



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:23 PM UTC

PDB ID : 3GNS / pdb_00003gns
Title : Crystal Structure of the Staphylococcus aureus Enoyl-Acyl Carrier Protein Reductase (FabI) in apo form (one molecule in AU)
Authors : Priyadarshi, A.; Hwang, K.Y.
Deposited on : 2009-03-18
Resolution : 2.71 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

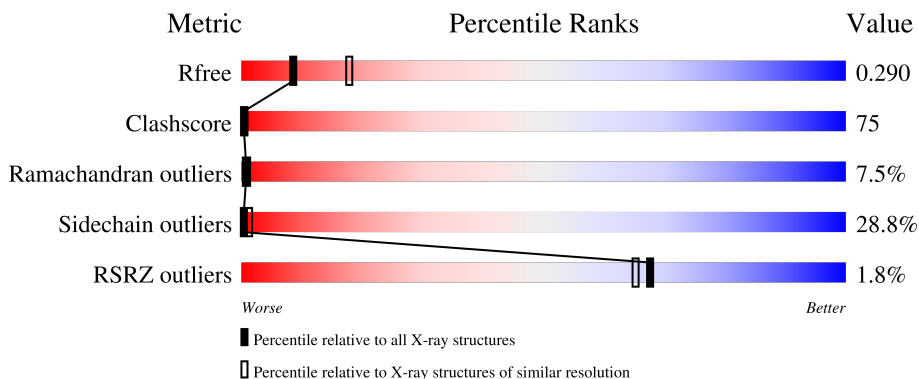
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	260	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1716 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 Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1704	1077	292	331	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	LEU	-	expression tag	UNP Q6GI75
A	-2	ALA	-	expression tag	UNP Q6GI75
A	-1	ALA	-	expression tag	UNP Q6GI75
A	0	ALA	-	expression tag	UNP Q6GI75

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

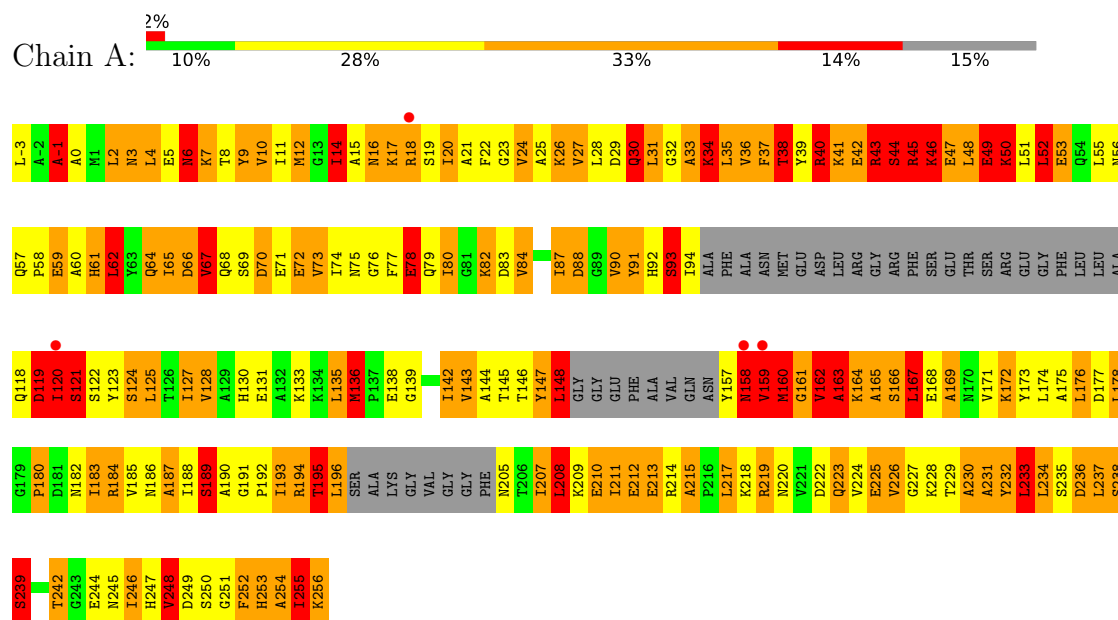
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		

3 Residue-property plots

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: Enoyl-[acyl-carrier-protein] reductase [NADH]



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	70.88Å 74.72Å 110.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.66 – 2.71 37.66 – 2.71	Depositor EDS
% Data completeness (in resolution range)	91.8 (37.66-2.71) 91.8 (37.66-2.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.28	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.289 0.219 , 0.290	Depositor DCC
R_{free} test set	347 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 81.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	1716	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	2.64	113/1723 (6.6%)	2.50	134/2322 (5.8%)

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	1	10

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	ILE	CA-CB	-12.52	1.39	1.54
1	A	187	ALA	N-CA	10.66	1.58	1.45
1	A	142	ILE	CA-CB	-9.67	1.42	1.54
1	A	60	ALA	N-CA	-9.54	1.35	1.46
1	A	14	ILE	N-CA	-9.47	1.34	1.46
1	A	176	LEU	CA-C	-9.39	1.41	1.52
1	A	187	ALA	CA-C	-8.99	1.42	1.52
1	A	34	LYS	N-CA	8.91	1.57	1.46
1	A	67	VAL	N-CA	8.78	1.57	1.46
1	A	169	ALA	CA-C	-8.73	1.41	1.52
1	A	211	ILE	CA-C	-8.48	1.42	1.52
1	A	189	SER	C-O	8.48	1.34	1.24
1	A	224	VAL	CA-CB	-8.35	1.45	1.54
1	A	166	SER	C-N	8.30	1.43	1.33
1	A	30	GLN	C-O	-8.27	1.14	1.24
1	A	30	GLN	N-CA	-8.18	1.36	1.46
1	A	38	THR	C-O	8.12	1.33	1.24
1	A	253	HIS	C-O	7.97	1.33	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	VAL	CA-CB	-7.80	1.44	1.54
1	A	-1	ALA	C-O	-7.75	1.13	1.24
1	A	17	LYS	N-CA	7.72	1.56	1.46
1	A	242	THR	CA-CB	-7.71	1.41	1.53
1	A	148	LEU	CG-CD2	7.53	1.77	1.52
1	A	230	ALA	CA-CB	-7.50	1.41	1.53
1	A	217	LEU	C-O	7.39	1.34	1.23
1	A	225	GLU	C-O	7.38	1.33	1.24
1	A	246	ILE	CA-CB	-7.20	1.45	1.54
1	A	166	SER	N-CA	-7.13	1.37	1.46
1	A	9	TYR	CA-C	-7.11	1.44	1.52
1	A	25	ALA	CA-CB	-7.04	1.42	1.53
1	A	33	ALA	CA-CB	-7.04	1.43	1.53
1	A	60	ALA	C-O	7.00	1.31	1.23
1	A	252	PHE	C-O	-6.99	1.15	1.24
1	A	190	ALA	C-O	6.95	1.32	1.24
1	A	66	ASP	N-CA	-6.92	1.37	1.46
1	A	91	TYR	C-O	-6.90	1.15	1.23
1	A	27	VAL	CA-CB	-6.89	1.47	1.54
1	A	148	LEU	CG-CD1	6.84	1.75	1.52
1	A	136	MET	N-CA	-6.83	1.36	1.46
1	A	33	ALA	N-CA	-6.79	1.37	1.46
1	A	169	ALA	CA-CB	-6.79	1.43	1.53
1	A	37	PHE	C-O	-6.74	1.16	1.23
1	A	15	ALA	N-CA	6.73	1.54	1.46
1	A	218	LYS	C-O	6.67	1.32	1.23
1	A	38	THR	N-CA	-6.57	1.38	1.46
1	A	46	LYS	CD-CE	6.48	1.71	1.52
1	A	139	GLY	C-O	6.46	1.29	1.23
1	A	80	ILE	CA-C	-6.38	1.43	1.52
1	A	119	ASP	N-CA	6.30	1.54	1.46
1	A	252	PHE	CA-C	-6.25	1.44	1.52
1	A	207	ILE	CA-C	6.21	1.58	1.52
1	A	94	ILE	N-CA	6.19	1.58	1.46
1	A	26	LYS	CD-CE	6.18	1.71	1.52
1	A	36	VAL	CA-C	-6.17	1.45	1.52
1	A	248	VAL	CA-CB	-6.11	1.45	1.53
1	A	182	ASN	CB-CG	-6.05	1.36	1.52
1	A	226	VAL	CA-C	-6.05	1.45	1.52
1	A	213	GLU	N-CA	-6.03	1.38	1.46
1	A	10	VAL	C-O	6.02	1.30	1.24
1	A	128	VAL	C-O	-6.00	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	LYS	C-O	5.99	1.31	1.23
1	A	173	TYR	CB-CG	5.97	1.64	1.51
1	A	2	LEU	N-CA	-5.94	1.38	1.46
1	A	195	THR	CB-CG2	5.93	1.72	1.52
1	A	182	ASN	CA-CB	-5.93	1.44	1.53
1	A	254	ALA	CA-CB	-5.92	1.43	1.53
1	A	52	LEU	CG-CD2	5.91	1.72	1.52
1	A	219	ARG	C-O	5.91	1.30	1.23
1	A	231	ALA	CA-CB	5.88	1.62	1.53
1	A	73	VAL	CA-CB	5.84	1.62	1.54
1	A	244	GLU	N-CA	5.84	1.53	1.45
1	A	91	TYR	N-CA	5.82	1.53	1.46
1	A	193	ILE	CA-CB	5.78	1.61	1.54
1	A	15	ALA	CA-CB	5.77	1.62	1.53
1	A	67	VAL	CA-CB	5.76	1.62	1.54
1	A	8	THR	C-O	5.75	1.30	1.24
1	A	3	ASN	CA-C	-5.71	1.45	1.52
1	A	167	LEU	CA-C	-5.69	1.45	1.52
1	A	167	LEU	C-O	-5.66	1.17	1.24
1	A	78	GLU	N-CA	5.65	1.53	1.46
1	A	62	LEU	CG-CD1	5.59	1.71	1.52
1	A	-1	ALA	N-CA	5.58	1.52	1.46
1	A	72	GLU	CG-CD	5.54	1.65	1.52
1	A	66	ASP	CG-OD2	5.52	1.35	1.25
1	A	124	SER	N-CA	-5.52	1.39	1.46
1	A	10	VAL	N-CA	-5.51	1.39	1.46
1	A	236	ASP	N-CA	5.49	1.54	1.46
1	A	180	PRO	N-CA	-5.48	1.40	1.47
1	A	219	ARG	N-CA	5.47	1.53	1.46
1	A	82	LYS	C-O	5.44	1.30	1.24
1	A	143	VAL	C-O	-5.42	1.16	1.24
1	A	16	ASN	N-CA	5.38	1.53	1.46
1	A	130	HIS	CA-C	5.37	1.59	1.52
1	A	239	SER	CA-CB	-5.36	1.44	1.53
1	A	184	ARG	CA-CB	-5.33	1.45	1.53
1	A	219	ARG	CD-NE	-5.32	1.38	1.46
1	A	71	GLU	CG-CD	5.32	1.65	1.52
1	A	53	GLU	CG-CD	5.25	1.65	1.52
1	A	168	GLU	C-O	5.24	1.30	1.24
1	A	223	GLN	C-O	5.20	1.30	1.24
1	A	224	VAL	N-CA	-5.20	1.40	1.46
1	A	131	GLU	CD-OE2	5.17	1.35	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	ILE	N-CA	-5.17	1.40	1.46
1	A	127	ILE	CA-CB	-5.17	1.48	1.54
1	A	36	VAL	N-CA	-5.15	1.39	1.46
1	A	130	HIS	N-CA	-5.12	1.40	1.46
1	A	135	LEU	N-CA	5.10	1.52	1.46
1	A	56	ASN	CA-C	-5.08	1.47	1.53
1	A	145	THR	CA-CB	-5.06	1.44	1.53
1	A	238	SER	C-O	5.06	1.30	1.24
1	A	162	VAL	CA-CB	-5.06	1.47	1.54
1	A	6	ASN	CA-C	-5.04	1.46	1.52
1	A	62	LEU	CA-C	-5.03	1.46	1.52

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	LYS	O-C-N	-20.21	100.56	122.38
1	A	169	ALA	N-CA-C	-14.01	95.60	113.12
1	A	84	VAL	CB-CA-C	-13.91	95.72	110.88
1	A	70	ASP	N-CA-C	11.94	124.30	111.28
1	A	159	VAL	N-CA-C	11.89	134.07	109.34
1	A	49	GLU	N-CA-C	-10.83	100.01	113.01
1	A	162	VAL	CB-CA-C	-9.76	95.28	111.29
1	A	71	GLU	N-CA-C	-9.47	101.15	112.89
1	A	191	GLY	CA-C-N	8.90	130.97	119.84
1	A	191	GLY	C-N-CA	8.90	130.97	119.84
1	A	47	GLU	N-CA-C	-8.52	100.84	111.75
1	A	21	ALA	N-CA-C	-8.40	102.29	112.54
1	A	244	GLU	N-CA-C	8.23	121.66	110.55
1	A	163	ALA	CB-CA-C	-8.21	94.08	110.42
1	A	61	HIS	N-CA-C	8.07	121.68	108.52
1	A	92	HIS	N-CA-C	7.92	122.31	109.40
1	A	128	VAL	CB-CA-C	-7.83	101.41	112.22
1	A	215	ALA	N-CA-C	-7.80	100.25	109.93
1	A	237	LEU	CA-CB-CG	7.80	143.59	116.30
1	A	236	ASP	N-CA-C	7.68	122.33	113.19
1	A	184	ARG	CA-C-N	-7.66	112.10	122.98
1	A	184	ARG	C-N-CA	-7.66	112.10	122.98
1	A	176	LEU	CA-CB-CG	-7.62	89.65	116.30
1	A	219	ARG	CG-CD-NE	-7.61	95.27	112.00
1	A	234	LEU	N-CA-C	-7.59	103.48	112.89
1	A	9	TYR	CA-C-N	-7.50	113.00	122.37
1	A	9	TYR	C-N-CA	-7.50	113.00	122.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	PHE	CA-C-N	-7.40	112.69	123.05
1	A	37	PHE	C-N-CA	-7.40	112.69	123.05
1	A	236	ASP	CB-CA-C	-7.38	95.96	110.27
1	A	70	ASP	CA-C-N	-7.33	108.31	121.14
1	A	70	ASP	C-N-CA	-7.33	108.31	121.14
1	A	47	GLU	CA-C-N	7.26	129.88	120.44
1	A	47	GLU	C-N-CA	7.26	129.88	120.44
1	A	72	GLU	N-CA-C	-7.22	103.41	111.28
1	A	208	LEU	N-CA-C	-7.16	95.54	110.80
1	A	247	HIS	N-CA-C	-7.14	95.99	108.20
1	A	61	HIS	CA-C-N	-7.11	111.53	122.62
1	A	61	HIS	C-N-CA	-7.11	111.53	122.62
1	A	238	SER	N-CA-C	-7.08	105.00	112.93
1	A	4	LEU	CB-CA-C	-7.04	96.41	110.42
1	A	73	VAL	N-CA-C	6.97	118.60	111.00
1	A	12	MET	N-CA-C	6.95	121.36	110.17
1	A	7	LYS	N-CA-C	-6.89	101.64	110.53
1	A	247	HIS	CA-C-O	-6.84	113.43	120.54
1	A	233	LEU	CD1-CG-CD2	-6.78	95.89	110.80
1	A	160	MET	N-CA-CB	-6.75	99.08	110.49
1	A	64	GLN	CA-C-N	-6.74	114.13	123.10
1	A	64	GLN	C-N-CA	-6.74	114.13	123.10
1	A	183	ILE	N-CA-CB	-6.69	103.03	111.46
1	A	24	VAL	CB-CA-C	-6.69	103.28	112.04
1	A	80	ILE	CB-CA-C	-6.63	101.52	112.26
1	A	182	ASN	CA-C-N	-6.60	114.54	123.12
1	A	182	ASN	C-N-CA	-6.60	114.54	123.12
1	A	127	ILE	CB-CA-C	-6.57	103.42	112.02
1	A	160	MET	N-CA-C	6.55	124.75	110.80
1	A	172	LYS	N-CA-C	-6.51	104.11	111.07
1	A	78	GLU	N-CA-CB	6.50	120.35	110.28
1	A	211	ILE	N-CA-C	-6.38	104.29	110.42
1	A	160	MET	CB-CA-C	6.36	123.08	110.42
1	A	32	GLY	CA-C-N	-6.30	113.79	122.30
1	A	32	GLY	C-N-CA	-6.30	113.79	122.30
1	A	130	HIS	CB-CA-C	6.22	120.73	110.90
1	A	58	PRO	CA-C-N	-6.16	112.92	122.59
1	A	58	PRO	C-N-CA	-6.16	112.92	122.59
1	A	232	TYR	CA-C-N	6.15	128.52	120.28
1	A	232	TYR	C-N-CA	6.15	128.52	120.28
1	A	158	ASN	N-CA-C	6.09	123.78	110.80
1	A	27	VAL	N-CA-C	-6.06	103.92	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	SER	CA-CB-OG	-6.00	99.10	111.10
1	A	207	ILE	N-CA-C	5.98	112.61	106.21
1	A	246	ILE	N-CA-C	-5.96	99.83	108.17
1	A	62	LEU	CA-C-O	-5.91	114.19	121.11
1	A	74	ILE	N-CA-C	5.87	116.06	110.42
1	A	120	ILE	N-CA-C	-5.87	105.31	112.76
1	A	176	LEU	N-CA-C	-5.86	103.69	111.24
1	A	65	ILE	CA-C-N	-5.85	112.97	122.34
1	A	65	ILE	C-N-CA	-5.85	112.97	122.34
1	A	84	VAL	N-CA-CB	5.77	120.31	112.35
1	A	167	LEU	CB-CA-C	-5.76	101.75	110.92
1	A	15	ALA	N-CA-C	5.76	120.82	111.37
1	A	174	LEU	N-CA-C	5.69	117.56	111.36
1	A	37	PHE	N-CA-C	5.69	117.91	108.13
1	A	20	ILE	O-C-N	5.67	127.60	121.87
1	A	190	ALA	N-CA-C	5.67	117.53	108.41
1	A	138	GLU	N-CA-C	-5.61	106.48	113.38
1	A	248	VAL	CA-C-O	-5.60	117.76	122.63
1	A	209	LYS	N-CA-C	-5.58	105.08	112.34
1	A	8	THR	CA-C-N	-5.58	114.57	122.94
1	A	8	THR	C-N-CA	-5.58	114.57	122.94
1	A	239	SER	CA-C-N	-5.55	110.53	121.41
1	A	239	SER	C-N-CA	-5.55	110.53	121.41
1	A	239	SER	N-CA-C	5.54	122.61	110.80
1	A	93	SER	CA-C-N	5.51	131.61	121.70
1	A	93	SER	C-N-CA	5.51	131.61	121.70
1	A	91	TYR	O-C-N	-5.47	116.20	122.93
1	A	223	GLN	N-CA-C	-5.46	104.73	111.40
1	A	167	LEU	O-C-N	5.41	127.87	122.08
1	A	48	LEU	N-CA-C	5.37	116.82	111.07
1	A	239	SER	N-CA-CB	-5.34	101.46	110.49
1	A	195	THR	N-CA-C	-5.34	106.62	113.02
1	A	145	THR	N-CA-CB	-5.32	102.12	110.69
1	A	40	ARG	N-CA-C	-5.30	106.98	113.50
1	A	47	GLU	O-C-N	5.29	128.23	122.20
1	A	38	THR	N-CA-C	5.23	117.05	108.52
1	A	73	VAL	CB-CA-C	5.23	119.25	112.24
1	A	93	SER	N-CA-C	5.22	117.45	109.62
1	A	142	ILE	N-CA-CB	-5.21	104.89	111.46
1	A	230	ALA	CA-C-N	-5.21	113.30	120.28
1	A	230	ALA	C-N-CA	-5.21	113.30	120.28
1	A	84	VAL	N-CA-C	5.20	119.51	113.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	TYR	CA-C-N	-5.20	115.14	122.94
1	A	91	TYR	C-N-CA	-5.20	115.14	122.94
1	A	233	LEU	CB-CG-CD1	5.19	126.28	110.70
1	A	12	MET	CB-CA-C	-5.17	100.75	109.50
1	A	59	GLU	CA-C-N	-5.16	115.52	122.95
1	A	59	GLU	C-N-CA	-5.16	115.52	122.95
1	A	30	GLN	CA-C-O	-5.16	115.09	120.55
1	A	207	ILE	CB-CA-C	5.11	118.95	113.22
1	A	-1	ALA	CA-C-N	5.11	131.30	121.54
1	A	-1	ALA	C-N-CA	5.11	131.30	121.54
1	A	189	SER	CA-C-N	5.11	129.22	122.42
1	A	189	SER	C-N-CA	5.11	129.22	122.42
1	A	119	ASP	CB-CA-C	-5.11	100.25	110.42
1	A	212	GLU	CA-C-N	-5.09	114.59	122.49
1	A	212	GLU	C-N-CA	-5.09	114.59	122.49
1	A	50	LYS	O-C-N	5.08	128.01	122.11
1	A	248	VAL	CB-CA-C	5.06	118.88	113.22
1	A	87	ILE	CA-C-O	-5.04	115.59	121.80
1	A	8	THR	CA-C-O	-5.04	114.92	120.36
1	A	148	LEU	CB-CG-CD2	5.03	125.80	110.70
1	A	207	ILE	CA-C-N	5.03	131.14	121.54
1	A	207	ILE	C-N-CA	5.03	131.14	121.54
1	A	3	ASN	N-CA-CB	5.00	118.94	110.49

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	159	VAL	CA

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-1	ALA	Peptide
1	A	120	ILE	Peptide
1	A	147	TYR	Peptide
1	A	158	ASN	Peptide
1	A	159	VAL	Peptide
1	A	161	GLY	Peptide
1	A	163	ALA	Peptide
1	A	208	LEU	Peptide
1	A	42	GLU	Peptide
1	A	43	ARG	Peptide

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	1704	0	1741	260	0
2	A	1	0	0	0	0
3	A	11	0	0	0	0
All	All	1716	0	1741	260	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 75.

All (260) 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:148:LEU:CD2	1:A:148:LEU:CG	1.77	1.59
1:A:148:LEU:CG	1:A:148:LEU:CD1	1.75	1.59
1:A:159:VAL:CG1	1:A:160:MET:HB3	1.58	1.33
1:A:161:GLY:CA	1:A:162:VAL:O	1.83	1.26
1:A:160:MET:HG2	1:A:161:GLY:CA	1.66	1.25
1:A:157:TYR:C	1:A:158:ASN:OD1	1.79	1.23
1:A:160:MET:CG	1:A:161:GLY:HA2	1.72	1.19
1:A:158:ASN:H	1:A:159:VAL:CG2	1.58	1.16
1:A:159:VAL:HG12	1:A:160:MET:CB	1.76	1.16
1:A:160:MET:HG2	1:A:162:VAL:O	1.49	1.09
1:A:158:ASN:N	1:A:159:VAL:HG23	1.66	1.09
1:A:159:VAL:CB	1:A:160:MET:HB3	1.82	1.09
1:A:16:ASN:ND2	1:A:18:ARG:H	1.51	1.08
1:A:162:VAL:HG12	1:A:163:ALA:N	1.69	1.08
1:A:159:VAL:CG1	1:A:160:MET:CB	2.30	1.08
1:A:161:GLY:HA2	1:A:162:VAL:O	1.50	1.08
1:A:255:ILE:HG22	1:A:256:LYS:HE3	1.26	1.07
1:A:120:ILE:HG13	1:A:121:SER:HB2	1.38	1.03
1:A:158:ASN:CA	1:A:159:VAL:HG23	1.86	1.03
1:A:255:ILE:CG2	1:A:256:LYS:HE3	1.89	1.02
1:A:148:LEU:CD2	1:A:148:LEU:HG	1.91	1.00
1:A:160:MET:HG2	1:A:161:GLY:HA2	1.00	0.99
1:A:160:MET:CG	1:A:161:GLY:CA	2.33	0.98
1:A:33:ALA:O	1:A:35:LEU:HD13	1.65	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ASN:C	1:A:159:VAL:HG23	1.90	0.95
1:A:159:VAL:HG12	1:A:160:MET:N	1.74	0.93
1:A:148:LEU:CD1	1:A:148:LEU:CB	2.45	0.93
1:A:159:VAL:HB	1:A:160:MET:HB3	1.47	0.93
1:A:160:MET:HG3	1:A:163:ALA:CB	1.99	0.93
1:A:158:ASN:H	1:A:159:VAL:HG23	1.21	0.92
1:A:16:ASN:HD21	1:A:18:ARG:CG	1.83	0.91
1:A:160:MET:SD	1:A:161:GLY:N	2.45	0.89
1:A:44:SER:C	1:A:46:LYS:H	1.75	0.89
1:A:123:TYR:CZ	1:A:127:ILE:HD11	2.08	0.89
1:A:16:ASN:HD21	1:A:18:ARG:HG3	1.38	0.87
1:A:44:SER:O	1:A:48:LEU:HD23	1.75	0.87
1:A:160:MET:CG	1:A:163:ALA:HB3	2.06	0.86
1:A:43:ARG:HG2	1:A:44:SER:N	1.89	0.86
1:A:162:VAL:O	1:A:163:ALA:HB3	1.75	0.85
1:A:162:VAL:HG12	1:A:163:ALA:H	1.39	0.84
1:A:160:MET:CG	1:A:163:ALA:CB	2.57	0.83
1:A:44:SER:C	1:A:46:LYS:N	2.31	0.83
1:A:161:GLY:HA3	1:A:162:VAL:O	1.78	0.82
1:A:75:ASN:O	1:A:79:GLN:HB2	1.79	0.82
1:A:123:TYR:CE1	1:A:127:ILE:HD11	2.16	0.81
1:A:205:ASN:N	1:A:207:ILE:HG13	1.95	0.81
1:A:157:TYR:O	1:A:158:ASN:OD1	1.98	0.79
1:A:158:ASN:N	1:A:159:VAL:CG2	2.29	0.79
1:A:18:ARG:HD3	1:A:195:THR:O	1.83	0.79
1:A:160:MET:SD	1:A:161:GLY:CA	2.70	0.79
1:A:186:ASN:HD21	1:A:242:THR:HA	1.48	0.78
1:A:164:LYS:O	1:A:165:ALA:C	2.23	0.77
1:A:48:LEU:HA	1:A:51:LEU:HB2	1.66	0.77
1:A:160:MET:HG2	1:A:163:ALA:HB3	1.66	0.77
1:A:253:HIS:O	1:A:256:LYS:HG2	1.84	0.77
1:A:7:LYS:HD2	1:A:88:ASP:OD1	1.83	0.77
1:A:172:LYS:O	1:A:176:LEU:HD12	1.85	0.76
1:A:205:ASN:C	1:A:207:ILE:N	2.39	0.75
1:A:162:VAL:O	1:A:163:ALA:CB	2.35	0.74
1:A:43:ARG:HG2	1:A:44:SER:CA	2.16	0.74
1:A:158:ASN:CA	1:A:159:VAL:CG2	2.64	0.74
1:A:159:VAL:HG12	1:A:160:MET:HB2	1.69	0.74
1:A:16:ASN:HD21	1:A:18:ARG:H	1.36	0.73
1:A:161:GLY:C	1:A:162:VAL:O	2.28	0.73
1:A:119:ASP:C	1:A:121:SER:H	1.96	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ASN:HB3	1:A:7:LYS:HE2	1.71	0.72
1:A:160:MET:HG3	1:A:163:ALA:HB3	1.70	0.71
1:A:205:ASN:C	1:A:207:ILE:H	1.98	0.71
1:A:47:GLU:O	1:A:50:LYS:HB3	1.91	0.71
1:A:52:LEU:O	1:A:52:LEU:HD23	1.91	0.70
1:A:119:ASP:HB3	1:A:123:TYR:H	1.55	0.70
1:A:40:ARG:HA	1:A:65:ILE:O	1.92	0.70
1:A:160:MET:HG2	1:A:161:GLY:HA3	1.71	0.70
1:A:118:GLN:O	1:A:120:ILE:N	2.25	0.70
1:A:158:ASN:C	1:A:159:VAL:CG2	2.62	0.70
1:A:159:VAL:HG11	1:A:160:MET:HB3	1.66	0.70
1:A:159:VAL:CG1	1:A:160:MET:N	2.49	0.69
1:A:77:PHE:HA	1:A:80:ILE:HD12	1.75	0.69
1:A:16:ASN:ND2	1:A:18:ARG:N	2.34	0.69
1:A:205:ASN:O	1:A:208:LEU:HD23	1.92	0.69
1:A:3:ASN:ND2	1:A:236:ASP:CG	2.51	0.69
1:A:184:ARG:NH1	1:A:238:SER:OG	2.21	0.68
1:A:43:ARG:HG2	1:A:44:SER:HA	1.76	0.68
1:A:164:LYS:O	1:A:166:SER:N	2.27	0.67
1:A:43:ARG:CG	1:A:44:SER:N	2.58	0.67
1:A:162:VAL:CG1	1:A:163:ALA:N	2.45	0.66
1:A:16:ASN:ND2	1:A:18:ARG:CG	2.57	0.66
1:A:160:MET:CB	1:A:161:GLY:HA2	2.23	0.66
1:A:70:ASP:N	1:A:70:ASP:OD2	2.28	0.66
1:A:69:SER:O	1:A:72:GLU:HB2	1.95	0.66
1:A:79:GLN:HG3	1:A:83:ASP:OD2	1.95	0.66
1:A:211:ILE:O	1:A:212:GLU:C	2.38	0.65
1:A:172:LYS:O	1:A:175:ALA:HB3	1.97	0.65
1:A:24:VAL:HG12	1:A:28:LEU:HD12	1.79	0.64
1:A:5:GLU:O	1:A:6:ASN:HB2	1.96	0.64
1:A:39:TYR:O	1:A:65:ILE:N	2.30	0.64
1:A:7:LYS:HB3	1:A:88:ASP:CG	2.23	0.64
1:A:158:ASN:OD1	1:A:158:ASN:N	2.30	0.64
1:A:47:GLU:O	1:A:50:LYS:CB	2.45	0.63
1:A:16:ASN:ND2	1:A:18:ARG:HG2	2.14	0.62
1:A:39:TYR:CE2	1:A:64:GLN:HB2	2.34	0.62
1:A:124:SER:O	1:A:128:VAL:HG23	2.00	0.62
1:A:211:ILE:HG23	1:A:215:ALA:HB2	1.82	0.62
1:A:164:LYS:O	1:A:167:LEU:N	2.33	0.62
1:A:177:ASP:HB3	1:A:178:LEU:HD23	1.81	0.62
1:A:22:PHE:O	1:A:26:LYS:HG3	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:VAL:HG12	1:A:160:MET:CA	2.29	0.61
1:A:14:ILE:O	1:A:14:ILE:CG1	2.47	0.61
1:A:29:ASP:OD2	1:A:57:GLN:NE2	2.27	0.61
1:A:39:TYR:O	1:A:64:GLN:HA	2.00	0.61
1:A:43:ARG:O	1:A:45:ARG:N	2.33	0.61
1:A:48:LEU:C	1:A:50:LYS:N	2.53	0.61
1:A:160:MET:HG3	1:A:163:ALA:HB2	1.83	0.60
1:A:48:LEU:C	1:A:50:LYS:H	2.02	0.60
1:A:157:TYR:N	1:A:158:ASN:OD1	2.33	0.60
1:A:67:VAL:HB	1:A:124:SER:OG	2.01	0.59
1:A:119:ASP:C	1:A:121:SER:N	2.56	0.59
1:A:159:VAL:HG12	1:A:160:MET:H	1.65	0.59
1:A:160:MET:SD	1:A:160:MET:C	2.86	0.59
1:A:160:MET:CG	1:A:163:ALA:HB2	2.33	0.59
1:A:50:LYS:O	1:A:53:GLU:HB2	2.02	0.59
1:A:67:VAL:CG1	1:A:124:SER:OG	2.51	0.59
1:A:3:ASN:ND2	1:A:236:ASP:OD2	2.35	0.58
1:A:119:ASP:N	1:A:119:ASP:OD1	2.35	0.58
1:A:44:SER:O	1:A:46:LYS:N	2.36	0.58
1:A:118:GLN:HA	1:A:118:GLN:OE1	2.03	0.58
1:A:46:LYS:C	1:A:48:LEU:N	2.52	0.58
1:A:178:LEU:HD23	1:A:178:LEU:N	2.19	0.58
1:A:16:ASN:HD22	1:A:17:LYS:H	1.52	0.58
1:A:217:LEU:O	1:A:219:ARG:HG2	2.04	0.57
1:A:46:LYS:O	1:A:47:GLU:C	2.46	0.57
1:A:44:SER:O	1:A:47:GLU:N	2.37	0.57
1:A:40:ARG:NE	1:A:66:ASP:OD1	2.33	0.57
1:A:24:VAL:CG1	1:A:28:LEU:HD12	2.35	0.57
1:A:123:TYR:O	1:A:127:ILE:HG12	2.05	0.56
1:A:211:ILE:O	1:A:213:GLU:N	2.37	0.56
1:A:20:ILE:HG21	1:A:226:VAL:HG11	1.87	0.56
1:A:44:SER:O	1:A:48:LEU:CD2	2.51	0.56
1:A:119:ASP:CB	1:A:122:SER:HB3	2.36	0.56
1:A:186:ASN:ND2	1:A:242:THR:HA	2.19	0.56
1:A:253:HIS:O	1:A:256:LYS:CG	2.53	0.56
1:A:147:TYR:CE1	1:A:193:ILE:HD12	2.41	0.56
1:A:3:ASN:O	1:A:4:LEU:HB2	2.06	0.55
1:A:159:VAL:CG1	1:A:160:MET:HB2	2.32	0.55
1:A:231:ALA:O	1:A:235:SER:HB3	2.06	0.55
1:A:162:VAL:CG1	1:A:163:ALA:H	2.16	0.55
1:A:44:SER:C	1:A:48:LEU:HD23	2.32	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LYS:O	1:A:50:LYS:HB2	2.08	0.54
1:A:37:PHE:HB2	1:A:62:LEU:HD12	1.89	0.54
1:A:90:VAL:HG22	1:A:90:VAL:O	2.05	0.54
1:A:159:VAL:CB	1:A:160:MET:CB	2.72	0.54
1:A:248:VAL:HG12	1:A:248:VAL:O	2.08	0.54
1:A:249:ASP:N	1:A:249:ASP:OD1	2.39	0.54
1:A:160:MET:SD	1:A:161:GLY:HA3	2.47	0.54
1:A:157:TYR:CA	1:A:158:ASN:OD1	2.54	0.53
1:A:46:LYS:HD3	1:A:49:GLU:OE2	2.08	0.53
1:A:205:ASN:C	1:A:205:ASN:OD1	2.51	0.53
1:A:26:LYS:O	1:A:30:GLN:HB2	2.08	0.53
1:A:159:VAL:HB	1:A:160:MET:CB	2.30	0.53
1:A:158:ASN:H	1:A:159:VAL:HG21	1.66	0.53
1:A:27:VAL:O	1:A:31:LEU:HD22	2.07	0.53
1:A:148:LEU:CD1	1:A:148:LEU:HB2	2.34	0.53
1:A:16:ASN:ND2	1:A:17:LYS:N	2.56	0.53
1:A:230:ALA:O	1:A:231:ALA:C	2.51	0.53
1:A:45:ARG:O	1:A:45:ARG:HG3	2.08	0.52
1:A:164:LYS:HA	1:A:167:LEU:HB3	1.90	0.52
1:A:160:MET:HG2	1:A:163:ALA:CB	2.32	0.52
1:A:10:VAL:HB	1:A:90:VAL:HB	1.92	0.52
1:A:17:LYS:HB2	1:A:51:LEU:HD21	1.91	0.52
1:A:68:GLN:HA	1:A:68:GLN:OE1	2.09	0.52
1:A:166:SER:O	1:A:169:ALA:HB3	2.09	0.52
1:A:79:GLN:O	1:A:82:LYS:HB2	2.09	0.52
1:A:76:GLY:O	1:A:79:GLN:HB3	2.10	0.51
1:A:40:ARG:HG2	1:A:40:ARG:HH11	1.76	0.51
1:A:75:ASN:O	1:A:79:GLN:CB	2.56	0.51
1:A:34:LYS:H	1:A:34:LYS:HD3	1.75	0.51
1:A:143:VAL:CG2	1:A:233:LEU:HB3	2.42	0.50
1:A:36:VAL:HG12	1:A:37:PHE:N	2.26	0.50
1:A:6:ASN:CG	1:A:34:LYS:HZ1	2.20	0.50
1:A:223:GLN:O	1:A:227:GLY:N	2.32	0.50
1:A:14:ILE:O	1:A:14:ILE:HG13	2.11	0.50
1:A:194:ARG:NH1	1:A:212:GLU:OE2	2.40	0.50
1:A:16:ASN:ND2	1:A:17:LYS:H	2.10	0.50
1:A:2:LEU:HG	1:A:237:LEU:CD2	2.43	0.49
1:A:33:ALA:O	1:A:35:LEU:CD1	2.50	0.49
1:A:119:ASP:HB3	1:A:122:SER:HB3	1.93	0.49
1:A:231:ALA:O	1:A:232:TYR:C	2.55	0.49
1:A:211:ILE:C	1:A:213:GLU:N	2.65	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:MET:O	1:A:93:SER:HB2	2.13	0.49
1:A:161:GLY:HA2	1:A:162:VAL:C	2.32	0.49
1:A:-1:ALA:O	1:A:2:LEU:HD13	2.13	0.49
1:A:24:VAL:HA	1:A:227:GLY:HA3	1.95	0.48
1:A:41:LYS:HG3	1:A:42:GLU:HG3	1.93	0.48
1:A:90:VAL:HG13	1:A:142:ILE:HG12	1.95	0.48
1:A:148:LEU:N	1:A:148:LEU:HD23	2.29	0.48
1:A:252:PHE:O	1:A:255:ILE:HB	2.14	0.48
1:A:24:VAL:HG21	1:A:91:TYR:CZ	2.49	0.48
1:A:26:LYS:O	1:A:27:VAL:C	2.57	0.47
1:A:41:LYS:HB2	1:A:41:LYS:HE2	1.63	0.47
1:A:160:MET:CG	1:A:161:GLY:HA3	2.37	0.47
1:A:133:LYS:C	1:A:135:LEU:N	2.70	0.47
1:A:36:VAL:HG12	1:A:37:PHE:H	1.79	0.46
1:A:193:ILE:HG12	1:A:222:ASP:HA	1.97	0.46
1:A:80:ILE:O	1:A:80:ILE:HG22	2.12	0.46
1:A:189:SER:OG	1:A:245:ASN:ND2	2.39	0.46
1:A:147:TYR:HE1	1:A:193:ILE:HD12	1.80	0.45
1:A:125:LEU:C	1:A:125:LEU:HD12	2.41	0.45
1:A:16:ASN:HD21	1:A:18:ARG:N	2.06	0.45
1:A:80:ILE:O	1:A:80:ILE:CG2	2.62	0.45
1:A:2:LEU:HG	1:A:237:LEU:HD22	1.99	0.44
1:A:3:ASN:HD22	1:A:236:ASP:CG	2.25	0.44
1:A:79:GLN:HA	1:A:79:GLN:NE2	2.32	0.44
1:A:20:ILE:O	1:A:20:ILE:HG22	2.17	0.44
1:A:24:VAL:HG21	1:A:91:TYR:CE1	2.52	0.44
1:A:232:TYR:CZ	1:A:238:SER:HB3	2.53	0.44
1:A:87:ILE:HD13	1:A:87:ILE:HG21	1.71	0.44
1:A:16:ASN:ND2	1:A:18:ARG:HG3	2.18	0.44
1:A:38:THR:HG21	1:A:65:ILE:HD12	2.00	0.44
1:A:47:GLU:O	1:A:51:LEU:HG	2.18	0.44
1:A:46:LYS:O	1:A:48:LEU:N	2.51	0.43
1:A:144:ALA:O	1:A:187:ALA:HA	2.18	0.43
1:A:210:GLU:O	1:A:214:ARG:HG3	2.18	0.43
1:A:205:ASN:O	1:A:205:ASN:OD1	2.36	0.43
1:A:3:ASN:ND2	1:A:236:ASP:OD1	2.52	0.43
1:A:28:LEU:O	1:A:31:LEU:N	2.49	0.43
1:A:119:ASP:HA	1:A:122:SER:CB	2.48	0.43
1:A:208:LEU:C	1:A:210:GLU:N	2.72	0.43
1:A:9:TYR:CD1	1:A:9:TYR:N	2.87	0.42
1:A:88:ASP:OD2	1:A:88:ASP:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:THR:O	1:A:195:THR:OG1	2.29	0.42
1:A:159:VAL:HG11	1:A:160:MET:CB	2.34	0.42
1:A:254:ALA:C	1:A:256:LYS:N	2.76	0.42
1:A:123:TYR:O	1:A:124:SER:C	2.63	0.42
1:A:222:ASP:HB2	1:A:223:GLN:OE1	2.20	0.42
1:A:19:SER:O	1:A:22:PHE:HB3	2.19	0.42
1:A:43:ARG:C	1:A:45:ARG:N	2.77	0.42
1:A:77:PHE:CZ	1:A:128:VAL:HG13	2.55	0.42
1:A:78:GLU:O	1:A:82:LYS:HG3	2.19	0.42
1:A:171:VAL:HG21	1:A:187:ALA:HB2	2.01	0.42
1:A:9:TYR:CD2	1:A:234:LEU:HD13	2.55	0.41
1:A:133:LYS:HA	1:A:136:MET:CG	2.50	0.41
1:A:40:ARG:HH11	1:A:40:ARG:CG	2.33	0.41
1:A:183:ILE:O	1:A:183:ILE:HG22	2.19	0.41
1:A:18:ARG:HD2	1:A:196:LEU:HA	2.03	0.41
1:A:6:ASN:OD1	1:A:34:LYS:NZ	2.47	0.41
1:A:40:ARG:CG	1:A:40:ARG:NH1	2.84	0.41
1:A:148:LEU:CD2	1:A:148:LEU:N	2.83	0.41
1:A:46:LYS:HD3	1:A:46:LYS:HA	1.89	0.41
1:A:119:ASP:HB3	1:A:123:TYR:N	2.31	0.41
1:A:119:ASP:CA	1:A:122:SER:HB3	2.50	0.41
1:A:18:ARG:HG2	1:A:18:ARG:NH1	2.37	0.41
1:A:194:ARG:C	1:A:196:LEU:H	2.29	0.41
1:A:20:ILE:O	1:A:23:GLY:N	2.54	0.40
1:A:36:VAL:CG1	1:A:37:PHE:N	2.84	0.40
1:A:118:GLN:O	1:A:119:ASP:C	2.64	0.40
1:A:188:ILE:CD1	1:A:229:THR:HG22	2.51	0.40
1:A:219:ARG:NH2	1:A:225:GLU:OE1	2.54	0.40
1:A:249:ASP:C	1:A:251:GLY:H	2.29	0.40
1:A:20:ILE:O	1:A:20:ILE:CG2	2.67	0.40
1:A:55:LEU:H	1:A:55:LEU:HG	1.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	213/260 (82%)	169 (79%)	28 (13%)	16 (8%)	1 1

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	119	ASP
1	A	121	SER
1	A	159	VAL
1	A	160	MET
1	A	162	VAL
1	A	250	SER
1	A	0	ALA
1	A	45	ARG
1	A	67	VAL
1	A	165	ALA
1	A	239	SER
1	A	255	ILE
1	A	6	ASN
1	A	208	LEU
1	A	44	SER

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	184/211 (87%)	131 (71%)	53 (29%)	0 1

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	LEU
1	A	11	ILE
1	A	14	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	18	ARG
1	A	30	GLN
1	A	31	LEU
1	A	34	LYS
1	A	35	LEU
1	A	38	THR
1	A	40	ARG
1	A	41	LYS
1	A	43	ARG
1	A	44	SER
1	A	45	ARG
1	A	46	LYS
1	A	49	GLU
1	A	50	LYS
1	A	52	LEU
1	A	59	GLU
1	A	61	HIS
1	A	62	LEU
1	A	67	VAL
1	A	73	VAL
1	A	78	GLU
1	A	84	VAL
1	A	88	ASP
1	A	90	VAL
1	A	93	SER
1	A	119	ASP
1	A	121	SER
1	A	125	LEU
1	A	136	MET
1	A	146	THR
1	A	148	LEU
1	A	158	ASN
1	A	159	VAL
1	A	167	LEU
1	A	178	LEU
1	A	180	PRO
1	A	189	SER
1	A	192	PRO
1	A	194	ARG
1	A	195	THR
1	A	196	LEU
1	A	210	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	220	ASN
1	A	228	LYS
1	A	233	LEU
1	A	239	SER
1	A	246	ILE
1	A	248	VAL
1	A	255	ILE
1	A	256	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	16	ASN
1	A	86	ASN
1	A	130	HIS
1	A	170	ASN
1	A	186	ASN
1	A	245	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](#)

Of 1 ligands modelled in this entry, 1 is 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	221/260 (85%)	-0.15	4 (1%) 67 65	13, 38, 69, 90	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	158	ASN	3.0
1	A	120	ILE	2.9
1	A	159	VAL	2.8
1	A	18	ARG	2.3

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NA	A	257	1/1	0.95	0.12	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.