



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:14 AM UTC

PDB ID : 1E4X / pdb_00001e4x
Title : crossreactive binding of a circularized peptide to an anti-TGFalpha antibody Fab-fragment
Authors : Hahn, M.; Winkler, D.; Misselwitz, R.; Wessner, H.; Welfle, K.; Zahn, G.; Schneider-Mergener, J.; Hoehne, W.
Deposited on : 2000-07-12
Resolution : 1.90 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

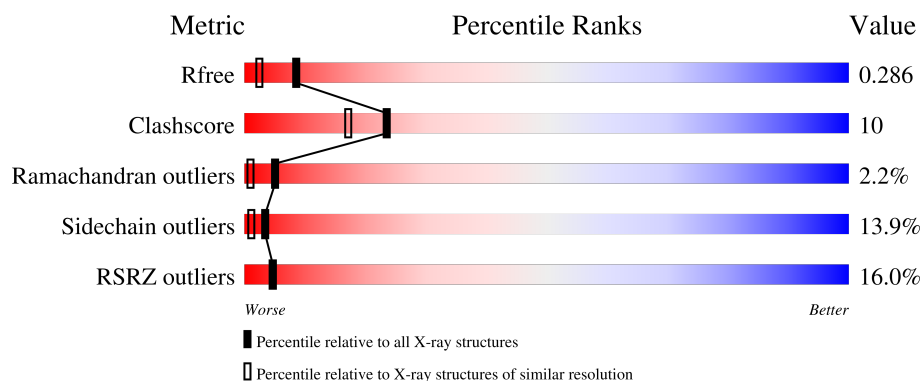
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	H	217	
2	I	217	
3	L	214	
3	M	214	
4	P	7	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	Q	7	29% 86% 14%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7115 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 TAB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	216	Total	C	N	O	S	0	0	0
			1634	1032	270	325	7			

- Molecule 2 is a protein called TAB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	217	Total	C	N	O	S	0	0	0
			1644	1040	271	326	7			

- Molecule 3 is a protein called TAB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1657	1032	276	342	7			
3	M	214	Total	C	N	O	S	0	0	0
			1657	1032	276	342	7			

- Molecule 4 is a protein called CYCLIC PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	7	Total	C	N	O	0	0	0
			58	36	10	12			
4	Q	7	Total	C	N	O	0	0	0
			58	36	10	12			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	67	Total	O	0	0
			67	67		
5	I	91	Total	O	0	0
			91	91		

Continued on next page...

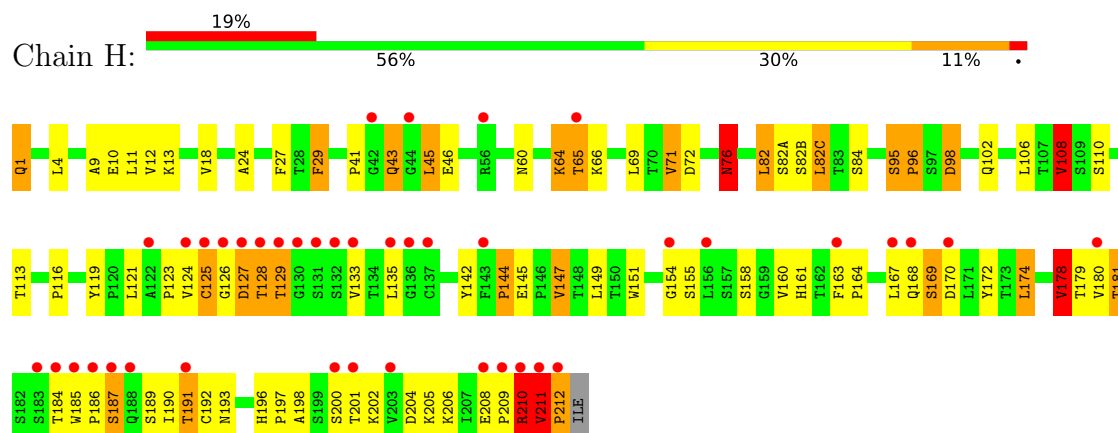
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	130	Total 130	O 130	0	0
5	M	116	Total 116	O 116	0	0
5	P	2	Total 2	O 2	0	0
5	Q	1	Total 1	O 1	0	0

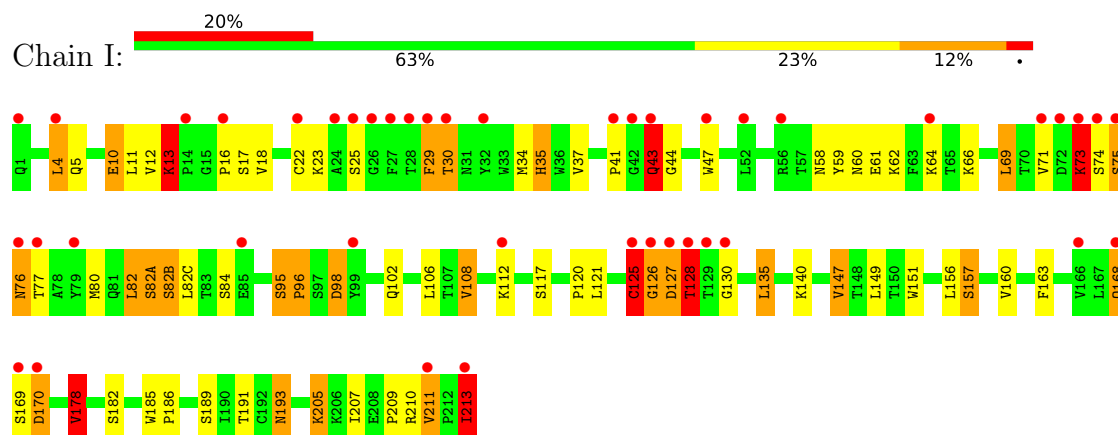
3 Residue-property plots [i](#)

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.

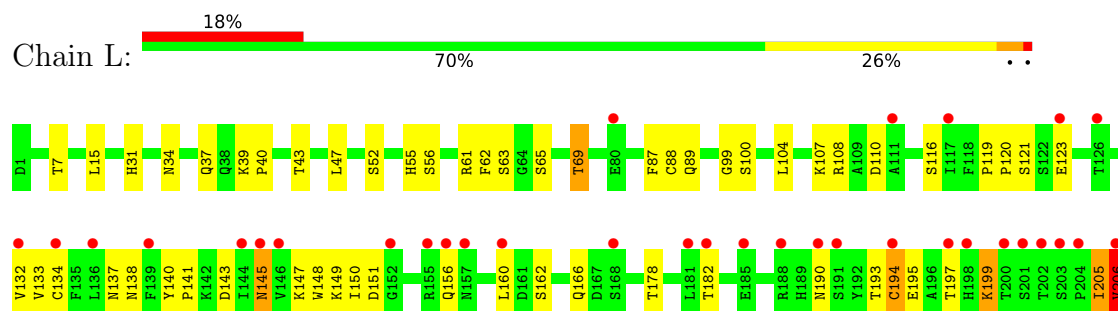
• Molecule 1: TAB2

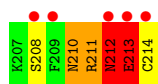


• Molecule 2: TAB2

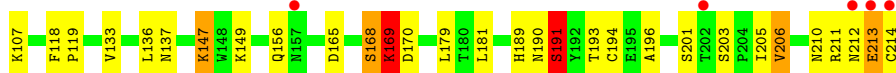
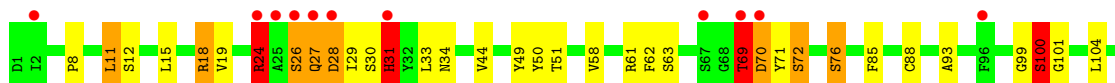


• Molecule 3: TAB2





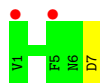
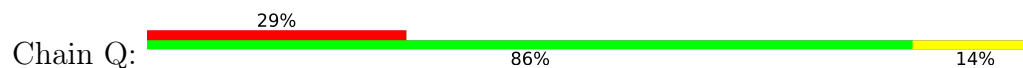
• Molecule 3: TAB2



• Molecule 4: CYCLIC PEPTIDE



• Molecule 4: CYCLIC PEPTIDE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.82Å 45.09Å 120.41Å 90.00° 99.13° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.6 (20.00-1.90) 92.7 (20.00-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.245 , 0.311 0.231 , 0.286	Depositor DCC
R_{free} test set	3426 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7115	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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	H	0.85	0/1677	1.91	39/2293 (1.7%)
2	I	0.86	0/1688	2.05	59/2309 (2.6%)
3	L	0.85	0/1694	1.84	44/2298 (1.9%)
3	M	0.91	0/1694	1.88	35/2298 (1.5%)
4	P	1.16	0/59	1.56	1/78 (1.3%)
4	Q	0.98	1/59 (1.7%)	1.38	0/78
All	All	0.87	1/6871 (0.0%)	1.92	178/9354 (1.9%)

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	H	0	2
2	I	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	7	ASP	C-OXT	5.26	1.34	1.23

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	76	ASN	CA-CB-CG	22.02	134.62	112.60
3	M	31	HIS	CA-CB-CG	21.90	135.70	113.80
1	H	127	ASP	CA-CB-CG	18.52	131.12	112.60
1	H	95	SER	CA-C-O	-15.42	103.49	119.22
2	I	127	ASP	CA-C-N	15.03	150.24	121.54
2	I	127	ASP	C-N-CA	15.03	150.24	121.54
2	I	211	VAL	N-CA-CB	-14.87	95.51	111.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	212	ASN	CA-CB-CG	14.76	127.36	112.60
3	M	18	ARG	CD-NE-CZ	14.01	144.02	124.40
2	I	95	SER	CA-C-O	-11.88	103.89	120.16
2	I	128	THR	N-CA-CB	11.74	130.33	110.49
2	I	76	ASN	N-CA-C	-11.47	97.49	110.91
3	L	69	THR	N-CA-CB	-11.41	93.87	110.65
1	H	65	THR	N-CA-CB	10.40	128.37	111.20
3	L	213	GLU	CA-C-N	9.56	138.91	121.70
3	L	213	GLU	C-N-CA	9.56	138.91	121.70
2	I	170	ASP	CA-CB-CG	9.13	121.73	112.60
1	H	211	VAL	CB-CA-C	9.03	127.80	111.36
2	I	96	PRO	N-CA-CB	8.99	112.69	103.25
1	H	210	ARG	CA-C-O	-8.88	111.48	120.80
2	I	178	VAL	CB-CA-C	-8.79	95.50	110.71
2	I	10	GLU	CA-CB-CG	8.41	130.93	114.10
3	M	206	VAL	CA-C-O	8.41	129.22	120.39
1	H	72	ASP	CA-CB-CG	8.16	120.76	112.60
1	H	209	PRO	CB-CA-C	8.04	122.14	110.63
2	I	147	VAL	N-CA-CB	-8.04	98.93	112.44
3	L	61	ARG	CD-NE-CZ	7.93	135.51	124.40
2	I	74	SER	CA-C-O	7.78	128.62	119.67
3	L	100	SER	CA-CB-OG	-7.69	95.72	111.10
1	H	64	LYS	O-C-N	-7.65	114.01	122.12
3	M	169	LYS	CA-C-O	-7.63	110.55	119.78
2	I	96	PRO	CA-N-CD	-7.60	101.36	112.00
3	M	211	ARG	CA-C-O	-7.56	112.46	120.63
1	H	178	VAL	CB-CA-C	-7.55	98.88	110.50
2	I	29	PHE	CA-CB-CG	7.49	121.29	113.80
1	H	76	ASN	CA-CB-CG	7.31	119.91	112.60
2	I	95	SER	CA-C-N	7.25	128.90	119.84
2	I	95	SER	C-N-CA	7.25	128.90	119.84
3	L	7	THR	O-C-N	7.25	127.02	121.88
2	I	178	VAL	N-CA-CB	7.24	123.33	111.45
1	H	71	VAL	N-CA-CB	-7.22	99.01	112.36
1	H	96	PRO	N-CA-CB	7.21	110.53	102.60
1	H	98	ASP	CA-CB-CG	7.17	119.77	112.60
2	I	157	SER	N-CA-CB	-7.17	100.01	110.40
2	I	210	ARG	CA-C-O	7.06	128.07	119.31
3	M	189	HIS	CA-CB-CG	-6.97	106.83	113.80
2	I	193	ASN	OD1-CG-ND2	6.95	129.55	122.60
2	I	29	PHE	N-CA-C	6.93	121.44	113.19
1	H	64	LYS	N-CA-C	6.93	119.72	111.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	76	SER	CA-C-O	-6.91	113.23	121.66
3	M	137	ASN	N-CA-C	6.85	120.84	109.95
3	L	206	VAL	CA-C-O	6.83	127.57	120.39
2	I	127	ASP	CA-C-O	6.82	130.26	120.51
1	H	1	GLN	CA-CB-CG	-6.82	100.47	114.10
2	I	75	SER	N-CA-C	-6.81	103.12	113.89
1	H	147	VAL	N-CA-CB	-6.71	102.14	111.41
3	L	206	VAL	N-CA-CB	6.71	120.67	111.41
3	L	31	HIS	O-C-N	-6.69	114.84	121.87
2	I	120	PRO	CA-C-O	-6.60	113.25	120.97
1	H	212	PRO	CA-N-CD	-6.52	102.87	112.00
2	I	41	PRO	CA-C-N	6.52	127.18	119.94
2	I	41	PRO	C-N-CA	6.52	127.18	119.94
2	I	213	ILE	N-CA-CB	6.51	122.56	111.50
3	L	178	THR	CA-C-N	-6.48	114.15	122.77
3	L	178	THR	C-N-CA	-6.48	114.15	122.77
2	I	73	LYS	CA-C-N	6.44	134.26	122.79
2	I	73	LYS	C-N-CA	6.44	134.26	122.79
2	I	98	ASP	CA-CB-CG	6.44	119.04	112.60
3	M	194	CYS	CA-C-O	-6.39	113.41	120.38
4	P	6	ASN	OD1-CG-ND2	6.34	128.94	122.60
1	H	108	VAL	CB-CA-C	6.32	119.20	110.99
3	L	145	ASN	CA-CB-CG	-6.32	106.28	112.60
2	I	210	ARG	CA-C-N	6.31	131.95	122.17
2	I	210	ARG	C-N-CA	6.31	131.95	122.17
3	L	69	THR	CA-CB-CG2	6.26	121.15	110.50
2	I	98	ASP	N-CA-C	6.24	119.27	110.23
3	M	93	ALA	CA-C-O	-6.23	114.04	120.89
3	M	69	THR	N-CA-CB	-6.23	100.99	110.33
3	L	166	GLN	O-C-N	-6.20	115.62	123.06
3	M	99	GLY	CA-C-N	6.17	131.03	120.72
3	M	99	GLY	C-N-CA	6.17	131.03	120.72
2	I	156	LEU	CA-C-O	6.16	127.72	120.70
1	H	45	LEU	CA-C-O	-6.16	114.05	120.70
2	I	178	VAL	CG1-CB-CG2	6.15	124.34	110.80
1	H	147	VAL	CB-CA-C	6.13	119.70	110.63
3	L	65	SER	O-C-N	6.12	130.23	123.25
3	M	18	ARG	CA-C-O	6.12	126.91	120.36
3	L	55	HIS	CA-CB-CG	6.11	119.91	113.80
3	L	213	GLU	CA-C-O	6.10	128.58	121.87
3	M	62	PHE	O-C-N	-6.08	116.29	123.22
1	H	66	LYS	N-CA-C	-6.06	104.01	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	127	ASP	O-C-N	-6.04	114.55	122.59
2	I	117	SER	N-CA-C	-6.02	100.68	110.20
3	M	72	SER	CA-CB-OG	-6.02	99.06	111.10
3	L	190	ASN	CA-CB-CG	-6.00	106.60	112.60
2	I	127	ASP	CA-CB-CG	6.00	118.60	112.60
2	I	13	LYS	CA-C-N	5.87	126.07	119.90
2	I	13	LYS	C-N-CA	5.87	126.07	119.90
2	I	205	LYS	O-C-N	5.83	130.72	123.14
2	I	60	ASN	CA-C-O	-5.83	114.11	120.81
3	M	44	VAL	O-C-N	-5.82	116.91	123.20
3	M	100	SER	N-CA-CB	-5.82	100.73	110.39
3	M	58	VAL	CB-CA-C	5.81	116.34	110.94
2	I	58	ASN	CA-CB-CG	5.80	118.40	112.60
3	L	178	THR	O-C-N	5.75	129.94	123.27
2	I	189	SER	O-C-N	-5.75	115.80	122.87
2	I	163	PHE	CA-CB-CG	-5.72	108.08	113.80
3	L	132	VAL	CA-C-N	-5.67	113.14	122.67
3	L	132	VAL	C-N-CA	-5.67	113.14	122.67
2	I	211	VAL	N-CA-C	5.66	115.41	109.01
1	H	65	THR	N-CA-C	-5.65	105.06	112.41
3	L	182	THR	N-CA-C	-5.65	102.92	110.55
2	I	147	VAL	CB-CA-C	5.64	119.13	110.55
3	M	170	ASP	CA-CB-CG	5.63	118.23	112.60
3	L	99	GLY	N-CA-C	-5.63	103.79	112.85
3	L	56	SER	O-C-N	-5.61	116.33	123.06
3	M	29	ILE	CA-C-N	5.59	130.30	122.36
3	M	29	ILE	C-N-CA	5.59	130.30	122.36
3	L	194	CYS	CB-CA-C	-5.57	99.35	109.38
1	H	209	PRO	CA-C-N	5.55	132.28	122.08
1	H	209	PRO	C-N-CA	5.55	132.28	122.08
3	M	26	SER	CA-CB-OG	5.52	122.15	111.10
3	L	87	PHE	CA-CB-CG	5.51	119.31	113.80
3	M	27	GLN	N-CA-C	5.49	117.05	107.49
2	I	96	PRO	N-CD-CG	5.47	111.41	103.20
2	I	182	SER	CA-CB-OG	-5.42	100.25	111.10
1	H	60	ASN	CA-CB-CG	5.42	118.02	112.60
2	I	213	ILE	CB-CA-C	-5.42	100.77	111.60
1	H	1	GLN	OE1-CD-NE2	5.41	128.01	122.60
1	H	60	ASN	N-CA-C	-5.40	100.99	109.25
3	M	211	ARG	CA-C-N	-5.39	113.62	122.79
3	M	211	ARG	C-N-CA	-5.39	113.62	122.79
3	L	212	ASN	N-CA-C	5.39	122.28	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	189	SER	CA-C-O	5.38	127.11	121.19
1	H	108	VAL	N-CA-CB	5.34	118.63	111.90
1	H	178	VAL	N-CA-CB	5.34	120.20	111.44
3	M	12	SER	N-CA-CB	5.34	118.98	110.65
1	H	64	LYS	CA-C-N	-5.33	114.11	122.49
1	H	64	LYS	C-N-CA	-5.33	114.11	122.49
2	I	30	THR	N-CA-C	5.32	117.49	111.11
3	L	210	ASN	CA-C-O	-5.32	114.58	120.38
3	M	214	CYS	CA-CB-SG	5.31	126.61	114.40
2	I	60	ASN	N-CA-C	-5.30	102.01	109.96
3	L	143	ASP	CA-CB-CG	-5.28	107.32	112.60
3	M	168	SER	CA-CB-OG	-5.28	100.53	111.10
1	H	191	THR	CA-C-N	-5.28	115.44	122.72
1	H	191	THR	C-N-CA	-5.28	115.44	122.72
3	L	108	ARG	N-CA-C	-5.26	101.44	108.86
3	L	69	THR	O-C-N	-5.26	115.89	122.35
3	L	213	GLU	N-CA-CB	5.25	117.77	110.26
3	L	89	GLN	OE1-CD-NE2	-5.25	117.35	122.60
2	I	35	HIS	N-CA-C	5.24	118.54	110.42
3	L	120	PRO	CA-C-O	-5.21	115.31	121.67
3	L	205	ILE	CA-C-O	-5.21	114.56	120.65
3	M	99	GLY	N-CA-C	-5.20	104.48	112.85
2	I	10	GLU	N-CA-CB	5.17	120.14	110.99
3	M	165	ASP	N-CA-C	-5.16	103.58	110.55
1	H	145	GLU	N-CA-C	-5.16	102.77	110.20
1	H	9	ALA	O-C-N	5.15	128.94	123.42
3	L	63	SER	CA-C-N	-5.15	117.15	121.58
3	L	63	SER	C-N-CA	-5.15	117.15	121.58
1	H	98	ASP	N-CA-C	5.15	117.69	110.23
3	L	213	GLU	N-CA-C	5.13	117.16	110.43
1	H	102	GLN	CA-C-O	5.12	125.67	119.31
3	L	52	SER	N-CA-CB	-5.11	101.82	111.43
2	I	76	ASN	CB-CA-C	5.10	121.19	112.27
3	M	49	TYR	CA-C-O	5.09	127.16	121.40
2	I	125	CYS	CA-C-O	5.09	127.78	120.51
1	H	46	GLU	O-C-N	5.08	129.26	123.31
3	L	190	ASN	CA-C-O	-5.06	113.24	120.07
3	L	62	PHE	CA-CB-CG	-5.05	108.75	113.80
3	M	76	SER	O-C-N	5.05	128.74	123.03
3	M	191	SER	O-C-N	-5.05	117.57	123.27
3	M	24	ARG	NE-CZ-NH1	5.04	126.54	121.50
2	I	140	LYS	N-CA-C	5.03	117.59	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	43	THR	CA-CB-OG1	5.01	117.12	109.60
3	L	137	ASN	N-CA-C	5.01	118.23	110.17
1	H	163	PHE	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	95	SER	Peptide,Mainchain
2	I	95	SER	Peptide,Mainchain

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	H	1634	0	1603	43	0
2	I	1644	0	1615	44	0
3	L	1657	0	1576	26	0
3	M	1657	0	1576	29	0
4	P	58	0	51	0	0
4	Q	58	0	51	0	0
5	H	67	0	0	1	0
5	I	91	0	0	3	0
5	L	130	0	0	3	0
5	M	116	0	0	6	0
5	P	2	0	0	0	0
5	Q	1	0	0	0	0
All	All	7115	0	6472	134	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 10.

All (134) 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:H:211:VAL:HG22	1:H:212:PRO:HD3	1.45	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:191:THR:HG22	1:H:206:LYS:HG3	1.51	0.91
2:I:126:GLY:H	2:I:211:VAL:HG21	1.35	0.89
2:I:125:CYS:HA	2:I:211:VAL:HG11	1.64	0.79
3:M:8:PRO:HG3	3:M:11:LEU:HD13	1.65	0.77
3:M:27:GLN:O	3:M:28:ASP:C	2.26	0.77
2:I:35:HIS:ND1	2:I:47:TRP:NE1	2.32	0.75
1:H:211:VAL:HG22	1:H:212:PRO:CD	2.17	0.74
1:H:160:VAL:HG22	1:H:178:VAL:HG13	1.68	0.74
3:L:193:THR:HG23	3:L:208:SER:HB3	1.71	0.73
1:H:196:HIS:HB3	1:H:201:THR:HG22	1.71	0.72
1:H:180:VAL:HG11	1:H:190:ILE:HD11	1.70	0.71
3:M:24:ARG:HD2	3:M:70:ASP:OD1	1.89	0.71
2:I:126:GLY:N	2:I:211:VAL:HG21	2.05	0.70
2:I:191:THR:HG23	5:I:2048:HOH:O	1.91	0.70
1:H:196:HIS:HB3	1:H:201:THR:CG2	2.22	0.69
3:L:211:ARG:O	3:L:212:ASN:HB2	1.91	0.69
2:I:135:LEU:HG	2:I:207:ILE:HG21	1.74	0.68
2:I:75:SER:HB2	2:I:77:THR:OG1	1.94	0.68
2:I:59:TYR:HB2	2:I:64:LYS:HE3	1.76	0.67
1:H:29:PHE:H	1:H:76:ASN:HD21	1.42	0.67
3:M:69:THR:HG22	3:M:70:ASP:OD1	1.98	0.63
3:M:30:SER:O	3:M:31:HIS:HB2	1.98	0.63
3:L:210:ASN:O	3:L:212:ASN:N	2.32	0.63
3:L:147:LYS:HE3	3:L:149:LYS:HE3	1.82	0.62
2:I:13:LYS:O	2:I:16:PRO:HD2	1.99	0.61
2:I:69:LEU:HD12	2:I:80:MET:HG3	1.84	0.59
2:I:160:VAL:HG22	2:I:178:VAL:HG13	1.83	0.59
1:H:169:SER:OG	1:H:170:ASP:N	2.34	0.59
2:I:126:GLY:H	2:I:211:VAL:CG2	2.11	0.59
3:M:11:LEU:HD23	3:M:19:VAL:HG13	1.86	0.58
2:I:4:LEU:HD11	2:I:34:MET:HE1	1.86	0.57
3:M:147:LYS:HD2	3:M:149:LYS:HE3	1.85	0.57
3:M:50:TYR:O	3:M:51:THR:HB	2.05	0.57
3:M:18:ARG:NE	5:M:2013:HOH:O	2.38	0.57
3:L:148:TRP:CH2	3:L:194:CYS:SG	2.99	0.56
3:L:211:ARG:O	3:L:212:ASN:CB	2.53	0.56
3:M:100:SER:HB2	5:M:2053:HOH:O	2.06	0.56
1:H:210:ARG:NH2	3:L:121:SER:HA	2.20	0.56
2:I:191:THR:HG21	5:I:2018:HOH:O	2.06	0.55
3:M:136:LEU:HD21	3:M:196:ALA:HB2	1.87	0.55
1:H:125:CYS:HA	1:H:210:ARG:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:154:GLY:HA3	2:I:16:PRO:HB3	1.89	0.55
2:I:23:LYS:HE2	2:I:75:SER:HB3	1.88	0.55
2:I:61:GLU:HA	2:I:64:LYS:HG3	1.89	0.55
3:M:169:LYS:HB3	3:M:169:LYS:NZ	2.22	0.54
3:M:149:LYS:HB2	3:M:193:THR:HB	1.90	0.54
1:H:161:HIS:HE1	3:L:138:ASN:OD1	1.91	0.54
1:H:18:VAL:HG12	1:H:82:LEU:HB2	1.90	0.53
1:H:125:CYS:SG	3:L:214:CYS:O	2.65	0.53
3:M:179:LEU:HG	3:M:181:LEU:HD13	1.91	0.51
1:H:193:ASN:HA	1:H:204:ASP:OD1	2.10	0.51
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.93	0.51
2:I:12:VAL:O	2:I:108:VAL:HA	2.11	0.51
1:H:127:ASP:O	1:H:128:THR:C	2.53	0.51
2:I:4:LEU:HG	2:I:22:CYS:SG	2.51	0.50
2:I:151:TRP:CE2	2:I:178:VAL:HG22	2.47	0.50
3:L:213:GLU:HG3	3:L:214:CYS:N	2.26	0.50
3:M:18:ARG:NH1	3:M:76:SER:OG	2.45	0.50
1:H:144:PRO:HD2	1:H:198:ALA:CB	2.42	0.50
3:L:123:GLU:HB2	5:L:2104:HOH:O	2.11	0.50
2:I:126:GLY:H	2:I:211:VAL:HG11	1.77	0.49
3:L:110:ASP:OD2	3:L:199:LYS:HD2	2.12	0.49
3:L:195:GLU:HG2	3:L:206:VAL:HB	1.93	0.49
2:I:169:SER:OG	2:I:170:ASP:N	2.45	0.49
1:H:144:PRO:O	1:H:196:HIS:HE1	1.96	0.49
1:H:181:THR:OG1	1:H:184:THR:HG23	2.13	0.49
1:H:185:TRP:HA	1:H:186:PRO:C	2.38	0.48
1:H:116:PRO:HB3	1:H:142:TYR:HB3	1.96	0.48
1:H:151:TRP:CZ3	1:H:192:CYS:HB3	2.49	0.48
2:I:209:PRO:HB3	2:I:213:ILE:HD11	1.96	0.48
2:I:61:GLU:HA	2:I:64:LYS:HZ3	1.78	0.48
3:L:210:ASN:O	3:L:211:ARG:C	2.57	0.47
3:L:197:THR:HG23	5:L:2128:HOH:O	2.15	0.47
3:M:205:ILE:HD11	5:M:2113:HOH:O	2.14	0.47
2:I:5:GLN:NE2	2:I:23:LYS:HD3	2.30	0.47
1:H:24:ALA:HB1	1:H:27:PHE:CE1	2.50	0.47
1:H:133:VAL:O	1:H:179:THR:HA	2.14	0.47
1:H:149:LEU:HD23	1:H:149:LEU:C	2.39	0.47
3:M:18:ARG:NH2	5:M:2013:HOH:O	2.47	0.47
2:I:59:TYR:HB3	2:I:64:LYS:HG2	1.97	0.47
1:H:189:SER:OG	1:H:206:LYS:HE3	2.15	0.47
2:I:5:GLN:HB3	2:I:23:LYS:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:12:VAL:HG12	2:I:16:PRO:HG2	1.96	0.46
1:H:197:PRO:O	1:H:198:ALA:C	2.59	0.46
1:H:155:SER:HB3	2:I:17:SER:OG	2.16	0.46
3:M:136:LEU:CD2	3:M:196:ALA:HB2	2.45	0.46
1:H:210:ARG:HG3	5:H:2054:HOH:O	2.16	0.46
2:I:43:GLN:HB3	2:I:44:GLY:H	1.53	0.46
1:H:12:VAL:O	1:H:108:VAL:HA	2.15	0.46
3:L:116:SER:O	3:L:134:CYS:HA	2.15	0.46
2:I:125:CYS:HA	2:I:211:VAL:CG1	2.42	0.45
3:M:201:SER:OG	3:M:203:SER:O	2.29	0.45
1:H:82:LEU:HB3	1:H:82(C):LEU:HD21	1.99	0.45
1:H:124:VAL:O	1:H:125:CYS:C	2.58	0.45
3:M:191:SER:HB2	3:M:210:ASN:ND2	2.32	0.45
2:I:69:LEU:CD1	2:I:80:MET:HG3	2.47	0.45
1:H:185:TRP:CG	1:H:186:PRO:HA	2.52	0.44
2:I:185:TRP:CG	2:I:186:PRO:HA	2.52	0.44
2:I:149:LEU:C	2:I:149:LEU:HD23	2.42	0.44
3:M:85:PHE:CZ	3:M:101:GLY:HA3	2.52	0.44
3:M:18:ARG:CZ	5:M:2013:HOH:O	2.65	0.44
1:H:164:PRO:HD2	3:L:162:SER:OG	2.18	0.44
3:L:213:GLU:HB3	5:L:2130:HOH:O	2.18	0.44
3:M:107:LYS:HE3	5:M:2006:HOH:O	2.18	0.44
2:I:157:SER:HB2	5:I:2050:HOH:O	2.17	0.44
3:M:33:LEU:HG	3:M:71:TYR:CB	2.48	0.43
2:I:66:LYS:O	2:I:82:LEU:HA	2.19	0.43
2:I:186:PRO:HG3	2:I:213:ILE:HD12	2.00	0.43
3:L:140:TYR:CG	3:L:141:PRO:HA	2.53	0.43
3:L:34:ASN:O	3:L:88:CYS:HA	2.19	0.43
3:L:150:ILE:O	3:L:151:ASP:HB2	2.18	0.43
3:M:34:ASN:O	3:M:88:CYS:HA	2.19	0.43
2:I:82(A):SER:O	2:I:82(B):SER:C	2.62	0.42
2:I:126:GLY:N	2:I:211:VAL:HG11	2.34	0.42
2:I:125:CYS:HB3	2:I:211:VAL:HG21	2.01	0.42
3:L:39:LYS:HB3	3:L:40:PRO:CD	2.50	0.42
2:I:211:VAL:O	2:I:211:VAL:HG13	2.18	0.42
3:M:118:PHE:HA	3:M:119:PRO:HD3	1.94	0.42
1:H:144:PRO:HD2	1:H:198:ALA:HB3	2.01	0.42
2:I:168:GLN:O	2:I:169:SER:C	2.63	0.42
1:H:119:TYR:CE1	3:L:123:GLU:HG2	2.55	0.41
3:L:39:LYS:HB3	3:L:40:PRO:HD2	2.01	0.41
1:H:174:LEU:C	1:H:174:LEU:HD12	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:13:LYS:HD2	1:H:110:SER:HA	2.02	0.41
3:M:27:GLN:O	3:M:27:GLN:HG3	2.20	0.41
1:H:186:PRO:O	1:H:187:SER:C	2.63	0.41
1:H:123:PRO:O	1:H:124:VAL:C	2.62	0.41
2:I:73:LYS:H	2:I:73:LYS:HG3	1.56	0.41
2:I:61:GLU:HA	2:I:64:LYS:NZ	2.36	0.40
1:H:167:LEU:HD13	1:H:172:TYR:CZ	2.56	0.40
3:M:18:ARG:CZ	3:M:76:SER:OG	2.69	0.40
1:H:124:VAL:HG22	3:L:119:PRO:HG3	2.03	0.40
3:M:61:ARG:HB2	3:M:76:SER:O	2.21	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	H	214/217 (99%)	191 (89%)	15 (7%)	8 (4%)	2	0
2	I	215/217 (99%)	199 (93%)	9 (4%)	7 (3%)	3	0
3	L	212/214 (99%)	205 (97%)	5 (2%)	2 (1%)	14	6
3	M	212/214 (99%)	206 (97%)	4 (2%)	2 (1%)	14	6
4	P	5/7 (71%)	5 (100%)	0	0	100	100
4	Q	5/7 (71%)	5 (100%)	0	0	100	100
All	All	863/876 (98%)	811 (94%)	33 (4%)	19 (2%)	5	1

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	126	GLY
1	H	129	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	211	VAL
2	I	126	GLY
2	I	128	THR
3	L	211	ARG
3	L	212	ASN
1	H	43	GLN
2	I	125	CYS
3	M	28	ASP
1	H	169	SER
2	I	73	LYS
2	I	130	GLY
3	M	213	GLU
1	H	113	THR
1	H	187	SER
2	I	43	GLN
2	I	96	PRO
1	H	96	PRO

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	H	188/189 (100%)	149 (79%)	39 (21%)	1	0
2	I	190/190 (100%)	156 (82%)	34 (18%)	2	0
3	L	190/190 (100%)	177 (93%)	13 (7%)	14	7
3	M	190/190 (100%)	169 (89%)	21 (11%)	6	2
4	P	7/7 (100%)	7 (100%)	0	100	100
4	Q	7/7 (100%)	7 (100%)	0	100	100
All	All	772/773 (100%)	665 (86%)	107 (14%)	3	1

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	4	LEU
1	H	10	GLU
1	H	11	LEU
1	H	29	PHE
1	H	41	PRO
1	H	43	GLN
1	H	45	LEU
1	H	64	LYS
1	H	65	THR
1	H	69	LEU
1	H	71	VAL
1	H	76	ASN
1	H	82	LEU
1	H	82(A)	SER
1	H	82(B)	SER
1	H	82(C)	LEU
1	H	84	SER
1	H	98	ASP
1	H	106	LEU
1	H	108	VAL
1	H	121	LEU
1	H	125	CYS
1	H	128	THR
1	H	129	THR
1	H	135	LEU
1	H	144	PRO
1	H	147	VAL
1	H	158	SER
1	H	168	GLN
1	H	174	LEU
1	H	178	VAL
1	H	181	THR
1	H	200	SER
1	H	202	LYS
1	H	205	LYS
1	H	208	GLU
1	H	210	ARG
1	H	211	VAL
2	I	4	LEU
2	I	10	GLU
2	I	11	LEU
2	I	13	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	18	VAL
2	I	25	SER
2	I	29	PHE
2	I	30	THR
2	I	37	VAL
2	I	43	GLN
2	I	62	LYS
2	I	69	LEU
2	I	71	VAL
2	I	76	ASN
2	I	82	LEU
2	I	82(A)	SER
2	I	82(B)	SER
2	I	82(C)	LEU
2	I	84	SER
2	I	98	ASP
2	I	102	GLN
2	I	106	LEU
2	I	108	VAL
2	I	112	LYS
2	I	121	LEU
2	I	127	ASP
2	I	128	THR
2	I	135	LEU
2	I	147	VAL
2	I	168	GLN
2	I	178	VAL
2	I	193	ASN
2	I	205	LYS
2	I	213	ILE
3	L	15	LEU
3	L	69	THR
3	L	104	LEU
3	L	107	LYS
3	L	133	VAL
3	L	145	ASN
3	L	156	GLN
3	L	160	LEU
3	L	199	LYS
3	L	205	ILE
3	L	206	VAL
3	L	212	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	213	GLU
3	M	11	LEU
3	M	15	LEU
3	M	24	ARG
3	M	26	SER
3	M	31	HIS
3	M	63	SER
3	M	69	THR
3	M	70	ASP
3	M	72	SER
3	M	100	SER
3	M	104	LEU
3	M	133	VAL
3	M	147	LYS
3	M	156	GLN
3	M	168	SER
3	M	169	LYS
3	M	190	ASN
3	M	191	SER
3	M	206	VAL
3	M	212	ASN
3	M	213	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	1	GLN
1	H	39	GLN
1	H	43	GLN
1	H	76	ASN
1	H	161	HIS
1	H	168	GLN
1	H	196	HIS
2	I	5	GLN
2	I	39	GLN
2	I	43	GLN
2	I	102	GLN
2	I	168	GLN
3	L	38	GLN
3	L	212	ASN
3	M	27	GLN
3	M	34	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	M	38	GLN
3	M	55	HIS
3	M	156	GLN
3	M	190	ASN
3	M	210	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 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	H	216/217 (99%)	1.14	41 (18%)	3 3	23, 38, 58, 79	0
2	I	217/217 (100%)	1.09	43 (19%)	3 3	21, 36, 59, 79	0
3	L	214/214 (100%)	0.88	38 (17%)	4 3	21, 35, 53, 69	0
3	M	214/214 (100%)	0.56	16 (7%)	20 21	21, 32, 47, 68	0
4	P	7/7 (100%)	-0.04	0	100 100	23, 25, 27, 27	0
4	Q	7/7 (100%)	1.22	2 (28%)	1 1	34, 35, 38, 42	0
All	All	875/876 (99%)	0.91	140 (16%)	5 5	21, 35, 55, 79	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	214	CYS	9.6
1	H	211	VAL	9.2
1	H	65	THR	6.8
2	I	128	THR	6.6
2	I	126	GLY	6.5
1	H	212	PRO	5.6
2	I	25	SER	5.4
1	H	126	GLY	5.3
1	H	129	THR	5.3
2	I	56	ARG	5.2
1	H	210	ARG	5.1
3	M	214	CYS	4.7
1	H	128	THR	4.6
3	M	31	HIS	4.6
3	M	212	ASN	4.6
3	L	194	CYS	4.4
1	H	125	CYS	4.2
3	L	212	ASN	4.2
2	I	213	ILE	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	I	129	THR	4.1
1	H	209	PRO	4.1
1	H	127	ASP	4.0
2	I	127	ASP	3.9
2	I	211	VAL	3.9
3	L	213	GLU	3.8
1	H	185	TRP	3.6
2	I	130	GLY	3.6
1	H	188	GLN	3.5
3	M	213	GLU	3.5
3	L	160	LEU	3.5
3	M	24	ARG	3.5
2	I	64	LYS	3.5
2	I	41	PRO	3.4
2	I	125	CYS	3.4
2	I	74	SER	3.4
2	I	75	SER	3.4
3	L	203	SER	3.4
2	I	76	ASN	3.3
1	H	156	LEU	3.3
2	I	27	PHE	3.3
2	I	1	GLN	3.3
1	H	130	GLY	3.3
3	L	181	LEU	3.2
1	H	122	ALA	3.2
2	I	16	PRO	3.2
2	I	71	VAL	3.2
3	M	27	GLN	3.2
1	H	154	GLY	3.0
3	M	28	ASP	3.0
1	H	170	ASP	3.0
1	H	201	THR	2.9
3	L	111	ALA	2.9
2	I	43	GLN	2.9
3	L	155	ARG	2.9
2	I	170	ASP	2.9
1	H	208	GLU	2.9
3	L	123	GLU	2.9
1	H	133	VAL	2.9
2	I	24	ALA	2.9
3	M	67	SER	2.9
2	I	4	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	187	SER	2.8
3	M	26	SER	2.8
3	L	197	THR	2.7
3	L	202	THR	2.7
2	I	28	THR	2.7
1	H	124	VAL	2.7
1	H	163	PHE	2.6
2	I	168	GLN	2.6
1	H	186	PRO	2.6
3	L	204	PRO	2.6
3	M	70	ASP	2.6
3	L	198	HIS	2.6
2	I	47	TRP	2.6
1	H	180	VAL	2.6
2	I	169	SER	2.6
1	H	42	GLY	2.5
2	I	26	GLY	2.5
2	I	166	VAL	2.5
4	Q	1	VAL	2.5
2	I	22	CYS	2.5
3	L	139	PHE	2.5
3	L	117	ILE	2.5
1	H	183	SER	2.5
3	L	182	THR	2.5
2	I	32	TYR	2.5
3	L	126	THR	2.5
2	I	112	LYS	2.5
1	H	167	LEU	2.4
1	H	184	THR	2.4
1	H	191	THR	2.4
2	I	73	LYS	2.4
3	L	188	ARG	2.4
1	H	131	SER	2.4
1	H	200	SER	2.4
3	L	209	PHE	2.4
3	L	157	ASN	2.4
3	L	191	SER	2.4
2	I	29	PHE	2.4
1	H	56	ARG	2.4
2	I	72	ASP	2.3
1	H	168	GLN	2.3
3	L	168	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	I	99	TYR	2.3
2	I	77	THR	2.3
3	M	69	THR	2.3
3	L	156	GLN	2.3
3	L	132	VAL	2.3
3	L	206	VAL	2.3
3	L	185	GLU	2.2
3	M	96	PHE	2.2
3	L	200	THR	2.2
1	H	44	GLY	2.2
2	I	42	GLY	2.2
3	L	152	GLY	2.2
2	I	85	GLU	2.2
3	L	134	CYS	2.2
1	H	135	LEU	2.2
3	M	157	ASN	2.2
3	L	144	ILE	2.1
3	L	201	SER	2.1
2	I	52	LEU	2.1
3	M	25	ALA	2.1
1	H	132	SER	2.1
3	L	208	SER	2.1
3	M	202	THR	2.1
3	L	80	GLU	2.1
3	L	136	LEU	2.1
3	L	190	ASN	2.1
2	I	30	THR	2.1
1	H	136	GLY	2.1
3	L	145	ASN	2.1
3	L	146	VAL	2.1
2	I	14	PRO	2.1
1	H	143	PHE	2.0
1	H	203	VAL	2.0
1	H	137	CYS	2.0
3	M	2	ILE	2.0
4	Q	5	PHE	2.0
2	I	79	TYR	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 [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.