



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:58 PM UTC

PDB ID : 8UJA / pdb_00008uja
Title : T33-fn10 - Designed Tetrahedral Protein Cage Using Fragment-based Hydrogen Bond Networks
Authors : Meador, K.; Sawaya, M.R.; Yeates, T.O.
Deposited on : 2023-10-11
Resolution : 6.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

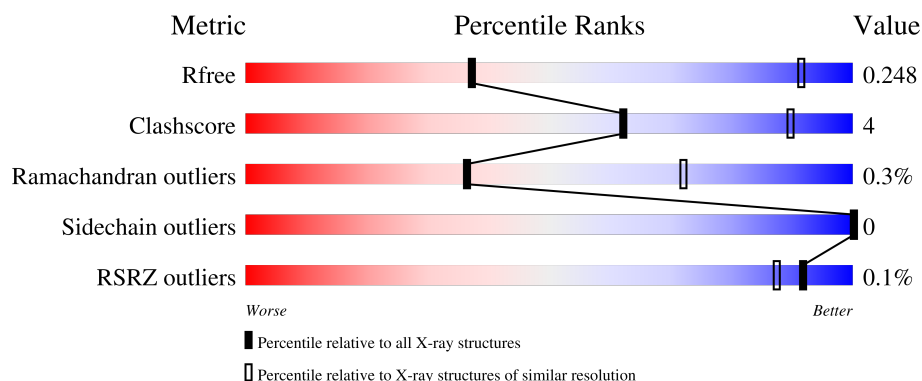
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

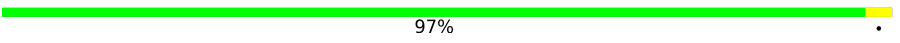
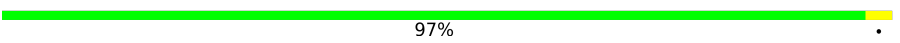
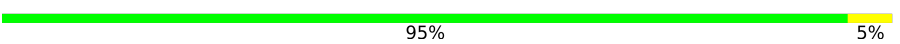
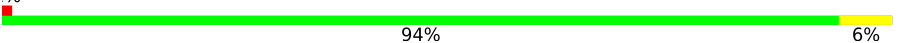
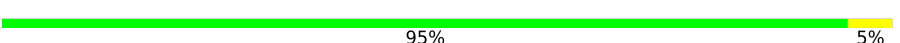
The reported resolution of this entry is 6.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



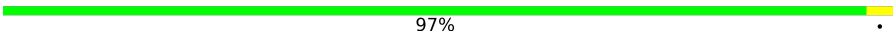
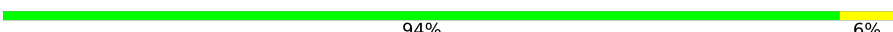
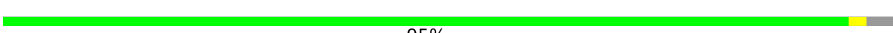
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1143 (8.00-4.00)
Clashscore	190562	1210 (8.00-4.00)
Ramachandran outliers	187476	1034 (8.00-4.00)
Sidechain outliers	187428	1000 (8.00-4.00)
RSRZ outliers	180081	1136 (8.00-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	108	 97% .
1	C	108	 97% .
1	E	108	 95% 5%
1	G	108	 94% 6%
1	I	108	 95% 5%

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Mol	Chain	Length	Quality of chain
1	K	108	 97% .
1	M	108	 92% 8%
1	O	108	 94% 6%
2	B	258	 86% 10% .
2	D	258	 95% . .
2	F	258	 87% 9% .
2	H	258	 86% 10% .
2	J	258	 86% 10% .
2	L	258	 88% 8% .
2	N	258	 86% 10% .
2	P	258	 93% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21720 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 T33-fn10: engineered DrsE like sulfur reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			852	546	149	155	2			
1	C	108	Total	C	N	O	S	0	0	0
			852	546	149	155	2			
1	E	108	Total	C	N	O	S	0	0	0
			852	546	149	155	2			
1	G	108	Total	C	N	O	S	0	0	0
			852	546	149	155	2			
1	I	108	Total	C	N	O	S	0	0	0
			852	546	149	155	2			
1	K	108	Total	C	N	O	S	0	0	0
			852	546	149	155	2			
1	M	108	Total	C	N	O	S	0	0	0
			852	546	149	155	2			
1	O	108	Total	C	N	O	S	0	0	0
			852	546	149	155	2			

- Molecule 2 is a protein called T33-fn10: engineered enoyl-CoA hydratase/isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	S	0	0	0
			1863	1170	336	347	10			
2	D	249	Total	C	N	O	S	0	0	0
			1863	1170	336	347	10			
2	F	249	Total	C	N	O	S	0	0	0
			1863	1170	336	347	10			
2	H	249	Total	C	N	O	S	0	0	0
			1863	1170	336	347	10			
2	J	249	Total	C	N	O	S	0	0	0
			1863	1170	336	347	10			
2	L	249	Total	C	N	O	S	0	0	0
			1863	1170	336	347	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	249	Total	C	N	O	S	0	0	0
			1863	1170	336	347	10			
2	P	249	Total	C	N	O	S	0	0	0
			1863	1170	336	347	10			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP A4XEF6
B	1	HIS	-	expression tag	UNP A4XEF6
B	2	HIS	-	expression tag	UNP A4XEF6
B	3	HIS	-	expression tag	UNP A4XEF6
B	4	HIS	-	expression tag	UNP A4XEF6
B	5	HIS	-	expression tag	UNP A4XEF6
B	6	HIS	-	expression tag	UNP A4XEF6
B	7	SER	-	expression tag	UNP A4XEF6
B	8	GLY	-	expression tag	UNP A4XEF6
B	87	LEU	ALA	engineered mutation	UNP A4XEF6
B	227	THR	ALA	engineered mutation	UNP A4XEF6
B	228	LEU	ASP	engineered mutation	UNP A4XEF6
B	231	CYS	ARG	engineered mutation	UNP A4XEF6
B	237	THR	PHE	engineered mutation	UNP A4XEF6
B	238	LEU	GLU	engineered mutation	UNP A4XEF6
D	0	MET	-	initiating methionine	UNP A4XEF6
D	1	HIS	-	expression tag	UNP A4XEF6
D	2	HIS	-	expression tag	UNP A4XEF6
D	3	HIS	-	expression tag	UNP A4XEF6
D	4	HIS	-	expression tag	UNP A4XEF6
D	5	HIS	-	expression tag	UNP A4XEF6
D	6	HIS	-	expression tag	UNP A4XEF6
D	7	SER	-	expression tag	UNP A4XEF6
D	8	GLY	-	expression tag	UNP A4XEF6
D	87	LEU	ALA	engineered mutation	UNP A4XEF6
D	227	THR	ALA	engineered mutation	UNP A4XEF6
D	228	LEU	ASP	engineered mutation	UNP A4XEF6
D	231	CYS	ARG	engineered mutation	UNP A4XEF6
D	237	THR	PHE	engineered mutation	UNP A4XEF6
D	238	LEU	GLU	engineered mutation	UNP A4XEF6
F	0	MET	-	initiating methionine	UNP A4XEF6
F	1	HIS	-	expression tag	UNP A4XEF6
F	2	HIS	-	expression tag	UNP A4XEF6
F	3	HIS	-	expression tag	UNP A4XEF6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	4	HIS	-	expression tag	UNP A4XEF6
F	5	HIS	-	expression tag	UNP A4XEF6
F	6	HIS	-	expression tag	UNP A4XEF6
F	7	SER	-	expression tag	UNP A4XEF6
F	8	GLY	-	expression tag	UNP A4XEF6
F	87	LEU	ALA	engineered mutation	UNP A4XEF6
F	227	THR	ALA	engineered mutation	UNP A4XEF6
F	228	LEU	ASP	engineered mutation	UNP A4XEF6
F	231	CYS	ARG	engineered mutation	UNP A4XEF6
F	237	THR	PHE	engineered mutation	UNP A4XEF6
F	238	LEU	GLU	engineered mutation	UNP A4XEF6
H	0	MET	-	initiating methionine	UNP A4XEF6
H	1	HIS	-	expression tag	UNP A4XEF6
H	2	HIS	-	expression tag	UNP A4XEF6
H	3	HIS	-	expression tag	UNP A4XEF6
H	4	HIS	-	expression tag	UNP A4XEF6
H	5	HIS	-	expression tag	UNP A4XEF6
H	6	HIS	-	expression tag	UNP A4XEF6
H	7	SER	-	expression tag	UNP A4XEF6
H	8	GLY	-	expression tag	UNP A4XEF6
H	87	LEU	ALA	engineered mutation	UNP A4XEF6
H	227	THR	ALA	engineered mutation	UNP A4XEF6
H	228	LEU	ASP	engineered mutation	UNP A4XEF6
H	231	CYS	ARG	engineered mutation	UNP A4XEF6
H	237	THR	PHE	engineered mutation	UNP A4XEF6
H	238	LEU	GLU	engineered mutation	UNP A4XEF6
J	0	MET	-	initiating methionine	UNP A4XEF6
J	1	HIS	-	expression tag	UNP A4XEF6
J	2	HIS	-	expression tag	UNP A4XEF6
J	3	HIS	-	expression tag	UNP A4XEF6
J	4	HIS	-	expression tag	UNP A4XEF6
J	5	HIS	-	expression tag	UNP A4XEF6
J	6	HIS	-	expression tag	UNP A4XEF6
J	7	SER	-	expression tag	UNP A4XEF6
J	8	GLY	-	expression tag	UNP A4XEF6
J	87	LEU	ALA	engineered mutation	UNP A4XEF6
J	227	THR	ALA	engineered mutation	UNP A4XEF6
J	228	LEU	ASP	engineered mutation	UNP A4XEF6
J	231	CYS	ARG	engineered mutation	UNP A4XEF6
J	237	THR	PHE	engineered mutation	UNP A4XEF6
J	238	LEU	GLU	engineered mutation	UNP A4XEF6
L	0	MET	-	initiating methionine	UNP A4XEF6

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Chain	Residue	Modelled	Actual	Comment	Reference
L	1	HIS	-	expression tag	UNP A4XEF6
L	2	HIS	-	expression tag	UNP A4XEF6
L	3	HIS	-	expression tag	UNP A4XEF6
L	4	HIS	-	expression tag	UNP A4XEF6
L	5	HIS	-	expression tag	UNP A4XEF6
L	6	HIS	-	expression tag	UNP A4XEF6
L	7	SER	-	expression tag	UNP A4XEF6
L	8	GLY	-	expression tag	UNP A4XEF6
L	87	LEU	ALA	engineered mutation	UNP A4XEF6
L	227	THR	ALA	engineered mutation	UNP A4XEF6
L	228	LEU	ASP	engineered mutation	UNP A4XEF6
L	231	CYS	ARG	engineered mutation	UNP A4XEF6
L	237	THR	PHE	engineered mutation	UNP A4XEF6
L	238	LEU	GLU	engineered mutation	UNP A4XEF6
N	0	MET	-	initiating methionine	UNP A4XEF6
N	1	HIS	-	expression tag	UNP A4XEF6
N	2	HIS	-	expression tag	UNP A4XEF6
N	3	HIS	-	expression tag	UNP A4XEF6
N	4	HIS	-	expression tag	UNP A4XEF6
N	5	HIS	-	expression tag	UNP A4XEF6
N	6	HIS	-	expression tag	UNP A4XEF6
N	7	SER	-	expression tag	UNP A4XEF6
N	8	GLY	-	expression tag	UNP A4XEF6
N	87	LEU	ALA	engineered mutation	UNP A4XEF6
N	227	THR	ALA	engineered mutation	UNP A4XEF6
N	228	LEU	ASP	engineered mutation	UNP A4XEF6
N	231	CYS	ARG	engineered mutation	UNP A4XEF6
N	237	THR	PHE	engineered mutation	UNP A4XEF6
N	238	LEU	GLU	engineered mutation	UNP A4XEF6
P	0	MET	-	initiating methionine	UNP A4XEF6
P	1	HIS	-	expression tag	UNP A4XEF6
P	2	HIS	-	expression tag	UNP A4XEF6
P	3	HIS	-	expression tag	UNP A4XEF6
P	4	HIS	-	expression tag	UNP A4XEF6
P	5	HIS	-	expression tag	UNP A4XEF6
P	6	HIS	-	expression tag	UNP A4XEF6
P	7	SER	-	expression tag	UNP A4XEF6
P	8	GLY	-	expression tag	UNP A4XEF6
P	87	LEU	ALA	engineered mutation	UNP A4XEF6
P	227	THR	ALA	engineered mutation	UNP A4XEF6
P	228	LEU	ASP	engineered mutation	UNP A4XEF6
P	231	CYS	ARG	engineered mutation	UNP A4XEF6

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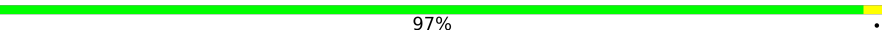
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Chain	Residue	Modelled	Actual	Comment	Reference
P	237	THR	PHE	engineered mutation	UNP A4XEF6
P	238	LEU	GLU	engineered mutation	UNP A4XEF6

3 Residue-property plots [i](#)

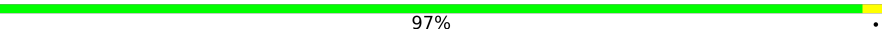
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: T33-fn10: engineered DrsE like sulfur reductase

Chain A:  97% .

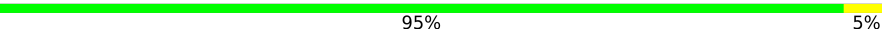


- Molecule 1: T33-fn10: engineered DrsE like sulfur reductase

Chain C:  97% .

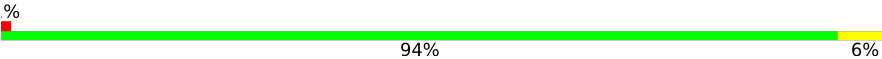


- Molecule 1: T33-fn10: engineered DrsE like sulfur reductase

Chain E:  95% 5%



- Molecule 1: T33-fn10: engineered DrsE like sulfur reductase

Chain G:  94% 6%



- Molecule 1: T33-fn10: engineered DrsE like sulfur reductase

Chain I:  95% 5%



- Molecule 1: T33-fn10: engineered DrsE like sulfur reductase

Chain K:  97% .



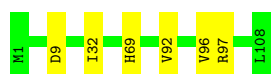
- Molecule 1: T33-fn10: engineered DrsE like sulfur reductase

Chain M: 92% 8%



- Molecule 1: T33-fn10: engineered DrsE like sulfur reductase

Chain O: 94% 6%



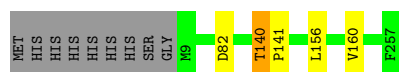
- Molecule 2: T33-fn10: engineered enoyl-CoA hydratase/isomerase

Chain B: 86% 10%



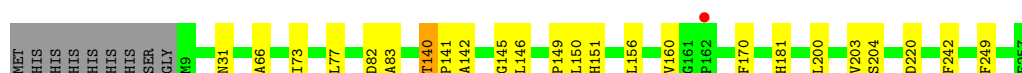
- Molecule 2: T33-fn10: engineered enoyl-CoA hydratase/isomerase

Chain D: 95%



- Molecule 2: T33-fn10: engineered enoyl-CoA hydratase/isomerase

Chain F: 87% 9%



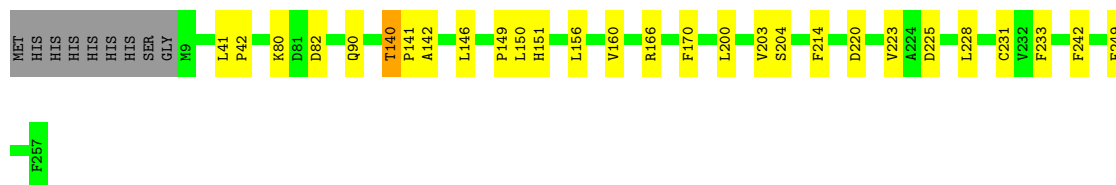
- Molecule 2: T33-fn10: engineered enoyl-CoA hydratase/isomerase

Chain H: 86% 10%



- Molecule 2: T33-fn10: engineered enoyl-CoA hydratase/isomerase

Chain J:  86% 10%



- Molecule 2: T33-fn10: engineered enoyl-CoA hydratase/isomerase

Chain L:  88% 8%

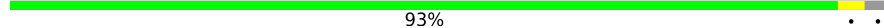


- Molecule 2: T33-fn10: engineered enoyl-CoA hydratase/isomerase

Chain N:  86% 10%



- Molecule 2: T33-fn10: engineered enoyl-CoA hydratase/isomerase

Chain P:  93%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	225.63Å 225.63Å 225.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.11 – 6.00 92.11 – 6.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (92.11-6.00) 99.9 (92.11-6.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 6.19Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.214 , 0.248 0.215 , 0.248	Depositor DCC
R_{free} test set	986 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	356.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 548.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.066 for l,-k,h	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	21720	wwPDB-VP
Average B, all atoms (Å ²)	401.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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	0.55	0/861	0.79	1/1161 (0.1%)
1	C	0.55	0/861	0.79	1/1161 (0.1%)
1	E	0.55	0/861	0.79	1/1161 (0.1%)
1	G	0.55	0/861	0.79	1/1161 (0.1%)
1	I	0.55	0/861	0.79	1/1161 (0.1%)
1	K	0.55	0/861	0.79	1/1161 (0.1%)
1	M	0.55	0/861	0.79	1/1161 (0.1%)
1	O	0.55	0/861	0.79	1/1161 (0.1%)
2	B	0.59	0/1889	0.68	0/2553
2	D	0.59	0/1889	0.68	0/2553
2	F	0.60	0/1889	0.69	0/2553
2	H	0.61	0/1889	0.71	0/2553
2	J	0.60	0/1889	0.69	0/2553
2	L	0.60	0/1889	0.68	0/2553
2	N	0.61	0/1889	0.71	0/2553
2	P	0.59	0/1889	0.69	0/2553
All	All	0.58	0/22000	0.72	8/29712 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	32	ILE	N-CA-C	5.92	117.12	108.53
1	A	32	ILE	N-CA-C	5.91	117.10	108.53
1	E	32	ILE	N-CA-C	5.91	117.10	108.53
1	K	32	ILE	N-CA-C	5.90	117.09	108.53
1	G	32	ILE	N-CA-C	5.89	117.07	108.53
1	I	32	ILE	N-CA-C	5.89	117.07	108.53
1	C	32	ILE	N-CA-C	5.85	117.01	108.53
1	O	32	ILE	N-CA-C	5.84	116.99	108.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	852	0	911	2	0
1	C	852	0	911	2	0
1	E	852	0	911	6	0
1	G	852	0	911	14	0
1	I	852	0	911	10	0
1	K	852	0	911	2	0
1	M	852	0	911	15	0
1	O	852	0	911	12	0
2	B	1863	0	1884	37	0
2	D	1863	0	1884	4	0
2	F	1863	0	1884	31	0
2	H	1863	0	1884	41	0
2	J	1863	0	1884	48	0
2	L	1863	0	1884	47	0
2	N	1863	0	1884	44	0
2	P	1863	0	1884	7	0
All	All	21720	0	22360	181	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 4.

All (181) 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:I:28:GLY:HA3	2:N:83:ALA:CB	1.70	1.21
1:I:28:GLY:HA3	2:N:83:ALA:HB1	1.27	1.16
2:J:146:LEU:HD21	2:L:242:PHE:CD1	2.00	0.97
2:J:150:LEU:HD13	2:L:214:PHE:CG	2.03	0.92
1:M:104:ILE:HG21	1:O:96:VAL:HG13	1.56	0.86
1:I:28:GLY:CA	2:N:83:ALA:HB1	2.06	0.85
1:M:106:LEU:HD21	1:O:92:VAL:HB	1.59	0.85
2:J:249:PHE:CE1	2:N:73:ILE:HG21	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:25:LEU:HB2	2:H:231:CYS:SG	2.17	0.84
2:J:249:PHE:CZ	2:N:73:ILE:HG21	2.14	0.82
2:B:242:PHE:CD1	2:F:146:LEU:HD21	2.16	0.81
1:E:28:GLY:HA3	2:H:83:ALA:CB	2.11	0.80
2:J:242:PHE:CD1	2:N:146:LEU:HD21	2.20	0.77
2:J:220:ASP:OD1	2:L:223:VAL:CG1	2.34	0.75
1:M:104:ILE:CG2	1:O:96:VAL:HG13	2.17	0.74
2:L:83:ALA:HB1	1:M:28:GLY:HA3	1.70	0.74
1:G:21:LEU:HD22	2:H:228:LEU:HD23	1.69	0.73
2:J:220:ASP:OD1	2:L:223:VAL:HG11	1.89	0.72
1:I:25:LEU:O	2:N:87:LEU:CD2	2.38	0.71
2:L:83:ALA:CB	1:M:28:GLY:HA3	2.20	0.71
1:M:12:LYS:NZ	1:O:9:ASP:OD1	2.24	0.70
1:E:25:LEU:O	2:H:87:LEU:HD11	1.92	0.70
2:J:146:LEU:HD21	2:L:242:PHE:CE1	2.27	0.69
1:M:22:ASN:CG	1:O:69:HIS:ND1	2.51	0.69
2:L:150:LEU:HD13	2:N:214:PHE:CG	2.28	0.68
1:K:89:ARG:HD2	2:P:91:GLN:HE22	1.60	0.67
2:B:214:PHE:CG	2:F:150:LEU:HD13	2.29	0.67
2:J:220:ASP:CG	2:L:223:VAL:HG11	2.20	0.66
2:J:146:LEU:CD2	2:L:242:PHE:CD1	2.79	0.66
1:I:25:LEU:O	2:N:87:LEU:HD22	1.96	0.65
2:L:146:LEU:HD21	2:N:242:PHE:CD1	2.32	0.65
2:B:249:PHE:CE1	2:F:73:ILE:HG21	2.31	0.65
1:G:29:ASN:H	2:H:238:LEU:HD11	1.62	0.64
1:E:28:GLY:HA3	2:H:83:ALA:HB2	1.79	0.64
1:E:25:LEU:O	2:H:87:LEU:CD1	2.46	0.64
2:J:150:LEU:HD13	2:L:214:PHE:CB	2.28	0.64
2:B:220:ASP:OD1	2:H:223:VAL:HG11	1.98	0.64
2:J:204:SER:CB	2:N:145:GLY:HA2	2.29	0.63
2:B:223:VAL:HG11	2:F:220:ASP:OD1	1.98	0.63
1:G:29:ASN:HA	2:H:238:LEU:HD13	1.81	0.62
2:J:150:LEU:CD1	2:L:214:PHE:HB3	2.29	0.62
2:J:214:PHE:CG	2:N:150:LEU:HD13	2.34	0.62
2:B:154:LYS:HG3	2:H:218:VAL:HG13	1.82	0.61
1:A:28:GLY:HA3	2:F:83:ALA:HB1	1.83	0.60
1:M:106:LEU:CD2	1:O:92:VAL:HB	2.30	0.60
2:B:223:VAL:CG1	2:F:220:ASP:OD1	2.49	0.60
1:C:26:ASP:OD2	1:E:97:ARG:NH1	2.28	0.60
2:J:151:HIS:HB2	2:L:225:ASP:OD2	2.02	0.59
2:J:150:LEU:CD1	2:L:214:PHE:CB	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:108:LEU:HD21	1:O:92:VAL:HG11	1.84	0.59
2:J:90:GLN:NE2	2:L:233:PHE:HD1	2.01	0.58
2:J:249:PHE:CD1	2:N:77:LEU:HD11	2.37	0.58
2:J:90:GLN:NE2	2:L:233:PHE:CD1	2.72	0.58
2:F:249:PHE:CZ	2:H:73:ILE:HG21	2.38	0.58
2:J:170:PHE:O	2:L:203:VAL:HG11	2.05	0.57
2:L:170:PHE:O	2:N:203:VAL:HG11	2.05	0.56
1:G:21:LEU:HD22	2:H:228:LEU:CD2	2.33	0.56
2:F:249:PHE:CE1	2:H:73:ILE:HG21	2.40	0.56
2:J:220:ASP:HA	2:L:223:VAL:CG2	2.36	0.56
2:J:150:LEU:HD12	2:L:214:PHE:HB3	1.88	0.55
2:J:166:ARG:NH2	2:L:127:ASP:O	2.39	0.55
2:B:94:ASN:ND2	2:H:230:LEU:CD2	2.69	0.55
2:L:220:ASP:OD1	2:N:223:VAL:CG1	2.55	0.55
1:G:25:LEU:HD13	2:H:231:CYS:SG	2.46	0.55
2:L:220:ASP:OD1	2:N:223:VAL:HG11	2.07	0.55
2:J:142:ALA:HB1	2:L:203:VAL:HB	1.89	0.54
1:M:22:ASN:HB3	1:O:69:HIS:ND1	2.23	0.53
1:I:28:GLY:HA3	2:N:83:ALA:HB2	1.81	0.53
2:J:223:VAL:HG11	2:N:220:ASP:OD1	2.09	0.53
2:B:225:ASP:OD2	2:F:151:HIS:HB2	2.08	0.52
2:J:220:ASP:OD1	2:L:223:VAL:HG13	2.08	0.52
2:B:204:SER:CB	2:F:145:GLY:HA2	2.40	0.52
2:J:150:LEU:HD13	2:L:214:PHE:CD1	2.45	0.52
1:M:108:LEU:HD21	1:O:92:VAL:CG1	2.41	0.51
2:L:140:THR:N	2:L:141:PRO:CD	2.74	0.51
1:K:56:GLU:HG3	2:L:228:LEU:HD22	1.92	0.51
2:B:146:LEU:HA	2:H:236:ALA:HB1	1.92	0.51
2:B:249:PHE:CZ	2:F:73:ILE:HG21	2.46	0.51
2:H:140:THR:N	2:H:141:PRO:CD	2.74	0.51
2:J:140:THR:N	2:J:141:PRO:CD	2.74	0.51
2:B:144:LEU:O	2:H:242:PHE:HA	2.10	0.51
2:J:223:VAL:CG1	2:N:220:ASP:OD1	2.59	0.51
2:B:154:LYS:HB2	2:H:218:VAL:HG22	1.92	0.51
2:F:140:THR:N	2:F:141:PRO:CD	2.74	0.51
2:P:140:THR:N	2:P:141:PRO:CD	2.74	0.50
2:D:140:THR:N	2:D:141:PRO:CD	2.74	0.50
2:H:73:ILE:O	2:H:77:LEU:HG	2.12	0.50
2:N:140:THR:N	2:N:141:PRO:CD	2.74	0.50
1:G:21:LEU:CD2	2:H:228:LEU:CD2	2.90	0.50
1:G:24:PHE:CE2	2:H:231:CYS:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:THR:N	2:B:141:PRO:CD	2.74	0.50
1:I:25:LEU:O	2:N:87:LEU:CD1	2.60	0.49
2:N:79:ASN:HB3	2:N:82:ASP:HB3	1.95	0.49
2:B:223:VAL:HG11	2:F:220:ASP:CG	2.38	0.49
2:B:249:PHE:CD1	2:F:77:LEU:HD11	2.47	0.49
2:B:220:ASP:OD1	2:H:223:VAL:CG1	2.60	0.49
2:J:149:PRO:HG3	2:L:233:PHE:CE2	2.48	0.49
2:J:200:LEU:CD2	2:N:170:PHE:HB3	2.43	0.48
1:I:56:GLU:HG3	2:J:228:LEU:HD22	1.95	0.48
2:F:204:SER:CB	2:H:145:GLY:HA2	2.45	0.47
2:B:203:VAL:HG21	2:F:170:PHE:O	2.14	0.47
2:J:225:ASP:OD2	2:N:151:HIS:HB2	2.15	0.47
2:J:203:VAL:HB	2:N:142:ALA:HB1	1.97	0.47
2:J:170:PHE:HB3	2:L:200:LEU:CD2	2.45	0.46
1:A:56:GLU:HB3	2:B:228:LEU:HD22	1.98	0.46
2:L:150:LEU:HD13	2:N:214:PHE:CB	2.45	0.46
2:N:79:ASN:HB2	2:N:85:PHE:CD2	2.51	0.46
1:G:21:LEU:CD1	2:H:228:LEU:HD21	2.45	0.45
2:L:151:HIS:HB2	2:N:225:ASP:OD2	2.15	0.45
1:M:22:ASN:CB	1:O:69:HIS:ND1	2.79	0.45
2:L:166:ARG:NH2	2:N:127:ASP:O	2.43	0.45
1:G:29:ASN:HA	2:H:238:LEU:CD1	2.46	0.45
2:L:166:ARG:NH2	2:N:127:ASP:HA	2.32	0.45
2:N:73:ILE:O	2:N:76:LEU:HB3	2.16	0.45
1:I:60:LEU:HD11	2:J:231:CYS:HB3	1.98	0.45
1:M:27:LEU:HD21	1:O:97:ARG:HH11	1.82	0.45
2:B:250:LEU:HD23	2:F:77:LEU:HD13	1.99	0.45
2:F:203:VAL:HG21	2:H:170:PHE:O	2.16	0.45
2:B:150:LEU:HD21	2:H:222:GLN:HG2	1.98	0.44
2:L:150:LEU:CD1	2:N:214:PHE:HB3	2.47	0.44
2:B:94:ASN:ND2	2:H:230:LEU:HD21	2.33	0.44
2:B:140:THR:N	2:B:141:PRO:HD2	2.32	0.44
2:H:140:THR:N	2:H:141:PRO:HD2	2.32	0.44
2:L:144:LEU:O	2:N:242:PHE:HA	2.17	0.44
2:P:140:THR:N	2:P:141:PRO:HD2	2.32	0.44
2:J:220:ASP:HA	2:L:223:VAL:HG21	2.00	0.44
2:B:203:VAL:HB	2:F:142:ALA:HB1	1.99	0.44
2:D:140:THR:N	2:D:141:PRO:HD2	2.32	0.44
2:F:140:THR:N	2:F:141:PRO:HD2	2.32	0.44
2:J:140:THR:N	2:J:141:PRO:HD2	2.32	0.44
2:L:140:THR:N	2:L:141:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:150:LEU:CD1	2:N:214:PHE:CB	2.96	0.44
2:B:233:PHE:CE2	2:F:149:PRO:HG3	2.53	0.43
1:G:21:LEU:CD2	2:H:228:LEU:HD21	2.48	0.43
2:L:220:ASP:CG	2:N:223:VAL:HG11	2.44	0.43
2:B:90:GLN:NE2	2:H:230:LEU:O	2.38	0.43
2:L:150:LEU:HD12	2:N:214:PHE:HB3	2.00	0.43
2:J:233:PHE:CD1	2:N:90:GLN:NE2	2.86	0.43
2:N:140:THR:N	2:N:141:PRO:HD2	2.32	0.43
2:J:90:GLN:HG3	2:L:233:PHE:CE1	2.54	0.43
1:M:56:GLU:HG3	2:N:228:LEU:HD22	2.01	0.43
2:B:242:PHE:CE1	2:F:146:LEU:HD21	2.54	0.42
2:J:220:ASP:HA	2:L:223:VAL:HG22	2.01	0.42
2:F:242:PHE:HA	2:H:144:LEU:O	2.20	0.42
1:I:25:LEU:O	2:N:87:LEU:HD21	2.15	0.42
2:P:82:ASP:OD1	2:P:82:ASP:C	2.63	0.42
2:J:249:PHE:CE1	2:N:73:ILE:CG2	2.96	0.42
2:B:82:ASP:OD1	2:B:82:ASP:C	2.63	0.42
2:F:181:HIS:CE1	2:H:182:ARG:CZ	3.03	0.41
2:H:82:ASP:OD1	2:H:82:ASP:C	2.63	0.41
2:L:82:ASP:OD1	2:L:82:ASP:C	2.63	0.41
2:B:83:ALA:HB1	1:G:28:GLY:HA3	2.02	0.41
2:B:223:VAL:CG2	2:F:220:ASP:HA	2.49	0.41
1:G:25:LEU:CB	2:H:231:CYS:SG	3.02	0.41
1:M:104:ILE:HG21	1:O:96:VAL:CG1	2.40	0.41
2:F:82:ASP:OD1	2:F:82:ASP:C	2.63	0.41
2:L:170:PHE:O	2:N:203:VAL:HG21	2.20	0.41
2:B:214:PHE:CD1	2:F:150:LEU:HD13	2.55	0.41
2:D:82:ASP:C	2:D:82:ASP:OD1	2.63	0.41
2:J:214:PHE:CB	2:N:150:LEU:HD13	2.51	0.41
1:C:23:LEU:HD11	1:E:96:VAL:HG21	2.02	0.41
1:G:25:LEU:HD22	2:H:227:THR:HG23	2.03	0.41
2:J:82:ASP:OD1	2:J:82:ASP:C	2.63	0.41
2:P:31:ASN:ND2	2:P:66:ALA:O	2.54	0.41
2:D:156:LEU:O	2:D:160:VAL:HG22	2.21	0.41
2:H:156:LEU:O	2:H:160:VAL:HG22	2.21	0.41
2:B:156:LEU:O	2:B:160:VAL:HG22	2.21	0.41
2:F:200:LEU:CD2	2:H:170:PHE:HB3	2.51	0.41
2:B:41:LEU:HB3	2:B:42:PRO:HD3	2.03	0.41
2:B:151:HIS:HB2	2:H:225:ASP:OD2	2.21	0.41
2:F:31:ASN:ND2	2:F:66:ALA:O	2.54	0.41
2:F:156:LEU:O	2:F:160:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:41:LEU:HB3	2:P:42:PRO:HD3	2.03	0.41
2:B:242:PHE:CD1	2:F:146:LEU:CD2	2.97	0.40
2:H:31:ASN:ND2	2:H:66:ALA:O	2.54	0.40
2:J:80:LYS:HE2	2:L:250:LEU:HD11	2.02	0.40
2:P:156:LEU:O	2:P:160:VAL:HG22	2.21	0.40
2:B:31:ASN:ND2	2:B:66:ALA:O	2.54	0.40
2:J:41:LEU:HB3	2:J:42:PRO:HD3	2.03	0.40
2:J:156:LEU:O	2:J:160:VAL:HG22	2.21	0.40
2:J:233:PHE:CE2	2:N:149:PRO:HG3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
1	C	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
1	E	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
1	G	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
1	I	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
1	K	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
1	M	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
1	O	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
2	B	247/258 (96%)	240 (97%)	6 (2%)	1 (0%)	30	67
2	D	247/258 (96%)	240 (97%)	6 (2%)	1 (0%)	30	67
2	F	247/258 (96%)	240 (97%)	6 (2%)	1 (0%)	30	67
2	H	247/258 (96%)	238 (96%)	8 (3%)	1 (0%)	30	67
2	J	247/258 (96%)	240 (97%)	6 (2%)	1 (0%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	247/258 (96%)	240 (97%)	6 (2%)	1 (0%)	30	67
2	N	247/258 (96%)	238 (96%)	7 (3%)	2 (1%)	16	54
2	P	247/258 (96%)	240 (97%)	6 (2%)	1 (0%)	30	67
All	All	2824/2928 (96%)	2748 (97%)	67 (2%)	9 (0%)	36	72

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	74	ALA
2	B	140	THR
2	D	140	THR
2	F	140	THR
2	H	140	THR
2	J	140	THR
2	L	140	THR
2	N	140	THR
2	P	140	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/97 (100%)	97 (100%)	0	100	100
1	C	97/97 (100%)	97 (100%)	0	100	100
1	E	97/97 (100%)	97 (100%)	0	100	100
1	G	97/97 (100%)	97 (100%)	0	100	100
1	I	97/97 (100%)	97 (100%)	0	100	100
1	K	97/97 (100%)	97 (100%)	0	100	100
1	M	97/97 (100%)	97 (100%)	0	100	100
1	O	97/97 (100%)	97 (100%)	0	100	100
2	B	188/196 (96%)	188 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	188/196 (96%)	188 (100%)	0	100	100
2	F	188/196 (96%)	188 (100%)	0	100	100
2	H	188/196 (96%)	188 (100%)	0	100	100
2	J	188/196 (96%)	188 (100%)	0	100	100
2	L	188/196 (96%)	188 (100%)	0	100	100
2	N	188/196 (96%)	188 (100%)	0	100	100
2	P	188/196 (96%)	188 (100%)	0	100	100
All	All	2280/2344 (97%)	2280 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	94	ASN
2	B	97	GLN
2	D	97	GLN
2	F	97	GLN
2	F	181	HIS
2	H	97	GLN
1	I	18	GLN
2	J	97	GLN
2	L	86	HIS
2	L	97	GLN
1	M	22	ASN
2	N	97	GLN
2	P	91	GLN
2	P	97	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 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	108/108 (100%)	-0.44	0	100	100	308, 346, 378, 405	0
1	C	108/108 (100%)	-0.37	0	100	100	329, 367, 394, 414	0
1	E	108/108 (100%)	-0.54	0	100	100	317, 352, 375, 387	0
1	G	108/108 (100%)	-0.46	1 (0%)	81	70	288, 332, 365, 386	0
1	I	108/108 (100%)	-0.54	0	100	100	299, 354, 396, 418	0
1	K	108/108 (100%)	-0.51	0	100	100	342, 409, 447, 466	0
1	M	108/108 (100%)	-0.55	0	100	100	354, 411, 440, 448	0
1	O	108/108 (100%)	-0.62	0	100	100	351, 418, 449, 469	0
2	B	249/258 (96%)	-0.60	0	100	100	304, 364, 413, 446	0
2	D	249/258 (96%)	-0.46	0	100	100	396, 469, 518, 541	0
2	F	249/258 (96%)	-0.56	1 (0%)	88	79	299, 370, 414, 446	0
2	H	249/258 (96%)	-0.59	1 (0%)	88	79	298, 347, 397, 449	0
2	J	249/258 (96%)	-0.58	0	100	100	359, 443, 492, 525	0
2	L	249/258 (96%)	-0.43	0	100	100	384, 465, 503, 532	0
2	N	249/258 (96%)	-0.58	1 (0%)	88	79	385, 438, 474, 513	0
2	P	249/258 (96%)	-0.51	0	100	100	375, 418, 455, 474	0
All	All	2856/2928 (97%)	-0.53	4 (0%)	92	87	288, 403, 490, 541	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	76	LEU	2.5
1	G	96	VAL	2.3
2	N	215	VAL	2.2
2	F	162	PRO	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.