



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:51 PM UTC

PDB ID : 1BM3 / pdb_00001bm3
Title : IMMUNOGLOBULIN OPG2 FAB-PEPTIDE COMPLEX
Authors : Kodandapani, R.; Veerapandian, L.; Ni, C.Z.; Chiou, C.-K.; Whital, R.; Kunicki, T.J.; Ely, K.R.
Deposited on : 1999-04-15
Resolution : 2.00 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

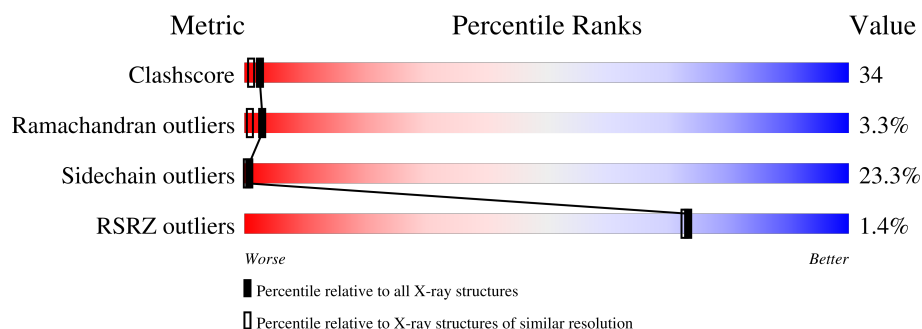
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	L	214	21% 45% 26% 8%
2	H	227	19% 41% 26% 9% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3589 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 IMMUNOGLOBULIN OPG2 FAB, CONSTANT DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1654	1023	280	344	7			

- Molecule 2 is a protein called IMMUNOGLOBULIN OPG2 FAB, VARIABLE DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1622	1016	280	317	9			

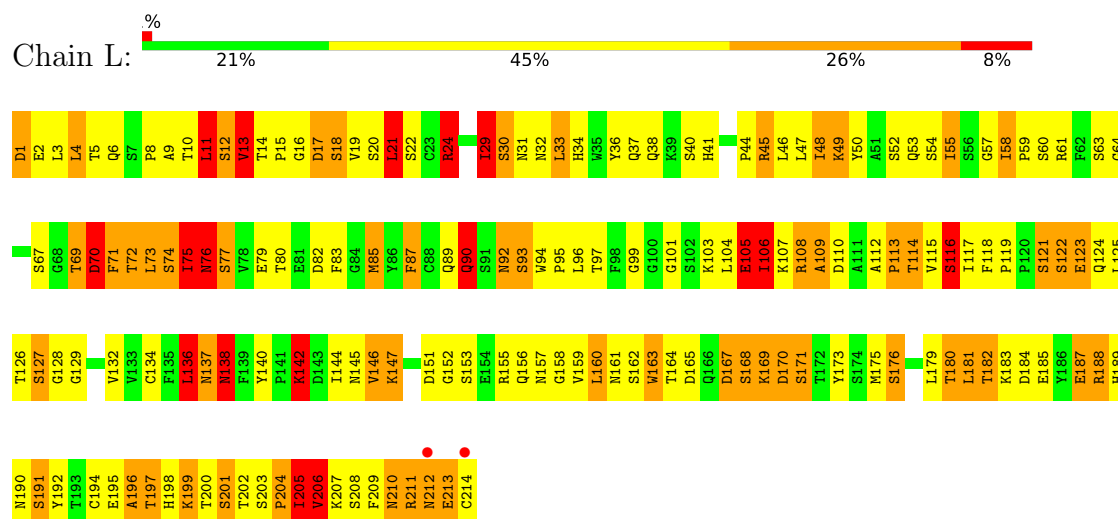
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	153	Total	O	0	0
			153	153		
3	H	160	Total	O	0	0
			160	160		

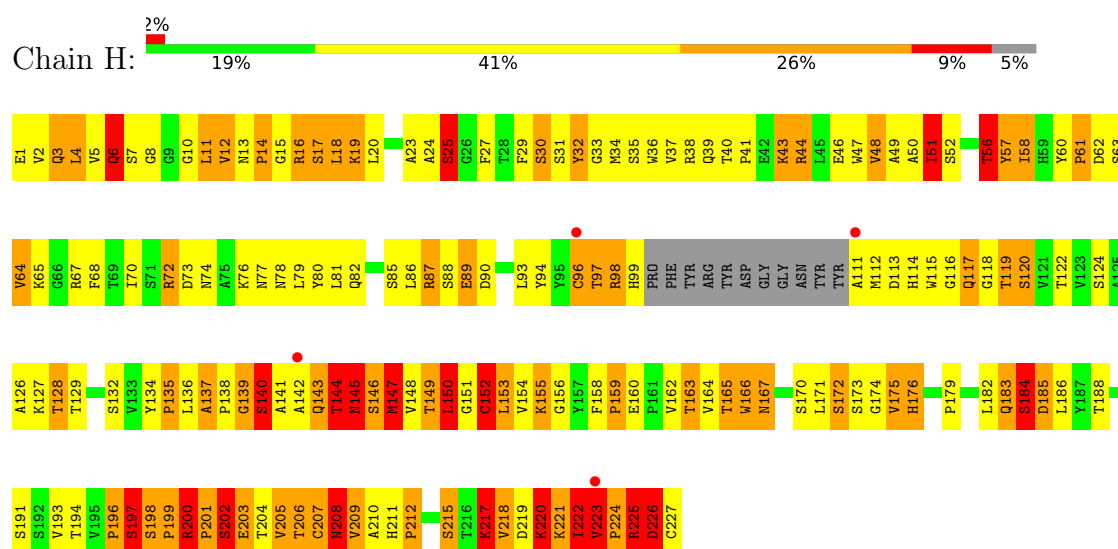
3 Residue-property plots [i](#)

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: IMMUNOGLOBULIN OPG2 FAB, CONSTANT DOMAIN



• Molecule 2: IMMUNOGLOBULIN OPG2 FAB, VARIABLE DOMAIN



4 Data and refinement statistics

Property	Value	Source
Space group	A 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	74.11Å 90.05Å 79.11Å 90.00° 115.30° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 8.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	78.0 (8.00-2.00) 81.5 (8.00-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.05Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.152 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 96.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3589	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L	1.28	1/1691 (0.1%)	3.16	248/2293 (10.8%)
2	H	1.28	2/1662 (0.1%)	3.11	223/2266 (9.8%)
All	All	1.28	3/3353 (0.1%)	3.14	471/4559 (10.3%)

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
2	H	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	67	ARG	NE-CZ	-7.21	1.25	1.33
2	H	115	TRP	NE1-CE2	-5.45	1.31	1.37
1	L	59	PRO	C-O	5.00	1.29	1.23

All (471) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	188	ARG	CD-NE-CZ	23.74	157.63	124.40
2	H	64	VAL	N-CA-CB	-21.12	88.98	112.21
2	H	77	ASN	CA-CB-CG	20.55	133.15	112.60
1	L	1	ASP	CA-CB-CG	18.70	131.30	112.60
1	L	212	ASN	N-CA-C	16.82	135.54	113.18
2	H	226	ASP	CA-CB-CG	13.71	126.31	112.60
2	H	67	ARG	CD-NE-CZ	13.39	143.15	124.40
1	L	138	ASN	CA-CB-CG	13.36	125.96	112.60
1	L	205	ILE	N-CA-CB	13.36	125.28	110.72
1	L	138	ASN	OD1-CG-ND2	-13.25	109.35	122.60
2	H	119	THR	N-CA-CB	12.88	133.08	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	59	PRO	CB-CA-C	12.81	127.76	110.98
1	L	211	ARG	CB-CA-C	12.71	131.86	112.03
2	H	60	TYR	O-C-N	12.63	130.85	121.88
2	H	184	SER	CA-C-N	11.70	139.27	122.08
2	H	184	SER	C-N-CA	11.70	139.27	122.08
2	H	226	ASP	N-CA-C	11.54	135.38	110.80
2	H	208	ASN	CA-CB-CG	11.49	124.09	112.60
1	L	49	LYS	CA-C-N	11.47	139.54	122.68
1	L	49	LYS	C-N-CA	11.47	139.54	122.68
1	L	11	LEU	CA-CB-CG	11.19	155.45	116.30
2	H	205	VAL	N-CA-CB	11.14	129.63	111.58
1	L	21	LEU	CA-C-O	-11.12	108.26	120.38
1	L	151	ASP	CA-CB-CG	11.03	123.63	112.60
1	L	162	SER	CA-CB-OG	-10.93	89.24	111.10
2	H	56	THR	CA-C-O	-10.90	109.16	120.71
2	H	200	ARG	N-CA-C	-10.77	86.01	109.81
1	L	123	GLU	CA-C-O	-10.72	109.19	120.55
2	H	67	ARG	NE-CZ-NH2	10.69	128.82	119.20
1	L	181	LEU	N-CA-CB	-10.66	93.86	111.66
1	L	211	ARG	CD-NE-CZ	10.64	139.30	124.40
2	H	73	ASP	CA-CB-CG	10.55	123.15	112.60
1	L	212	ASN	CA-CB-CG	10.19	122.79	112.60
1	L	1	ASP	N-CA-CB	10.18	127.81	110.50
1	L	2	GLU	CB-CG-CD	-10.12	95.39	112.60
2	H	162	VAL	CA-C-O	-10.03	109.65	121.28
2	H	15	GLY	CA-C-O	-9.99	108.88	119.27
2	H	8	GLY	CA-C-O	-9.92	107.96	118.97
1	L	213	GLU	N-CA-C	9.85	125.58	113.17
2	H	57	TYR	CA-CB-CG	9.79	131.52	113.90
2	H	167	ASN	CA-CB-CG	9.71	122.31	112.60
1	L	72	THR	CA-C-N	9.57	136.45	123.05
1	L	72	THR	C-N-CA	9.57	136.45	123.05
1	L	204	PRO	CA-C-O	-9.50	110.62	121.36
2	H	163	THR	CA-C-O	-9.43	110.17	120.36
2	H	183	GLN	CB-CG-CD	9.43	128.63	112.60
1	L	76	ASN	CA-CB-CG	-9.36	103.24	112.60
2	H	132	SER	CA-C-O	-9.33	110.32	120.30
2	H	199	PRO	CA-C-O	9.23	142.37	120.20
2	H	199	PRO	CA-C-N	9.23	144.32	121.80
2	H	199	PRO	C-N-CA	9.23	144.32	121.80
2	H	222	ILE	CA-C-O	9.21	132.29	120.78
1	L	153	SER	CA-CB-OG	9.16	129.42	111.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	64	VAL	CB-CA-C	9.10	122.22	110.84
2	H	72	ARG	NE-CZ-NH1	-9.10	112.40	121.50
2	H	36	TRP	CA-C-O	-9.05	110.75	120.80
2	H	39	GLN	CA-C-O	-9.00	110.42	120.32
2	H	184	SER	CA-C-O	8.98	133.35	120.51
1	L	71	PHE	CA-C-O	-8.93	110.66	121.11
2	H	90	ASP	CB-CG-OD1	8.93	138.94	118.40
2	H	49	ALA	CA-C-O	-8.87	110.82	120.75
1	L	13	VAL	CA-CB-CG1	8.85	125.45	110.40
2	H	19	LYS	CA-C-O	-8.84	111.12	120.40
2	H	226	ASP	CA-C-O	8.75	133.02	120.51
2	H	68	PHE	CA-CB-CG	8.73	122.53	113.80
1	L	107	LYS	CA-CB-CG	8.71	131.51	114.10
1	L	77	SER	CA-C-O	-8.64	111.55	120.54
1	L	54	SER	N-CA-CB	8.62	122.64	109.97
2	H	67	ARG	CB-CG-CD	8.59	131.05	111.30
1	L	184	ASP	CA-CB-CG	8.56	121.16	112.60
1	L	63	SER	CA-C-O	-8.53	111.50	120.89
2	H	87	ARG	CD-NE-CZ	-8.51	112.48	124.40
2	H	146	SER	N-CA-C	-8.49	93.78	108.56
1	L	90	GLN	CB-CG-CD	8.44	126.94	112.60
2	H	40	THR	CA-CB-CG2	8.40	124.78	110.50
1	L	123	GLU	CB-CG-CD	8.37	126.84	112.60
1	L	206	VAL	N-CA-C	8.36	120.82	108.45
2	H	4	LEU	CA-C-O	-8.36	110.00	120.28
2	H	155	LYS	CA-CB-CG	8.35	130.81	114.10
1	L	153	SER	CA-C-O	-8.30	111.91	120.71
1	L	109	ALA	CA-C-N	8.30	132.52	120.82
1	L	109	ALA	C-N-CA	8.30	132.52	120.82
1	L	136	LEU	CA-CB-CG	8.29	145.33	116.30
1	L	60	SER	CA-C-O	-8.26	110.95	120.20
2	H	164	VAL	O-C-N	8.23	131.54	123.14
1	L	105	GLU	CB-CG-CD	8.21	126.57	112.60
1	L	87	PHE	CA-CB-CG	8.16	121.96	113.80
2	H	33	GLY	N-CA-C	-8.12	101.66	112.14
2	H	150	LEU	CA-C-O	-8.10	111.61	121.89
2	H	225	ARG	CB-CG-CD	8.09	129.90	111.30
1	L	123	GLU	N-CA-CB	8.07	121.98	110.12
2	H	217	LYS	N-CA-CB	8.01	124.65	110.80
2	H	143	GLN	CB-CG-CD	8.00	126.21	112.60
1	L	58	ILE	O-C-N	7.92	129.69	121.14
1	L	211	ARG	CA-C-O	7.90	131.46	122.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	166	TRP	CB-CA-C	7.90	123.67	110.79
1	L	137	ASN	CA-C-O	7.88	130.81	121.36
2	H	46	GLU	N-CA-CB	7.87	124.42	110.80
1	L	3	LEU	O-C-N	7.86	132.18	123.22
1	L	90	GLN	CA-CB-CG	7.84	129.78	114.10
1	L	110	ASP	CA-CB-CG	7.83	120.43	112.60
2	H	137	ALA	N-CA-C	-7.79	99.55	110.31
1	L	55	ILE	CB-CA-C	7.75	122.34	111.34
2	H	217	LYS	N-CA-C	-7.75	95.67	108.76
2	H	139	GLY	N-CA-C	-7.73	94.86	113.18
1	L	73	LEU	CA-C-O	7.71	128.80	120.32
2	H	19	LYS	CA-CB-CG	-7.68	98.74	114.10
1	L	124	GLN	OE1-CD-NE2	7.68	130.28	122.60
1	L	205	ILE	CB-CA-C	-7.65	101.43	110.91
1	L	212	ASN	CB-CA-C	-7.62	96.82	110.23
2	H	225	ARG	NE-CZ-NH1	7.61	129.11	121.50
2	H	140	SER	CA-C-O	7.60	131.37	120.51
2	H	18	LEU	N-CA-CB	7.58	123.29	111.24
2	H	140	SER	CA-C-N	7.58	136.01	121.54
2	H	140	SER	C-N-CA	7.58	136.01	121.54
1	L	37	GLN	CA-C-O	-7.54	112.44	120.80
1	L	147	LYS	CA-C-O	-7.53	111.57	120.60
1	L	74	SER	N-CA-CB	-7.53	98.57	110.69
1	L	10	THR	CA-C-O	7.51	129.62	120.60
1	L	1	ASP	CB-CG-OD1	7.50	135.66	118.40
1	L	11	LEU	CA-C-O	7.49	129.59	120.60
2	H	82	GLN	OE1-CD-NE2	-7.45	115.15	122.60
2	H	197	SER	N-CA-CB	-7.45	97.91	110.49
1	L	190	ASN	CA-CB-CG	7.44	120.04	112.60
1	L	4	LEU	N-CA-C	-7.43	96.79	108.90
2	H	205	VAL	N-CA-C	-7.43	97.32	108.17
1	L	152	GLY	CA-C-O	-7.37	110.75	119.00
2	H	87	ARG	NH1-CZ-NH2	-7.37	109.72	119.30
1	L	124	GLN	O-C-N	7.36	129.65	122.07
1	L	127	SER	CB-CA-C	7.35	123.83	109.72
2	H	25	SER	CB-CA-C	-7.34	97.48	109.89
2	H	63	SER	CA-C-O	7.33	128.32	120.55
2	H	51	ILE	CB-CA-C	7.32	121.02	110.33
1	L	73	LEU	N-CA-CB	7.32	122.04	110.55
2	H	209	VAL	CA-C-O	7.31	128.86	120.67
1	L	17	ASP	CA-CB-CG	7.30	119.90	112.60
2	H	6	GLN	O-C-N	7.28	131.21	123.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	59	PRO	N-CA-CB	-7.25	96.59	103.33
1	L	64	GLY	CA-C-O	-7.24	114.30	121.76
2	H	48	VAL	N-CA-CB	-7.23	98.21	110.86
1	L	13	VAL	CA-C-O	-7.23	114.22	121.45
1	L	123	GLU	O-C-N	7.23	129.78	122.12
1	L	169	LYS	CA-C-O	-7.20	110.84	119.27
2	H	176	HIS	CB-CA-C	-7.20	99.75	110.62
2	H	87	ARG	NE-CZ-NH1	7.19	128.69	121.50
2	H	175	VAL	CA-CB-CG1	7.19	122.62	110.40
2	H	225	ARG	CB-CA-C	-7.19	105.42	114.40
2	H	188	THR	CA-C-O	-7.19	112.40	120.66
2	H	23	ALA	CA-C-O	-7.17	112.91	120.58
1	L	180	THR	CB-CA-C	7.16	121.54	109.80
1	L	161	ASN	OD1-CG-ND2	7.14	129.74	122.60
1	L	89	GLN	CA-C-N	7.09	132.51	122.72
1	L	89	GLN	C-N-CA	7.09	132.51	122.72
2	H	145	ASN	CA-C-O	7.07	130.46	121.55
2	H	152	CYS	CA-C-O	-7.07	111.59	120.28
1	L	15	PRO	N-CA-CB	7.04	109.53	103.19
2	H	119	THR	CA-C-O	-7.04	112.50	120.32
1	L	97	THR	CA-C-N	6.95	133.46	122.62
1	L	97	THR	C-N-CA	6.95	133.46	122.62
1	L	155	ARG	CD-NE-CZ	6.95	134.13	124.40
1	L	1	ASP	OD1-CG-OD2	-6.93	106.26	122.90
1	L	127	SER	N-CA-C	-6.93	104.82	113.28
1	L	58	ILE	CA-C-O	-6.92	113.39	119.62
2	H	43	LYS	N-CA-C	6.92	121.09	112.24
2	H	78	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	L	132	VAL	N-CA-C	-6.90	98.49	108.36
2	H	4	LEU	O-C-N	6.89	131.77	123.36
2	H	220	LYS	N-CA-CB	6.89	121.59	110.77
2	H	164	VAL	CA-C-O	-6.88	112.87	120.72
1	L	164	THR	CA-C-O	6.88	129.24	122.01
2	H	48	VAL	CB-CA-C	6.88	119.46	111.55
1	L	146	VAL	CB-CA-C	6.87	120.85	110.62
2	H	29	PHE	CA-CB-CG	6.83	120.63	113.80
1	L	145	ASN	O-C-N	6.82	131.59	123.27
1	L	192	TYR	CB-CG-CD2	-6.82	110.57	120.80
1	L	192	TYR	CB-CG-CD1	6.81	131.02	120.80
2	H	37	VAL	CA-C-O	-6.80	113.01	120.43
1	L	153	SER	CB-CA-C	-6.80	97.14	109.38
2	H	80	TYR	O-C-N	6.77	131.53	123.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	207	CYS	N-CA-CB	6.77	121.70	110.52
1	L	190	ASN	OD1-CG-ND2	6.76	129.36	122.60
2	H	24	ALA	O-C-N	-6.75	115.50	123.06
1	L	168	SER	CB-CA-C	-6.75	99.58	110.79
2	H	2	VAL	CA-C-O	-6.74	112.36	120.78
1	L	103	LYS	CA-CB-CG	6.73	127.56	114.10
1	L	194	CYS	CA-C-O	-6.72	113.34	120.40
2	H	175	VAL	N-CA-C	6.71	118.08	109.30
2	H	132	SER	N-CA-C	-6.69	97.50	108.41
1	L	2	GLU	CG-CD-OE2	-6.69	103.01	118.40
1	L	117	ILE	N-CA-CB	6.67	120.33	111.25
1	L	119	PRO	O-C-N	6.67	129.34	121.46
1	L	153	SER	O-C-N	6.67	131.68	123.21
2	H	24	ALA	CA-C-N	6.67	132.97	121.64
2	H	24	ALA	C-N-CA	6.67	132.97	121.64
1	L	96	LEU	O-C-N	6.66	131.12	122.93
2	H	218	VAL	O-C-N	6.65	130.43	123.05
1	L	213	GLU	CB-CG-CD	6.65	123.91	112.60
2	H	18	LEU	CB-CA-C	-6.65	99.29	109.99
1	L	206	VAL	N-CA-CB	-6.65	100.55	111.45
1	L	115	VAL	N-CA-C	6.64	117.86	108.36
2	H	205	VAL	CA-CB-CG2	6.64	121.69	110.40
2	H	224	PRO	CB-CA-C	6.64	122.51	111.56
2	H	164	VAL	CA-C-N	-6.62	112.19	122.59
2	H	164	VAL	C-N-CA	-6.62	112.19	122.59
1	L	105	GLU	CA-CB-CG	6.62	127.34	114.10
2	H	185	ASP	CB-CA-C	6.62	122.06	111.66
1	L	208	SER	O-C-N	6.62	130.95	123.27
1	L	132	VAL	CA-C-O	-6.61	113.50	120.57
1	L	121	SER	N-CA-C	-6.61	101.63	110.55
1	L	92	ASN	N-CA-CB	6.60	119.55	109.98
1	L	59	PRO	CA-C-N	6.60	130.01	120.38
1	L	59	PRO	C-N-CA	6.60	130.01	120.38
2	H	191	SER	O-C-N	6.59	131.30	123.33
2	H	149	THR	CA-C-N	6.57	134.04	122.67
2	H	149	THR	C-N-CA	6.57	134.04	122.67
1	L	189	HIS	N-CA-C	6.57	119.86	109.81
2	H	31	SER	CA-C-N	-6.57	113.41	122.93
2	H	31	SER	C-N-CA	-6.57	113.41	122.93
2	H	150	LEU	O-C-N	6.54	130.43	122.84
1	L	165	ASP	N-CA-C	-6.52	100.82	110.46
2	H	145	ASN	N-CA-C	6.51	120.16	109.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	40	THR	CA-CB-OG1	-6.49	99.86	109.60
1	L	3	LEU	CA-C-N	-6.48	113.85	122.99
1	L	3	LEU	C-N-CA	-6.48	113.85	122.99
1	L	75	ILE	N-CA-C	-6.46	98.82	108.12
1	L	208	SER	CA-C-O	-6.45	113.58	121.06
1	L	94	TRP	CB-CG-CD2	-6.45	117.77	126.80
1	L	94	TRP	N-CA-CB	6.44	120.74	110.11
1	L	204	PRO	N-CD-CG	-6.44	93.54	103.20
1	L	190	ASN	CA-C-O	-6.43	111.39	120.07
1	L	33	LEU	CA-C-O	-6.42	113.20	120.32
2	H	67	ARG	NH1-CZ-NH2	-6.38	111.00	119.30
1	L	158	GLY	N-CA-C	6.38	124.12	115.32
1	L	129	GLY	N-CA-C	-6.36	101.39	111.18
1	L	140	TYR	CA-CB-CG	-6.36	102.45	113.90
2	H	135	PRO	CA-C-O	-6.35	113.69	121.31
1	L	210	ASN	CA-C-O	-6.35	113.92	121.60
1	L	211	ARG	NH1-CZ-NH2	-6.35	111.05	119.30
2	H	56	THR	N-CA-C	-6.33	99.39	109.59
1	L	29	ILE	CB-CG1-CD1	6.32	127.07	113.80
1	L	82	ASP	CA-C-O	-6.32	111.94	119.15
2	H	16	ARG	N-CA-CB	6.31	119.53	110.45
1	L	57	GLY	CA-C-O	-6.29	112.54	119.27
1	L	75	ILE	CA-CB-CG1	6.29	121.09	110.40
1	L	59	PRO	CA-C-O	6.29	129.34	121.67
2	H	50	ALA	CA-C-O	-6.29	113.43	120.66
1	L	94	TRP	CB-CG-CD1	6.25	136.28	126.90
2	H	116	GLY	CA-C-O	-6.25	116.03	122.28
2	H	8	GLY	O-C-N	6.22	129.61	122.33
2	H	30	SER	O-C-N	6.22	130.86	122.59
2	H	17	SER	CA-C-O	-6.21	114.37	121.58
2	H	120	SER	CA-C-N	6.21	131.37	123.10
2	H	120	SER	C-N-CA	6.21	131.37	123.10
2	H	72	ARG	NH1-CZ-NH2	6.21	127.37	119.30
2	H	7	SER	CA-C-O	6.20	127.86	121.23
1	L	90	GLN	CB-CA-C	6.19	119.96	109.75
1	L	106	ILE	CB-CA-C	6.18	118.09	111.35
2	H	179	PRO	CA-C-N	6.18	130.65	120.94
2	H	179	PRO	C-N-CA	6.18	130.65	120.94
1	L	118	PHE	CA-CB-CG	-6.18	107.62	113.80
1	L	113	PRO	CA-C-O	-6.18	114.13	121.67
2	H	196	PRO	CB-CA-C	6.17	119.03	110.95
1	L	2	GLU	OE1-CD-OE2	6.16	137.68	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	90	ASP	CA-C-N	6.16	131.17	121.99
2	H	90	ASP	C-N-CA	6.16	131.17	121.99
1	L	45	ARG	CA-C-N	6.15	130.12	121.02
1	L	45	ARG	C-N-CA	6.15	130.12	121.02
1	L	71	PHE	O-C-N	6.15	130.80	123.24
2	H	154	VAL	CA-CB-CG2	6.14	120.84	110.40
1	L	153	SER	N-CA-CB	6.13	120.57	110.69
1	L	85	MET	N-CA-CB	-6.13	100.41	110.52
2	H	218	VAL	CA-C-O	-6.12	114.03	120.76
2	H	197	SER	CA-CB-OG	-6.11	98.87	111.10
2	H	220	LYS	CA-C-O	6.11	126.71	120.24
1	L	70	ASP	O-C-N	6.10	130.35	123.27
1	L	116	SER	CA-C-O	-6.09	113.78	120.36
2	H	191	SER	CA-C-O	-6.09	113.29	120.60
1	L	201	SER	N-CA-C	6.08	118.32	109.07
2	H	88	SER	CA-C-O	-6.08	112.98	119.97
2	H	185	ASP	N-CA-C	6.07	119.92	111.90
2	H	31	SER	O-C-N	6.06	130.73	122.37
1	L	113	PRO	O-C-N	6.05	130.51	123.06
1	L	188	ARG	CB-CA-C	6.05	122.29	110.67
2	H	32	TYR	CA-C-O	-6.04	114.31	120.71
2	H	11	LEU	CB-CA-C	6.03	119.69	109.80
2	H	210	ALA	CA-C-O	6.03	126.87	120.36
2	H	46	GLU	O-C-N	6.03	130.36	123.31
2	H	223	VAL	CB-CA-C	6.02	122.31	111.36
2	H	41	PRO	CB-CA-C	6.01	120.46	111.68
1	L	75	ILE	CB-CG1-CD1	-6.01	101.18	113.80
2	H	32	TYR	O-C-N	5.99	130.82	123.21
1	L	97	THR	CA-CB-OG1	-5.98	100.64	109.60
1	L	115	VAL	N-CA-CB	-5.97	103.82	110.99
2	H	172	SER	O-C-N	5.97	129.20	122.27
1	L	90	GLN	CA-C-N	5.97	131.56	122.37
1	L	90	GLN	C-N-CA	5.97	131.56	122.37
1	L	137	ASN	CA-C-N	5.95	132.91	121.54
1	L	137	ASN	C-N-CA	5.95	132.91	121.54
2	H	5	VAL	CB-CA-C	5.95	117.81	110.73
2	H	206	THR	CA-C-N	-5.95	113.78	122.65
2	H	206	THR	C-N-CA	-5.95	113.78	122.65
1	L	59	PRO	O-C-N	-5.94	115.75	123.06
1	L	58	ILE	CB-CG1-CD1	5.94	126.28	113.80
1	L	132	VAL	CB-CA-C	5.94	118.92	110.84
1	L	52	SER	N-CA-C	5.93	121.30	112.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	211	ARG	O-C-N	-5.93	115.40	122.46
1	L	203	SER	CA-C-N	5.93	125.95	119.90
1	L	203	SER	C-N-CA	5.93	125.95	119.90
2	H	57	TYR	CA-C-O	5.93	128.99	120.51
2	H	29	PHE	CA-C-N	5.90	132.80	121.54
2	H	29	PHE	C-N-CA	5.90	132.80	121.54
2	H	23	ALA	O-C-N	5.89	130.00	122.93
1	L	209	PHE	N-CA-C	-5.89	100.10	109.23
1	L	55	ILE	CA-C-N	5.88	129.47	121.05
1	L	55	ILE	C-N-CA	5.88	129.47	121.05
1	L	189	HIS	CB-CG-CD2	-5.86	123.58	131.20
2	H	32	TYR	N-CA-C	5.85	119.01	109.59
1	L	48	ILE	O-C-N	5.85	129.54	123.05
1	L	22	SER	CB-CA-C	-5.85	99.62	109.50
1	L	142	LYS	CA-CB-CG	5.84	125.78	114.10
2	H	137	ALA	N-CA-CB	5.83	119.73	110.11
2	H	5	VAL	N-CA-CB	-5.81	104.66	112.10
1	L	117	ILE	CA-CB-CG1	5.80	120.27	110.40
1	L	204	PRO	N-CA-C	5.80	120.32	111.15
2	H	196	PRO	N-CA-C	-5.78	102.74	111.41
1	L	5	THR	CA-C-O	-5.77	113.97	120.32
2	H	70	ILE	O-C-N	5.77	129.05	122.93
1	L	157	ASN	N-CA-CB	5.77	118.52	109.69
2	H	200	ARG	CB-CA-C	5.75	121.50	110.17
2	H	18	LEU	CA-CB-CG	5.75	136.41	116.30
1	L	90	GLN	N-CA-CB	-5.74	101.07	110.43
1	L	184	ASP	CB-CA-C	5.73	120.59	110.85
1	L	48	ILE	CA-C-O	-5.73	114.46	120.76
2	H	4	LEU	N-CA-C	-5.73	98.55	108.69
1	L	44	PRO	CB-CA-C	5.72	118.55	111.23
2	H	128	THR	CA-CB-CG2	5.72	120.22	110.50
1	L	37	GLN	CB-CG-CD	-5.71	102.88	112.60
2	H	162	VAL	CA-C-N	-5.70	114.95	122.99
2	H	162	VAL	C-N-CA	-5.70	114.95	122.99
1	L	199	LYS	CA-C-O	-5.70	114.47	120.63
1	L	9	ALA	CA-C-N	5.70	132.17	122.37
1	L	9	ALA	C-N-CA	5.70	132.17	122.37
1	L	77	SER	O-C-N	5.68	129.81	123.05
1	L	13	VAL	N-CA-CB	-5.67	100.37	112.00
2	H	24	ALA	CB-CA-C	5.67	119.21	109.51
2	H	165	THR	N-CA-CB	5.66	121.40	111.55
1	L	70	ASP	CA-CB-CG	-5.64	106.96	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	29	ILE	N-CA-C	5.63	117.52	112.17
2	H	46	GLU	CG-CD-OE2	-5.61	105.49	118.40
1	L	159	VAL	N-CA-CB	-5.61	104.60	110.72
1	L	29	ILE	CA-CB-CG2	-5.61	100.96	110.50
2	H	151	GLY	CA-C-O	5.61	127.50	121.61
1	L	167	ASP	CA-CB-CG	-5.61	106.99	112.60
1	L	127	SER	CA-CB-OG	-5.60	99.90	111.10
2	H	10	GLY	CA-C-O	-5.60	115.47	121.35
2	H	37	VAL	O-C-N	5.59	129.11	123.07
1	L	185	GLU	CA-C-O	5.59	126.47	120.55
1	L	176	SER	CA-CB-OG	5.58	122.27	111.10
2	H	174	GLY	CA-C-N	5.58	128.84	120.69
2	H	174	GLY	C-N-CA	5.58	128.84	120.69
1	L	17	ASP	CA-C-N	5.57	130.96	122.65
1	L	17	ASP	C-N-CA	5.57	130.96	122.65
1	L	32	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	L	204	PRO	CB-CA-C	-5.57	104.49	111.56
2	H	29	PHE	CA-C-O	5.57	127.53	121.02
2	H	199	PRO	O-C-N	-5.55	110.55	121.10
1	L	212	ASN	N-CA-CB	-5.54	97.75	110.83
2	H	58	ILE	CA-C-O	-5.53	114.19	120.67
1	L	20	SER	CA-C-O	-5.52	114.20	120.32
1	L	16	GLY	CA-C-O	-5.51	114.76	119.56
2	H	61	PRO	O-C-N	-5.51	116.27	123.00
1	L	197	THR	N-CA-CB	5.50	119.19	110.55
2	H	173	SER	CB-CA-C	5.50	118.83	109.80
2	H	124	SER	N-CA-CB	-5.50	102.47	111.66
1	L	114	THR	N-CA-C	-5.50	98.80	108.20
1	L	108	ARG	CA-C-O	-5.50	115.30	121.40
1	L	123	GLU	CG-CD-OE1	5.49	131.03	118.40
2	H	124	SER	CA-C-O	-5.48	115.41	121.33
2	H	93	LEU	N-CA-CB	5.48	119.36	110.42
1	L	147	LYS	O-C-N	5.48	129.96	123.33
2	H	167	ASN	N-CA-CB	-5.47	103.99	112.30
1	L	16	GLY	N-CA-C	-5.45	107.41	113.79
1	L	54	SER	N-CA-C	-5.45	102.22	110.28
2	H	160	GLU	CA-CB-CG	5.43	124.96	114.10
1	L	96	LEU	CA-C-O	-5.43	114.57	120.81
2	H	115	TRP	CA-C-O	-5.42	114.98	121.11
2	H	81	LEU	N-CA-CB	5.42	119.21	110.65
2	H	115	TRP	CA-C-N	-5.42	116.91	122.27
2	H	115	TRP	C-N-CA	-5.42	116.91	122.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	94	TRP	CA-C-O	-5.41	115.16	120.19
1	L	12	SER	CA-C-O	-5.40	114.52	120.30
1	L	4	LEU	O-C-N	5.40	129.73	123.30
2	H	220	LYS	CA-C-N	5.40	129.60	122.42
2	H	220	LYS	C-N-CA	5.40	129.60	122.42
2	H	60	TYR	CA-C-O	-5.39	114.72	120.28
1	L	24	ARG	CA-CB-CG	-5.39	103.32	114.10
2	H	48	VAL	CA-CB-CG1	5.39	119.56	110.40
2	H	143	GLN	CG-CD-OE1	5.38	131.56	120.80
2	H	208	ASN	O-C-N	5.37	129.69	123.30
1	L	5	THR	O-C-N	5.35	129.59	123.27
1	L	137	ASN	N-CA-C	5.35	118.82	110.32
2	H	117	GLN	N-CA-C	5.35	119.52	112.89
1	L	171	SER	N-CA-CB	-5.35	105.79	113.65
2	H	41	PRO	CA-C-O	5.34	126.47	119.00
1	L	126	THR	CA-CB-OG1	-5.33	101.61	109.60
1	L	145	ASN	CA-C-N	-5.30	115.75	123.06
1	L	145	ASN	C-N-CA	-5.30	115.75	123.06
1	L	164	THR	N-CA-C	-5.30	103.62	110.19
2	H	85	SER	N-CA-CB	5.30	119.44	110.49
2	H	98	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	L	16	GLY	O-C-N	5.28	127.73	122.77
2	H	30	SER	N-CA-C	5.28	122.05	110.80
2	H	41	PRO	O-C-N	-5.27	115.13	122.30
2	H	173	SER	N-CA-C	-5.26	100.73	109.46
2	H	20	LEU	CA-C-O	-5.25	115.07	121.36
1	L	132	VAL	CA-CB-CG1	-5.24	101.50	110.40
2	H	184	SER	N-CA-CB	-5.23	101.64	110.49
1	L	160	LEU	CA-C-O	-5.23	114.70	120.30
2	H	140	SER	O-C-N	-5.23	115.63	122.59
1	L	73	LEU	CA-C-N	5.23	130.51	122.93
1	L	73	LEU	C-N-CA	5.23	130.51	122.93
1	L	75	ILE	CA-C-O	-5.23	114.82	120.36
1	L	122	SER	CA-C-O	-5.23	114.88	120.42
2	H	129	THR	CA-CB-CG2	5.23	119.39	110.50
1	L	22	SER	N-CA-CB	5.21	119.13	110.63
2	H	188	THR	N-CA-CB	5.20	120.42	111.00
1	L	72	THR	CB-CA-C	5.20	119.94	109.38
2	H	155	LYS	N-CA-CB	-5.20	102.53	110.85
1	L	182	THR	N-CA-C	-5.20	103.67	110.53
1	L	138	ASN	CB-CG-OD1	5.19	131.18	120.80
2	H	86	LEU	CA-C-N	5.19	131.52	122.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	86	LEU	C-N-CA	5.19	131.52	122.81
2	H	171	LEU	N-CA-CB	-5.18	102.62	110.35
2	H	226	ASP	CA-C-N	5.18	131.03	121.70
2	H	226	ASP	C-N-CA	5.18	131.03	121.70
2	H	225	ARG	N-CA-CB	-5.17	102.60	108.96
2	H	49	ALA	O-C-N	5.17	129.04	123.56
2	H	88	SER	CB-CA-C	5.16	120.57	110.67
2	H	215	SER	CA-C-O	5.15	126.40	120.32
2	H	224	PRO	N-CD-CG	-5.15	95.47	103.20
2	H	18	LEU	O-C-N	5.14	129.01	123.56
1	L	12	SER	N-CA-CB	-5.14	102.64	110.65
2	H	27	PHE	CA-CB-CG	5.13	118.93	113.80
2	H	153	LEU	CB-CA-C	5.12	118.59	109.72
1	L	22	SER	CA-C-O	-5.12	115.23	121.28
1	L	29	ILE	CA-CB-CG1	5.12	119.10	110.40
1	L	179	LEU	CD1-CG-CD2	5.12	122.06	110.80
2	H	72	ARG	CD-NE-CZ	-5.12	117.23	124.40
1	L	196	ALA	N-CA-CB	-5.11	102.55	110.57
2	H	223	VAL	N-CA-C	-5.10	97.86	108.88
2	H	136	LEU	CA-C-O	-5.10	114.15	120.57
2	H	199	PRO	CA-N-CD	-5.10	104.36	111.50
1	L	64	GLY	O-C-N	5.09	128.06	123.42
1	L	69	THR	CA-CB-OG1	-5.09	101.96	109.60
1	L	63	SER	CA-C-N	-5.07	117.22	121.58
1	L	63	SER	C-N-CA	-5.07	117.22	121.58
1	L	170	ASP	CB-CA-C	5.07	117.95	109.80
1	L	38	GLN	CB-CG-CD	5.06	121.21	112.60
1	L	101	GLY	CA-C-N	5.06	130.84	122.33
1	L	101	GLY	C-N-CA	5.06	130.84	122.33
1	L	103	LYS	CA-C-O	5.05	125.94	120.43
1	L	201	SER	CA-C-O	5.05	126.79	121.33
2	H	36	TRP	N-CA-C	-5.04	101.50	109.76
1	L	18	SER	CA-CB-OG	-5.04	101.03	111.10
1	L	79	GLU	CA-C-O	-5.03	115.53	121.66
1	L	106	ILE	CA-CB-CG2	5.02	119.03	110.50
1	L	124	GLN	CA-C-O	-5.02	115.55	120.82
1	L	211	ARG	N-CA-C	-5.01	99.84	108.56
2	H	188	THR	N-CA-C	-5.01	100.88	109.24
2	H	6	GLN	N-CA-CB	5.01	118.57	110.41
1	L	121	SER	O-C-N	5.00	128.55	122.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	225	ARG	Sidechain

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	L	1654	0	1569	83	6
2	H	1622	0	1589	145	1
3	H	160	0	0	18	6
3	L	153	0	0	17	3
All	All	3589	0	3158	221	9

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 34.

All (221) 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)
2:H:16:ARG:HG3	2:H:17:SER:H	1.08	1.08
1:L:36:TYR:OH	2:H:111:ALA:HB1	1.67	0.94
1:L:8:PRO:HG2	1:L:11:LEU:HD22	1.50	0.92
1:L:11:LEU:HD21	1:L:21:LEU:CD1	1.99	0.92
1:L:1:ASP:HB2	1:L:95:PRO:HD2	1.53	0.91
1:L:11:LEU:HD21	1:L:21:LEU:HD11	1.51	0.90
1:L:90:GLN:HE21	1:L:92:ASN:H	1.20	0.89
2:H:137:ALA:HB2	2:H:225:ARG:HD3	1.54	0.89
2:H:97:THR:HA	2:H:114:HIS:O	1.72	0.89
2:H:182:LEU:HD11	2:H:185:ASP:HA	1.54	0.88
2:H:147:MET:HE3	2:H:194:THR:HG22	1.57	0.85
1:L:34:HIS:CD2	2:H:111:ALA:HB2	2.13	0.82
1:L:198:HIS:HB3	3:L:901:HOH:O	1.81	0.80
2:H:97:THR:CG2	2:H:112:MET:HB3	2.11	0.80
2:H:16:ARG:HG3	2:H:17:SER:N	1.92	0.80
2:H:98:ARG:O	2:H:113:ASP:OD1	2.00	0.79
1:L:40:SER:HA	3:L:697:HOH:O	1.82	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:137:ASN:ND2	3:L:706:HOH:O	2.13	0.78
2:H:4:LEU:HD11	3:H:637:HOH:O	1.82	0.77
1:L:205:ILE:HD12	1:L:205:ILE:N	2.01	0.76
2:H:96:CYS:O	2:H:97:THR:HG23	1.85	0.76
2:H:44:ARG:HG3	3:H:930:HOH:O	1.87	0.74
2:H:16:ARG:HG2	3:H:767:HOH:O	1.85	0.74
2:H:185:ASP:HA	3:H:858:HOH:O	1.86	0.74
2:H:143:GLN:HB2	3:H:689:HOH:O	1.89	0.72
2:H:199:PRO:HB3	2:H:203:GLU:N	2.05	0.71
1:L:12:SER:HA	1:L:105:GLU:O	1.91	0.71
2:H:199:PRO:HB3	2:H:203:GLU:H	1.56	0.71
2:H:98:ARG:NH2	2:H:113:ASP:OD2	2.23	0.71
2:H:203:GLU:O	2:H:223:VAL:HG13	1.90	0.70
1:L:50:TYR:HB2	3:L:840:HOH:O	1.93	0.69
2:H:51:ILE:HG13	2:H:58:ILE:HG12	1.76	0.68
1:L:77:SER:HB2	3:L:748:HOH:O	1.93	0.68
1:L:125:LEU:O	1:L:128:GLY:N	2.27	0.67
2:H:97:THR:HB	2:H:112:MET:HB3	1.76	0.67
1:L:90:GLN:HE21	1:L:92:ASN:N	1.92	0.66
2:H:225:ARG:HG2	2:H:226:ASP:HB3	1.77	0.66
1:L:113:PRO:HD2	3:L:901:HOH:O	1.95	0.66
2:H:139:GLY:O	2:H:142:ALA:N	2.29	0.65
2:H:225:ARG:HG3	3:H:908:HOH:O	1.96	0.65
2:H:32:TYR:CG	2:H:98:ARG:HD2	2.31	0.64
2:H:143:GLN:HG2	2:H:200:ARG:NH2	2.12	0.64
2:H:200:ARG:C	2:H:202:SER:H	2.05	0.64
1:L:205:ILE:HD12	1:L:205:ILE:H	1.62	0.64
2:H:196:PRO:C	2:H:198:SER:H	2.04	0.64
2:H:38:ARG:HG2	2:H:48:VAL:CG2	2.28	0.63
2:H:200:ARG:O	2:H:202:SER:N	2.32	0.62
2:H:6:GLN:HE21	2:H:6:GLN:H	1.47	0.62
2:H:97:THR:CB	2:H:112:MET:HB3	2.30	0.62
2:H:199:PRO:HG3	2:H:203:GLU:HB2	1.82	0.62
2:H:145:ASN:HD22	2:H:146:SER:H	1.48	0.62
1:L:205:ILE:HD11	3:L:773:HOH:O	2.00	0.61
1:L:205:ILE:HD11	3:L:901:HOH:O	1.99	0.61
2:H:139:GLY:O	2:H:141:ALA:N	2.28	0.61
2:H:97:THR:CB	2:H:112:MET:HG2	2.30	0.61
2:H:200:ARG:C	2:H:202:SER:N	2.57	0.61
2:H:223:VAL:O	2:H:225:ARG:HD2	2.01	0.61
2:H:217:LYS:HB2	3:H:846:HOH:O	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:97:THR:HG21	2:H:112:MET:CB	2.31	0.60
2:H:135:PRO:HG2	2:H:225:ARG:NH2	2.17	0.60
2:H:199:PRO:CG	2:H:203:GLU:HB2	2.31	0.60
1:L:147:LYS:HB2	3:L:828:HOH:O	2.01	0.60
1:L:6:GLN:HE21	1:L:99:GLY:HA3	1.66	0.60
1:L:214:CYS:HA	2:H:227:CYS:HB2	1.83	0.60
2:H:25:SER:HB2	3:H:659:HOH:O	2.02	0.59
2:H:97:THR:CG2	2:H:112:MET:CB	2.78	0.59
1:L:211:ARG:HA	3:L:822:HOH:O	2.01	0.59
2:H:223:VAL:O	2:H:225:ARG:N	2.34	0.59
1:L:19:VAL:HG22	1:L:75:ILE:HD12	1.85	0.59
1:L:90:GLN:NE2	1:L:92:ASN:H	1.94	0.59
2:H:143:GLN:HG2	2:H:200:ARG:HH21	1.68	0.58
1:L:90:GLN:NE2	1:L:92:ASN:N	2.50	0.58
2:H:11:LEU:HD22	2:H:159:PRO:HG3	1.85	0.58
2:H:205:VAL:H	2:H:223:VAL:HG22	1.68	0.58
2:H:16:ARG:CG	2:H:17:SER:H	1.91	0.57
2:H:225:ARG:HG2	2:H:226:ASP:N	2.18	0.57
1:L:127:SER:HB3	3:L:864:HOH:O	2.04	0.57
2:H:128:THR:HA	2:H:158:PHE:O	2.05	0.57
2:H:97:THR:HG21	2:H:112:MET:HG2	1.87	0.56
2:H:52:SER:OG	2:H:56:THR:O	2.23	0.56
2:H:144:THR:HG23	3:H:920:HOH:O	2.05	0.56
2:H:76:LYS:HD3	3:H:870:HOH:O	2.05	0.56
2:H:223:VAL:HG21	3:H:843:HOH:O	2.04	0.56
2:H:150:LEU:HG	2:H:222:ILE:HG21	1.87	0.56
2:H:96:CYS:O	2:H:97:THR:CG2	2.53	0.55
1:L:19:VAL:CG2	1:L:75:ILE:HD12	2.35	0.55
1:L:11:LEU:HG	1:L:104:LEU:HD12	1.88	0.55
1:L:29:ILE:CD1	1:L:33:LEU:HD23	2.37	0.55
3:L:707:HOH:O	2:H:43:LYS:HD2	2.05	0.55
2:H:12:VAL:HG23	2:H:16:ARG:HB3	1.88	0.55
1:L:108:ARG:NE	1:L:109:ALA:O	2.40	0.55
2:H:12:VAL:HG11	2:H:18:LEU:HG	1.89	0.55
2:H:201:PRO:HD3	2:H:224:PRO:O	2.07	0.54
2:H:87:ARG:HB3	2:H:89:GLU:HG3	1.90	0.54
2:H:32:TYR:O	2:H:72:ARG:NH2	2.36	0.54
2:H:145:ASN:ND2	3:H:680:HOH:O	2.40	0.54
2:H:200:ARG:HH11	2:H:224:PRO:CB	2.21	0.54
2:H:201:PRO:HA	2:H:223:VAL:HG12	1.90	0.54
2:H:96:CYS:O	2:H:97:THR:OG1	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:108:ARG:HG2	1:L:171:SER:HB3	1.91	0.53
2:H:167:ASN:HA	2:H:206:THR:HG23	1.89	0.53
2:H:207:CYS:N	2:H:220:LYS:O	2.42	0.53
2:H:140:SER:HA	2:H:200:ARG:NH2	2.24	0.53
2:H:38:ARG:HG2	2:H:48:VAL:HG21	1.91	0.53
1:L:1:ASP:HB2	1:L:95:PRO:CD	2.34	0.53
2:H:47:TRP:CZ3	2:H:61:PRO:HD3	2.43	0.53
1:L:1:ASP:CB	1:L:95:PRO:HD2	2.34	0.52
1:L:195:GLU:HB2	1:L:206:VAL:CG2	2.40	0.52
2:H:145:ASN:ND2	2:H:146:SER:H	2.08	0.52
2:H:196:PRO:O	2:H:198:SER:N	2.35	0.51
2:H:182:LEU:HD11	2:H:185:ASP:CA	2.35	0.51
2:H:34:MET:HB3	2:H:79:LEU:HD22	1.93	0.50
2:H:167:ASN:OD1	2:H:206:THR:HG22	2.11	0.50
2:H:200:ARG:HB3	2:H:201:PRO:HD2	1.92	0.50
2:H:96:CYS:O	2:H:97:THR:CB	2.59	0.50
1:L:18:SER:HA	1:L:76:ASN:O	2.11	0.50
1:L:138:ASN:OD1	2:H:176:HIS:HE1	1.95	0.50
2:H:156:GLY:HA2	2:H:186:LEU:HB3	1.93	0.50
2:H:196:PRO:C	2:H:198:SER:N	2.69	0.50
2:H:6:GLN:NE2	2:H:118:GLY:H	2.10	0.50
2:H:97:THR:HB	2:H:112:MET:CB	2.41	0.50
1:L:127:SER:OG	3:L:723:HOH:O	2.14	0.49
1:L:175:MET:HG2	1:L:176:SER:N	2.26	0.49
2:H:97:THR:OG1	2:H:112:MET:HG2	2.12	0.49
2:H:200:ARG:CA	2:H:224:PRO:HG2	2.42	0.49
2:H:200:ARG:NH1	2:H:224:PRO:HB3	2.27	0.49
2:H:126:ALA:HB2	2:H:185:ASP:HB3	1.95	0.49
2:H:145:ASN:O	2:H:197:SER:HB3	2.13	0.49
2:H:16:ARG:HB2	2:H:16:ARG:CZ	2.43	0.49
1:L:136:LEU:CD1	1:L:196:ALA:HB2	2.43	0.48
1:L:136:LEU:HD21	1:L:146:VAL:HG21	1.94	0.48
2:H:32:TYR:CD1	2:H:98:ARG:HD2	2.47	0.48
2:H:146:SER:HA	2:H:197:SER:OG	2.13	0.48
2:H:200:ARG:O	2:H:201:PRO:C	2.56	0.48
1:L:195:GLU:HG3	1:L:204:PRO:HB2	1.94	0.48
2:H:6:GLN:HE22	2:H:117:GLN:N	2.12	0.48
1:L:142:LYS:HE3	3:L:814:HOH:O	2.14	0.48
2:H:4:LEU:HD13	2:H:96:CYS:HB3	1.93	0.48
2:H:97:THR:CB	2:H:112:MET:CG	2.91	0.48
2:H:97:THR:HG21	2:H:112:MET:CG	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:55:ILE:O	1:L:58:ILE:HG12	2.13	0.48
1:L:210:ASN:HB2	1:L:212:ASN:HB2	1.96	0.48
1:L:33:LEU:HG	1:L:71:PHE:CG	2.49	0.47
1:L:30:SER:HB3	1:L:31:ASN:H	1.57	0.47
1:L:108:ARG:NH2	1:L:109:ALA:O	2.45	0.47
1:L:142:LYS:HG2	3:L:928:HOH:O	2.15	0.47
1:L:213:GLU:HG2	2:H:141:ALA:HB2	1.96	0.47
1:L:213:GLU:HG2	2:H:141:ALA:CB	2.46	0.46
2:H:87:ARG:HG2	3:H:951:HOH:O	2.15	0.46
2:H:97:THR:HG22	2:H:112:MET:HB3	1.95	0.46
2:H:200:ARG:HH11	2:H:224:PRO:HB3	1.78	0.46
1:L:90:GLN:HE22	1:L:93:SER:H	1.61	0.46
2:H:138:PRO:HD3	2:H:150:LEU:HD12	1.97	0.46
2:H:6:GLN:H	2:H:6:GLN:NE2	2.13	0.46
2:H:200:ARG:HA	2:H:224:PRO:HG2	1.98	0.46
2:H:97:THR:CG2	2:H:112:MET:HG2	2.45	0.46
2:H:221:LYS:H	2:H:221:LYS:HD2	1.80	0.46
2:H:147:MET:CB	3:H:609:HOH:O	2.63	0.46
2:H:200:ARG:HD3	2:H:201:PRO:HD2	1.98	0.46
2:H:137:ALA:CB	2:H:225:ARG:HD3	2.35	0.45
2:H:98:ARG:HB2	3:H:637:HOH:O	2.16	0.45
2:H:199:PRO:O	2:H:224:PRO:HG2	2.17	0.45
2:H:99:HIS:HE1	2:H:112:MET:HE3	1.81	0.45
2:H:204:THR:HA	2:H:223:VAL:HG22	1.99	0.45
2:H:217:LYS:HD2	2:H:218:VAL:N	2.32	0.45
1:L:61:ARG:HG3	1:L:75:ILE:HG23	1.98	0.45
2:H:199:PRO:HA	2:H:202:SER:HB2	1.99	0.45
1:L:163:TRP:N	1:L:163:TRP:CD1	2.84	0.45
1:L:167:ASP:OD1	1:L:169:LYS:N	2.47	0.45
1:L:85:MET:HG2	1:L:87:PHE:CZ	2.51	0.45
1:L:205:ILE:CD1	3:L:901:HOH:O	2.59	0.45
2:H:134:TYR:HA	2:H:135:PRO:HD3	1.80	0.45
2:H:208:ASN:HB3	2:H:219:ASP:OD1	2.17	0.44
2:H:221:LYS:O	2:H:221:LYS:HD3	2.17	0.44
2:H:97:THR:HB	2:H:112:MET:CG	2.47	0.44
1:L:125:LEU:C	1:L:128:GLY:H	2.23	0.44
1:L:116:SER:O	1:L:134:CYS:HA	2.18	0.44
2:H:211:HIS:O	2:H:212:PRO:C	2.60	0.44
1:L:55:ILE:HD11	1:L:58:ILE:HD11	1.99	0.43
2:H:200:ARG:C	2:H:224:PRO:HD2	2.42	0.43
1:L:113:PRO:HG3	1:L:144:ILE:CD1	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:183:LYS:O	1:L:187:GLU:HG2	2.19	0.43
1:L:29:ILE:HG22	1:L:92:ASN:HB3	2.01	0.43
2:H:13:ASN:HA	2:H:14:PRO:HD3	1.87	0.43
1:L:8:PRO:CG	1:L:11:LEU:HD22	2.36	0.43
1:L:55:ILE:C	1:L:55:ILE:HD12	2.44	0.43
2:H:147:MET:HB3	3:H:609:HOH:O	2.19	0.43
1:L:112:ALA:HB2	1:L:200:THR:OG1	2.18	0.43
2:H:62:ASP:OD1	2:H:65:LYS:HE3	2.19	0.43
2:H:117:GLN:HG3	3:H:635:HOH:O	2.17	0.43
1:L:80:THR:HA	1:L:83:PHE:CE2	2.54	0.42
1:L:13:VAL:HG11	1:L:19:VAL:HG11	2.02	0.42
1:L:24:ARG:HG3	1:L:70:ASP:OD1	2.19	0.42
1:L:49:LYS:HG3	1:L:53:GLN:HB2	2.01	0.42
2:H:11:LEU:HA	2:H:122:THR:O	2.19	0.42
1:L:204:PRO:O	3:L:733:HOH:O	2.21	0.42
2:H:222:ILE:O	2:H:225:ARG:HD2	2.19	0.42
1:L:34:HIS:CG	2:H:111:ALA:HB2	2.54	0.42
1:L:113:PRO:HG3	1:L:144:ILE:HD11	2.01	0.42
2:H:152:CYS:HB2	2:H:166:TRP:CZ2	2.55	0.42
1:L:106:ILE:HD13	1:L:106:ILE:HG21	1.93	0.42
2:H:147:MET:HG2	3:H:625:HOH:O	2.19	0.42
1:L:191:SER:HB3	1:L:210:ASN:OD1	2.19	0.42
1:L:170:ASP:O	1:L:171:SER:HB2	2.20	0.41
2:H:94:TYR:O	2:H:118:GLY:HA2	2.20	0.41
2:H:200:ARG:HD3	2:H:201:PRO:CD	2.51	0.41
1:L:14:THR:O	1:L:17:ASP:HB2	2.21	0.41
1:L:90:GLN:NE2	1:L:93:SER:H	2.19	0.41
2:H:200:ARG:HH11	2:H:224:PRO:HB2	1.83	0.41
2:H:3:GLN:HB2	2:H:25:SER:HB3	2.02	0.41
2:H:183:GLN:O	2:H:184:SER:C	2.63	0.41
2:H:220:LYS:HD2	2:H:220:LYS:HA	1.77	0.41
1:L:19:VAL:O	1:L:74:SER:HA	2.20	0.41
2:H:150:LEU:HD11	2:H:224:PRO:HG3	2.02	0.41
1:L:12:SER:O	1:L:13:VAL:HG23	2.20	0.41
2:H:149:THR:HA	2:H:193:VAL:O	2.21	0.41
2:H:221:LYS:H	2:H:221:LYS:CD	2.32	0.41
1:L:142:LYS:HB2	1:L:173:TYR:CE2	2.55	0.41
2:H:135:PRO:HG2	2:H:225:ARG:HH22	1.86	0.41
2:H:72:ARG:HE	2:H:74:ASN:HD21	1.69	0.40
1:L:205:ILE:N	1:L:205:ILE:CD1	2.79	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:834:HOH:O	3:H:829:HOH:O[2_657]	1.26	0.94
3:L:763:HOH:O	3:L:763:HOH:O[2_556]	1.36	0.84
1:L:181:LEU:CA	3:H:952:HOH:O[2_657]	1.53	0.67
1:L:181:LEU:CB	3:H:952:HOH:O[2_657]	1.69	0.51
1:L:156:GLN:OE1	3:L:712:HOH:O[2_657]	1.84	0.36
2:H:57:TYR:OH	2:H:140:SER:CB[1_455]	1.84	0.36
1:L:181:LEU:C	3:H:952:HOH:O[2_657]	1.93	0.27
1:L:182:THR:N	3:H:952:HOH:O[2_657]	2.06	0.14
1:L:181:LEU:CG	3:H:952:HOH:O[2_657]	2.18	0.02

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	L	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	24	21
2	H	212/227 (93%)	180 (85%)	19 (9%)	13 (6%)	1	0
All	All	424/441 (96%)	383 (90%)	27 (6%)	14 (3%)	3	1

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	97	THR
2	H	140	SER
2	H	147	MET
2	H	226	ASP
1	L	76	ASN
2	H	144	THR
2	H	184	SER
2	H	197	SER
2	H	202	SER
2	H	200	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	222	ILE
2	H	223	VAL
2	H	201	PRO
2	H	159	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	L	193/193 (100%)	149 (77%)	44 (23%)	1	0
2	H	184/193 (95%)	140 (76%)	44 (24%)	1	0
All	All	377/386 (98%)	289 (77%)	88 (23%)	1	0

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	LEU
1	L	11	LEU
1	L	13	VAL
1	L	21	LEU
1	L	24	ARG
1	L	29	ILE
1	L	30	SER
1	L	41	HIS
1	L	45	ARG
1	L	46	LEU
1	L	47	LEU
1	L	48	ILE
1	L	67	SER
1	L	69	THR
1	L	70	ASP
1	L	72	THR
1	L	73	LEU
1	L	75	ILE
1	L	90	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	93	SER
1	L	105	GLU
1	L	106	ILE
1	L	114	THR
1	L	116	SER
1	L	121	SER
1	L	122	SER
1	L	123	GLU
1	L	136	LEU
1	L	138	ASN
1	L	142	LYS
1	L	160	LEU
1	L	163	TRP
1	L	168	SER
1	L	180	THR
1	L	187	GLU
1	L	188	ARG
1	L	191	SER
1	L	197	THR
1	L	199	LYS
1	L	201	SER
1	L	202	THR
1	L	205	ILE
1	L	206	VAL
1	L	207	LYS
2	H	1	GLU
2	H	3	GLN
2	H	6	GLN
2	H	12	VAL
2	H	14	PRO
2	H	19	LYS
2	H	25	SER
2	H	30	SER
2	H	35	SER
2	H	44	ARG
2	H	51	ILE
2	H	56	THR
2	H	64	VAL
2	H	89	GLU
2	H	96	CYS
2	H	119	THR
2	H	120	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	127	LYS
2	H	144	THR
2	H	145	ASN
2	H	147	MET
2	H	148	VAL
2	H	150	LEU
2	H	152	CYS
2	H	153	LEU
2	H	155	LYS
2	H	163	THR
2	H	165	THR
2	H	170	SER
2	H	172	SER
2	H	175	VAL
2	H	184	SER
2	H	198	SER
2	H	200	ARG
2	H	202	SER
2	H	203	GLU
2	H	208	ASN
2	H	209	VAL
2	H	212	PRO
2	H	215	SER
2	H	217	LYS
2	H	220	LYS
2	H	221	LYS
2	H	226	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	38	GLN
1	L	90	GLN
1	L	157	ASN
1	L	161	ASN
1	L	212	ASN
2	H	6	GLN
2	H	39	GLN
2	H	74	ASN
2	H	145	ASN
2	H	176	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	183	GLN

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 [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	L	214/214 (100%)	-0.53	2 (0%) 81 80	4, 17, 36, 126	0
2	H	216/227 (95%)	-0.34	4 (1%) 66 66	4, 21, 56, 112	0
All	All	430/441 (97%)	-0.44	6 (1%) 73 73	4, 18, 46, 126	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	111	ALA	5.0
2	H	96	CYS	2.9
1	L	212	ASN	2.4
2	H	223	VAL	2.3
2	H	142	ALA	2.2
1	L	214	CYS	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 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.