SER:O	1:B:75:LYS:HB2	1.86	0.75
1:B:24:LEU:HD12	1:B:24:LEU:N	2.02	0.75
1:D:74:SER:O	1:D:75:LYS:HB3	1.85	0.74
1:I:74:SER:O	1:I:75:LYS:HB2	1.87	0.74
1:R:74:SER:O	1:R:75:LYS:HB2	1.88	0.73
1:L:74:SER:O	1:L:75:LYS:HB2	1.88	0.73
1:I:45:ILE:HD12	1:I:45:ILE:N	2.04	0.73
1:M:32:PHE:N	1:M:32:PHE:CD1	2.57	0.73
1:H:11:VAL:HB	1:H:64:GLN:HB2	1.71	0.73
1:Q:62:LEU:HD21	1:Q:71:LYS:HE3	1.70	0.73
1:L:11:VAL:HB	1:L:64:GLN:HB2	1.69	0.72
1:N:30:THR:HG1	2:O:80:TRP:N	1.86	0.72
1:N:56:LYS:HE3	1:O:42:GLU:OE1	1.89	0.72
1:F:22:ILE:HG21	1:F:32:PHE:CD2	2.24	0.72
1:K:74:SER:O	1:K:75:LYS:HB2	1.90	0.72
1:H:20:ASN:ND2	1:H:35:SER:OG	2.22	0.72
1:R:60:GLU:HA	1:R:72:SER:O	1.90	0.71
1:U:60:GLU:HA	1:U:72:SER:O	1.90	0.71
1:P:74:SER:O	1:P:75:LYS:HB2	1.89	0.71
1:Q:24:LEU:HD12	1:Q:24:LEU:N	2.05	0.71
1:R:26:ARG:HH22	1:S:47:GLN:HE22	1.39	0.71
1:B:34:HIS:ND1	3:B:2016:HOH:O	2.24	0.70
1:F:22:ILE:HG21	1:F:32:PHE:HD2	1.54	0.70
1:L:50[B]:GLU:OE1	1:L:50[B]:GLU:HA	1.90	0.70
1:G:30:THR:HG1	2:H:80:TRP:N	1.90	0.69
1:I:25:THR:HG23	1:I:31:ARG:O	1.92	0.69
1:J:22:ILE:HB	1:J:56:LYS:HB3	1.74	0.69
1:J:60:GLU:HA	1:J:72:SER:O	1.91	0.69
1:I:15:VAL:HG23	1:I:61:ALA:HA	1.75	0.69
1:M:59:GLY:HA2	1:M:74:SER:HB3	1.73	0.69
1:Q:30:THR:HG1	2:R:80:TRP:N	1.90	0.69
1:A:15:VAL:HB	1:A:60:GLU:HG2	1.75	0.68
1:F:60:GLU:HA	1:F:72:SER:O	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:56:LYS:HE3	1:S:38:LEU:CD2	2.22	0.68
1:Q:22:ILE:HG21	1:Q:32:PHE:HD2	1.58	0.68
1:C:28:THR:HG22	1:C:29:ASP:OD1	1.93	0.67
1:N:20:ASN:ND2	1:N:35:SER:OG	2.22	0.66
1:V:74:SER:O	1:V:75:LYS:CB	2.42	0.66
1:F:48:PHE:HZ	1:G:45:ILE:HG22	1.60	0.66
1:M:74:SER:O	1:M:75:LYS:CB	2.44	0.66
1:G:32:PHE:H	1:G:32:PHE:HD1	1.42	0.66
1:E:74:SER:O	1:E:75:LYS:HB2	1.94	0.66
1:A:30:THR:HG1	2:B:80:TRP:N	1.94	0.66
3:J:2010:HOH:O	1:K:33:HIS:HB2	1.96	0.66
1:T:16:GLU:HG2	1:T:60:GLU:HB3	1.77	0.65
1:N:74:SER:O	1:N:75:LYS:CB	2.45	0.65
1:P:74:SER:O	1:P:75:LYS:CB	2.44	0.65
1:A:60:GLU:HA	1:A:72:SER:O	1.97	0.65
1:S:48:PHE:HZ	1:T:45:ILE:HG22	1.61	0.64
1:Q:32:PHE:HD1	1:Q:32:PHE:H	1.44	0.64
1:O:30:THR:HG1	2:P:80:TRP:N	1.96	0.64
1:G:24:LEU:HD12	1:G:24:LEU:N	2.13	0.64
1:G:32:PHE:CD1	1:G:32:PHE:N	2.66	0.63
1:C:26:ARG:HB2	1:C:53:SER:HB3	1.79	0.63
1:Q:11:VAL:HB	1:Q:64:GLN:HB2	1.80	0.63
1:G:32:PHE:HD1	1:G:32:PHE:N	1.97	0.63
1:H:48:PHE:HZ	1:I:45:ILE:HG22	1.63	0.63
1:R:22:ILE:HD12	1:R:22:ILE:N	2.13	0.62
1:P:13:LYS:HG2	1:P:62:LEU:HD12	1.81	0.62
1:I:71:LYS:O	1:J:13:LYS:HD2	1.99	0.62
1:P:20:ASN:OD1	1:P:35:SER:OG	2.17	0.62
1:Q:32:PHE:CD1	1:Q:32:PHE:N	2.68	0.62
1:M:13:LYS:HG2	1:M:43:VAL:HG22	1.82	0.61
1:I:16:GLU:HG2	1:I:60:GLU:HB3	1.81	0.61
1:J:16:GLU:OE2	1:T:71:LYS:NZ	2.27	0.61
1:Q:60:GLU:HA	1:Q:72:SER:O	2.00	0.61
1:S:74:SER:O	1:S:75:LYS:C	2.39	0.61
1:Q:45:ILE:N	1:Q:45:ILE:HD12	2.15	0.61
1:A:24:LEU:N	1:A:24:LEU:HD12	2.15	0.61
1:S:15:VAL:HG23	1:S:61:ALA:HA	1.83	0.60
1:P:60:GLU:OE1	1:P:73:GLU:HA	2.01	0.60
1:Q:62:LEU:CD2	1:Q:71:LYS:HE3	2.30	0.60
1:B:24:LEU:N	1:B:24:LEU:CD1	2.65	0.60
1:L:30:THR:HG1	2:M:80:TRP:N	1.99	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:30:THR:HG1	2:T:80:TRP:N	2.00	0.60
1:E:74:SER:O	1:E:75:LYS:CB	2.50	0.60
2:L:80:TRP:N	1:V:30:THR:HG1	1.99	0.60
1:O:64:GLN:HG2	1:O:69:GLU:HG2	1.83	0.60
1:T:10:VAL:CG1	1:T:46:CYS:SG	2.90	0.60
1:F:22:ILE:HD12	1:F:22:ILE:H	1.67	0.59
1:F:30:THR:HG1	2:G:80:TRP:N	2.00	0.59
1:A:34:HIS:ND1	1:K:30:THR:HB	2.17	0.59
1:K:20:ASN:ND2	1:K:35:SER:OG	2.27	0.59
1:P:30:THR:HG1	2:Q:80:TRP:N	2.00	0.59
1:C:30:THR:HG1	2:D:80:TRP:N	2.01	0.59
1:M:30:THR:HG1	2:N:80:TRP:N	2.00	0.59
1:C:60:GLU:HA	1:C:72:SER:O	2.02	0.58
1:T:26:ARG:HD3	3:T:2007:HOH:O	2.02	0.58
1:U:24:LEU:HD12	1:U:24:LEU:N	2.18	0.58
1:E:64:GLN:HG2	1:E:69:GLU:HG2	1.84	0.58
1:R:45:ILE:N	1:R:45:ILE:HD12	2.19	0.58
1:D:32:PHE:CD1	1:D:32:PHE:C	2.77	0.58
1:F:27:GLY:HA2	1:G:51:HIS:CD2	2.39	0.58
1:B:74:SER:HB2	3:B:2028:HOH:O	2.03	0.58
1:F:64:GLN:HG2	1:F:69:GLU:HG2	1.84	0.58
1:Q:50:GLU:HG2	3:Q:2009:HOH:O	2.03	0.58
1:A:15:VAL:HG12	1:A:15:VAL:O	2.05	0.57
1:H:49:THR:OG1	2:H:80:TRP:OXT	2.18	0.57
1:H:34:HIS:HE2	1:H:36:GLU:HB2	1.69	0.57
1:D:64:GLN:HG2	1:D:69:GLU:HG2	1.85	0.57
1:H:60:GLU:HA	1:H:72:SER:O	2.05	0.56
1:H:22:ILE:CG2	1:H:32:PHE:HB2	2.36	0.56
1:Q:15:VAL:HG12	1:Q:16:GLU:HG2	1.88	0.56
1:F:22:ILE:HD12	1:F:22:ILE:N	2.20	0.56
1:E:62:LEU:HD21	1:E:71:LYS:NZ	2.21	0.55
1:S:38:LEU:HD11	1:S:44:MET:CB	2.36	0.55
1:A:74:SER:O	1:A:75:LYS:CB	2.48	0.55
1:H:15:VAL:HB	1:H:60:GLU:HG2	1.88	0.55
1:U:74:SER:O	1:U:75:LYS:HB2	2.06	0.55
1:S:24:LEU:HB2	1:S:54:ALA:HB3	1.89	0.55
1:S:38:LEU:HD11	1:S:44:MET:HB2	1.89	0.55
1:N:11:VAL:HB	1:N:64:GLN:HB2	1.89	0.55
1:Q:74:SER:O	1:Q:75:LYS:C	2.44	0.55
1:R:32:PHE:HD1	1:R:32:PHE:H	1.53	0.54
1:O:74:SER:O	1:O:75:LYS:HB2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:NH1	3:A:2013:HOH:O	2.40	0.54
1:U:11:VAL:HB	1:U:64:GLN:HB2	1.88	0.54
1:Q:22:ILE:HG21	1:Q:32:PHE:CD2	2.42	0.54
1:Q:45:ILE:HD12	1:Q:45:ILE:H	1.72	0.54
1:B:74:SER:O	1:B:75:LYS:CB	2.56	0.54
1:J:20:ASN:ND2	1:J:35:SER:HB3	2.23	0.53
1:J:64:GLN:HG2	1:J:69:GLU:HG2	1.90	0.53
1:R:11:VAL:HB	1:R:64:GLN:HB2	1.90	0.53
1:N:56:LYS:CE	1:O:42:GLU:OE1	2.56	0.53
1:U:74:SER:O	1:U:75:LYS:CB	2.56	0.53
1:V:20:ASN:ND2	1:V:35:SER:OG	2.36	0.53
1:P:33:HIS:HA	3:P:2012:HOH:O	2.08	0.53
1:R:32:PHE:CD1	1:R:32:PHE:N	2.76	0.53
1:V:64:GLN:HG2	1:V:69:GLU:HG2	1.91	0.53
1:K:74:SER:O	1:K:75:LYS:CB	2.56	0.53
1:S:15:VAL:HG22	1:S:62:LEU:HD13	1.90	0.52
1:B:62:LEU:HD23	1:B:71:LYS:HG2	1.90	0.52
1:H:38:LEU:HD11	1:H:44:MET:HB3	1.91	0.52
1:N:15:VAL:HG12	1:N:15:VAL:O	2.08	0.52
1:O:26:ARG:HD2	1:O:50:GLU:O	2.09	0.52
1:S:11:VAL:HB	1:S:64:GLN:HB2	1.92	0.52
1:I:74:SER:O	1:I:75:LYS:CB	2.56	0.52
1:T:30:THR:HG1	2:U:80:TRP:N	2.08	0.52
1:S:48:PHE:CZ	1:T:45:ILE:HG22	2.45	0.51
1:O:11:VAL:HB	1:O:64:GLN:HB2	1.91	0.51
1:T:56:LYS:HE3	1:U:38:LEU:HD23	1.92	0.51
1:G:24:LEU:HB2	1:G:54:ALA:HB3	1.93	0.51
1:G:15:VAL:O	1:G:16:GLU:HG3	2.10	0.51
1:R:8:ASP:N	3:R:2001:HOH:O	2.43	0.51
1:F:32:PHE:CD1	1:F:32:PHE:N	2.78	0.51
1:I:11:VAL:HB	1:I:64:GLN:HB2	1.93	0.51
1:L:74:SER:O	1:L:75:LYS:CB	2.58	0.51
1:Q:24:LEU:N	1:Q:24:LEU:CD1	2.75	0.50
1:L:24:LEU:HD12	1:L:24:LEU:N	2.26	0.50
1:P:67:ASN:ND2	1:Q:9:PHE:CE1	2.79	0.50
1:K:45:ILE:HD12	1:K:45:ILE:N	2.27	0.50
1:K:73:GLU:OE2	1:R:71:LYS:NZ	2.44	0.50
1:V:25:THR:HG23	1:V:31:ARG:O	2.11	0.50
1:L:26:ARG:NH2	1:M:47:GLN:OE1	2.38	0.50
1:E:8:ASP:N	3:E:2001:HOH:O	2.45	0.50
1:B:23:GLY:C	1:B:24:LEU:HD12	2.31	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:56:LYS:HE3	1:I:38:LEU:HD23	1.94	0.49
1:T:72:SER:HB3	1:U:43:VAL:HG23	1.94	0.49
1:D:45:ILE:HD12	1:D:45:ILE:N	2.27	0.49
1:G:64:GLN:HG2	1:G:69:GLU:HG2	1.93	0.49
1:F:62:LEU:HD23	1:F:71:LYS:HG2	1.93	0.49
1:T:15:VAL:HB	1:T:60:GLU:HG2	1.94	0.49
1:E:22:ILE:HB	1:E:56:LYS:HB3	1.94	0.49
1:G:74:SER:OG	1:G:75:LYS:N	2.45	0.49
1:J:32:PHE:CD1	1:J:32:PHE:C	2.85	0.49
1:O:22:ILE:HB	1:O:56:LYS:HB3	1.94	0.49
1:D:13:LYS:HD3	1:D:62:LEU:HD12	1.94	0.49
1:F:10:VAL:HG22	1:F:65:THR:HG22	1.95	0.49
1:P:48:PHE:HZ	1:Q:45:ILE:HG22	1.78	0.48
1:R:45:ILE:HD12	1:R:45:ILE:H	1.79	0.48
1:A:24:LEU:HB2	1:A:54:ALA:HB3	1.95	0.48
1:T:10:VAL:HG12	1:T:46:CYS:SG	2.53	0.48
1:F:34:HIS:CD2	1:F:35:SER:N	2.82	0.48
1:O:72:SER:HB3	1:P:43:VAL:HG23	1.95	0.48
1:B:71:LYS:NZ	3:B:2026:HOH:O	2.35	0.48
1:N:22:ILE:CG2	1:N:32:PHE:HB2	2.44	0.48
1:D:12:ILE:HD13	1:D:21:VAL:HG22	1.96	0.48
1:M:64:GLN:HG2	1:M:69:GLU:HG2	1.96	0.48
1:P:56:LYS:HD2	1:Q:38:LEU:CD2	2.44	0.48
1:D:70:MET:HG3	1:D:71:LYS:N	2.29	0.48
1:E:58:ARG:NH1	3:E:2008:HOH:O	2.47	0.48
1:H:15:VAL:CG2	1:H:62:LEU:HD13	2.44	0.48
1:H:24:LEU:HB2	1:H:54:ALA:HB3	1.95	0.48
1:V:23:GLY:O	1:V:32:PHE:HA	2.14	0.47
1:H:15:VAL:HG22	1:H:62:LEU:HD13	1.96	0.47
1:R:26:ARG:HG2	1:R:27:GLY:N	2.29	0.47
1:L:24:LEU:HB2	1:L:54:ALA:HB3	1.95	0.47
1:A:34:HIS:CE1	1:K:30:THR:HB	2.49	0.47
1:I:30:THR:HG1	2:J:80:TRP:N	2.12	0.47
1:K:12:ILE:HD12	1:K:12:ILE:N	2.30	0.47
1:L:60:GLU:HA	1:L:72:SER:O	2.14	0.47
1:M:56:LYS:NZ	1:M:58:ARG:NH2	2.61	0.47
1:C:27:GLY:HA2	1:D:51:HIS:CE1	2.50	0.47
1:H:48:PHE:CZ	1:I:45:ILE:HG22	2.47	0.47
1:H:74:SER:O	1:H:75:LYS:HB2	2.14	0.47
1:S:15:VAL:O	1:S:40:LYS:HG3	2.15	0.47
1:A:22:ILE:HB	1:A:56:LYS:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:11:VAL:HB	1:V:64:GLN:HB2	1.96	0.47
1:N:38:LEU:HD22	1:N:42:GLU:HB3	1.97	0.46
1:B:62:LEU:HD21	1:B:71:LYS:HE2	1.96	0.46
1:O:13:LYS:HD3	1:O:62:LEU:HD12	1.97	0.46
1:A:45:ILE:N	1:A:45:ILE:HD12	2.30	0.46
1:D:75:LYS:HB3	1:D:75:LYS:HE2	1.67	0.46
1:O:38:LEU:HD21	1:O:44:MET:HB2	1.97	0.46
1:P:46:CYS:HB2	2:P:80:TRP:NE1	2.30	0.46
1:B:20:ASN:ND2	3:B:2009:HOH:O	2.07	0.46
1:Q:27:GLY:HA2	1:R:51:HIS:CD2	2.51	0.46
1:T:58:ARG:NE	1:U:42:GLU:OE2	2.49	0.46
1:R:22:ILE:HG21	1:R:32:PHE:HD2	1.80	0.46
1:R:74:SER:O	1:R:75:LYS:CB	2.61	0.46
1:P:17:ASP:OD1	1:P:40:LYS:N	2.45	0.46
1:D:30:THR:HB	1:E:34:HIS:ND1	2.31	0.46
1:L:56:LYS:HE3	1:M:38:LEU:HD23	1.98	0.46
1:N:64:GLN:HG2	1:N:69:GLU:HG2	1.98	0.46
1:G:24:LEU:N	1:G:24:LEU:CD1	2.79	0.46
1:B:11:VAL:HB	1:B:64:GLN:HB2	1.98	0.45
1:A:11:VAL:HB	1:A:64:GLN:HB2	1.98	0.45
1:C:34:HIS:HE2	1:C:36:GLU:HB2	1.80	0.45
1:D:32:PHE:CD1	1:D:32:PHE:O	2.70	0.45
1:I:11:VAL:C	1:I:12:ILE:HG13	2.36	0.45
1:R:22:ILE:HD12	1:R:22:ILE:H	1.80	0.45
1:I:30:THR:HB	1:J:34:HIS:ND1	2.31	0.45
1:J:13:LYS:HB2	1:J:43:VAL:HG22	1.98	0.45
1:Q:15:VAL:C	1:Q:16:GLU:HG2	2.37	0.45
1:I:22:ILE:HB	1:I:56:LYS:HB3	1.97	0.45
1:Q:15:VAL:O	1:Q:15:VAL:CG1	2.65	0.45
1:U:24:LEU:HB2	1:U:54:ALA:HB3	1.98	0.45
1:U:27:GLY:O	2:V:80:TRP:N	2.49	0.45
1:H:72:SER:HB3	1:I:43:VAL:HG23	1.99	0.45
1:C:11:VAL:HB	1:C:64:GLN:HB2	1.99	0.45
1:L:51:HIS:CD2	1:V:28:THR:HG22	2.52	0.45
1:U:30:THR:HG1	2:V:80:TRP:N	2.15	0.45
1:C:15:VAL:HG12	1:C:15:VAL:O	2.16	0.45
1:N:60:GLU:HA	1:N:72:SER:O	2.17	0.45
1:G:56:LYS:HE3	1:H:38:LEU:HD23	1.98	0.45
1:O:26:ARG:HD3	3:O:2008:HOH:O	2.16	0.45
1:T:56:LYS:HE2	1:T:58:ARG:HH21	1.83	0.44
1:I:38:LEU:HD21	1:I:44:MET:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:25:THR:HG23	1:N:31:ARG:O	2.17	0.44
1:O:70:MET:HG3	1:O:71:LYS:N	2.33	0.44
1:E:62:LEU:HD21	1:E:71:LYS:HZ3	1.82	0.44
1:L:7:ASN:HA	3:L:2002:HOH:O	2.18	0.44
1:S:24:LEU:HD12	1:S:24:LEU:N	2.32	0.44
1:K:26:ARG:HD2	1:K:50:GLU:O	2.17	0.44
1:P:23:GLY:O	1:P:32:PHE:HA	2.18	0.44
1:V:10:VAL:HG12	1:V:12:ILE:HG13	1.99	0.44
1:D:34:HIS:ND1	3:D:2015:HOH:O	2.34	0.44
1:O:15:VAL:HG23	1:O:61:ALA:HA	2.00	0.44
1:I:45:ILE:N	1:I:45:ILE:CD1	2.74	0.43
1:N:53:SER:OG	2:O:80:TRP:HB3	2.18	0.43
1:F:75:LYS:HD3	1:F:75:LYS:HA	1.86	0.43
1:A:56:LYS:HE3	1:B:38:LEU:HD23	2.01	0.43
1:G:74:SER:O	1:G:75:LYS:HB2	2.19	0.43
1:Q:13:LYS:O	1:Q:61:ALA:HB1	2.19	0.43
1:S:33:HIS:NE2	1:S:52:THR:OG1	2.45	0.43
1:N:22:ILE:HG22	1:N:32:PHE:HB2	2.00	0.43
1:I:16:GLU:HB3	3:I:2002:HOH:O	2.18	0.43
1:L:36:GLU:OE2	1:V:56:LYS:NZ	2.45	0.43
1:H:38:LEU:HD11	1:H:44:MET:CB	2.49	0.43
1:I:48:PHE:HZ	1:J:45:ILE:HG22	1.83	0.43
1:A:24:LEU:N	1:A:24:LEU:CD1	2.82	0.43
1:D:30:THR:HG23	2:E:80:TRP:HB2	2.01	0.43
1:T:46:CYS:HB2	2:T:80:TRP:NE1	2.34	0.43
1:T:56:LYS:HE3	1:U:38:LEU:CD2	2.48	0.43
1:M:48:PHE:HZ	1:N:45:ILE:HG22	1.84	0.42
1:H:34:HIS:NE2	1:H:36:GLU:OE1	2.49	0.42
1:H:38:LEU:HD21	1:H:44:MET:HB2	2.00	0.42
1:H:74:SER:HB3	3:H:2011:HOH:O	2.18	0.42
1:F:48:PHE:HZ	1:G:45:ILE:CG2	2.31	0.42
1:P:11:VAL:C	1:P:12:ILE:HG13	2.40	0.42
1:Q:30:THR:OG1	2:R:80:TRP:HB2	2.20	0.42
1:R:30:THR:HG1	2:S:80:TRP:N	2.17	0.42
1:C:53:SER:OG	2:D:80:TRP:HB3	2.18	0.42
1:H:20:ASN:ND2	1:H:35:SER:HG	2.13	0.42
1:Q:15:VAL:HG12	1:Q:15:VAL:O	2.20	0.42
1:R:15:VAL:O	1:R:15:VAL:HG12	2.18	0.42
1:C:45:ILE:N	1:C:45:ILE:HD12	2.35	0.42
1:U:22:ILE:HB	1:U:56:LYS:HB3	2.01	0.42
1:A:15:VAL:HG23	1:A:61:ALA:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:37:LYS:HG3	3:S:2010:HOH:O	2.19	0.42
1:S:56:LYS:CE	1:T:38:LEU:HD23	2.49	0.42
1:E:15:VAL:O	1:E:15:VAL:HG12	2.20	0.42
1:H:22:ILE:HG23	1:H:32:PHE:HB2	2.02	0.42
1:J:30:THR:HG1	2:K:80:TRP:N	2.17	0.42
1:M:24:LEU:HB2	1:M:54:ALA:HB3	2.02	0.42
1:S:56:LYS:HE2	1:T:38:LEU:HD23	2.02	0.42
1:A:25:THR:HA	1:A:51:HIS:O	2.20	0.42
1:P:31[B]:ARG:NH2	3:P:2010:HOH:O	2.52	0.42
1:I:32:PHE:HD1	1:I:32:PHE:H	1.67	0.41
1:F:13:LYS:HB2	1:F:43:VAL:HG22	2.02	0.41
1:I:15:VAL:HG12	1:I:15:VAL:O	2.19	0.41
1:L:38:LEU:HD11	1:L:44:MET:CB	2.50	0.41
1:T:74:SER:O	1:T:76:LYS:N	2.53	0.41
1:F:45:ILE:H	1:F:45:ILE:HD12	1.85	0.41
1:L:38:LEU:HD11	1:L:44:MET:HB2	2.02	0.41
1:U:71:LYS:O	1:V:13:LYS:HD2	2.21	0.41
1:K:64:GLN:HG2	1:K:69:GLU:HG2	2.03	0.41
1:S:19:VAL:O	1:S:37:LYS:HA	2.21	0.41
1:P:57:VAL:HG11	1:P:63:ILE:HD11	2.02	0.41
1:R:26:ARG:HH22	1:S:47:GLN:NE2	2.13	0.41
1:L:24:LEU:N	1:L:24:LEU:CD1	2.83	0.41
1:A:16:GLU:OE2	1:A:74:SER:HB3	2.20	0.41
1:D:71:LYS:O	1:E:13:LYS:NZ	2.50	0.41
1:F:16[A]:GLU:HG3	1:F:17:ASP:O	2.21	0.41
1:H:15:VAL:CG2	1:H:62:LEU:CD1	2.99	0.41
1:H:34:HIS:NE2	1:H:36:GLU:HB2	2.34	0.41
1:H:71:LYS:O	1:I:13:LYS:CE	2.69	0.41
1:P:11:VAL:HB	1:P:64:GLN:HB2	2.02	0.41
1:P:56:LYS:HD2	1:Q:38:LEU:HD23	2.02	0.41
1:U:72:SER:HB3	1:V:43:VAL:HG23	2.02	0.41
1:L:13:LYS:HB2	1:L:43:VAL:HG22	2.03	0.41
1:C:75:LYS:HG3	1:C:75:LYS:O	2.22	0.40
1:F:70:MET:HG3	1:F:71:LYS:N	2.35	0.40
1:L:70:MET:SD	1:M:13:LYS:HB2	2.61	0.40
1:C:48:PHE:HZ	1:D:45:ILE:HG22	1.86	0.40
1:K:22:ILE:CG2	1:K:32:PHE:HB2	2.52	0.40
1:L:15:VAL:O	1:L:40:LYS:HG3	2.21	0.40
1:O:48:PHE:HZ	1:P:45:ILE:HG22	1.85	0.40
1:O:75:LYS:NZ	1:O:75:LYS:HB3	2.36	0.40
1:V:32:PHE:CD1	1:V:32:PHE:C	2.94	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLY:C	1:A:24:LEU:HD12	2.40	0.40
1:C:22:ILE:CG2	1:C:32:PHE:HB2	2.52	0.40
1:E:72:SER:HB2	1:F:41:GLY:O	2.22	0.40
3:J:2019:HOH:O	1:K:13:LYS:NZ	2.50	0.40
1:O:32[A]:PHE:HD1	1:O:32[A]:PHE:H	1.68	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	67/78 (86%)	66 (98%)	0	1 (2%)	10	13
1	B	68/78 (87%)	65 (96%)	2 (3%)	1 (2%)	10	13
1	C	67/78 (86%)	66 (98%)	0	1 (2%)	10	13
1	D	67/78 (86%)	65 (97%)	2 (3%)	0	100	100
1	E	67/78 (86%)	65 (97%)	1 (2%)	1 (2%)	10	13
1	F	68/78 (87%)	65 (96%)	2 (3%)	1 (2%)	10	13
1	G	67/78 (86%)	66 (98%)	1 (2%)	0	100	100
1	H	67/78 (86%)	63 (94%)	4 (6%)	0	100	100
1	I	67/78 (86%)	64 (96%)	2 (3%)	1 (2%)	10	13
1	J	68/78 (87%)	66 (97%)	2 (3%)	0	100	100
1	K	67/78 (86%)	65 (97%)	1 (2%)	1 (2%)	10	13
1	L	70/78 (90%)	67 (96%)	1 (1%)	2 (3%)	4	3
1	M	67/78 (86%)	65 (97%)	1 (2%)	1 (2%)	10	13
1	N	67/78 (86%)	66 (98%)	0	1 (2%)	10	13
1	O	68/78 (87%)	67 (98%)	1 (2%)	0	100	100
1	P	68/78 (87%)	67 (98%)	0	1 (2%)	10	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	67/78 (86%)	66 (98%)	0	1 (2%)	10	13
1	R	67/78 (86%)	66 (98%)	0	1 (2%)	10	13
1	S	67/78 (86%)	64 (96%)	1 (2%)	2 (3%)	4	3
1	T	67/78 (86%)	64 (96%)	2 (3%)	1 (2%)	10	13
1	U	68/78 (87%)	67 (98%)	0	1 (2%)	10	13
1	V	67/78 (86%)	66 (98%)	0	1 (2%)	10	13
All	All	1483/1716 (86%)	1441 (97%)	23 (2%)	19 (1%)	12	16

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	75	LYS
1	C	75	LYS
1	I	75	LYS
1	K	75	LYS
1	L	7	ASN
1	L	75	LYS
1	M	75	LYS
1	N	75	LYS
1	P	75	LYS
1	Q	75	LYS
1	R	75	LYS
1	S	74	SER
1	S	75	LYS
1	U	75	LYS
1	A	75	LYS
1	E	75	LYS
1	F	75	LYS
1	V	75	LYS
1	T	75	LYS

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	58/68 (85%)	58 (100%)	0	100	100
1	B	59/68 (87%)	59 (100%)	0	100	100
1	C	58/68 (85%)	56 (97%)	2 (3%)	37	54
1	D	58/68 (85%)	57 (98%)	1 (2%)	60	77
1	E	58/68 (85%)	56 (97%)	2 (3%)	37	54
1	F	59/68 (87%)	58 (98%)	1 (2%)	60	77
1	G	58/68 (85%)	57 (98%)	1 (2%)	60	77
1	H	58/68 (85%)	58 (100%)	0	100	100
1	I	58/68 (85%)	58 (100%)	0	100	100
1	J	59/68 (87%)	58 (98%)	1 (2%)	60	77
1	K	58/68 (85%)	56 (97%)	2 (3%)	37	54
1	L	61/68 (90%)	60 (98%)	1 (2%)	62	78
1	M	58/68 (85%)	56 (97%)	2 (3%)	37	54
1	N	58/68 (85%)	57 (98%)	1 (2%)	60	77
1	O	59/68 (87%)	59 (100%)	0	100	100
1	P	59/68 (87%)	58 (98%)	1 (2%)	60	77
1	Q	58/68 (85%)	56 (97%)	2 (3%)	37	54
1	R	58/68 (85%)	57 (98%)	1 (2%)	60	77
1	S	58/68 (85%)	58 (100%)	0	100	100
1	T	58/68 (85%)	58 (100%)	0	100	100
1	U	59/68 (87%)	58 (98%)	1 (2%)	60	77
1	V	58/68 (85%)	56 (97%)	2 (3%)	37	54
All	All	1285/1496 (86%)	1264 (98%)	21 (2%)	62	78

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	20	ASN
1	C	50	GLU
1	D	32	PHE
1	E	8	ASP
1	E	32	PHE
1	F	32	PHE
1	G	32	PHE
1	J	32	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	20	ASN
1	K	31	ARG
1	L	16	GLU
1	M	13	LYS
1	M	32	PHE
1	N	20	ASN
1	P	13	LYS
1	Q	32	PHE
1	Q	73	GLU
1	R	32	PHE
1	U	32	PHE
1	V	20	ASN
1	V	32	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	51	HIS
1	H	20	ASN
1	J	7	ASN
1	J	20	ASN
1	K	20	ASN
1	L	7	ASN
1	N	20	ASN
1	O	20	ASN
1	S	47	GLN
1	V	20	ASN
1	V	67	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

22 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TRP	G	80	-	14,16,16	1.18	1 (7%)	16,22,22	1.34	3 (18%)
2	TRP	V	80	-	14,16,16	1.19	1 (7%)	16,22,22	1.39	4 (25%)
2	TRP	C	80	-	14,16,16	1.19	1 (7%)	16,22,22	1.47	4 (25%)
2	TRP	H	80	-	14,16,16	1.19	1 (7%)	16,22,22	1.42	4 (25%)
2	TRP	U	80	-	14,16,16	1.20	2 (14%)	16,22,22	1.45	4 (25%)
2	TRP	Q	80	-	14,16,16	1.18	1 (7%)	16,22,22	1.36	4 (25%)
2	TRP	K	80	-	14,16,16	1.18	1 (7%)	16,22,22	1.44	4 (25%)
2	TRP	B	80	-	14,16,16	1.17	1 (7%)	16,22,22	1.41	4 (25%)
2	TRP	A	80	-	14,16,16	1.20	1 (7%)	16,22,22	1.48	4 (25%)
2	TRP	F	80	-	14,16,16	1.17	1 (7%)	16,22,22	1.37	3 (18%)
2	TRP	R	80	-	14,16,16	1.19	1 (7%)	16,22,22	1.38	3 (18%)
2	TRP	L	80	-	14,16,16	1.20	1 (7%)	16,22,22	1.44	4 (25%)
2	TRP	I	80	-	14,16,16	1.18	1 (7%)	16,22,22	1.45	4 (25%)
2	TRP	N	80	-	14,16,16	1.20	1 (7%)	16,22,22	1.41	4 (25%)
2	TRP	D	80	-	14,16,16	1.19	1 (7%)	16,22,22	1.38	4 (25%)
2	TRP	E	80	-	14,16,16	1.19	1 (7%)	16,22,22	1.50	4 (25%)
2	TRP	O	80	-	14,16,16	1.20	1 (7%)	16,22,22	1.46	4 (25%)
2	TRP	T	80	-	14,16,16	1.18	1 (7%)	16,22,22	1.43	4 (25%)
2	TRP	S	80	-	14,16,16	1.16	1 (7%)	16,22,22	1.35	4 (25%)
2	TRP	M	80	-	14,16,16	1.17	1 (7%)	16,22,22	1.37	4 (25%)
2	TRP	J	80	-	14,16,16	1.20	1 (7%)	16,22,22	1.39	4 (25%)
2	TRP	P	80	-	14,16,16	1.16	0	16,22,22	1.38	4 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRP	G	80	-	-	2/7/8/8	0/2/2/2
2	TRP	V	80	-	-	2/7/8/8	0/2/2/2
2	TRP	C	80	-	-	1/7/8/8	0/2/2/2
2	TRP	H	80	-	-	2/7/8/8	0/2/2/2
2	TRP	U	80	-	-	2/7/8/8	0/2/2/2
2	TRP	Q	80	-	-	0/7/8/8	0/2/2/2
2	TRP	K	80	-	-	1/7/8/8	0/2/2/2
2	TRP	B	80	-	-	2/7/8/8	0/2/2/2
2	TRP	A	80	-	-	1/7/8/8	0/2/2/2
2	TRP	F	80	-	-	0/7/8/8	0/2/2/2
2	TRP	R	80	-	-	1/7/8/8	0/2/2/2
2	TRP	L	80	-	-	1/7/8/8	0/2/2/2
2	TRP	I	80	-	-	1/7/8/8	0/2/2/2
2	TRP	N	80	-	-	1/7/8/8	0/2/2/2
2	TRP	D	80	-	-	1/7/8/8	0/2/2/2
2	TRP	E	80	-	-	0/7/8/8	0/2/2/2
2	TRP	O	80	-	-	2/7/8/8	0/2/2/2
2	TRP	T	80	-	-	1/7/8/8	0/2/2/2
2	TRP	S	80	-	-	1/7/8/8	0/2/2/2
2	TRP	M	80	-	-	0/7/8/8	0/2/2/2
2	TRP	J	80	-	-	2/7/8/8	0/2/2/2
2	TRP	P	80	-	-	2/7/8/8	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	80	TRP	OXT-C	-2.20	1.23	1.30
2	A	80	TRP	OXT-C	-2.17	1.23	1.30
2	R	80	TRP	OXT-C	-2.16	1.23	1.30
2	H	80	TRP	OXT-C	-2.16	1.23	1.30
2	G	80	TRP	OXT-C	-2.15	1.23	1.30
2	I	80	TRP	OXT-C	-2.14	1.23	1.30
2	V	80	TRP	OXT-C	-2.13	1.23	1.30
2	D	80	TRP	OXT-C	-2.13	1.23	1.30
2	T	80	TRP	OXT-C	-2.11	1.23	1.30
2	N	80	TRP	OXT-C	-2.11	1.23	1.30
2	C	80	TRP	OXT-C	-2.10	1.23	1.30
2	L	80	TRP	OXT-C	-2.09	1.23	1.30
2	F	80	TRP	OXT-C	-2.09	1.23	1.30
2	S	80	TRP	OXT-C	-2.08	1.23	1.30
2	M	80	TRP	OXT-C	-2.08	1.23	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	80	TRP	OXT-C	-2.08	1.23	1.30
2	K	80	TRP	OXT-C	-2.07	1.23	1.30
2	J	80	TRP	OXT-C	-2.07	1.23	1.30
2	O	80	TRP	OXT-C	-2.06	1.23	1.30
2	Q	80	TRP	OXT-C	-2.06	1.23	1.30
2	U	80	TRP	OXT-C	-2.04	1.23	1.30
2	U	80	TRP	CD2-CE2	2.01	1.48	1.42

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	80	TRP	OXT-C-O	-2.97	117.35	124.09
2	I	80	TRP	OXT-C-O	-2.93	117.43	124.09
2	F	80	TRP	OXT-C-O	-2.93	117.44	124.09
2	L	80	TRP	OXT-C-O	-2.92	117.47	124.09
2	A	80	TRP	OXT-C-O	-2.91	117.49	124.09
2	E	80	TRP	CE3-CD2-CE2	2.88	121.99	118.17
2	H	80	TRP	OXT-C-O	-2.86	117.59	124.09
2	R	80	TRP	OXT-C-O	-2.86	117.60	124.09
2	V	80	TRP	OXT-C-O	-2.83	117.67	124.09
2	C	80	TRP	OXT-C-O	-2.82	117.70	124.09
2	K	80	TRP	OXT-C-O	-2.80	117.73	124.09
2	E	80	TRP	OXT-C-O	-2.78	117.79	124.09
2	U	80	TRP	OXT-C-O	-2.76	117.83	124.09
2	D	80	TRP	OXT-C-O	-2.74	117.87	124.09
2	A	80	TRP	CE3-CD2-CE2	2.73	121.79	118.17
2	C	80	TRP	CE3-CD2-CE2	2.72	121.77	118.17
2	O	80	TRP	CE3-CD2-CE2	2.71	121.76	118.17
2	L	80	TRP	CE3-CD2-CE2	2.67	121.71	118.17
2	B	80	TRP	OXT-C-O	-2.66	118.05	124.09
2	N	80	TRP	OXT-C-O	-2.66	118.05	124.09
2	O	80	TRP	OXT-C-O	-2.64	118.09	124.09
2	N	80	TRP	CE3-CD2-CE2	2.64	121.67	118.17
2	U	80	TRP	CE3-CD2-CE2	2.60	121.62	118.17
2	G	80	TRP	OXT-C-O	-2.60	118.19	124.09
2	B	80	TRP	CE3-CD2-CE2	2.59	121.60	118.17
2	I	80	TRP	CE3-CD2-CE2	2.58	121.60	118.17
2	J	80	TRP	OXT-C-O	-2.56	118.27	124.09
2	M	80	TRP	CE3-CD2-CE2	2.55	121.54	118.17
2	S	80	TRP	CE3-CD2-CE2	2.54	121.53	118.17
2	K	80	TRP	CE3-CD2-CE2	2.54	121.53	118.17
2	C	80	TRP	CZ3-CE3-CD2	-2.53	117.39	120.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	80	TRP	OXT-C-O	-2.52	118.38	124.09
2	M	80	TRP	OXT-C-O	-2.51	118.38	124.09
2	S	80	TRP	OXT-C-O	-2.50	118.41	124.09
2	H	80	TRP	CE3-CD2-CE2	2.49	121.47	118.17
2	T	80	TRP	CE3-CD2-CE2	2.48	121.46	118.17
2	J	80	TRP	CE3-CD2-CE2	2.47	121.44	118.17
2	P	80	TRP	OXT-C-O	-2.44	118.54	124.09
2	E	80	TRP	CZ3-CE3-CD2	-2.44	117.50	120.89
2	Q	80	TRP	CE3-CD2-CE2	2.44	121.41	118.17
2	P	80	TRP	CE3-CD2-CE2	2.42	121.38	118.17
2	A	80	TRP	CZ3-CE3-CD2	-2.36	117.62	120.89
2	U	80	TRP	CZ3-CE3-CD2	-2.35	117.64	120.89
2	O	80	TRP	CZ3-CE3-CD2	-2.34	117.64	120.89
2	R	80	TRP	CE3-CD2-CE2	2.33	121.26	118.17
2	B	80	TRP	OXT-C-CA	2.33	121.32	113.38
2	K	80	TRP	CZ3-CE3-CD2	-2.32	117.68	120.89
2	G	80	TRP	CE3-CD2-CE2	2.32	121.24	118.17
2	V	80	TRP	CE3-CD2-CE2	2.31	121.23	118.17
2	O	80	TRP	OXT-C-CA	2.30	121.23	113.38
2	D	80	TRP	CE3-CD2-CE2	2.30	121.22	118.17
2	K	80	TRP	OXT-C-CA	2.30	121.21	113.38
2	R	80	TRP	OXT-C-CA	2.30	121.21	113.38
2	F	80	TRP	OXT-C-CA	2.29	121.20	113.38
2	H	80	TRP	OXT-C-CA	2.29	121.17	113.38
2	T	80	TRP	OXT-C-CA	2.28	121.15	113.38
2	I	80	TRP	CZ3-CE3-CD2	-2.27	117.74	120.89
2	N	80	TRP	CZ3-CE3-CD2	-2.27	117.75	120.89
2	J	80	TRP	CZ3-CE3-CD2	-2.26	117.76	120.89
2	L	80	TRP	CZ3-CE3-CD2	-2.26	117.76	120.89
2	P	80	TRP	OXT-C-CA	2.26	121.08	113.38
2	A	80	TRP	OXT-C-CA	2.24	121.03	113.38
2	U	80	TRP	OXT-C-CA	2.24	121.01	113.38
2	G	80	TRP	OXT-C-CA	2.22	120.96	113.38
2	F	80	TRP	CE3-CD2-CE2	2.22	121.11	118.17
2	I	80	TRP	OXT-C-CA	2.22	120.94	113.38
2	D	80	TRP	OXT-C-CA	2.22	120.93	113.38
2	V	80	TRP	OXT-C-CA	2.21	120.92	113.38
2	V	80	TRP	CZ3-CE3-CD2	-2.20	117.84	120.89
2	E	80	TRP	OXT-C-CA	2.19	120.85	113.38
2	H	80	TRP	CZ3-CE3-CD2	-2.19	117.86	120.89
2	J	80	TRP	OXT-C-CA	2.18	120.82	113.38
2	M	80	TRP	OXT-C-CA	2.17	120.76	113.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	80	TRP	CZ3-CE3-CD2	-2.16	117.90	120.89
2	S	80	TRP	CZ3-CE3-CD2	-2.15	117.92	120.89
2	Q	80	TRP	CZ3-CE3-CD2	-2.14	117.92	120.89
2	Q	80	TRP	OXT-C-CA	2.14	120.66	113.38
2	B	80	TRP	CZ3-CE3-CD2	-2.13	117.94	120.89
2	N	80	TRP	OXT-C-CA	2.13	120.64	113.38
2	C	80	TRP	OXT-C-CA	2.12	120.62	113.38
2	L	80	TRP	OXT-C-CA	2.12	120.60	113.38
2	D	80	TRP	CZ3-CE3-CD2	-2.10	117.98	120.89
2	M	80	TRP	CZ3-CE3-CD2	-2.08	118.01	120.89
2	T	80	TRP	CZ3-CE3-CD2	-2.04	118.06	120.89
2	S	80	TRP	OXT-C-CA	2.03	120.30	113.38

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	80	TRP	OXT-C-CA-N
2	H	80	TRP	OXT-C-CA-N
2	P	80	TRP	OXT-C-CA-N
2	G	80	TRP	OXT-C-CA-N
2	J	80	TRP	OXT-C-CA-N
2	V	80	TRP	OXT-C-CA-N
2	B	80	TRP	O-C-CA-N
2	O	80	TRP	OXT-C-CA-N
2	T	80	TRP	OXT-C-CA-N
2	L	80	TRP	OXT-C-CA-N
2	U	80	TRP	OXT-C-CA-N
2	K	80	TRP	OXT-C-CA-N
2	N	80	TRP	OXT-C-CA-N
2	C	80	TRP	OXT-C-CA-N
2	G	80	TRP	O-C-CA-N
2	H	80	TRP	O-C-CA-N
2	J	80	TRP	O-C-CA-N
2	O	80	TRP	O-C-CA-N
2	P	80	TRP	O-C-CA-N
2	U	80	TRP	O-C-CA-N
2	V	80	TRP	O-C-CA-N
2	D	80	TRP	OXT-C-CA-N
2	A	80	TRP	OXT-C-CA-N
2	S	80	TRP	OXT-C-CA-N
2	R	80	TRP	OXT-C-CA-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	I	80	TRP	OXT-C-CA-N

There are no ring outliers.

19 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	80	TRP	1	0
2	V	80	TRP	2	0
2	H	80	TRP	2	0
2	U	80	TRP	1	0
2	Q	80	TRP	1	0
2	K	80	TRP	1	0
2	B	80	TRP	1	0
2	R	80	TRP	2	0
2	L	80	TRP	1	0
2	I	80	TRP	1	0
2	N	80	TRP	1	0
2	D	80	TRP	2	0
2	E	80	TRP	1	0
2	O	80	TRP	2	0
2	T	80	TRP	2	0
2	S	80	TRP	1	0
2	M	80	TRP	1	0
2	J	80	TRP	1	0
2	P	80	TRP	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	69/78 (88%)	0.30	2 (2%)	51	49	22, 33, 44, 53	0
1	B	69/78 (88%)	0.14	0	100	100	23, 34, 45, 52	0
1	C	69/78 (88%)	0.28	3 (4%)	35	32	22, 30, 46, 63	0
1	D	69/78 (88%)	0.08	2 (2%)	51	49	20, 29, 37, 46	0
1	E	69/78 (88%)	0.03	1 (1%)	75	73	21, 28, 36, 45	0
1	F	69/78 (88%)	0.16	1 (1%)	75	73	23, 34, 47, 60	0
1	G	69/78 (88%)	0.40	2 (2%)	51	49	26, 34, 47, 52	0
1	H	69/78 (88%)	0.38	2 (2%)	51	49	24, 32, 45, 53	1 (1%)
1	I	69/78 (88%)	0.26	4 (5%)	23	21	25, 34, 47, 51	0
1	J	70/78 (89%)	0.24	1 (1%)	75	73	24, 34, 44, 50	0
1	K	69/78 (88%)	0.32	2 (2%)	51	49	21, 31, 41, 53	1 (1%)
1	L	71/78 (91%)	0.37	3 (4%)	36	34	24, 33, 47, 52	0
1	M	69/78 (88%)	0.15	1 (1%)	75	73	24, 33, 46, 53	0
1	N	69/78 (88%)	0.13	0	100	100	21, 31, 44, 54	0
1	O	69/78 (88%)	0.09	2 (2%)	51	49	21, 29, 38, 45	0
1	P	69/78 (88%)	0.15	1 (1%)	75	73	22, 30, 38, 47	0
1	Q	69/78 (88%)	0.26	1 (1%)	75	73	23, 35, 46, 51	0
1	R	69/78 (88%)	0.08	0	100	100	25, 33, 44, 50	0
1	S	69/78 (88%)	0.15	1 (1%)	75	73	19, 33, 45, 61	0
1	T	69/78 (88%)	0.10	0	100	100	24, 34, 45, 51	0
1	U	70/78 (89%)	-0.09	0	100	100	21, 31, 42, 50	0
1	V	69/78 (88%)	0.08	0	100	100	22, 31, 39, 46	0
All	All	1522/1716 (88%)	0.19	29 (1%)	66	64	19, 32, 46, 63	2 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	LYS	11.5
1	C	76	LYS	6.6
1	K	76	LYS	6.1
1	G	76	LYS	5.2
1	L	6	SER	4.7
1	Q	18	GLY	4.6
1	P	76	LYS	4.2
1	I	76	LYS	4.1
1	K	31	ARG	3.7
1	D	76	LYS	3.6
1	E	76	LYS	3.1
1	C	75	LYS	3.1
1	C	74	SER	2.7
1	I	32	PHE	2.5
1	L	7	ASN	2.4
1	I	51	HIS	2.3
1	O	32[A]	PHE	2.3
1	A	32	PHE	2.3
1	H	31	ARG	2.2
1	J	75	LYS	2.2
1	D	66	ALA	2.2
1	S	66	ALA	2.2
1	H	29	ASP	2.1
1	F	75	LYS	2.1
1	I	75	LYS	2.1
1	M	51	HIS	2.0
1	O	51	HIS	2.0
1	L	73	GLU	2.0
1	G	75	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TRP	N	80	15/15	0.88	0.19	21,22,26,27	0
2	TRP	T	80	15/15	0.89	0.17	23,26,31,33	0
2	TRP	O	80	15/15	0.90	0.20	28,30,32,33	0
2	TRP	D	80	15/15	0.91	0.14	25,26,28,29	0
2	TRP	I	80	15/15	0.91	0.16	28,31,35,35	0
2	TRP	J	80	15/15	0.91	0.20	22,25,26,27	0
2	TRP	A	80	15/15	0.92	0.16	23,25,27,27	0
2	TRP	Q	80	15/15	0.92	0.14	22,27,34,35	0
2	TRP	B	80	15/15	0.92	0.15	24,26,30,30	0
2	TRP	L	80	15/15	0.93	0.14	20,25,27,27	0
2	TRP	M	80	15/15	0.93	0.14	27,29,31,33	0
2	TRP	R	80	15/15	0.93	0.15	27,29,31,31	0
2	TRP	H	80	15/15	0.93	0.14	18,20,26,27	0
2	TRP	P	80	15/15	0.94	0.15	13,16,22,23	0
2	TRP	E	80	15/15	0.94	0.14	12,17,21,21	0
2	TRP	F	80	15/15	0.94	0.13	22,24,28,29	0
2	TRP	C	80	15/15	0.94	0.14	16,22,24,24	0
2	TRP	U	80	15/15	0.94	0.16	23,25,27,28	0
2	TRP	S	80	15/15	0.95	0.13	20,23,24,27	0
2	TRP	K	80	15/15	0.95	0.14	14,22,24,24	0
2	TRP	G	80	15/15	0.95	0.15	25,27,31,32	0
2	TRP	V	80	15/15	0.95	0.16	19,21,26,27	0

6.5 Other polymers (i)

There are no such residues in this entry.