



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:39 PM UTC

PDB ID : 3CAD / pdb_00003cad
Title : Crystal structure of Natural Killer Cell Receptor, Ly49G
Authors : Cho, S.
Deposited on : 2008-02-19
Resolution : 2.60 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

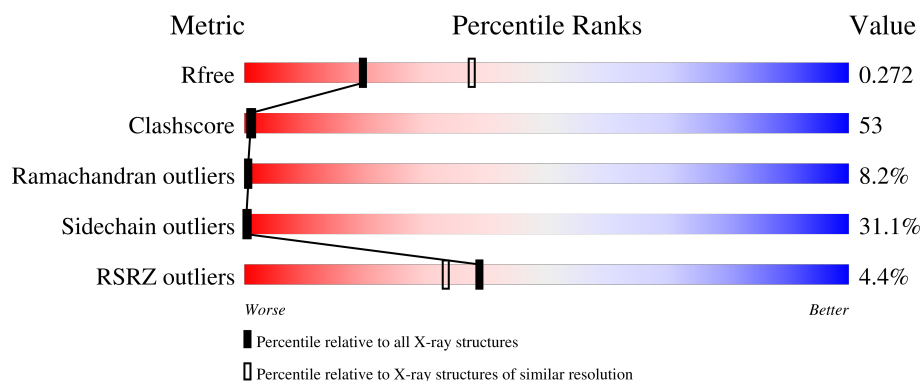
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	125	
1	B	125	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2097 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 Lectin-related NK cell receptor LY49G1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	0	0	0
			1006	642	167	187	10			
1	B	125	Total	C	N	O	S	0	0	0
			1021	653	169	189	10			

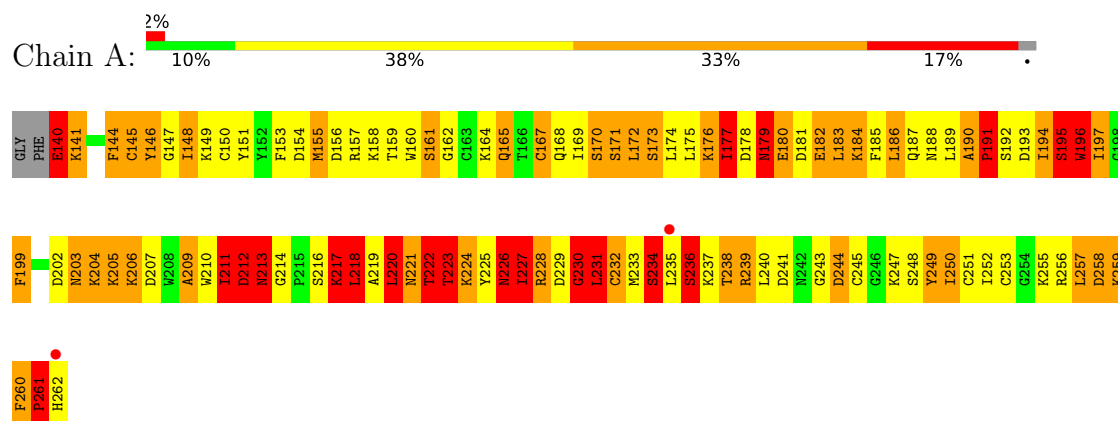
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	45	Total	O	0	0
			45	45		
2	B	25	Total	O	0	0
			25	25		

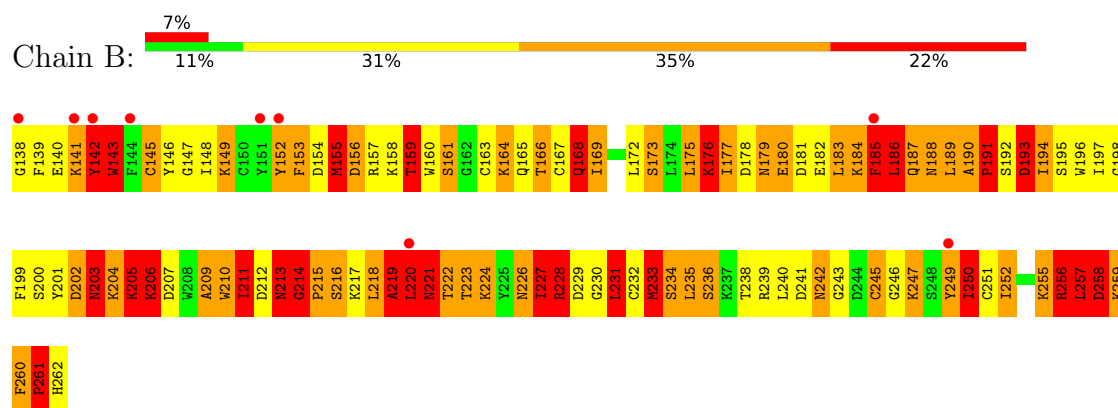
3 Residue-property plots [i](#)

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: Lectin-related NK cell receptor LY49G1



- Molecule 1: Lectin-related NK cell receptor LY49G1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.38Å 56.20Å 33.76Å 90.00° 100.29° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.8 (50.00-2.60) 90.3 (50.00-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.89 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.227 , 0.286 0.268 , 0.272	Depositor DCC
R_{free} test set	363 reflections (3.68%)	wwPDB-VP
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 119.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2097	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.99% 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	A	1.99	25/1031 (2.4%)	2.54	87/1385 (6.3%)
1	B	2.05	28/1047 (2.7%)	2.96	128/1406 (9.1%)
All	All	2.02	53/2078 (2.6%)	2.76	215/2791 (7.7%)

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	A	0	9
1	B	0	23
All	All	0	32

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	ASP	C-N	-13.43	1.20	1.33
1	A	199	PHE	C-O	-10.67	1.12	1.23
1	B	213	ASN	C-O	9.49	1.32	1.24
1	B	255	LYS	C-N	-9.08	1.23	1.33
1	A	219	ALA	CA-C	9.00	1.64	1.52
1	A	195	SER	CA-C	-8.97	1.41	1.52
1	B	214	GLY	C-N	8.88	1.45	1.33
1	B	158	LYS	C-N	8.76	1.45	1.33
1	A	180	GLU	CA-C	8.68	1.60	1.52
1	A	167	CYS	CA-C	-8.57	1.41	1.52
1	B	165	GLN	N-CA	-8.33	1.36	1.46
1	B	166	THR	N-CA	8.31	1.56	1.46
1	B	209	ALA	C-N	-8.04	1.23	1.33
1	A	222	THR	CA-CB	7.84	1.66	1.53
1	A	177	ILE	CA-CB	-7.60	1.45	1.54
1	A	173	SER	N-CA	-7.55	1.37	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	LYS	N-CA	-7.43	1.37	1.46
1	A	220	LEU	N-CA	7.33	1.55	1.46
1	A	197	ILE	C-O	-7.23	1.16	1.24
1	B	236	SER	CA-C	7.18	1.62	1.53
1	B	177	ILE	C-O	7.03	1.31	1.24
1	A	213	ASN	CA-C	6.90	1.61	1.53
1	A	196	TRP	CA-C	6.88	1.60	1.52
1	A	204	LYS	CA-C	-6.79	1.44	1.52
1	B	168	GLN	C-O	6.77	1.32	1.24
1	B	252	ILE	CA-CB	-6.62	1.46	1.54
1	B	233	MET	C-O	-6.62	1.15	1.23
1	A	184	LYS	CA-C	-6.57	1.44	1.52
1	A	167	CYS	C-O	-6.54	1.15	1.24
1	B	234	SER	C-O	6.49	1.31	1.23
1	A	195	SER	N-CA	-6.42	1.38	1.46
1	B	149	LYS	CA-C	6.27	1.60	1.52
1	B	232	CYS	N-CA	-6.19	1.39	1.46
1	B	250	ILE	C-N	6.15	1.42	1.33
1	B	165	GLN	C-O	-6.15	1.17	1.24
1	A	173	SER	CA-C	6.10	1.59	1.52
1	B	262	HIS	CA-C	6.03	1.65	1.52
1	A	154	ASP	CA-C	-5.96	1.45	1.52
1	B	179	ASN	C-N	-5.84	1.26	1.34
1	B	172	LEU	C-O	-5.80	1.17	1.23
1	A	179	ASN	C-O	5.60	1.31	1.24
1	A	229	ASP	C-N	5.48	1.41	1.33
1	B	199	PHE	CA-CB	-5.37	1.43	1.53
1	B	147	GLY	C-O	-5.37	1.16	1.23
1	A	253	CYS	N-CA	-5.35	1.39	1.46
1	B	168	GLN	CA-C	5.34	1.60	1.52
1	B	260	PHE	C-O	5.29	1.31	1.24
1	A	176	LYS	CA-CB	5.21	1.60	1.53
1	A	140	GLU	CA-CB	5.18	1.63	1.53
1	B	233	MET	CA-CB	-5.10	1.45	1.53
1	A	190	ALA	C-O	-5.08	1.17	1.24
1	B	191	PRO	N-CD	5.07	1.54	1.47
1	B	199	PHE	N-CA	-5.06	1.39	1.46

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	ASN	CA-C-N	14.43	149.10	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	ASN	C-N-CA	14.43	149.10	121.54
1	B	257	LEU	CA-C-N	13.71	147.73	121.54
1	B	257	LEU	C-N-CA	13.71	147.73	121.54
1	B	212	ASP	CA-C-N	13.05	146.09	122.08
1	B	212	ASP	C-N-CA	13.05	146.09	122.08
1	A	190	ALA	CA-C-N	-11.33	108.61	120.85
1	A	190	ALA	C-N-CA	-11.33	108.61	120.85
1	A	227	ILE	CA-C-N	11.25	135.36	120.28
1	A	227	ILE	C-N-CA	11.25	135.36	120.28
1	B	156	ASP	CA-CB-CG	11.00	123.60	112.60
1	B	222	THR	CA-C-N	10.88	134.85	120.28
1	B	222	THR	C-N-CA	10.88	134.85	120.28
1	B	214	GLY	CA-C-N	-10.60	109.64	120.98
1	B	214	GLY	C-N-CA	-10.60	109.64	120.98
1	B	250	ILE	O-C-N	-10.41	110.43	122.72
1	B	220	LEU	O-C-N	-10.28	110.22	122.86
1	B	216	SER	CA-C-N	10.12	140.87	121.54
1	B	216	SER	C-N-CA	10.12	140.87	121.54
1	B	260	PHE	CA-C-N	10.11	132.47	119.84
1	B	260	PHE	C-N-CA	10.11	132.47	119.84
1	B	206	LYS	CA-C-O	10.00	134.81	120.51
1	B	202	ASP	CA-C-N	9.99	134.48	120.29
1	B	202	ASP	C-N-CA	9.99	134.48	120.29
1	B	214	GLY	O-C-N	9.96	131.73	121.77
1	B	255	LYS	CA-C-N	9.75	138.97	122.20
1	B	255	LYS	C-N-CA	9.75	138.97	122.20
1	A	225	TYR	N-CA-C	9.61	125.07	109.59
1	B	142	TYR	CA-C-O	9.41	133.04	122.03
1	B	175	LEU	CA-C-N	9.37	135.24	122.77
1	B	175	LEU	C-N-CA	9.37	135.24	122.77
1	B	213	ASN	CA-C-O	-9.37	110.96	120.80
1	B	215	PRO	CA-C-N	9.20	135.78	122.44
1	B	215	PRO	C-N-CA	9.20	135.78	122.44
1	B	230	GLY	O-C-N	-9.19	113.83	123.58
1	A	252	ILE	O-C-N	-9.05	109.94	122.62
1	A	232	CYS	O-C-N	-8.91	112.25	122.68
1	B	251	CYS	CA-C-N	-8.91	111.50	122.90
1	B	251	CYS	C-N-CA	-8.91	111.50	122.90
1	A	153	PHE	O-C-N	-8.68	111.67	123.12
1	B	203	ASN	CA-C-N	8.51	132.61	120.79
1	B	203	ASN	C-N-CA	8.51	132.61	120.79
1	B	165	GLN	CA-C-O	-8.49	111.73	121.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	ASN	CA-CB-CG	8.22	120.82	112.60
1	A	170	SER	CA-C-O	8.20	131.02	121.34
1	A	170	SER	O-C-N	-7.97	111.19	121.95
1	A	153	PHE	CA-C-O	7.94	128.74	120.40
1	B	245	CYS	CA-C-N	7.92	128.74	119.94
1	B	245	CYS	C-N-CA	7.92	128.74	119.94
1	B	211	ILE	CA-C-N	-7.87	110.23	122.42
1	B	211	ILE	C-N-CA	-7.87	110.23	122.42
1	B	251	CYS	N-CA-C	7.87	121.47	108.96
1	B	241	ASP	CA-CB-CG	7.83	120.43	112.60
1	B	152	TYR	O-C-N	-7.79	114.24	123.28
1	A	156	ASP	N-CA-C	7.71	122.61	108.58
1	B	259	LYS	O-C-N	-7.71	113.42	123.13
1	A	223	THR	N-CA-C	-7.65	103.78	113.72
1	A	224	LYS	CA-C-N	-7.63	111.87	122.93
1	A	224	LYS	C-N-CA	-7.63	111.87	122.93
1	B	191	PRO	CA-N-CD	-7.62	101.33	112.00
1	A	258	ASP	CA-CB-CG	7.60	120.20	112.60
1	A	165	GLN	CA-C-N	7.59	131.84	120.31
1	A	165	GLN	C-N-CA	7.59	131.84	120.31
1	A	184	LYS	N-CA-C	-7.49	102.71	111.03
1	B	177	ILE	CB-CA-C	-7.43	100.79	110.98
1	A	203	ASN	CA-CB-CG	7.42	120.02	112.60
1	B	246	GLY	CA-C-N	7.32	131.52	121.05
1	B	246	GLY	C-N-CA	7.32	131.52	121.05
1	A	167	CYS	N-CA-C	-7.23	102.40	112.45
1	A	239	ARG	O-C-N	-7.13	114.52	122.72
1	B	256	ARG	CA-C-O	-7.11	113.82	121.14
1	B	250	ILE	N-CA-CB	7.00	119.84	110.26
1	B	192	SER	CA-C-N	6.96	134.84	121.54
1	B	192	SER	C-N-CA	6.96	134.84	121.54
1	B	193	ASP	CA-CB-CG	6.95	119.55	112.60
1	A	154	ASP	N-CA-C	-6.95	97.90	108.67
1	A	157	ARG	NE-CZ-NH2	6.93	125.44	119.20
1	B	223	THR	N-CA-C	6.90	118.80	111.28
1	A	195	SER	O-C-N	6.87	130.18	123.04
1	B	139	PHE	N-CA-C	6.84	117.67	108.23
1	A	232	CYS	CA-C-N	6.83	132.63	122.99
1	A	232	CYS	C-N-CA	6.83	132.63	122.99
1	B	249	TYR	CA-C-N	6.81	131.93	121.71
1	B	249	TYR	C-N-CA	6.81	131.93	121.71
1	B	158	LYS	CA-C-O	-6.77	114.03	121.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ASP	CA-C-N	-6.68	108.32	121.41
1	A	229	ASP	C-N-CA	-6.68	108.32	121.41
1	B	212	ASP	O-C-N	6.67	130.06	122.19
1	B	141	LYS	CA-C-N	6.66	131.85	122.46
1	B	141	LYS	C-N-CA	6.66	131.85	122.46
1	A	182	GLU	N-CA-C	-6.64	96.66	110.80
1	A	226	ASN	CA-CB-CG	6.60	119.20	112.60
1	B	176	LYS	CB-CA-C	-6.54	99.59	110.19
1	A	172	LEU	CA-C-N	6.49	132.67	121.64
1	A	172	LEU	C-N-CA	6.49	132.67	121.64
1	B	256	ARG	CA-C-N	6.43	133.82	121.54
1	B	256	ARG	C-N-CA	6.43	133.82	121.54
1	A	191	PRO	CA-C-O	-6.40	114.09	121.96
1	B	141	LYS	N-CA-CB	6.37	121.85	111.27
1	B	167	CYS	N-CA-C	-6.31	104.69	112.38
1	B	143	TRP	O-C-N	-6.30	114.96	122.46
1	A	226	ASN	CA-C-N	6.30	133.31	121.97
1	A	226	ASN	C-N-CA	6.30	133.31	121.97
1	B	204	LYS	CA-C-O	-6.28	114.16	121.07
1	A	180	GLU	CA-C-O	6.28	127.40	119.61
1	A	226	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	B	153	PHE	CA-CB-CG	6.25	120.05	113.80
1	B	223	THR	CA-C-N	6.25	128.95	120.38
1	B	223	THR	C-N-CA	6.25	128.95	120.38
1	B	220	LEU	CA-C-O	6.20	129.83	122.14
1	B	231	LEU	CB-CG-CD2	-6.20	92.10	110.70
1	B	226	ASN	CA-C-N	6.18	128.93	120.46
1	B	226	ASN	C-N-CA	6.18	128.93	120.46
1	B	186	LEU	N-CA-C	-6.17	105.40	113.12
1	A	260	PHE	O-C-N	6.17	128.41	121.32
1	A	205	LYS	N-CA-C	-6.16	105.25	112.89
1	B	152	TYR	CA-C-O	6.16	128.72	120.89
1	A	194	ILE	CA-C-N	-6.09	111.60	122.45
1	A	194	ILE	C-N-CA	-6.09	111.60	122.45
1	B	156	ASP	CA-C-N	6.05	133.10	121.54
1	B	156	ASP	C-N-CA	6.05	133.10	121.54
1	B	228	ARG	CD-NE-CZ	6.05	132.87	124.40
1	A	203	ASN	N-CA-C	6.04	117.67	111.14
1	B	209	ALA	O-C-N	6.03	130.61	122.59
1	A	216	SER	CA-C-N	6.02	128.95	120.28
1	A	216	SER	C-N-CA	6.02	128.95	120.28
1	A	250	ILE	CA-C-N	-6.00	112.35	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ILE	C-N-CA	-6.00	112.35	122.92
1	B	260	PHE	O-C-N	5.95	126.11	121.47
1	A	171	SER	CB-CA-C	-5.93	99.09	110.65
1	B	250	ILE	N-CA-C	5.92	117.26	109.21
1	A	261	PRO	CA-C-N	5.91	132.34	121.70
1	A	261	PRO	C-N-CA	5.91	132.34	121.70
1	B	179	ASN	N-CA-C	5.90	117.82	108.79
1	B	258	ASP	N-CA-C	5.89	123.34	110.80
1	B	169	ILE	N-CA-C	-5.85	104.10	112.35
1	B	175	LEU	CA-C-O	5.79	126.32	120.88
1	B	180	GLU	CA-C-N	5.79	127.97	120.44
1	B	180	GLU	C-N-CA	5.79	127.97	120.44
1	A	214	GLY	CA-C-N	-5.77	112.62	119.84
1	A	214	GLY	C-N-CA	-5.77	112.62	119.84
1	B	219	ALA	CA-C-N	-5.74	114.24	122.68
1	B	219	ALA	C-N-CA	-5.74	114.24	122.68
1	A	260	PHE	CA-C-O	-5.70	112.36	120.16
1	B	172	LEU	CA-C-O	-5.69	115.33	121.36
1	A	203	ASN	N-CA-CB	5.69	118.31	110.07
1	A	155	MET	N-CA-C	5.67	119.30	112.38
1	A	209	ALA	O-C-N	5.64	129.54	123.56
1	B	141	LYS	CB-CA-C	5.62	119.88	110.44
1	A	217	LYS	CA-C-N	5.60	131.66	121.97
1	A	217	LYS	C-N-CA	5.60	131.66	121.97
1	A	154	ASP	CA-C-O	-5.59	114.28	120.60
1	B	243	GLY	N-CA-C	5.58	119.70	110.55
1	B	260	PHE	N-CA-C	-5.56	101.81	109.71
1	A	192	SER	N-CA-C	-5.52	105.34	111.36
1	A	229	ASP	CA-CB-CG	5.50	118.10	112.60
1	B	236	SER	N-CA-C	5.50	117.79	110.53
1	B	197	ILE	O-C-N	-5.49	115.71	122.57
1	B	156	ASP	CA-C-O	5.48	128.34	120.51
1	B	224	LYS	N-CA-C	5.48	117.96	111.33
1	B	188	ASN	O-C-N	-5.46	115.32	122.59
1	B	212	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	172	LEU	O-C-N	5.44	128.87	121.74
1	B	155	MET	CA-C-N	5.43	131.91	121.54
1	B	155	MET	C-N-CA	5.43	131.91	121.54
1	B	250	ILE	CA-C-N	5.42	129.62	122.30
1	B	250	ILE	C-N-CA	5.42	129.62	122.30
1	A	234	SER	CA-CB-OG	5.41	121.92	111.10
1	B	211	ILE	CA-CB-CG1	5.39	119.57	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	PRO	CA-C-N	5.38	131.39	121.70
1	B	261	PRO	C-N-CA	5.38	131.39	121.70
1	A	227	ILE	CA-C-O	-5.36	114.08	120.78
1	A	245	CYS	CA-C-N	5.32	130.25	120.79
1	A	245	CYS	C-N-CA	5.32	130.25	120.79
1	A	252	ILE	CA-C-O	5.31	127.92	120.86
1	A	236	SER	CA-C-O	5.28	127.14	121.44
1	B	156	ASP	CB-CA-C	5.25	120.87	110.42
1	A	162	GLY	CA-C-N	5.22	127.54	120.38
1	A	162	GLY	C-N-CA	5.22	127.54	120.38
1	B	169	ILE	CG1-CB-CG2	5.22	126.36	110.70
1	A	224	LYS	N-CA-C	-5.21	106.75	113.01
1	B	259	LYS	N-CA-C	5.21	117.22	107.99
1	A	205	LYS	CD-CE-NZ	-5.19	95.29	111.90
1	A	153	PHE	CA-C-N	-5.19	114.26	121.99
1	A	153	PHE	C-N-CA	-5.19	114.26	121.99
1	A	156	ASP	CB-CA-C	-5.19	102.99	111.50
1	B	213	ASN	O-C-N	-5.18	116.20	122.68
1	A	202	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	205	LYS	CA-C-N	5.17	131.42	121.54
1	B	205	LYS	C-N-CA	5.17	131.42	121.54
1	A	154	ASP	CB-CG-OD2	5.17	130.28	118.40
1	B	185	PHE	CA-CB-CG	5.16	118.96	113.80
1	B	149	LYS	CG-CD-CE	5.15	123.16	111.30
1	B	176	LYS	N-CA-C	5.15	117.13	108.73
1	A	211	ILE	CA-CB-CG1	5.15	119.16	110.40
1	A	195	SER	CB-CA-C	-5.15	101.59	111.78
1	A	238	THR	CA-C-N	5.14	131.36	122.32
1	A	238	THR	C-N-CA	5.14	131.36	122.32
1	B	232	CYS	N-CA-C	5.12	117.14	108.02
1	B	219	ALA	O-C-N	-5.11	115.80	122.59
1	A	218	LEU	N-CA-C	5.10	118.19	110.64
1	B	159	THR	CA-C-N	-5.10	113.66	120.54
1	B	159	THR	C-N-CA	-5.10	113.66	120.54
1	B	189	LEU	O-C-N	-5.10	110.39	121.35
1	B	189	LEU	CA-C-O	5.09	128.98	122.31
1	B	227	ILE	O-C-N	-5.09	116.93	121.87
1	A	204	LYS	CA-CB-CG	-5.08	103.93	114.10
1	A	212	ASP	CB-CA-C	5.08	119.87	109.55
1	B	190	ALA	CA-C-N	-5.08	113.50	119.84
1	B	190	ALA	C-N-CA	-5.08	113.50	119.84
1	A	157	ARG	CD-NE-CZ	5.07	131.50	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	ARG	NE-CZ-NH1	5.07	126.56	121.50
1	A	156	ASP	N-CA-CB	-5.04	102.06	110.42
1	B	256	ARG	CA-CB-CG	5.04	124.17	114.10
1	A	146	TYR	CA-CB-CG	5.01	122.92	113.90

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	CYS	Mainchain
1	A	191	PRO	Mainchain
1	A	193	ASP	Mainchain
1	A	226	ASN	Mainchain
1	A	230	GLY	Mainchain
1	A	231	LEU	Mainchain
1	A	236	SER	Mainchain
1	A	249	TYR	Mainchain
1	A	260	PHE	Mainchain
1	B	138	GLY	Mainchain
1	B	142	TYR	Mainchain
1	B	143	TRP	Mainchain
1	B	145	CYS	Mainchain
1	B	155	MET	Mainchain
1	B	159	THR	Mainchain
1	B	161	SER	Mainchain
1	B	173	SER	Mainchain
1	B	185	PHE	Mainchain
1	B	186	LEU	Mainchain
1	B	189	LEU	Mainchain
1	B	190	ALA	Mainchain
1	B	207	ASP	Mainchain
1	B	210	TRP	Mainchain
1	B	213	ASN	Peptide,Mainchain
1	B	214	GLY	Mainchain
1	B	215	PRO	Mainchain
1	B	219	ALA	Mainchain
1	B	220	LEU	Mainchain
1	B	221	ASN	Mainchain
1	B	227	ILE	Mainchain
1	B	238	THR	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	A	1006	0	976	120	2
1	B	1021	0	983	94	5
2	A	45	0	0	2	3
2	B	25	0	0	1	0
All	All	2097	0	1959	210	5

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 53.

All (210) 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:A:179:ASN:O	1:A:218:LEU:HD12	1.23	1.32
1:B:203:ASN:O	1:B:206:LYS:HD2	1.14	1.28
1:A:217:LYS:NZ	1:A:217:LYS:HB2	1.37	1.26
1:A:140:GLU:OE1	1:A:144:PHE:HE1	1.22	1.21
1:B:180:GLU:O	1:B:184:LYS:HG3	1.41	1.16
1:A:230:GLY:HA3	1:A:243:GLY:HA2	1.18	1.12
1:A:231:LEU:HD23	1:B:227:ILE:HD13	1.29	1.12
1:A:140:GLU:OE1	1:A:144:PHE:CE1	2.04	1.08
1:A:148:ILE:H	1:A:148:ILE:HD12	1.16	1.05
1:A:179:ASN:O	1:A:218:LEU:CD1	2.03	1.04
1:B:205:LYS:HE2	1:B:209:ALA:HB2	1.39	1.03
1:A:217:LYS:NZ	1:A:217:LYS:CB	2.24	1.01
1:A:194:ILE:CG2	1:A:234:SER:OG	2.09	1.01
1:B:235:LEU:HD12	1:B:239:ARG:O	1.61	1.01
1:B:203:ASN:O	1:B:206:LYS:CD	2.08	1.00
1:B:196:TRP:HZ2	1:B:247:LYS:O	1.42	1.00
1:B:226:ASN:O	1:B:229:ASP:HB2	1.60	0.98
1:A:182:GLU:O	1:A:186:LEU:HB2	1.67	0.95
1:A:217:LYS:HB2	1:A:217:LYS:HZ3	0.90	0.95
1:B:184:LYS:O	1:B:188:ASN:HB2	1.67	0.94
1:A:247:LYS:NZ	2:A:32:HOH:O	2.01	0.92
1:B:195:SER:OG	1:B:250:ILE:HG13	1.70	0.92
1:A:217:LYS:CB	1:A:217:LYS:HZ3	1.80	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLU:C	1:A:182:GLU:H	1.79	0.90
1:A:203:ASN:C	1:A:206:LYS:H	1.79	0.89
1:A:203:ASN:O	1:A:206:LYS:HG3	1.72	0.89
1:B:235:LEU:CD1	1:B:239:ARG:O	2.21	0.88
1:A:217:LYS:HB2	1:A:217:LYS:HZ2	1.38	0.87
1:A:231:LEU:CD2	1:B:227:ILE:HD13	2.05	0.87
1:B:180:GLU:O	1:B:184:LYS:CG	2.20	0.87
1:B:202:ASP:O	1:B:206:LYS:HA	1.75	0.86
1:A:194:ILE:HG21	1:A:234:SER:OG	1.74	0.86
1:B:235:LEU:HD13	1:B:240:LEU:HB3	1.55	0.85
1:A:183:LEU:O	1:A:183:LEU:HD12	1.76	0.84
1:A:148:ILE:HD12	1:A:148:ILE:N	1.90	0.84
1:A:230:GLY:HA3	1:A:243:GLY:CA	2.06	0.84
1:B:193:ASP:O	1:B:236:SER:HA	1.77	0.84
1:A:195:SER:HB3	1:A:250:ILE:HG13	1.58	0.84
1:B:194:ILE:HG12	1:B:249:TYR:CD1	2.14	0.83
1:A:203:ASN:OD1	1:B:226:ASN:ND2	2.12	0.83
1:B:175:LEU:CD2	1:B:177:ILE:HD11	2.09	0.82
1:A:221:ASN:O	1:A:223:THR:N	2.14	0.81
1:B:216:SER:C	1:B:218:LEU:H	1.86	0.81
1:A:203:ASN:O	1:A:206:LYS:N	2.15	0.80
1:A:210:TRP:C	1:A:212:ASP:H	1.87	0.78
1:A:158:LYS:C	1:A:248:SER:OG	2.26	0.78
1:A:230:GLY:CA	1:A:243:GLY:HA2	2.10	0.76
1:B:175:LEU:HD23	1:B:177:ILE:HD11	1.67	0.76
1:A:233:MET:HE3	1:A:241:ASP:O	1.85	0.76
1:A:221:ASN:C	1:A:223:THR:H	1.91	0.75
1:A:180:GLU:O	1:A:184:LYS:N	2.16	0.75
1:A:194:ILE:HG22	1:A:195:SER:N	2.01	0.75
1:A:227:ILE:HG22	1:A:231:LEU:HD11	1.69	0.75
1:A:205:LYS:NZ	1:A:213:ASN:HB3	2.02	0.74
1:B:183:LEU:HD22	1:B:187:GLN:NE2	2.01	0.74
1:A:140:GLU:HB2	1:A:141:LYS:HE3	1.69	0.74
1:B:160:TRP:CZ2	1:B:200:SER:HB3	2.24	0.73
1:A:180:GLU:O	1:A:182:GLU:N	2.22	0.72
1:A:255:LYS:HD3	1:A:256:ARG:H	1.52	0.72
1:A:177:ILE:HG23	1:A:182:GLU:HG2	1.72	0.71
1:A:210:TRP:C	1:A:212:ASP:N	2.45	0.71
1:A:185:PHE:O	1:A:188:ASN:HB3	1.91	0.71
1:B:196:TRP:CZ2	1:B:247:LYS:O	2.35	0.70
1:B:233:MET:HE3	1:B:234:SER:N	2.05	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:LYS:HA	1:B:210:TRP:CZ3	2.26	0.70
1:B:177:ILE:O	1:B:216:SER:OG	2.10	0.69
1:A:199:PHE:HD2	1:A:233:MET:HG3	1.56	0.69
1:A:194:ILE:HG22	1:A:195:SER:H	1.56	0.69
1:B:205:LYS:CE	1:B:209:ALA:HB2	2.19	0.68
1:A:233:MET:CE	1:A:241:ASP:O	2.42	0.68
1:A:235:LEU:HA	1:A:240:LEU:HG	1.76	0.66
1:B:228:ARG:HB2	1:B:228:ARG:HH11	1.61	0.66
1:B:175:LEU:CD2	1:B:177:ILE:CD1	2.74	0.65
1:A:183:LEU:HD12	1:A:183:LEU:C	2.16	0.65
1:A:205:LYS:HZ1	1:A:213:ASN:HB3	1.59	0.65
1:B:175:LEU:HD21	1:B:177:ILE:HD11	1.79	0.65
1:B:229:ASP:HB3	1:B:242:ASN:ND2	2.11	0.64
1:B:142:TYR:O	1:B:152:TYR:HA	1.97	0.64
1:A:187:GLN:O	1:A:188:ASN:C	2.39	0.64
1:B:229:ASP:HB3	1:B:242:ASN:HD21	1.63	0.64
1:A:155:MET:HE1	1:A:191:PRO:CB	2.27	0.62
1:A:165:GLN:O	1:A:169:ILE:HG13	1.99	0.62
1:B:233:MET:HE3	1:B:233:MET:C	2.25	0.62
1:A:151:TYR:HE2	1:A:175:LEU:HD13	1.63	0.62
1:A:180:GLU:C	1:A:182:GLU:N	2.46	0.62
1:A:199:PHE:CD2	1:A:233:MET:HG3	2.35	0.62
1:A:188:ASN:C	1:A:188:ASN:OD1	2.42	0.61
1:A:195:SER:O	1:A:234:SER:HA	2.02	0.59
1:A:194:ILE:CG2	1:A:195:SER:H	2.16	0.59
1:A:194:ILE:CG2	1:A:195:SER:N	2.65	0.59
1:B:164:LYS:HD2	1:B:211:ILE:CD1	2.33	0.59
1:B:183:LEU:HD22	1:B:187:GLN:CD	2.28	0.58
1:A:199:PHE:HB3	1:A:233:MET:HG3	1.84	0.58
1:B:229:ASP:CB	1:B:242:ASN:HD21	2.16	0.58
1:A:230:GLY:HA3	1:A:244:ASP:H	1.68	0.58
1:B:180:GLU:C	1:B:184:LYS:HG3	2.24	0.58
1:A:221:ASN:C	1:A:223:THR:N	2.59	0.57
1:B:219:ALA:O	1:B:220:LEU:C	2.42	0.57
1:A:227:ILE:HD12	1:A:228:ARG:N	2.20	0.56
1:A:167:CYS:HB3	1:A:172:LEU:HB2	1.87	0.56
1:A:160:TRP:CG	1:A:232:CYS:SG	2.99	0.56
1:B:155:MET:HE1	1:B:191:PRO:HB2	1.86	0.56
1:A:203:ASN:O	1:A:206:LYS:CG	2.52	0.56
1:A:159:THR:N	1:A:248:SER:OG	2.39	0.55
1:B:256:ARG:O	1:B:257:LEU:HB2	2.04	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ASP:O	1:B:206:LYS:CA	2.53	0.55
1:A:148:ILE:N	1:A:148:ILE:CD1	2.65	0.55
1:A:213:ASN:OD1	1:A:213:ASN:N	2.39	0.55
1:A:217:LYS:CB	1:A:217:LYS:HZ2	2.06	0.54
1:A:199:PHE:CD1	1:A:209:ALA:C	2.85	0.54
1:B:180:GLU:N	1:B:218:LEU:HD22	2.22	0.54
1:B:157:ARG:HD3	1:B:249:TYR:HA	1.89	0.54
1:A:227:ILE:HD11	1:B:203:ASN:OD1	2.08	0.54
1:B:203:ASN:HD22	1:B:204:LYS:H	1.55	0.54
1:A:184:LYS:HE2	2:A:47:HOH:O	2.08	0.53
1:B:228:ARG:HH11	1:B:228:ARG:CB	2.22	0.53
1:B:155:MET:CE	1:B:191:PRO:HB2	2.39	0.53
1:A:257:LEU:CD1	1:A:261:PRO:HG3	2.38	0.53
1:B:176:LYS:HE2	2:B:48:HOH:O	2.08	0.53
1:A:230:GLY:CA	1:A:244:ASP:H	2.22	0.52
1:B:177:ILE:HG22	1:B:218:LEU:HD23	1.91	0.52
1:A:160:TRP:CD1	1:A:232:CYS:HB3	2.45	0.52
1:B:194:ILE:HG12	1:B:249:TYR:CE1	2.45	0.52
1:A:227:ILE:HG22	1:A:231:LEU:CD1	2.40	0.51
1:B:233:MET:HE3	1:B:233:MET:CA	2.39	0.51
1:A:230:GLY:HA3	1:A:244:ASP:N	2.25	0.51
1:B:257:LEU:HG	1:B:258:ASP:HB2	1.91	0.51
1:A:228:ARG:O	1:A:228:ARG:HD2	2.10	0.51
1:A:259:LYS:N	1:A:259:LYS:HD3	2.26	0.51
1:B:194:ILE:HD12	1:B:194:ILE:H	1.76	0.50
1:B:240:LEU:C	1:B:240:LEU:HD12	2.36	0.50
1:B:159:THR:O	1:B:160:TRP:C	2.53	0.50
1:B:233:MET:HE3	1:B:234:SER:H	1.74	0.50
1:A:149:LYS:HG2	1:A:255:LYS:O	2.11	0.50
1:A:164:LYS:HE2	1:A:211:ILE:CG2	2.42	0.50
1:B:149:LYS:HG2	1:B:255:LYS:O	2.11	0.50
1:B:175:LEU:HD21	1:B:177:ILE:CD1	2.41	0.49
1:A:194:ILE:HG23	1:A:234:SER:OG	2.05	0.49
1:A:180:GLU:O	1:A:184:LYS:HB2	2.12	0.49
1:B:146:TYR:CD2	1:B:146:TYR:C	2.91	0.49
1:B:176:LYS:HA	1:B:210:TRP:CE3	2.48	0.49
1:B:255:LYS:HG3	1:B:256:ARG:O	2.13	0.49
1:B:213:ASN:OD1	1:B:214:GLY:N	2.46	0.49
1:B:183:LEU:HD12	1:B:218:LEU:HD11	1.94	0.48
1:B:216:SER:C	1:B:218:LEU:N	2.60	0.48
1:A:155:MET:SD	1:A:191:PRO:HG3	2.54	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:LYS:HZ2	1:A:213:ASN:HB3	1.76	0.48
1:A:141:LYS:HZ2	1:A:141:LYS:HB2	1.79	0.48
1:A:170:SER:O	1:A:171:SER:CB	2.57	0.48
1:A:197:ILE:O	1:A:197:ILE:HG13	2.10	0.47
1:A:170:SER:O	1:A:171:SER:HB2	2.15	0.47
1:B:175:LEU:HD23	1:B:177:ILE:CD1	2.37	0.47
1:A:151:TYR:CE2	1:A:175:LEU:HD13	2.46	0.46
1:B:145:CYS:HB3	1:B:149:LYS:O	2.15	0.46
1:A:199:PHE:CE1	1:A:209:ALA:C	2.94	0.46
1:B:185:PHE:CD2	1:B:186:LEU:HD23	2.51	0.46
1:B:233:MET:HA	1:B:242:ASN:HA	1.96	0.46
1:B:168:GLN:HA	1:B:168:GLN:OE1	2.14	0.46
1:A:199:PHE:HB3	1:A:233:MET:CG	2.46	0.46
1:B:185:PHE:C	1:B:188:ASN:H	2.25	0.45
1:B:198:GLY:O	1:B:210:TRP:HA	2.15	0.45
1:B:203:ASN:C	1:B:206:LYS:HD2	2.19	0.45
1:B:227:ILE:HD12	1:B:228:ARG:N	2.32	0.45
1:B:195:SER:OG	1:B:250:ILE:CG1	2.52	0.45
1:A:145:CYS:HA	1:A:150:CYS:HA	2.00	0.44
1:B:233:MET:HE1	1:B:240:LEU:HD13	1.99	0.44
1:B:260:PHE:HA	1:B:261:PRO:HD2	1.58	0.44
1:A:174:LEU:HD12	1:A:174:LEU:HA	1.85	0.44
1:A:189:LEU:HD23	1:A:189:LEU:N	2.32	0.44
1:A:141:LYS:NZ	1:A:144:PHE:CE1	2.85	0.44
1:A:220:LEU:H	1:A:220:LEU:HD12	1.82	0.44
1:B:227:ILE:C	1:B:229:ASP:N	2.69	0.44
1:B:250:ILE:C	1:B:250:ILE:HD12	2.42	0.44
1:B:179:ASN:OD1	1:B:181:ASP:HB2	2.18	0.44
1:A:183:LEU:O	1:A:187:GLN:HG2	2.17	0.44
1:A:194:ILE:C	1:A:195:SER:OG	2.57	0.44
1:A:258:ASP:C	1:A:259:LYS:HD3	2.42	0.43
1:A:227:ILE:HA	1:A:231:LEU:HD12	2.00	0.43
1:A:185:PHE:HA	1:A:188:ASN:CB	2.48	0.43
1:B:182:GLU:O	1:B:186:LEU:HG	2.19	0.43
1:B:163:CYS:SG	1:B:196:TRP:HD1	2.42	0.43
1:B:166:THR:C	1:B:168:GLN:N	2.72	0.43
1:B:194:ILE:CG1	1:B:249:TYR:CD1	2.96	0.43
1:A:210:TRP:O	1:A:212:ASP:N	2.50	0.42
1:A:151:TYR:CZ	1:A:186:LEU:HD21	2.54	0.42
1:A:247:LYS:HD3	1:A:249:TYR:OH	2.19	0.42
1:A:160:TRP:O	1:A:161:SER:C	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:TYR:HB3	1:B:231:LEU:HB3	2.00	0.42
1:A:182:GLU:O	1:A:183:LEU:C	2.61	0.42
1:B:160:TRP:HB3	1:B:245:CYS:HB3	2.02	0.42
1:B:179:ASN:C	1:B:218:LEU:CD2	2.93	0.42
1:A:141:LYS:HZ1	1:A:144:PHE:HE1	1.67	0.42
1:A:226:ASN:HB2	1:A:228:ARG:H	1.85	0.42
1:A:167:CYS:HB3	1:A:173:SER:N	2.35	0.41
1:A:197:ILE:HG21	1:A:235:LEU:HD12	2.01	0.41
1:A:258:ASP:HB2	1:A:259:LYS:NZ	2.35	0.41
1:B:164:LYS:HD2	1:B:211:ILE:HD11	2.00	0.41
1:B:195:SER:CB	1:B:250:ILE:HG13	2.48	0.41
1:B:235:LEU:HA	1:B:240:LEU:HA	2.03	0.41
1:B:235:LEU:HD13	1:B:239:ARG:O	2.11	0.41
1:A:183:LEU:HD13	1:A:183:LEU:HA	1.74	0.41
1:B:140:GLU:C	1:B:141:LYS:HD3	2.46	0.41
1:B:234:SER:OG	1:B:235:LEU:N	2.54	0.41
1:A:255:LYS:CD	1:A:256:ARG:H	2.30	0.40
1:A:233:MET:HE1	1:A:241:ASP:C	2.46	0.40
1:A:179:ASN:OD1	1:A:180:GLU:N	2.53	0.40
1:A:146:TYR:O	1:A:147:GLY:C	2.63	0.40
1:A:160:TRP:HD1	1:A:196:TRP:CE3	2.39	0.40
1:A:196:TRP:CZ2	1:A:247:LYS:O	2.75	0.40
1:A:227:ILE:HA	1:A:231:LEU:CD1	2.52	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ASP:OD1	2:A:34:HOH:O[4_554]	0.78	1.42
1:B:258:ASP:CG	2:A:34:HOH:O[4_554]	1.14	1.06
1:A:262:HIS:CE1	1:B:141:LYS:NZ[4_545]	1.62	0.58
1:B:258:ASP:OD2	2:A:34:HOH:O[4_554]	1.70	0.50
1:A:262:HIS:ND1	1:B:141:LYS:NZ[4_545]	1.96	0.24

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	121/125 (97%)	88 (73%)	23 (19%)	10 (8%)	0	0
1	B	123/125 (98%)	86 (70%)	27 (22%)	10 (8%)	1	0
All	All	244/250 (98%)	174 (71%)	50 (20%)	20 (8%)	0	0

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	181	ASP
1	A	222	THR
1	A	231	LEU
1	A	244	ASP
1	B	191	PRO
1	B	217	LYS
1	B	222	THR
1	B	257	LEU
1	B	258	ASP
1	B	261	PRO
1	A	230	GLY
1	A	261	PRO
1	B	184	LYS
1	B	219	ALA
1	A	190	ALA
1	B	155	MET
1	B	193	ASP
1	A	211	ILE
1	A	227	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	112/113 (99%)	77 (69%)	35 (31%)	0	0
1	B	113/113 (100%)	78 (69%)	35 (31%)	0	0
All	All	225/226 (100%)	155 (69%)	70 (31%)	0	0

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	GLU
1	A	141	LYS
1	A	144	PHE
1	A	148	ILE
1	A	161	SER
1	A	168	GLN
1	A	176	LYS
1	A	177	ILE
1	A	178	ASP
1	A	183	LEU
1	A	186	LEU
1	A	195	SER
1	A	196	TRP
1	A	204	LYS
1	A	206	LYS
1	A	207	ASP
1	A	211	ILE
1	A	212	ASP
1	A	213	ASN
1	A	217	LYS
1	A	218	LEU
1	A	220	LEU
1	A	221	ASN
1	A	222	THR
1	A	223	THR
1	A	224	LYS
1	A	228	ARG
1	A	234	SER
1	A	236	SER
1	A	237	LYS
1	A	238	THR
1	A	239	ARG
1	A	251	CYS
1	A	257	LEU
1	A	259	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	143	TRP
1	B	148	ILE
1	B	153	PHE
1	B	154	ASP
1	B	156	ASP
1	B	161	SER
1	B	164	LYS
1	B	168	GLN
1	B	169	ILE
1	B	173	SER
1	B	176	LYS
1	B	178	ASP
1	B	183	LEU
1	B	187	GLN
1	B	191	PRO
1	B	194	ILE
1	B	203	ASN
1	B	205	LYS
1	B	206	LYS
1	B	211	ILE
1	B	218	LEU
1	B	220	LEU
1	B	221	ASN
1	B	223	THR
1	B	224	LYS
1	B	228	ARG
1	B	231	LEU
1	B	233	MET
1	B	235	LEU
1	B	242	ASN
1	B	247	LYS
1	B	250	ILE
1	B	252	ILE
1	B	256	ARG
1	B	259	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	ASN
1	B	187	GLN
1	B	188	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	123/125 (98%)	0.24	2 (1%) 70 66	37, 54, 74, 82	0
1	B	125/125 (100%)	0.53	9 (7%) 21 17	24, 53, 76, 112	0
All	All	248/250 (99%)	0.39	11 (4%) 39 33	24, 54, 76, 112	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	138	GLY	5.8
1	B	141	LYS	3.0
1	B	185	PHE	2.9
1	B	142	TYR	2.9
1	A	262	HIS	2.7
1	B	220	LEU	2.6
1	B	151	TYR	2.4
1	A	235	LEU	2.3
1	B	144	PHE	2.3
1	B	152	TYR	2.2
1	B	249	TYR	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.