



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:29 pm BST

PDB ID : 1SPD
Title : AMYOTROPHIC LATERAL SCLEROSIS AND STRUCTURAL DEFECTS
IN CU,ZN SUPEROXIDE DISMUTASE
Authors : Parge, H.E.; Tainer, J.A.
Deposited on : 1993-07-21
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

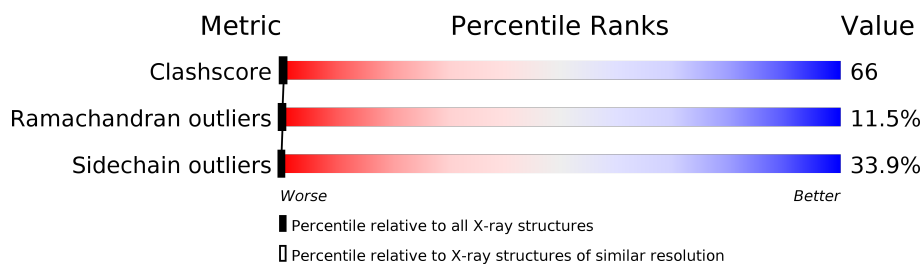
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	154	 8% 32% 39% 20%
1	B	154	 • 35% 45% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2230 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 SUPEROXIDE DISMUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	154	1113	681	203	225	4	0	0	0
1	B	154	1113	681	203	225	4	0	0	0

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cu	0	0
			1	1		
2	A	1	Total	Cu	0	0
			1	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

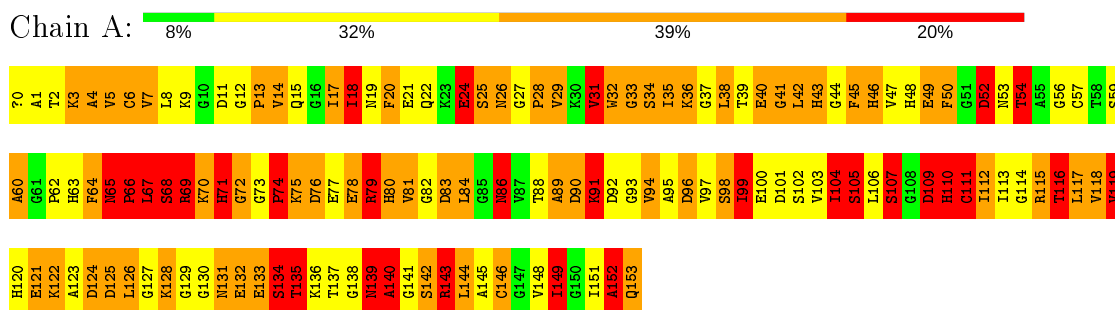
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

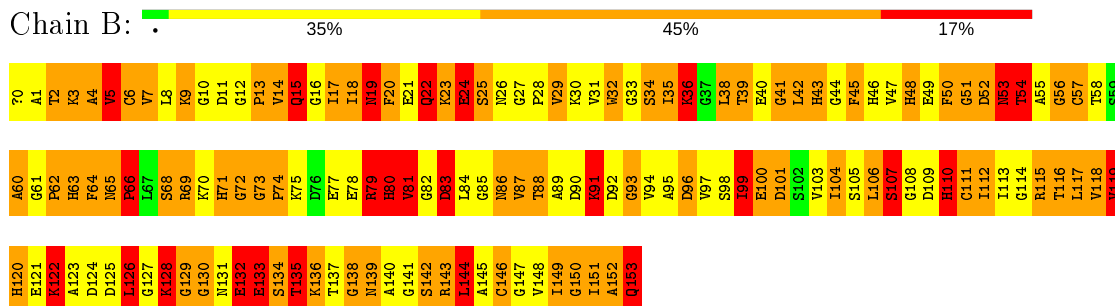
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

- Molecule 1: SUPEROXIDE DISMUTASE



- Molecule 1: SUPEROXIDE DISMUTASE



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	113.57Å 113.57Å 71.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	5.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.224 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2230	wwPDB-VP
Average B, all atoms (Å ²)	7.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CU, ACE

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	2.04	26/1129 (2.3%)	3.40	214/1522 (14.1%)
1	B	2.11	26/1129 (2.3%)	3.51	214/1522 (14.1%)
All	All	2.07	52/2258 (2.3%)	3.46	428/3044 (14.1%)

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	0	ACE	C-N	22.21	1.85	1.34
1	B	0	ACE	C-N	20.24	1.80	1.34
1	B	33	GLY	N-CA	11.84	1.63	1.46
1	B	14	VAL	C-N	-9.12	1.13	1.34
1	B	150	GLY	N-CA	8.88	1.59	1.46
1	B	41	GLY	N-CA	8.32	1.58	1.46
1	B	12	GLY	CA-C	7.25	1.63	1.51
1	B	132	GLU	CD-OE2	7.24	1.33	1.25
1	A	56	GLY	CA-C	6.94	1.62	1.51
1	A	41	GLY	CA-C	6.61	1.62	1.51
1	A	24	GLU	CD-OE2	6.49	1.32	1.25
1	B	27	GLY	N-CA	6.35	1.55	1.46
1	A	72	GLY	N-CA	-6.32	1.36	1.46
1	A	27	GLY	CA-C	6.29	1.61	1.51
1	A	2	THR	CB-OG1	6.27	1.55	1.43
1	A	44	GLY	N-CA	6.19	1.55	1.46
1	B	17	ILE	N-CA	6.11	1.58	1.46
1	A	98	SER	CB-OG	6.05	1.50	1.42
1	B	146	CYS	CB-SG	5.96	1.92	1.82
1	B	121	GLU	CD-OE2	-5.95	1.19	1.25
1	B	93	GLY	C-O	5.80	1.32	1.23
1	A	34	SER	C-O	5.79	1.34	1.23
1	A	99	ILE	C-O	5.75	1.34	1.23
1	B	73	GLY	CA-C	5.73	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	GLY	N-CA	5.72	1.54	1.46
1	B	4	ALA	C-O	5.69	1.34	1.23
1	B	51	GLY	CA-C	5.67	1.60	1.51
1	B	5	VAL	N-CA	5.56	1.57	1.46
1	B	129	GLY	N-CA	5.55	1.54	1.46
1	B	79	ARG	NE-CZ	5.54	1.40	1.33
1	A	53	ASN	N-CA	5.51	1.57	1.46
1	A	143	ARG	CZ-NH2	5.49	1.40	1.33
1	A	18	ILE	C-O	5.41	1.33	1.23
1	B	93	GLY	N-CA	-5.41	1.38	1.46
1	A	4	ALA	C-O	5.33	1.33	1.23
1	B	79	ARG	CG-CD	-5.27	1.38	1.51
1	A	68	SER	CA-CB	5.26	1.60	1.52
1	A	88	THR	CB-OG1	5.25	1.53	1.43
1	B	57	CYS	CB-SG	5.23	1.91	1.82
1	A	80	HIS	CG-CD2	5.20	1.44	1.35
1	A	89	ALA	C-O	5.19	1.33	1.23
1	A	134	SER	CB-OG	5.18	1.49	1.42
1	B	36	LYS	C-O	5.16	1.33	1.23
1	A	47	VAL	C-N	-5.16	1.22	1.34
1	B	40	GLU	C-N	5.14	1.42	1.33
1	B	111	CYS	CB-SG	5.12	1.91	1.82
1	A	76	ASP	N-CA	5.11	1.56	1.46
1	A	28	PRO	C-N	5.08	1.45	1.34
1	B	34	SER	CB-OG	5.04	1.48	1.42
1	A	17	ILE	C-O	5.03	1.32	1.23
1	A	73	GLY	N-CA	5.03	1.53	1.46
1	B	118	VAL	C-O	5.02	1.32	1.23

All (428) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	ARG	NE-CZ-NH1	22.31	131.45	120.30
1	A	115	ARG	NE-CZ-NH2	-20.02	110.29	120.30
1	B	14	VAL	O-C-N	-16.55	96.21	122.70
1	B	14	VAL	C-N-CA	15.60	160.69	121.70
1	A	69	ARG	NE-CZ-NH1	-15.38	112.61	120.30
1	A	115	ARG	NE-CZ-NH1	13.01	126.80	120.30
1	A	26	ASN	C-N-CA	-12.68	95.68	122.30
1	B	101	ASP	O-C-N	12.37	142.50	122.70
1	B	143	ARG	NE-CZ-NH2	-12.27	114.17	120.30
1	A	4	ALA	O-C-N	12.26	142.32	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	ARG	NE-CZ-NH1	12.24	126.42	120.30
1	B	144	LEU	CA-CB-CG	12.05	143.01	115.30
1	A	77	GLU	OE1-CD-OE2	-12.01	108.89	123.30
1	A	78	GLU	N-CA-CB	11.65	131.57	110.60
1	B	87	VAL	CA-CB-CG1	11.46	128.10	110.90
1	B	110	HIS	CA-CB-CG	11.43	133.02	113.60
1	A	125	ASP	CB-CG-OD2	-11.23	108.19	118.30
1	A	146	CYS	O-C-N	11.08	142.04	123.20
1	B	4	ALA	O-C-N	11.08	140.43	122.70
1	B	79	ARG	CB-CG-CD	11.04	140.29	111.60
1	B	101	ASP	CB-CG-OD2	10.75	127.97	118.30
1	B	19	ASN	O-C-N	10.68	139.78	122.70
1	B	100	GLU	N-CA-CB	10.38	129.29	110.60
1	A	143	ARG	NE-CZ-NH1	-10.36	115.12	120.30
1	A	69	ARG	NH1-CZ-NH2	10.26	130.69	119.40
1	B	55	ALA	N-CA-CB	10.01	124.11	110.10
1	A	52	ASP	CB-CG-OD2	9.93	127.24	118.30
1	A	98	SER	N-CA-CB	9.92	125.38	110.50
1	A	109	ASP	CB-CG-OD2	9.76	127.08	118.30
1	B	58	THR	CA-CB-CG2	-9.60	98.95	112.40
1	B	29	VAL	O-C-N	9.58	138.03	122.70
1	A	28	PRO	N-CA-C	9.56	136.96	112.10
1	A	14	VAL	CA-CB-CG1	-9.54	96.58	110.90
1	A	38	LEU	C-N-CA	9.54	145.55	121.70
1	B	55	ALA	N-CA-C	-9.53	85.26	111.00
1	A	116	THR	CA-CB-CG2	9.47	125.65	112.40
1	A	4	ALA	C-N-CA	-9.41	98.17	121.70
1	A	124	ASP	CB-CG-OD2	-9.38	109.86	118.30
1	B	45	PHE	O-C-N	9.29	137.56	122.70
1	B	45	PHE	CA-C-N	-9.26	96.83	117.20
1	A	8	LEU	O-C-N	9.24	137.49	122.70
1	B	14	VAL	CA-C-O	9.23	139.49	120.10
1	B	71	HIS	CA-C-N	-9.22	97.76	116.20
1	B	83	ASP	CB-CG-OD1	-9.17	110.05	118.30
1	A	14	VAL	CA-CB-CG2	9.13	124.59	110.90
1	B	42	LEU	N-CA-CB	-9.12	92.16	110.40
1	B	32	TRP	C-N-CA	-9.10	103.20	122.30
1	B	87	VAL	CG1-CB-CG2	-9.09	96.36	110.90
1	B	115	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	B	40	GLU	C-N-CA	-9.06	103.28	122.30
1	B	149	ILE	CA-CB-CG1	9.03	128.16	111.00
1	A	107	SER	O-C-N	8.91	138.35	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	VAL	CG1-CB-CG2	-8.91	96.65	110.90
1	B	32	TRP	O-C-N	8.89	138.31	123.20
1	A	125	ASP	C-N-CA	8.87	143.89	121.70
1	A	56	GLY	C-N-CA	8.78	143.65	121.70
1	A	60	ALA	N-CA-CB	-8.63	98.02	110.10
1	B	21	GLU	N-CA-CB	8.62	126.12	110.60
1	A	115	ARG	CD-NE-CZ	8.55	135.56	123.60
1	B	149	ILE	C-N-CA	-8.49	104.47	122.30
1	B	72	GLY	CA-C-N	-8.47	99.25	116.20
1	A	91	LYS	CD-CE-NZ	-8.47	92.23	111.70
1	B	135	THR	CA-CB-OG1	-8.46	91.22	109.00
1	A	1	ALA	CA-C-O	8.42	137.78	120.10
1	B	36	LYS	O-C-N	8.36	137.41	123.20
1	B	144	LEU	CB-CG-CD1	8.34	125.17	111.00
1	A	86	ASN	CB-CA-C	8.33	127.06	110.40
1	B	34	SER	N-CA-CB	8.33	122.99	110.50
1	A	2	THR	N-CA-CB	-8.31	94.50	110.30
1	B	4	ALA	C-N-CA	-8.30	100.94	121.70
1	B	18	ILE	CA-CB-CG2	8.27	127.43	110.90
1	B	72	GLY	C-N-CA	-8.19	105.10	122.30
1	B	12	GLY	N-CA-C	-8.19	92.64	113.10
1	B	135	THR	OG1-CB-CG2	8.16	128.77	110.00
1	A	50	PHE	O-C-N	8.15	137.06	123.20
1	B	85	GLY	CA-C-O	8.14	135.25	120.60
1	A	78	GLU	N-CA-C	-8.12	89.08	111.00
1	B	15	GLN	CA-CB-CG	8.10	131.21	113.40
1	B	40	GLU	CA-C-N	-8.07	100.07	116.20
1	B	55	ALA	O-C-N	8.06	136.91	123.20
1	A	76	ASP	N-CA-CB	-8.06	96.10	110.60
1	A	121	GLU	OE1-CD-OE2	8.05	132.96	123.30
1	B	77	GLU	CA-CB-CG	8.02	131.03	113.40
1	A	1	ALA	CA-C-N	-7.98	99.64	117.20
1	A	68	SER	N-CA-C	7.97	132.51	111.00
1	A	68	SER	CA-C-N	-7.90	99.83	117.20
1	A	15	GLN	CA-CB-CG	7.82	130.61	113.40
1	B	96	ASP	C-N-CA	-7.82	102.14	121.70
1	B	95	ALA	N-CA-CB	7.80	121.02	110.10
1	B	63	HIS	CA-CB-CG	-7.76	100.42	113.60
1	A	67	LEU	N-CA-CB	7.74	125.88	110.40
1	B	148	VAL	CA-CB-CG2	7.72	122.48	110.90
1	A	110	HIS	N-CA-CB	-7.72	96.71	110.60
1	A	74	PRO	N-CD-CG	-7.70	91.65	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ALA	O-C-N	7.69	135.00	122.70
1	A	29	VAL	O-C-N	7.62	134.90	122.70
1	B	125	ASP	CB-CG-OD2	7.62	125.16	118.30
1	B	93	GLY	O-C-N	7.60	134.85	122.70
1	A	66	PRO	N-CA-CB	-7.58	94.21	103.30
1	B	136	LYS	CA-C-N	-7.55	100.59	117.20
1	B	64	PHE	CA-C-N	-7.55	100.59	117.20
1	A	125	ASP	CB-CG-OD1	7.54	125.09	118.30
1	A	75	LYS	CA-CB-CG	7.53	129.97	113.40
1	B	64	PHE	N-CA-CB	7.52	124.14	110.60
1	B	136	LYS	CB-CG-CD	7.50	131.09	111.60
1	A	117	LEU	O-C-N	7.48	134.66	122.70
1	B	60	ALA	N-CA-CB	-7.47	99.64	110.10
1	B	2	THR	C-N-CA	7.43	140.28	121.70
1	B	66	PRO	C-N-CA	7.39	140.18	121.70
1	A	122	LYS	C-N-CA	7.39	140.17	121.70
1	A	124	ASP	O-C-N	7.38	134.51	122.70
1	B	122	LYS	CA-CB-CG	7.34	129.55	113.40
1	B	19	ASN	CA-C-N	-7.33	101.07	117.20
1	B	123	ALA	N-CA-CB	-7.32	99.85	110.10
1	B	91	LYS	N-CA-CB	7.30	123.74	110.60
1	A	45	PHE	CA-C-N	-7.28	101.18	117.20
1	A	34	SER	O-C-N	7.28	134.34	122.70
1	A	78	GLU	CA-CB-CG	7.26	129.38	113.40
1	A	8	LEU	CA-CB-CG	7.25	131.98	115.30
1	B	40	GLU	OE1-CD-OE2	-7.24	114.61	123.30
1	B	75	LYS	O-C-N	-7.24	111.12	122.70
1	B	73	GLY	N-CA-C	-7.24	95.01	113.10
1	A	91	LYS	O-C-N	7.23	134.26	122.70
1	A	131	ASN	CB-CG-ND2	7.22	134.04	116.70
1	A	69	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	B	107	SER	CA-C-O	-7.21	104.96	120.10
1	A	28	PRO	CA-C-N	-7.20	101.36	117.20
1	A	49	GLU	OE1-CD-OE2	-7.19	114.67	123.30
1	A	59	SER	N-CA-CB	-7.17	99.75	110.50
1	B	42	LEU	N-CA-C	7.11	130.20	111.00
1	A	80	HIS	CA-CB-CG	7.11	125.68	113.60
1	B	96	ASP	O-C-N	7.06	134.00	122.70
1	A	80	HIS	CB-CG-ND1	7.06	140.85	123.20
1	A	96	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	A	43	HIS	CA-CB-CG	-7.03	101.64	113.60
1	B	107	SER	N-CA-CB	7.03	121.04	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	GLU	N-CA-CB	6.99	123.19	110.60
1	A	14	VAL	C-N-CA	-6.97	104.28	121.70
1	A	117	LEU	CA-C-N	-6.94	101.93	117.20
1	A	109	ASP	OD1-CG-OD2	-6.90	110.20	123.30
1	B	40	GLU	CG-CD-OE1	6.89	132.08	118.30
1	A	52	ASP	CA-CB-CG	6.88	128.54	113.40
1	A	143	ARG	N-CA-C	-6.88	92.42	111.00
1	B	80	HIS	C-N-CA	6.88	138.90	121.70
1	A	123	ALA	N-CA-CB	-6.83	100.54	110.10
1	A	116	THR	O-C-N	6.83	133.62	122.70
1	A	65	ASN	CA-C-N	6.82	136.19	117.10
1	A	68	SER	CA-C-O	6.81	134.40	120.10
1	B	116	THR	O-C-N	6.81	133.60	122.70
1	B	40	GLU	CA-C-O	6.80	134.38	120.10
1	B	38	LEU	CB-CG-CD1	6.80	122.56	111.00
1	B	101	ASP	N-CA-CB	6.78	122.80	110.60
1	B	124	ASP	O-C-N	6.77	133.54	122.70
1	B	40	GLU	CA-CB-CG	6.77	128.29	113.40
1	A	32	TRP	O-C-N	6.75	134.68	123.20
1	B	27	GLY	N-CA-C	-6.75	96.22	113.10
1	B	99	ILE	N-CA-CB	6.74	126.30	110.80
1	A	76	ASP	O-C-N	-6.74	111.92	122.70
1	B	62	PRO	N-CD-CG	-6.74	93.10	103.20
1	B	42	LEU	CA-C-O	6.73	134.23	120.10
1	A	65	ASN	CA-C-O	-6.72	106.00	120.10
1	A	19	ASN	C-N-CA	-6.71	104.93	121.70
1	B	52	ASP	N-CA-C	-6.70	92.92	111.00
1	A	122	LYS	O-C-N	-6.69	111.99	122.70
1	B	92	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	B	122	LYS	N-CA-CB	-6.67	98.59	110.60
1	A	28	PRO	CA-C-O	6.66	136.19	120.20
1	A	19	ASN	O-C-N	6.63	133.31	122.70
1	B	119	VAL	CA-CB-CG1	6.62	120.83	110.90
1	A	3	LYS	CD-CE-NZ	-6.61	96.49	111.70
1	B	151	ILE	N-CA-CB	6.59	125.96	110.80
1	A	129	GLY	C-N-CA	6.59	136.14	122.30
1	B	81	VAL	N-CA-CB	6.58	125.97	111.50
1	B	104	ILE	N-CA-CB	-6.58	95.67	110.80
1	A	77	GLU	CG-CD-OE1	6.57	131.45	118.30
1	B	79	ARG	CA-CB-CG	6.56	127.84	113.40
1	A	145	ALA	C-N-CA	-6.55	105.32	121.70
1	B	91	LYS	CB-CA-C	-6.55	97.30	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	THR	OG1-CB-CG2	6.52	125.00	110.00
1	B	32	TRP	CA-C-N	-6.52	103.16	116.20
1	A	86	ASN	N-CA-C	-6.52	93.40	111.00
1	B	149	ILE	N-CA-CB	6.50	125.75	110.80
1	A	65	ASN	N-CA-C	6.47	128.46	111.00
1	A	140	ALA	N-CA-CB	-6.46	101.05	110.10
1	A	2	THR	N-CA-C	6.46	128.44	111.00
1	B	143	ARG	N-CA-C	-6.46	93.57	111.00
1	A	6	CYS	O-C-N	6.44	133.00	122.70
1	B	149	ILE	CB-CA-C	-6.42	98.75	111.60
1	B	64	PHE	CA-C-O	6.41	133.56	120.10
1	A	42	LEU	O-C-N	6.40	132.94	122.70
1	B	2	THR	CB-CA-C	6.40	128.87	111.60
1	B	77	GLU	N-CA-C	-6.39	93.75	111.00
1	B	43	HIS	CA-CB-CG	-6.39	102.74	113.60
1	A	9	LYS	CA-C-N	6.37	128.94	116.20
1	A	142	SER	C-N-CA	6.36	137.60	121.70
1	B	54	THR	N-CA-CB	-6.35	98.23	110.30
1	A	31	VAL	CA-C-N	-6.35	103.22	117.20
1	B	115	ARG	O-C-N	6.34	132.85	122.70
1	B	54	THR	CA-CB-OG1	-6.32	95.72	109.00
1	B	123	ALA	CB-CA-C	6.31	119.57	110.10
1	B	132	GLU	N-CA-CB	6.31	121.95	110.60
1	A	67	LEU	N-CA-C	-6.30	93.99	111.00
1	A	111	CYS	CB-CA-C	6.30	123.00	110.40
1	B	7	VAL	N-CA-C	-6.29	94.02	111.00
1	B	71	HIS	O-C-N	6.29	133.89	123.20
1	A	4	ALA	CA-C-N	-6.28	103.39	117.20
1	B	100	GLU	CB-CA-C	-6.27	97.86	110.40
1	B	3	LYS	N-CA-CB	-6.26	99.33	110.60
1	B	120	HIS	CA-CB-CG	-6.25	102.98	113.60
1	A	116	THR	OG1-CB-CG2	-6.25	95.63	110.00
1	B	90	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	A	71	HIS	C-N-CA	6.25	135.41	122.30
1	A	2	THR	CA-CB-OG1	-6.24	95.90	109.00
1	A	20	PHE	CA-CB-CG	6.23	128.85	113.90
1	A	1	ALA	CB-CA-C	-6.23	100.76	110.10
1	B	43	HIS	N-CA-CB	-6.22	99.41	110.60
1	B	117	LEU	CB-CA-C	6.20	121.98	110.20
1	A	9	LYS	CA-CB-CG	6.20	127.03	113.40
1	A	14	VAL	N-CA-CB	-6.18	97.91	111.50
1	B	40	GLU	N-CA-C	6.15	127.61	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	ILE	CA-CB-CG1	-6.14	99.34	111.00
1	A	24	GLU	CA-C-O	6.12	132.96	120.10
1	A	94	VAL	N-CA-C	-6.12	94.47	111.00
1	A	110	HIS	CB-CA-C	6.12	122.64	110.40
1	B	107	SER	CA-CB-OG	6.11	127.70	111.20
1	A	66	PRO	CA-C-N	6.09	130.61	117.20
1	A	138	GLY	N-CA-C	-6.09	97.87	113.10
1	B	104	ILE	CA-C-O	6.09	132.89	120.10
1	B	121	GLU	OE1-CD-OE2	6.09	130.60	123.30
1	B	50	PHE	O-C-N	6.08	133.54	123.20
1	A	38	LEU	CA-C-N	-6.08	103.82	117.20
1	B	48	HIS	CA-C-N	-6.08	103.83	117.20
1	A	29	VAL	CA-C-N	-6.08	103.84	117.20
1	B	13	PRO	CA-C-O	-6.07	105.62	120.20
1	A	90	ASP	N-CA-C	-6.06	94.63	111.00
1	A	99	ILE	O-C-N	6.06	132.40	122.70
1	A	48	HIS	CB-CA-C	6.04	122.47	110.40
1	A	68	SER	N-CA-CB	-6.02	101.47	110.50
1	A	133	GLU	O-C-N	6.02	132.33	122.70
1	A	129	GLY	N-CA-C	6.01	128.12	113.10
1	A	89	ALA	CA-C-N	6.01	130.42	117.20
1	A	62	PRO	O-C-N	-6.01	113.09	122.70
1	B	20	PHE	O-C-N	6.00	132.31	122.70
1	A	45	PHE	CB-CG-CD1	-5.99	116.61	120.80
1	A	32	TRP	C-N-CA	-5.98	109.74	122.30
1	A	36	LYS	CA-CB-CG	5.98	126.56	113.40
1	A	42	LEU	CB-CG-CD2	-5.98	100.83	111.00
1	B	72	GLY	O-C-N	5.98	133.37	123.20
1	B	71	HIS	CB-CG-ND1	5.98	138.15	123.20
1	B	13	PRO	CA-C-N	5.98	130.35	117.20
1	A	91	LYS	CA-C-N	-5.97	104.07	117.20
1	A	34	SER	C-N-CA	-5.95	106.82	121.70
1	B	5	VAL	N-CA-CB	5.95	124.59	111.50
1	A	46	HIS	CA-CB-CG	-5.95	103.49	113.60
1	B	138	GLY	CA-C-O	-5.94	109.91	120.60
1	A	139	ASN	CB-CA-C	-5.94	98.52	110.40
1	A	143	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	B	96	ASP	N-CA-C	-5.93	94.98	111.00
1	B	5	VAL	O-C-N	5.93	132.19	122.70
1	B	83	ASP	N-CA-CB	5.92	121.26	110.60
1	B	87	VAL	CB-CA-C	5.91	122.63	111.40
1	B	101	ASP	C-N-CA	5.91	136.47	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	77	GLU	N-CA-C	-5.90	95.07	111.00
1	A	109	ASP	CA-CB-CG	5.89	126.36	113.40
1	A	32	TRP	CA-CB-CG	5.89	124.89	113.70
1	B	13	PRO	C-N-CA	-5.88	106.99	121.70
1	B	65	ASN	CB-CG-OD1	5.88	133.36	121.60
1	A	50	PHE	CB-CG-CD2	-5.86	116.70	120.80
1	B	83	ASP	O-C-N	5.84	132.05	122.70
1	A	111	CYS	O-C-N	5.83	132.03	122.70
1	B	32	TRP	CA-CB-CG	5.83	124.78	113.70
1	A	105	SER	O-C-N	5.81	132.00	122.70
1	B	21	GLU	CA-C-N	5.80	129.97	117.20
1	A	89	ALA	O-C-N	-5.80	113.42	122.70
1	A	86	ASN	N-CA-CB	-5.80	100.17	110.60
1	B	115	ARG	CA-C-N	-5.80	104.45	117.20
1	B	1	ALA	CA-C-N	-5.79	104.47	117.20
1	B	5	VAL	CA-CB-CG2	5.78	119.57	110.90
1	B	126	LEU	N-CA-CB	-5.78	98.84	110.40
1	B	79	ARG	CG-CD-NE	5.77	123.92	111.80
1	B	138	GLY	CA-C-N	5.76	129.87	117.20
1	A	32	TRP	CB-CG-CD1	5.76	134.49	127.00
1	B	17	ILE	CB-CA-C	5.76	123.12	111.60
1	B	58	THR	CA-CB-OG1	5.75	121.08	109.00
1	A	17	ILE	N-CA-C	-5.75	95.48	111.00
1	A	139	ASN	N-CA-C	5.75	126.52	111.00
1	A	143	ARG	CA-CB-CG	5.74	126.03	113.40
1	B	18	ILE	CG1-CB-CG2	-5.74	98.78	111.40
1	A	41	GLY	CA-C-N	-5.73	104.59	117.20
1	A	33	GLY	CA-C-O	-5.73	110.28	120.60
1	A	9	LYS	O-C-N	-5.73	113.46	123.20
1	A	111	CYS	CA-CB-SG	-5.73	103.69	114.00
1	B	94	VAL	N-CA-C	-5.72	95.54	111.00
1	B	21	GLU	CA-C-O	-5.72	108.08	120.10
1	A	34	SER	CA-C-N	-5.72	104.62	117.20
1	A	134	SER	N-CA-C	-5.71	95.57	111.00
1	B	26	ASN	CB-CA-C	5.71	121.82	110.40
1	B	81	VAL	CA-C-N	-5.70	104.79	116.20
1	A	49	GLU	CG-CD-OE1	5.69	129.68	118.30
1	A	96	ASP	O-C-N	5.69	131.81	122.70
1	B	20	PHE	N-CA-CB	-5.68	100.37	110.60
1	B	11	ASP	CB-CA-C	5.68	121.76	110.40
1	B	10	GLY	O-C-N	5.66	131.76	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	LEU	N-CA-CB	5.66	121.71	110.40
1	B	107	SER	O-C-N	5.66	132.81	123.20
1	B	101	ASP	N-CA-C	-5.65	95.74	111.00
1	A	152	ALA	N-CA-CB	5.65	118.01	110.10
1	B	86	ASN	N-CA-CB	-5.64	100.44	110.60
1	B	81	VAL	O-C-N	5.64	132.79	123.20
1	A	127	GLY	CA-C-O	5.63	130.73	120.60
1	B	4	ALA	CA-C-O	-5.63	108.28	120.10
1	A	21	GLU	OE1-CD-OE2	-5.62	116.55	123.30
1	B	69	ARG	CA-CB-CG	-5.61	101.05	113.40
1	A	59	SER	N-CA-C	5.60	126.13	111.00
1	A	7	VAL	CB-CA-C	5.60	122.03	111.40
1	A	110	HIS	CA-C-O	5.59	131.85	120.10
1	A	40	GLU	CA-CB-CG	5.59	125.70	113.40
1	B	71	HIS	N-CA-CB	5.59	120.65	110.60
1	B	36	LYS	CA-C-N	-5.58	105.03	116.20
1	A	81	VAL	CA-CB-CG2	5.58	119.26	110.90
1	B	141	GLY	O-C-N	-5.57	113.79	122.70
1	B	71	HIS	CA-CB-CG	5.57	123.06	113.60
1	B	14	VAL	N-CA-CB	-5.56	99.26	111.50
1	B	101	ASP	CA-C-N	-5.56	104.96	117.20
1	B	6	CYS	CA-C-O	5.56	131.77	120.10
1	B	35	ILE	CG1-CB-CG2	-5.55	99.20	111.40
1	A	131	ASN	CA-CB-CG	5.53	125.57	113.40
1	B	15	GLN	CB-CA-C	5.53	121.46	110.40
1	B	118	VAL	N-CA-CB	5.52	123.64	111.50
1	A	21	GLU	CB-CG-CD	5.52	129.09	114.20
1	A	73	GLY	N-CA-C	-5.52	99.31	113.10
1	B	153	GLN	CB-CG-CD	5.52	125.94	111.60
1	A	128	LYS	CA-CB-CG	5.51	125.53	113.40
1	B	74	PRO	N-CA-C	-5.51	97.76	112.10
1	A	88	THR	CA-C-O	5.51	131.67	120.10
1	B	40	GLU	CB-CA-C	-5.50	99.41	110.40
1	B	35	ILE	CA-C-O	-5.48	108.59	120.10
1	B	137	THR	N-CA-CB	-5.48	99.89	110.30
1	A	146	CYS	CA-C-N	-5.48	105.25	116.20
1	A	28	PRO	N-CA-CB	-5.47	96.59	102.60
1	B	53	ASN	O-C-N	5.46	131.44	122.70
1	B	150	GLY	N-CA-C	-5.43	99.52	113.10
1	A	134	SER	CB-CA-C	5.43	120.42	110.10
1	A	149	ILE	CA-C-O	5.42	131.49	120.10
1	A	69	ARG	CG-CD-NE	-5.42	100.42	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ALA	CB-CA-C	5.42	118.23	110.10
1	A	101	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	119	VAL	N-CA-C	-5.40	96.42	111.00
1	A	80	HIS	CB-CG-CD2	-5.39	114.08	130.80
1	A	46	HIS	CA-C-N	-5.39	105.34	117.20
1	A	49	GLU	N-CA-C	5.38	125.52	111.00
1	A	5	VAL	O-C-N	5.37	131.30	122.70
1	A	131	ASN	OD1-CG-ND2	-5.36	109.56	121.90
1	A	66	PRO	CA-N-CD	-5.36	104.00	111.50
1	A	139	ASN	O-C-N	5.36	131.27	122.70
1	B	35	ILE	O-C-N	5.36	131.27	122.70
1	B	131	ASN	CB-CG-ND2	5.35	129.54	116.70
1	A	45	PHE	CA-C-O	5.35	131.34	120.10
1	B	5	VAL	CA-CB-CG1	5.35	118.92	110.90
1	B	28	PRO	C-N-CA	-5.35	108.33	121.70
1	A	42	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	50	PHE	CA-C-O	-5.35	108.87	120.10
1	B	2	THR	N-CA-CB	-5.34	100.15	110.30
1	B	152	ALA	CB-CA-C	-5.34	102.09	110.10
1	A	118	VAL	CG1-CB-CG2	-5.33	102.36	110.90
1	A	127	GLY	CA-C-N	-5.33	105.46	117.20
1	A	149	ILE	CB-CA-C	5.33	122.26	111.60
1	B	101	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	B	85	GLY	CA-C-N	-5.32	105.50	117.20
1	B	128	LYS	CA-CB-CG	5.32	125.10	113.40
1	A	76	ASP	N-CA-C	5.31	125.34	111.00
1	A	115	ARG	N-CA-CB	5.30	120.14	110.60
1	B	149	ILE	O-C-N	5.30	132.21	123.20
1	A	5	VAL	CA-C-N	-5.29	105.56	117.20
1	A	98	SER	N-CA-C	-5.29	96.71	111.00
1	B	104	ILE	N-CA-C	5.29	125.29	111.00
1	B	15	GLN	CA-C-O	5.29	131.21	120.10
1	A	135	THR	N-CA-CB	5.27	120.32	110.30
1	A	53	ASN	CA-C-O	5.27	131.17	120.10
1	A	79	ARG	N-CA-CB	5.27	120.09	110.60
1	B	66	PRO	O-C-N	-5.25	114.29	122.70
1	A	62	PRO	N-CA-CB	5.25	109.60	103.30
1	A	54	THR	N-CA-C	5.25	125.17	111.00
1	B	115	ARG	NH1-CZ-NH2	5.23	125.16	119.40
1	B	9	LYS	CA-C-O	5.22	131.07	120.10
1	A	32	TRP	CB-CG-CD2	-5.22	119.81	126.60
1	A	36	LYS	CA-C-N	-5.22	105.77	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	ILE	O-C-N	5.21	131.04	122.70
1	A	17	ILE	CB-CA-C	5.20	122.01	111.60
1	B	26	ASN	CA-CB-CG	5.20	124.83	113.40
1	B	45	PHE	CB-CA-C	5.20	120.80	110.40
1	B	85	GLY	N-CA-C	5.20	126.09	113.10
1	A	5	VAL	C-N-CA	-5.20	108.71	121.70
1	A	104	ILE	CA-CB-CG1	5.17	120.83	111.00
1	B	16	GLY	N-CA-C	5.17	126.04	113.10
1	B	110	HIS	N-CA-C	5.17	124.96	111.00
1	B	1	ALA	O-C-N	5.15	130.93	122.70
1	B	79	ARG	N-CA-C	5.14	124.87	111.00
1	A	33	GLY	C-N-CA	-5.13	108.86	121.70
1	B	92	ASP	CA-CB-CG	-5.13	102.11	113.40
1	A	111	CYS	N-CA-CB	-5.12	101.38	110.60
1	A	112	ILE	CA-CB-CG2	5.12	121.14	110.90
1	B	134	SER	O-C-N	5.12	130.89	122.70
1	A	14	VAL	O-C-N	5.10	130.86	122.70
1	A	137	THR	C-N-CA	-5.10	111.58	122.30
1	B	100	GLU	N-CA-C	-5.10	97.23	111.00
1	A	119	VAL	CA-CB-CG1	5.10	118.55	110.90
1	B	55	ALA	CA-C-N	-5.10	106.01	116.20
1	B	3	LYS	C-N-CA	-5.09	108.98	121.70
1	A	149	ILE	CA-CB-CG2	5.08	121.06	110.90
1	A	39	THR	N-CA-C	-5.08	97.28	111.00
1	A	31	VAL	C-N-CA	-5.08	109.01	121.70
1	B	62	PRO	CA-N-CD	-5.08	104.39	111.50
1	A	140	ALA	N-CA-C	5.07	124.68	111.00
1	B	21	GLU	CB-CA-C	-5.07	100.27	110.40
1	A	105	SER	CB-CA-C	-5.06	100.49	110.10
1	B	86	ASN	O-C-N	5.05	130.79	122.70
1	A	137	THR	O-C-N	-5.05	114.61	123.20
1	A	8	LEU	CA-C-O	-5.05	109.50	120.10
1	A	145	ALA	CA-C-N	-5.05	106.10	117.20
1	B	41	GLY	CA-C-O	-5.05	111.52	120.60
1	B	69	ARG	NH1-CZ-NH2	-5.04	113.85	119.40
1	A	14	VAL	CB-CA-C	5.04	120.98	111.40
1	A	47	VAL	CA-CB-CG1	5.03	118.45	110.90
1	B	87	VAL	N-CA-CB	-5.02	100.47	111.50
1	B	79	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	B	112	ILE	CG1-CB-CG2	5.00	122.41	111.40

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	1113	0	1071	141	0
1	B	1113	0	1075	157	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	2230	0	2146	290	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 66.

All (290) 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:B:118:VAL:HG21	1:B:143:ARG:HB3	1.33	1.10
1:B:42:LEU:HD22	1:B:86:ASN:OD1	1.59	1.03
1:A:152:ALA:HA	1:B:52:ASP:HB2	1.41	1.02
1:B:18:ILE:HD13	1:B:45:PHE:HZ	1.29	0.97
1:A:35:ILE:HD11	1:A:119:VAL:HG21	1.44	0.97
1:A:66:PRO:HG2	1:A:81:VAL:HG11	1.46	0.96
1:B:72:GLY:HA2	1:B:79:ARG:HA	1.45	0.96
1:B:31:VAL:O	1:B:98:SER:HA	1.70	0.91
1:A:125:ASP:O	1:A:128:LYS:NZ	2.05	0.88
1:A:122:LYS:NZ	1:A:139:ASN:HD22	1.72	0.88
1:B:18:ILE:HD13	1:B:45:PHE:CZ	2.10	0.85
1:B:6:CYS:SG	1:B:147:GLY:HA3	2.17	0.83
1:A:5:VAL:HG22	1:A:6:CYS:H	1.44	0.82
1:A:122:LYS:HZ2	1:A:139:ASN:HD22	1.25	0.81
1:A:52:ASP:HB3	1:A:54:THR:OG1	1.81	0.80
1:A:6:CYS:HB2	1:A:149:ILE:HG13	1.64	0.80
1:B:97:VAL:HG12	1:B:98:SER:H	1.47	0.79
1:B:41:GLY:O	1:B:88:THR:HA	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:PHE:HA	1:B:30:LYS:O	1.82	0.79
1:B:43:HIS:O	1:B:86:ASN:HA	1.82	0.79
1:A:152:ALA:HB1	1:A:153:GLN:NE2	1.99	0.78
1:B:89:ALA:HB1	1:B:93:GLY:HA2	1.65	0.78
1:A:118:VAL:HG22	1:A:146:CYS:HB3	1.64	0.77
1:B:118:VAL:HG21	1:B:143:ARG:CB	2.12	0.77
1:B:31:VAL:HG22	1:B:99:ILE:HB	1.65	0.77
1:A:104:ILE:HD13	1:A:112:ILE:HD13	1.66	0.77
1:B:74:PRO:HD2	1:B:126:LEU:CD2	2.16	0.74
1:B:38:LEU:HD23	1:B:93:GLY:O	1.87	0.74
1:B:50:PHE:O	1:B:60:ALA:HA	1.86	0.74
1:A:122:LYS:NZ	1:A:139:ASN:ND2	2.35	0.74
1:A:64:PHE:CD2	1:A:81:VAL:HG13	2.22	0.74
1:A:112:ILE:O	1:A:115:ARG:HB2	1.89	0.73
1:A:118:VAL:HG11	1:A:143:ARG:HG3	1.69	0.73
1:B:97:VAL:HG12	1:B:98:SER:N	2.05	0.72
1:B:18:ILE:CD1	1:B:45:PHE:HZ	2.00	0.71
1:B:39:THR:O	1:B:43:HIS:NE2	2.21	0.71
1:A:122:LYS:HZ2	1:A:139:ASN:ND2	1.89	0.71
1:A:57:CYS:HB3	1:A:143:ARG:HG2	1.72	0.70
1:B:71:HIS:HA	1:B:80:HIS:CE1	2.26	0.70
1:B:72:GLY:HA2	1:B:79:ARG:CA	2.18	0.70
1:A:109:ASP:O	1:A:111:CYS:HB2	1.92	0.70
1:B:74:PRO:HD2	1:B:126:LEU:HD23	1.74	0.69
1:A:105:SER:OG	1:A:110:HIS:HB2	1.93	0.68
1:A:79:ARG:HH11	1:A:79:ARG:HB2	1.56	0.68
1:A:22:GLN:OE1	1:A:106:LEU:HB2	1.95	0.67
1:A:14:VAL:HG12	1:A:37:GLY:HA3	1.75	0.67
1:A:117:LEU:HB2	1:A:149:ILE:CD1	2.24	0.67
1:A:109:ASP:O	1:A:111:CYS:N	2.28	0.66
1:B:80:HIS:HB2	1:B:83:ASP:OD1	1.96	0.66
1:A:118:VAL:CG1	1:A:143:ARG:HG3	2.26	0.66
1:A:4:ALA:HB3	1:A:20:PHE:HB2	1.77	0.65
1:B:18:ILE:CD1	1:B:45:PHE:CZ	2.78	0.65
1:B:71:HIS:HA	1:B:80:HIS:ND1	2.12	0.65
1:A:105:SER:O	1:A:106:LEU:HD23	1.96	0.65
1:A:84:LEU:HD21	1:A:104:ILE:HG12	1.79	0.64
1:A:81:VAL:HG23	1:A:103:VAL:HG12	1.79	0.64
1:A:5:VAL:O	1:A:149:ILE:HA	1.98	0.64
1:B:64:PHE:CD2	1:B:112:ILE:HG22	2.32	0.64
1:B:5:VAL:HG13	1:B:6:CYS:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ASN:HD21	1:B:68:SER:H	1.46	0.63
1:B:118:VAL:HG11	1:B:143:ARG:HG2	1.79	0.63
1:A:79:ARG:HH11	1:A:79:ARG:CB	2.12	0.63
1:B:46:HIS:HB3	1:B:63:HIS:CD2	2.33	0.63
1:B:19:ASN:ND2	1:B:32:TRP:NE1	2.46	0.62
1:A:106:LEU:HD22	1:A:113:ILE:HD11	1.81	0.62
1:A:18:ILE:HD12	1:A:45:PHE:CZ	2.34	0.62
1:B:122:LYS:HB3	1:B:140:ALA:O	1.99	0.62
1:A:52:ASP:C	1:A:54:THR:H	2.02	0.62
1:B:72:GLY:CA	1:B:79:ARG:HA	2.26	0.62
1:B:46:HIS:HB3	1:B:63:HIS:HD2	1.64	0.62
1:A:74:PRO:HD2	1:A:75:LYS:H	1.65	0.61
1:B:112:ILE:HA	1:B:115:ARG:HE	1.63	0.61
1:B:65:ASN:HD21	1:B:68:SER:N	1.98	0.61
1:A:18:ILE:HD12	1:A:45:PHE:HZ	1.66	0.60
1:A:106:LEU:HD22	1:A:113:ILE:CD1	2.32	0.60
1:A:43:HIS:O	1:A:86:ASN:HA	2.01	0.60
1:A:117:LEU:HB2	1:A:149:ILE:HD11	1.82	0.60
1:A:121:GLU:HB2	1:A:144:LEU:HG	1.84	0.60
1:B:64:PHE:O	1:B:81:VAL:HB	2.02	0.60
1:A:124:ASP:OD1	1:A:126:LEU:HD23	2.01	0.60
1:B:80:HIS:HB2	1:B:83:ASP:CG	2.21	0.60
1:A:50:PHE:O	1:A:60:ALA:HA	2.02	0.60
1:B:45:PHE:HD2	1:B:119:VAL:HG23	1.67	0.59
1:A:122:LYS:HE3	1:A:139:ASN:O	2.01	0.59
1:A:118:VAL:HG11	1:A:143:ARG:CG	2.32	0.59
1:A:125:ASP:HB2	1:A:139:ASN:HB2	1.84	0.59
1:A:31:VAL:HG13	1:A:99:ILE:HB	1.84	0.59
1:B:64:PHE:CE2	1:B:112:ILE:HG22	2.38	0.59
1:B:113:ILE:HG23	1:B:150:GLY:HA2	1.85	0.59
1:B:81:VAL:HG13	1:B:103:VAL:CG1	2.33	0.59
1:A:64:PHE:HB3	1:A:82:GLY:HA3	1.84	0.58
1:A:118:VAL:HG22	1:A:146:CYS:CB	2.32	0.58
1:B:15:GLN:O	1:B:36:LYS:HB2	2.03	0.58
1:A:118:VAL:HG11	1:A:143:ARG:CD	2.33	0.58
1:B:46:HIS:CE1	1:B:71:HIS:HE1	2.21	0.58
1:A:13:PRO:HG2	1:A:14:VAL:HG13	1.84	0.58
1:A:46:HIS:HD1	1:A:120:HIS:CD2	2.11	0.57
1:B:31:VAL:CG2	1:B:99:ILE:HB	2.34	0.57
1:A:64:PHE:HB3	1:A:82:GLY:CA	2.34	0.57
1:A:84:LEU:HD21	1:A:104:ILE:CG1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:GLN:O	1:B:36:LYS:HE2	2.06	0.56
1:B:65:ASN:ND2	1:B:68:SER:H	2.03	0.56
1:A:49:GLU:HG3	1:A:115:ARG:HH21	1.70	0.56
1:A:65:ASN:ND2	1:A:68:SER:HA	2.20	0.56
1:A:40:GLU:HA	1:A:89:ALA:HB3	1.85	0.56
1:B:81:VAL:HG13	1:B:103:VAL:HG12	1.86	0.56
1:B:43:HIS:O	1:B:87:VAL:HG22	2.06	0.56
1:A:6:CYS:SG	1:A:149:ILE:HD12	2.45	0.56
1:A:35:ILE:CD1	1:A:119:VAL:HG21	2.26	0.56
1:A:134:SER:O	1:A:136:LYS:N	2.39	0.56
1:B:32:TRP:HA	1:B:97:VAL:O	2.06	0.55
1:B:14:VAL:O	1:B:36:LYS:O	2.25	0.55
1:B:118:VAL:HG23	1:B:145:ALA:O	2.06	0.55
1:B:53:ASN:HA	1:B:56:GLY:O	2.07	0.55
1:B:71:HIS:O	1:B:128:LYS:NZ	2.21	0.55
1:A:118:VAL:HG11	1:A:143:ARG:HD2	1.88	0.55
1:A:65:ASN:ND2	1:A:69:ARG:N	2.54	0.55
1:B:109:ASP:OD1	1:B:110:HIS:N	2.40	0.55
1:A:42:LEU:HB3	1:A:86:ASN:OD1	2.06	0.55
1:B:79:ARG:O	1:B:79:ARG:HD3	2.07	0.54
1:B:57:CYS:SG	1:B:145:ALA:C	2.86	0.54
1:B:35:ILE:CG2	1:B:38:LEU:HD13	2.39	0.53
1:A:124:ASP:HB3	1:A:126:LEU:CD2	2.38	0.53
1:B:42:LEU:HD13	1:B:86:ASN:OD1	2.08	0.53
1:B:74:PRO:CD	1:B:126:LEU:HD23	2.39	0.53
1:A:113:ILE:HA	1:A:149:ILE:HG22	1.90	0.53
1:A:106:LEU:O	1:A:107:SER:HB2	2.08	0.53
1:A:13:PRO:C	1:A:14:VAL:HG13	2.28	0.53
1:A:5:VAL:HG22	1:A:6:CYS:N	2.21	0.53
1:B:4:ALA:HB3	1:B:20:PHE:HB2	1.91	0.53
1:B:29:VAL:HG11	1:B:104:ILE:HG22	1.91	0.52
1:B:46:HIS:O	1:B:117:LEU:HG	2.10	0.52
1:B:73:GLY:O	1:B:74:PRO:C	2.48	0.52
1:B:48:HIS:CD2	1:B:118:VAL:HG12	2.43	0.52
1:B:134:SER:O	1:B:138:GLY:HA2	2.10	0.52
1:A:132:GLU:O	1:A:136:LYS:HG3	2.10	0.51
1:B:9:LYS:HB3	1:B:9:LYS:HZ2	1.74	0.51
1:A:46:HIS:ND1	1:A:120:HIS:CD2	2.78	0.51
1:B:111:CYS:SG	1:B:113:ILE:HD13	2.51	0.51
1:B:63:HIS:HB3	1:B:82:GLY:HA3	1.91	0.51
1:A:98:SER:O	1:A:99:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LYS:HZ1	1:A:139:ASN:HD22	1.57	0.50
1:A:116:THR:HG22	1:A:118:VAL:HG23	1.93	0.50
1:A:79:ARG:HH11	1:A:79:ARG:CG	2.22	0.50
1:B:19:ASN:O	1:B:31:VAL:HA	2.12	0.50
1:B:97:VAL:CG1	1:B:98:SER:N	2.76	0.49
1:B:127:GLY:C	1:B:129:GLY:N	2.65	0.49
1:B:35:ILE:HG21	1:B:38:LEU:HD13	1.93	0.49
1:A:45:PHE:CE2	1:A:117:LEU:HD21	2.47	0.49
1:A:120:HIS:O	1:A:144:LEU:HD11	2.12	0.49
1:B:128:LYS:C	1:B:130:GLY:H	2.15	0.49
1:B:34:SER:OG	1:B:36:LYS:NZ	2.45	0.49
1:B:29:VAL:HG11	1:B:104:ILE:O	2.12	0.48
1:A:104:ILE:HD12	1:A:104:ILE:O	2.12	0.48
1:B:5:VAL:CG1	1:B:6:CYS:N	2.77	0.48
1:B:23:LYS:HB3	1:B:24:GLU:OE1	2.14	0.48
1:A:124:ASP:HB3	1:A:126:LEU:HD21	1.95	0.48
1:A:66:PRO:HG2	1:A:81:VAL:CG1	2.33	0.48
1:B:38:LEU:HG	1:B:89:ALA:HB2	1.96	0.48
1:B:69:ARG:NH2	1:B:78:GLU:HG2	2.29	0.48
1:A:72:GLY:HA3	1:A:78:GLU:O	2.14	0.47
1:A:99:ILE:HG22	1:A:100:GLU:N	2.29	0.47
1:B:45:PHE:CD2	1:B:119:VAL:HG23	2.47	0.47
1:A:98:SER:C	1:A:99:ILE:HG12	2.35	0.47
1:A:124:ASP:CG	1:A:126:LEU:HD23	2.35	0.47
1:A:133:GLU:CD	1:A:136:LYS:HZ3	2.18	0.47
1:B:51:GLY:HA2	1:B:116:THR:OG1	2.13	0.47
1:B:71:HIS:HB2	1:B:135:THR:O	2.14	0.47
1:A:153:GLN:NE2	1:A:153:GLN:H	2.12	0.47
1:A:24:GLU:O	1:A:25:SER:C	2.53	0.47
1:B:14:VAL:HG11	1:B:144:LEU:O	2.14	0.47
1:A:74:PRO:HG3	1:A:84:LEU:O	2.14	0.47
1:B:48:HIS:HB3	1:B:60:ALA:O	2.15	0.47
1:B:74:PRO:HD2	1:B:126:LEU:HD21	1.94	0.47
1:B:14:VAL:HA	1:B:36:LYS:O	2.15	0.47
1:B:69:ARG:NH1	1:B:78:GLU:CD	2.68	0.47
1:B:42:LEU:CD2	1:B:86:ASN:OD1	2.46	0.47
1:A:29:VAL:HG22	1:A:106:LEU:HG	1.97	0.47
1:A:5:VAL:HG13	1:A:6:CYS:N	2.30	0.46
1:A:91:LYS:HA	1:A:91:LYS:HE3	1.97	0.46
1:A:65:ASN:OD1	1:A:80:HIS:HB3	2.15	0.46
1:B:112:ILE:HA	1:B:115:ARG:NE	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:GLY:O	1:B:129:GLY:N	2.48	0.46
1:A:34:SER:C	1:A:35:ILE:HG22	2.35	0.46
1:A:70:LYS:HB3	1:A:135:THR:HG22	1.98	0.46
1:A:89:ALA:HA	1:A:95:ALA:HB2	1.98	0.46
1:B:112:ILE:O	1:B:115:ARG:HG3	2.16	0.46
1:B:19:ASN:HD21	1:B:32:TRP:HE1	1.63	0.46
1:B:106:LEU:HD22	1:B:113:ILE:HD11	1.97	0.46
1:B:46:HIS:NE2	1:B:83:ASP:HB3	2.31	0.46
1:A:65:ASN:ND2	1:A:69:ARG:H	2.13	0.46
1:B:138:GLY:O	1:B:140:ALA:N	2.49	0.45
1:A:151:ILE:N	1:B:114:GLY:O	2.50	0.45
1:B:9:LYS:HB3	1:B:9:LYS:NZ	2.31	0.45
1:B:72:GLY:H	1:B:80:HIS:HD1	1.65	0.45
1:B:99:ILE:CG2	1:B:100:GLU:N	2.80	0.45
1:A:109:ASP:HB2	1:A:110:HIS:H	1.13	0.45
1:A:14:VAL:HG12	1:A:37:GLY:CA	2.44	0.45
1:B:48:HIS:ND1	1:B:61:GLY:O	2.45	0.45
1:A:104:ILE:HD12	1:A:104:ILE:C	2.38	0.45
1:A:152:ALA:HB1	1:A:153:GLN:HE22	1.77	0.45
1:A:54:THR:HG22	1:B:17:ILE:HD11	1.98	0.45
1:B:127:GLY:C	1:B:129:GLY:H	2.19	0.44
1:B:49:GLU:OE2	1:B:50:PHE:CZ	2.70	0.44
1:B:65:ASN:HD21	1:B:68:SER:CA	2.30	0.44
1:B:97:VAL:CG1	1:B:98:SER:H	2.25	0.44
1:A:151:ILE:HB	1:B:114:GLY:O	2.17	0.44
1:A:45:PHE:CE1	1:A:119:VAL:HB	2.52	0.44
1:B:132:GLU:O	1:B:133:GLU:HB2	2.15	0.44
1:A:151:ILE:O	1:B:51:GLY:N	2.50	0.44
1:A:65:ASN:HD21	1:A:69:ARG:N	2.15	0.44
1:B:128:LYS:C	1:B:130:GLY:N	2.70	0.44
1:B:9:LYS:CD	1:B:15:GLN:HG3	2.46	0.44
1:A:17:ILE:HG23	1:B:54:THR:HG22	1.99	0.44
1:A:13:PRO:HD2	1:A:14:VAL:HG22	1.99	0.44
1:A:46:HIS:HB3	1:A:63:HIS:CD2	2.52	0.44
1:A:79:ARG:NH1	1:A:83:ASP:O	2.49	0.44
1:B:106:LEU:CD2	1:B:113:ILE:HD11	2.48	0.44
1:A:114:GLY:HA3	1:B:150:GLY:HA2	1.99	0.44
1:B:80:HIS:HB2	1:B:83:ASP:OD2	2.17	0.44
1:B:8:LEU:HD11	1:B:119:VAL:HB	2.00	0.44
1:B:29:VAL:HG11	1:B:104:ILE:C	2.38	0.44
1:B:39:THR:O	1:B:43:HIS:CD2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:CYS:HB3	1:A:143:ARG:CG	2.44	0.43
1:A:95:ALA:O	1:A:97:VAL:HG23	2.18	0.43
1:B:106:LEU:HA	1:B:111:CYS:HA	2.00	0.43
1:A:99:ILE:HG22	1:A:100:GLU:H	1.82	0.43
1:A:122:LYS:HZ1	1:A:139:ASN:ND2	2.10	0.43
1:A:79:ARG:NH1	1:A:79:ARG:CG	2.74	0.43
1:B:133:GLU:OE1	1:B:139:ASN:ND2	2.52	0.43
1:A:151:ILE:O	1:B:50:PHE:HB3	2.18	0.43
1:B:139:ASN:HD22	1:B:139:ASN:HA	1.57	0.43
1:B:46:HIS:CD2	1:B:83:ASP:HB3	2.53	0.43
1:A:12:GLY:C	1:A:14:VAL:H	2.21	0.43
1:A:106:LEU:CD2	1:A:112:ILE:HD11	2.49	0.43
1:B:50:PHE:C	1:B:52:ASP:H	2.22	0.43
1:B:127:GLY:HA2	1:B:134:SER:O	2.19	0.43
1:B:48:HIS:CD2	1:B:118:VAL:CG1	3.02	0.43
1:B:44:GLY:HA3	1:B:120:HIS:HB2	2.00	0.43
1:B:4:ALA:C	1:B:152:ALA:HB2	2.40	0.43
1:B:38:LEU:CG	1:B:89:ALA:HB2	2.48	0.43
1:A:52:ASP:HB3	1:A:54:THR:HG1	1.81	0.42
1:A:5:VAL:O	1:A:6:CYS:HB2	2.19	0.42
1:A:33:GLY:C	1:A:34:SER:OG	2.58	0.42
1:B:46:HIS:CD2	1:B:83:ASP:HA	2.55	0.42
1:B:35:ILE:HD11	1:B:45:PHE:HE2	1.84	0.42
1:A:65:ASN:O	1:A:67:LEU:N	2.52	0.42
1:B:79:ARG:NH2	1:B:83:ASP:O	2.53	0.42
1:A:118:VAL:HG12	1:A:120:HIS:CD2	2.54	0.42
1:A:131:ASN:ND2	1:A:134:SER:OG	2.53	0.42
1:B:3:LYS:HD3	1:B:153:GLN:OXT	2.19	0.42
1:A:70:LYS:CB	1:A:135:THR:HG22	2.49	0.42
1:A:133:GLU:OE1	1:A:136:LYS:NZ	2.52	0.42
1:A:36:LYS:HB3	1:A:37:GLY:H	1.57	0.41
1:B:52:ASP:OD1	1:B:54:THR:HG23	2.20	0.41
1:B:66:PRO:HD3	1:B:81:VAL:HG21	2.02	0.41
1:B:78:GLU:O	1:B:128:LYS:NZ	2.53	0.41
1:B:69:ARG:CZ	1:B:78:GLU:HG2	2.50	0.41
1:B:8:LEU:HD21	1:B:119:VAL:HG11	2.02	0.41
1:B:22:GLN:HB2	1:B:29:VAL:HG23	2.01	0.41
1:B:61:GLY:HA3	1:B:62:PRO:HD3	1.72	0.41
1:A:71:HIS:O	1:A:78:GLU:HG3	2.20	0.41
1:B:122:LYS:NZ	1:B:122:LYS:HB2	2.35	0.41
1:B:134:SER:HA	1:B:139:ASN:ND2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ASN:HD21	1:B:68:SER:HA	1.85	0.41
1:A:81:VAL:O	1:A:104:ILE:HG22	2.20	0.41
1:A:6:CYS:SG	1:A:148:VAL:C	2.98	0.41
1:A:109:ASP:HB2	1:A:110:HIS:CG	2.55	0.41
1:A:134:SER:O	1:A:135:THR:C	2.59	0.41
1:B:23:LYS:HB3	1:B:24:GLU:H	1.71	0.41
1:A:40:GLU:CG	1:A:41:GLY:N	2.84	0.41
1:A:52:ASP:C	1:A:54:THR:N	2.73	0.41
1:B:80:HIS:O	1:B:81:VAL:HG23	2.21	0.41
1:A:6:CYS:CB	1:A:149:ILE:HG13	2.44	0.41
1:B:13:PRO:O	1:B:13:PRO:CG	2.68	0.41
1:B:9:LYS:HD2	1:B:15:GLN:HG3	2.03	0.41
1:B:6:CYS:SG	1:B:147:GLY:CA	3.01	0.41
1:A:120:HIS:HB3	1:A:140:ALA:O	2.21	0.41
1:A:6:CYS:SG	1:A:149:ILE:CD1	3.08	0.41
1:A:40:GLU:HG3	1:A:89:ALA:O	2.21	0.40
1:B:52:ASP:OD1	1:B:54:THR:CG2	2.69	0.40
1:A:36:LYS:HD3	1:A:94:VAL:HG22	2.02	0.40
1:B:47:VAL:HG22	1:B:117:LEU:HD12	2.02	0.40
1:B:79:ARG:NH1	1:B:83:ASP:O	2.54	0.40
1:B:7:VAL:HG23	1:B:17:ILE:HD12	2.03	0.40
1:B:45:PHE:CD2	1:B:87:VAL:HG11	2.55	0.40
1:A:124:ASP:CB	1:A:126:LEU:HD23	2.51	0.40
1:B:35:ILE:HD11	1:B:45:PHE:CE2	2.56	0.40
1:B:47:VAL:HA	1:B:117:LEU:HA	2.03	0.40
1:A:124:ASP:HB3	1:A:126:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	152/154 (99%)	96 (63%)	37 (24%)	19 (12%)	0	0
1	B	152/154 (99%)	110 (72%)	26 (17%)	16 (10%)	0	0
All	All	304/308 (99%)	206 (68%)	63 (21%)	35 (12%)	0	0

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	66	PRO
1	A	93	GLY
1	A	107	SER
1	B	56	GLY
1	B	80	HIS
1	B	81	VAL
1	B	91	LYS
1	B	108	GLY
1	B	126	LEU
1	B	139	ASN
1	A	24	GLU
1	A	135	THR
1	A	140	ALA
1	A	141	GLY
1	B	130	GLY
1	B	133	GLU
1	A	3	LYS
1	A	68	SER
1	A	126	LEU
1	B	22	GLN
1	B	24	GLU
1	B	66	PRO
1	B	107	SER
1	B	142	SER
1	A	152	ALA
1	A	64	PHE
1	A	74	PRO
1	A	84	LEU
1	A	110	HIS
1	B	68	SER
1	B	25	SER
1	A	130	GLY
1	A	28	PRO
1	A	65	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	118/118 (100%)	76 (64%)	42 (36%)	0	0
1	B	118/118 (100%)	80 (68%)	38 (32%)	0	0
All	All	236/236 (100%)	156 (66%)	80 (34%)	0	0

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	11	ASP
1	A	13	PRO
1	A	18	ILE
1	A	26	ASN
1	A	31	VAL
1	A	32	TRP
1	A	35	ILE
1	A	38	LEU
1	A	52	ASP
1	A	54	THR
1	A	65	ASN
1	A	66	PRO
1	A	67	LEU
1	A	69	ARG
1	A	70	LYS
1	A	71	HIS
1	A	76	ASP
1	A	79	ARG
1	A	83	ASP
1	A	86	ASN
1	A	90	ASP
1	A	91	LYS
1	A	92	ASP
1	A	96	ASP
1	A	99	ILE
1	A	102	SER

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Mol	Chain	Res	Type
1	A	104	ILE
1	A	105	SER
1	A	109	ASP
1	A	111	CYS
1	A	116	THR
1	A	119	VAL
1	A	132	GLU
1	A	134	SER
1	A	135	THR
1	A	139	ASN
1	A	142	SER
1	A	143	ARG
1	A	144	LEU
1	A	149	ILE
1	A	153	GLN
1	B	2	THR
1	B	5	VAL
1	B	15	GLN
1	B	19	ASN
1	B	22	GLN
1	B	23	LYS
1	B	24	GLU
1	B	25	SER
1	B	36	LYS
1	B	39	THR
1	B	53	ASN
1	B	54	THR
1	B	70	LYS
1	B	79	ARG
1	B	83	ASP
1	B	84	LEU
1	B	88	THR
1	B	91	LYS
1	B	96	ASP
1	B	99	ILE
1	B	101	ASP
1	B	105	SER
1	B	106	LEU
1	B	107	SER
1	B	110	HIS
1	B	119	VAL
1	B	122	LYS

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Mol	Chain	Res	Type
1	B	128	LYS
1	B	132	GLU
1	B	133	GLU
1	B	135	THR
1	B	136	LYS
1	B	142	SER
1	B	144	LEU
1	B	146	CYS
1	B	149	ILE
1	B	151	ILE
1	B	153	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	131	ASN
1	A	139	ASN
1	A	153	GLN
1	B	19	ASN
1	B	53	ASN
1	B	65	ASN
1	B	139	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	0:ACE	C	1:ALA	N	1.85
1	B	0:ACE	C	1:ALA	N	1.80
1	B	14:VAL	C	15:GLN	N	1.13

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.