



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:50 PM UTC

PDB ID : 1GUB / pdb_00001gub
Title : Hinge-bending motion of D-allose binding protein from Escherichia coli: three open conformations
Authors : Magnusson, U.; Chaudhuri, B.N.; Ko, J.; Park, C.; Jones, T.A.; Mowbray, S.L.
Deposited on : 2002-01-24
Resolution : 3.10 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

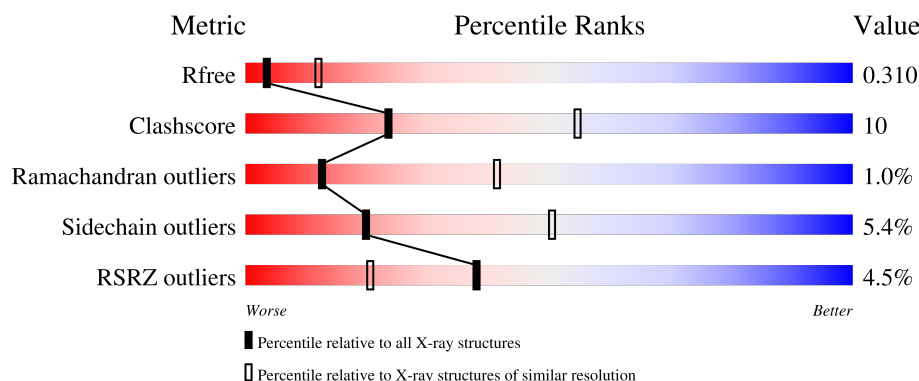
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	288	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NI	A	1289	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2144 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 D-ALLOSE-BINDING PERIPLASMIC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2133	1346	362	416	9			

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

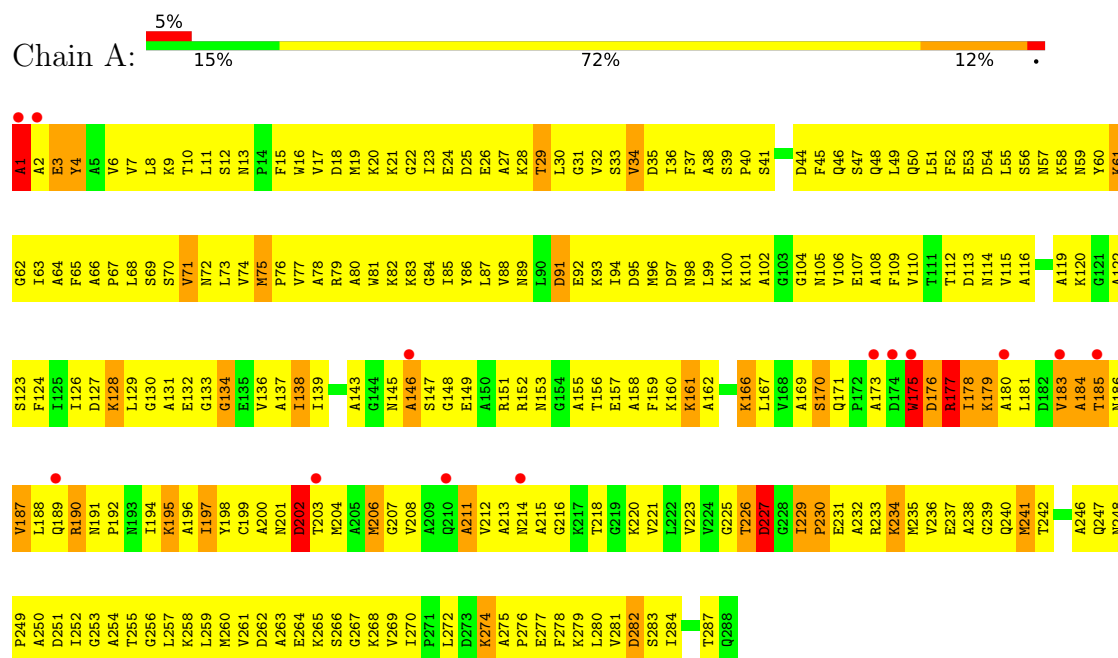
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		

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: D-ALLOSE-BINDING PERIPLASMIC PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	133.10Å 133.10Å 133.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 3.10 29.75 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.75-3.10) 99.2 (29.75-3.10)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.62 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.280 , 0.339 0.251 , 0.310	Depositor DCC
R_{free} test set	606 reflections (7.12%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 25.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	2144	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: NI

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	4.15	414/2161 (19.2%)	2.13	84/2920 (2.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2

All (414) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	ALA	CA-CB	27.63	2.43	1.52
1	A	1	ALA	C-O	25.10	1.73	1.23
1	A	9	LYS	C-O	22.28	1.50	1.24
1	A	1	ALA	CA-C	-20.80	1.09	1.52
1	A	72	ASN	CA-C	-20.25	1.25	1.52
1	A	44	ASP	CA-C	-15.45	1.37	1.53
1	A	146	ALA	CA-CB	13.84	1.76	1.53
1	A	38	ALA	CA-CB	-13.76	1.31	1.53
1	A	110	VAL	CA-CB	-13.73	1.36	1.53
1	A	241	MET	SD-CE	-13.62	1.45	1.79
1	A	35	ASP	C-O	-13.48	1.08	1.24
1	A	115	VAL	N-CA	-13.44	1.30	1.46
1	A	95	ASP	C-O	-13.27	1.07	1.24
1	A	58	LYS	C-O	13.26	1.37	1.23
1	A	181	LEU	CA-C	13.02	1.69	1.52
1	A	196	ALA	CA-CB	-12.74	1.32	1.53
1	A	206	MET	SD-CE	12.57	2.10	1.79
1	A	169	ALA	CA-CB	12.50	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	ALA	CA-CB	-12.18	1.33	1.53
1	A	95	ASP	CA-C	-12.10	1.36	1.52
1	A	255	THR	C-O	-12.04	1.08	1.24
1	A	1	ALA	N-CA	11.88	1.68	1.46
1	A	33	SER	N-CA	-11.84	1.32	1.45
1	A	36	ILE	C-O	-11.38	1.11	1.24
1	A	251	ASP	CA-C	-11.28	1.36	1.52
1	A	136	VAL	CA-CB	11.25	1.74	1.55
1	A	51	LEU	C-O	-11.21	1.11	1.24
1	A	70	SER	C-O	-11.20	1.09	1.24
1	A	37	PHE	CD1-CE1	-11.18	1.05	1.38
1	A	218	THR	CA-CB	11.16	1.69	1.53
1	A	10	THR	CA-C	-11.02	1.39	1.52
1	A	275	ALA	CA-C	-10.96	1.39	1.53
1	A	85	ILE	CA-CB	-10.90	1.40	1.54
1	A	254	ALA	CA-CB	-10.90	1.35	1.53
1	A	215	ALA	C-O	10.89	1.38	1.24
1	A	184	ALA	CA-C	-10.88	1.39	1.52
1	A	24	GLU	C-O	-10.87	1.11	1.24
1	A	33	SER	CA-C	-10.80	1.39	1.52
1	A	61	LYS	C-O	-10.74	1.11	1.24
1	A	102	ALA	CA-CB	-10.65	1.34	1.53
1	A	110	VAL	N-CA	-10.61	1.31	1.46
1	A	279	LYS	C-O	-10.54	1.11	1.24
1	A	38	ALA	CA-C	-10.42	1.39	1.52
1	A	16	TRP	C-O	-10.38	1.10	1.24
1	A	27	ALA	CA-CB	10.36	1.69	1.53
1	A	248	ASN	C-O	-10.35	1.10	1.24
1	A	284	ILE	C-O	-10.26	1.12	1.24
1	A	249	PRO	C-O	-10.25	1.10	1.24
1	A	3	GLU	CA-C	-10.16	1.38	1.52
1	A	26	GLU	CA-C	-10.13	1.38	1.52
1	A	246	ALA	CA-CB	-10.11	1.36	1.53
1	A	184	ALA	CA-CB	10.09	1.69	1.53
1	A	122	ALA	C-O	-10.09	1.12	1.24
1	A	6	VAL	CA-CB	-10.05	1.41	1.54
1	A	185	THR	CA-CB	10.04	1.69	1.53
1	A	112	THR	C-O	-9.99	1.11	1.24
1	A	221	VAL	CA-C	9.94	1.64	1.52
1	A	223	VAL	CA-C	-9.78	1.40	1.52
1	A	185	THR	N-CA	9.68	1.58	1.46
1	A	281	VAL	CA-CB	-9.57	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	ASP	C-O	-9.55	1.11	1.24
1	A	190	ARG	NE-CZ	9.55	1.43	1.33
1	A	73	LEU	N-CA	9.48	1.56	1.46
1	A	66	ALA	C-O	-9.46	1.16	1.25
1	A	86	TYR	N-CA	-9.45	1.34	1.46
1	A	261	VAL	CA-CB	-9.43	1.41	1.54
1	A	158	ALA	CA-CB	-9.42	1.38	1.53
1	A	223	VAL	CA-CB	9.38	1.66	1.54
1	A	136	VAL	C-O	9.35	1.33	1.23
1	A	17	VAL	CA-CB	9.29	1.66	1.54
1	A	234	LYS	CD-CE	9.28	1.80	1.52
1	A	9	LYS	CA-C	9.28	1.64	1.52
1	A	173	ALA	CA-CB	9.27	1.69	1.52
1	A	109	PHE	CA-C	9.27	1.64	1.52
1	A	57	ASN	CA-CB	9.26	1.70	1.53
1	A	102	ALA	CA-C	-9.24	1.39	1.52
1	A	75	MET	SD-CE	-9.22	1.56	1.79
1	A	77	VAL	C-O	-9.14	1.13	1.24
1	A	62	GLY	C-O	-9.12	1.11	1.23
1	A	34	VAL	CA-C	-9.11	1.41	1.52
1	A	61	LYS	CE-NZ	9.10	1.76	1.49
1	A	6	VAL	C-O	-9.03	1.14	1.24
1	A	54	ASP	CA-C	-9.00	1.41	1.52
1	A	52	PHE	C-O	-8.98	1.13	1.24
1	A	13	ASN	CG-ND2	8.97	1.52	1.33
1	A	69	SER	CA-C	-8.97	1.41	1.52
1	A	187	VAL	CA-CB	8.90	1.66	1.54
1	A	78	ALA	N-CA	-8.90	1.34	1.46
1	A	157	GLU	N-CA	-8.81	1.35	1.46
1	A	87	LEU	CA-C	-8.79	1.41	1.52
1	A	220	LYS	CA-C	-8.78	1.40	1.52
1	A	19	MET	C-O	-8.76	1.13	1.24
1	A	52	PHE	CA-C	-8.75	1.41	1.52
1	A	80	ALA	C-O	-8.74	1.13	1.24
1	A	266	SER	CB-OG	-8.63	1.24	1.42
1	A	20	LYS	C-O	-8.62	1.14	1.24
1	A	91	ASP	N-CA	8.61	1.57	1.46
1	A	266	SER	CA-C	-8.58	1.41	1.52
1	A	50	GLN	CG-CD	-8.56	1.30	1.52
1	A	80	ALA	CA-CB	-8.50	1.39	1.53
1	A	50	GLN	C-O	-8.48	1.13	1.24
1	A	68	LEU	CG-CD1	-8.48	1.24	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	ASP	CA-C	-8.47	1.41	1.52
1	A	87	LEU	C-O	-8.47	1.13	1.23
1	A	130	GLY	C-O	8.37	1.35	1.23
1	A	52	PHE	CE2-CZ	-8.36	1.13	1.38
1	A	250	ALA	N-CA	-8.36	1.36	1.46
1	A	75	MET	CA-C	-8.35	1.42	1.52
1	A	183	VAL	N-CA	8.34	1.56	1.46
1	A	119	ALA	CA-C	-8.30	1.41	1.52
1	A	74	VAL	CA-CB	-8.29	1.43	1.54
1	A	18	ASP	N-CA	-8.28	1.35	1.46
1	A	122	ALA	N-CA	8.21	1.56	1.46
1	A	262	ASP	CA-CB	-8.20	1.40	1.53
1	A	215	ALA	C-N	8.18	1.43	1.33
1	A	270	ILE	CB-CG1	-8.16	1.37	1.53
1	A	79	ARG	C-O	-8.13	1.14	1.24
1	A	45	PHE	C-O	-8.13	1.14	1.24
1	A	221	VAL	CB-CG2	-8.13	1.25	1.52
1	A	11	LEU	CA-CB	-8.13	1.42	1.53
1	A	64	ALA	CA-CB	-8.07	1.41	1.53
1	A	12	SER	CA-C	-8.06	1.42	1.52
1	A	36	ILE	CA-C	-8.06	1.42	1.52
1	A	44	ASP	CA-CB	8.05	1.65	1.53
1	A	189	GLN	C-O	-8.05	1.13	1.24
1	A	2	ALA	N-CA	8.04	1.56	1.45
1	A	270	ILE	C-O	-8.03	1.14	1.24
1	A	100	LYS	C-O	-8.01	1.14	1.24
1	A	32	VAL	CA-C	7.94	1.62	1.52
1	A	67	PRO	C-O	7.91	1.32	1.23
1	A	202	ASP	C-O	7.90	1.34	1.24
1	A	254	ALA	C-O	-7.90	1.14	1.24
1	A	256	GLY	C-O	-7.87	1.14	1.23
1	A	37	PHE	CD2-CE2	-7.86	1.15	1.38
1	A	189	GLN	CG-CD	7.86	1.71	1.52
1	A	6	VAL	CA-C	-7.86	1.43	1.52
1	A	50	GLN	CD-OE1	-7.85	1.08	1.23
1	A	132	GLU	CD-OE2	7.83	1.40	1.25
1	A	167	LEU	CA-C	7.81	1.62	1.52
1	A	226	THR	N-CA	-7.81	1.35	1.45
1	A	283	SER	C-O	-7.80	1.14	1.23
1	A	29	THR	C-O	-7.78	1.14	1.24
1	A	105	ASN	N-CA	-7.78	1.35	1.46
1	A	15	PHE	CA-C	-7.77	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	ASP	CB-CG	7.74	1.71	1.52
1	A	274	LYS	CE-NZ	7.73	1.72	1.49
1	A	166	LYS	CD-CE	7.72	1.75	1.52
1	A	277	GLU	C-O	-7.71	1.13	1.23
1	A	180	ALA	N-CA	7.70	1.55	1.46
1	A	17	VAL	N-CA	7.69	1.55	1.46
1	A	74	VAL	CB-CG2	-7.68	1.27	1.52
1	A	161	LYS	CD-CE	7.68	1.75	1.52
1	A	256	GLY	CA-C	-7.66	1.43	1.52
1	A	47	SER	C-O	7.61	1.33	1.24
1	A	33	SER	C-O	-7.60	1.15	1.23
1	A	177	ARG	CZ-NH2	7.59	1.43	1.33
1	A	187	VAL	CA-C	7.57	1.63	1.52
1	A	106	VAL	CA-C	-7.57	1.43	1.52
1	A	221	VAL	N-CA	7.55	1.55	1.46
1	A	85	ILE	CA-C	-7.53	1.43	1.52
1	A	56	SER	CA-CB	-7.51	1.40	1.53
1	A	242	THR	CA-C	7.35	1.62	1.52
1	A	204	MET	SD-CE	-7.32	1.61	1.79
1	A	22	GLY	C-O	-7.32	1.15	1.23
1	A	25	ASP	CG-OD1	7.29	1.39	1.25
1	A	15	PHE	CA-CB	-7.29	1.42	1.53
1	A	259	LEU	N-CA	-7.27	1.36	1.46
1	A	16	TRP	N-CA	7.26	1.55	1.46
1	A	108	ALA	C-O	-7.26	1.14	1.23
1	A	58	LYS	CA-CB	-7.25	1.42	1.53
1	A	82	LYS	CA-C	-7.21	1.43	1.52
1	A	13	ASN	C-O	-7.21	1.15	1.24
1	A	183	VAL	CA-C	7.20	1.60	1.52
1	A	29	THR	N-CA	-7.20	1.37	1.46
1	A	114	ASN	CA-C	7.19	1.62	1.52
1	A	28	LYS	C-O	-7.18	1.14	1.24
1	A	81	TRP	CA-C	-7.18	1.43	1.52
1	A	71	VAL	CA-C	-7.17	1.43	1.52
1	A	24	GLU	N-CA	-7.15	1.37	1.46
1	A	249	PRO	N-CA	-7.15	1.38	1.47
1	A	282	ASP	C-O	-7.13	1.15	1.23
1	A	109	PHE	C-O	-7.13	1.15	1.24
1	A	1	ALA	C-N	7.12	1.43	1.33
1	A	65	PHE	CA-CB	-7.12	1.42	1.53
1	A	128	LYS	C-O	7.09	1.32	1.24
1	A	216	GLY	CA-C	7.06	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	SER	C-N	-7.05	1.24	1.33
1	A	250	ALA	CA-C	-7.05	1.43	1.52
1	A	240	GLN	CG-CD	7.02	1.69	1.52
1	A	274	LYS	CA-C	-6.98	1.43	1.52
1	A	204	MET	CA-C	-6.90	1.43	1.52
1	A	175	TRP	C-O	6.89	1.32	1.24
1	A	199	CYS	CA-CB	-6.89	1.41	1.53
1	A	180	ALA	CA-C	6.88	1.61	1.52
1	A	88	VAL	CA-CB	-6.87	1.45	1.54
1	A	53	GLU	CA-C	6.86	1.61	1.52
1	A	32	VAL	N-CA	6.84	1.54	1.46
1	A	70	SER	N-CA	6.82	1.55	1.46
1	A	129	LEU	C-O	6.82	1.32	1.24
1	A	265	LYS	CB-CG	6.82	1.73	1.52
1	A	69	SER	N-CA	6.79	1.54	1.45
1	A	11	LEU	CG-CD2	-6.77	1.30	1.52
1	A	7	VAL	CA-C	-6.76	1.44	1.52
1	A	113	ASP	C-O	-6.76	1.15	1.24
1	A	255	THR	CA-CB	6.75	1.64	1.53
1	A	19	MET	CG-SD	-6.74	1.63	1.80
1	A	69	SER	CB-OG	-6.73	1.28	1.42
1	A	51	LEU	CA-C	-6.73	1.44	1.52
1	A	238	ALA	N-CA	6.69	1.54	1.46
1	A	72	ASN	N-CA	6.68	1.54	1.46
1	A	123	SER	C-N	-6.67	1.24	1.33
1	A	277	GLU	CD-OE1	6.67	1.38	1.25
1	A	277	GLU	CD-OE2	6.65	1.38	1.25
1	A	236	VAL	CA-CB	-6.64	1.43	1.54
1	A	169	ALA	C-O	-6.63	1.16	1.23
1	A	40	PRO	C-O	6.60	1.32	1.24
1	A	149	GLU	CD-OE2	6.60	1.37	1.25
1	A	160	LYS	C-O	6.57	1.32	1.24
1	A	4	TYR	CA-CB	-6.57	1.40	1.54
1	A	268	LYS	CB-CG	6.57	1.72	1.52
1	A	240	GLN	CB-CG	6.55	1.72	1.52
1	A	124	PHE	CE1-CZ	6.54	1.58	1.38
1	A	257	LEU	N-CA	6.53	1.54	1.46
1	A	63	ILE	CA-CB	6.53	1.63	1.54
1	A	268	LYS	C-O	6.52	1.32	1.23
1	A	60	TYR	CA-C	-6.51	1.44	1.52
1	A	63	ILE	C-O	-6.51	1.16	1.24
1	A	229	ILE	CB-CG1	-6.51	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	ALA	N-CA	-6.50	1.38	1.46
1	A	9	LYS	N-CA	-6.50	1.38	1.46
1	A	162	ALA	C-O	-6.49	1.15	1.23
1	A	116	ALA	CA-C	-6.48	1.44	1.52
1	A	109	PHE	CE1-CZ	-6.45	1.19	1.38
1	A	106	VAL	N-CA	6.44	1.53	1.46
1	A	179	LYS	CE-NZ	6.42	1.68	1.49
1	A	20	LYS	CA-C	-6.41	1.44	1.52
1	A	249	PRO	C-N	-6.37	1.25	1.33
1	A	21	LYS	C-O	-6.36	1.16	1.24
1	A	68	LEU	C-N	-6.36	1.24	1.33
1	A	26	GLU	C-O	-6.34	1.15	1.24
1	A	153	ASN	C-O	-6.34	1.16	1.24
1	A	143	ALA	CA-C	6.33	1.61	1.53
1	A	143	ALA	CA-CB	6.32	1.63	1.53
1	A	156	THR	C-O	-6.31	1.16	1.24
1	A	216	GLY	N-CA	6.29	1.54	1.45
1	A	89	ASN	CG-OD1	-6.28	1.11	1.23
1	A	35	ASP	CG-OD1	6.26	1.37	1.25
1	A	91	ASP	CG-OD1	-6.26	1.13	1.25
1	A	104	GLY	N-CA	-6.25	1.39	1.45
1	A	134	GLY	C-O	6.24	1.29	1.23
1	A	44	ASP	CG-OD1	6.24	1.37	1.25
1	A	102	ALA	C-O	6.24	1.32	1.24
1	A	281	VAL	CB-CG1	-6.23	1.31	1.52
1	A	162	ALA	N-CA	6.22	1.54	1.46
1	A	263	ALA	CA-CB	-6.22	1.43	1.53
1	A	31	GLY	CA-C	-6.21	1.43	1.51
1	A	272	LEU	CA-C	6.20	1.60	1.52
1	A	96	MET	SD-CE	-6.20	1.64	1.79
1	A	264	GLU	N-CA	-6.20	1.38	1.46
1	A	211	ALA	CA-CB	6.20	1.64	1.53
1	A	257	LEU	CB-CG	-6.19	1.41	1.53
1	A	235	MET	C-N	-6.17	1.27	1.34
1	A	229	ILE	CB-CG2	6.16	1.72	1.52
1	A	233	ARG	CZ-NH1	6.12	1.41	1.32
1	A	17	VAL	CB-CG1	-6.11	1.32	1.52
1	A	198	TYR	CA-C	-6.11	1.45	1.52
1	A	13	ASN	CA-C	6.11	1.59	1.52
1	A	53	GLU	CD-OE1	-6.10	1.13	1.25
1	A	126	ILE	CB-CG1	-6.10	1.41	1.53
1	A	91	ASP	CB-CG	-6.09	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	ASN	CA-C	-6.08	1.44	1.53
1	A	40	PRO	CA-C	6.07	1.61	1.52
1	A	131	ALA	CA-C	-6.07	1.45	1.52
1	A	7	VAL	C-O	-6.04	1.16	1.24
1	A	16	TRP	CE3-CZ3	-6.03	1.20	1.38
1	A	287	THR	N-CA	6.03	1.53	1.45
1	A	190	ARG	CA-C	6.03	1.60	1.52
1	A	278	PHE	C-O	6.02	1.32	1.23
1	A	189	GLN	CD-NE2	6.01	1.45	1.33
1	A	46	GLN	CD-NE2	-6.00	1.20	1.33
1	A	109	PHE	CE2-CZ	-5.98	1.20	1.38
1	A	279	LYS	CB-CG	-5.97	1.34	1.52
1	A	23	ILE	CB-CG2	-5.97	1.32	1.52
1	A	74	VAL	CA-C	5.97	1.60	1.52
1	A	93	LYS	CA-C	-5.97	1.45	1.52
1	A	221	VAL	CA-CB	-5.97	1.46	1.54
1	A	239	GLY	CA-C	-5.96	1.43	1.51
1	A	220	LYS	C-O	5.96	1.31	1.24
1	A	147	SER	C-O	-5.95	1.16	1.24
1	A	93	LYS	CB-CG	-5.95	1.34	1.52
1	A	212	VAL	CA-C	-5.93	1.45	1.52
1	A	86	TYR	CG-CD1	-5.92	1.26	1.39
1	A	229	ILE	CA-C	-5.92	1.46	1.52
1	A	24	GLU	CD-OE1	-5.91	1.14	1.25
1	A	161	LYS	CA-C	-5.89	1.44	1.52
1	A	269	VAL	CA-CB	-5.88	1.48	1.54
1	A	48	GLN	CD-OE1	-5.87	1.12	1.23
1	A	92	GLU	N-CA	-5.86	1.39	1.45
1	A	21	LYS	C-N	-5.84	1.26	1.33
1	A	227	ASP	C-O	5.81	1.31	1.24
1	A	96	MET	C-O	-5.79	1.16	1.24
1	A	55	LEU	C-O	5.77	1.31	1.24
1	A	171	GLN	CG-CD	5.77	1.66	1.52
1	A	235	MET	CA-C	-5.76	1.45	1.52
1	A	15	PHE	CE2-CZ	-5.74	1.21	1.38
1	A	69	SER	C-O	-5.73	1.16	1.23
1	A	88	VAL	C-O	5.72	1.30	1.24
1	A	223	VAL	CB-CG2	5.69	1.71	1.52
1	A	234	LYS	C-O	5.69	1.31	1.24
1	A	73	LEU	CG-CD2	-5.67	1.33	1.52
1	A	208	VAL	CA-CB	-5.67	1.46	1.54
1	A	213	ALA	C-O	5.65	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	GLY	C-N	-5.64	1.26	1.33
1	A	188	LEU	CA-C	5.64	1.60	1.52
1	A	231	GLU	C-O	5.64	1.31	1.24
1	A	84	GLY	C-O	5.63	1.31	1.23
1	A	49	LEU	C-O	-5.63	1.16	1.24
1	A	107	GLU	CA-C	5.62	1.60	1.52
1	A	59	ASN	CG-ND2	5.62	1.45	1.33
1	A	66	ALA	C-N	-5.62	1.27	1.33
1	A	173	ALA	CA-C	5.61	1.58	1.52
1	A	282	ASP	CG-OD1	5.60	1.35	1.25
1	A	15	PHE	N-CA	-5.60	1.39	1.46
1	A	105	ASN	CB-CG	5.60	1.66	1.52
1	A	204	MET	C-O	-5.59	1.17	1.24
1	A	60	TYR	CG-CD2	-5.58	1.27	1.39
1	A	226	THR	CA-C	5.56	1.59	1.52
1	A	120	LYS	C-N	-5.55	1.27	1.34
1	A	45	PHE	N-CA	5.55	1.53	1.46
1	A	175	TRP	CG-CD1	5.55	1.50	1.36
1	A	225	GLY	C-O	-5.53	1.17	1.23
1	A	147	SER	CA-C	-5.52	1.45	1.52
1	A	269	VAL	CB-CG2	-5.51	1.34	1.52
1	A	148	GLY	CA-C	5.51	1.59	1.51
1	A	176	ASP	CG-OD2	5.50	1.35	1.25
1	A	146	ALA	CA-C	5.48	1.60	1.52
1	A	211	ALA	N-CA	5.48	1.53	1.46
1	A	201	ASN	N-CA	5.48	1.52	1.45
1	A	85	ILE	C-O	-5.46	1.17	1.24
1	A	155	ALA	CA-C	5.46	1.60	1.52
1	A	48	GLN	N-CA	5.46	1.53	1.46
1	A	109	PHE	CG-CD1	-5.45	1.27	1.38
1	A	263	ALA	C-N	-5.45	1.26	1.34
1	A	88	VAL	CA-C	5.43	1.59	1.52
1	A	260	MET	N-CA	5.43	1.53	1.46
1	A	4	TYR	N-CA	5.43	1.52	1.45
1	A	112	THR	CA-C	-5.43	1.46	1.52
1	A	189	GLN	CD-OE1	5.42	1.33	1.23
1	A	12	SER	N-CA	-5.40	1.39	1.46
1	A	24	GLU	C-N	-5.40	1.26	1.33
1	A	19	MET	SD-CE	-5.39	1.66	1.79
1	A	33	SER	C-N	5.39	1.40	1.33
1	A	187	VAL	C-O	5.38	1.31	1.24
1	A	188	LEU	C-O	5.38	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	ALA	C-O	5.37	1.31	1.24
1	A	71	VAL	CB-CG1	5.36	1.70	1.52
1	A	237	GLU	CD-OE2	5.35	1.35	1.25
1	A	284	ILE	N-CA	-5.33	1.39	1.46
1	A	68	LEU	CA-C	-5.33	1.45	1.52
1	A	214	ASN	C-O	5.32	1.30	1.24
1	A	152	ARG	CA-CB	-5.32	1.44	1.53
1	A	89	ASN	C-O	-5.30	1.17	1.23
1	A	116	ALA	C-O	-5.29	1.17	1.24
1	A	171	GLN	CD-NE2	5.29	1.44	1.33
1	A	79	ARG	CZ-NH2	5.26	1.40	1.33
1	A	55	LEU	CG-CD1	-5.26	1.35	1.52
1	A	57	ASN	CG-ND2	5.26	1.44	1.33
1	A	33	SER	CA-CB	-5.26	1.45	1.53
1	A	238	ALA	CA-C	5.25	1.59	1.52
1	A	110	VAL	CB-CG1	5.25	1.69	1.52
1	A	114	ASN	CB-CG	-5.25	1.39	1.52
1	A	214	ASN	N-CA	5.25	1.52	1.46
1	A	257	LEU	C-O	-5.24	1.17	1.24
1	A	202	ASP	C-N	5.22	1.40	1.33
1	A	136	VAL	N-CA	5.22	1.51	1.46
1	A	262	ASP	C-O	5.22	1.30	1.24
1	A	71	VAL	CA-CB	5.21	1.60	1.54
1	A	109	PHE	CA-CB	-5.21	1.46	1.53
1	A	138	ILE	CA-C	5.18	1.58	1.52
1	A	39	SER	N-CA	5.18	1.54	1.45
1	A	254	ALA	CA-C	-5.17	1.46	1.52
1	A	157	GLU	CD-OE2	5.17	1.35	1.25
1	A	199	CYS	CA-C	5.17	1.58	1.52
1	A	107	GLU	CD-OE2	5.16	1.35	1.25
1	A	112	THR	CA-CB	-5.16	1.46	1.53
1	A	94	ILE	CA-C	-5.16	1.46	1.52
1	A	170	SER	C-O	5.16	1.29	1.23
1	A	50	GLN	C-N	-5.16	1.27	1.33
1	A	194	ILE	CA-C	5.16	1.58	1.52
1	A	238	ALA	CA-CB	5.15	1.62	1.53
1	A	151	ARG	N-CA	-5.14	1.39	1.46
1	A	27	ALA	C-O	-5.14	1.17	1.24
1	A	35	ASP	C-N	5.13	1.40	1.33
1	A	23	ILE	C-O	-5.09	1.17	1.24
1	A	173	ALA	C-O	5.09	1.29	1.23
1	A	100	LYS	CG-CD	5.09	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	MET	C-O	5.09	1.30	1.23
1	A	159	PHE	N-CA	-5.08	1.39	1.46
1	A	177	ARG	CZ-NH1	5.08	1.39	1.32
1	A	83	LYS	C-O	5.07	1.30	1.24
1	A	190	ARG	CA-CB	5.07	1.61	1.53
1	A	93	LYS	C-O	-5.06	1.17	1.24
1	A	249	PRO	CA-C	5.06	1.59	1.52
1	A	235	MET	CG-SD	5.05	1.93	1.80
1	A	258	LYS	C-O	-5.04	1.18	1.24
1	A	229	ILE	CA-CB	5.04	1.60	1.54
1	A	191	ASN	C-O	-5.04	1.18	1.24
1	A	37	PHE	CE1-CZ	-5.04	1.23	1.38
1	A	93	LYS	C-N	-5.04	1.27	1.33
1	A	282	ASP	CB-CG	-5.03	1.39	1.52
1	A	37	PHE	CE2-CZ	-5.02	1.23	1.38
1	A	41	SER	CB-OG	5.01	1.52	1.42
1	A	101	LYS	CA-CB	-5.00	1.45	1.53
1	A	267	GLY	N-CA	5.00	1.52	1.45

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	ALA	N-CA-C	10.96	141.70	111.00
1	A	1	ALA	O-C-N	-10.76	105.78	123.00
1	A	1	ALA	CA-C-O	-10.56	102.84	120.80
1	A	234	LYS	N-CA-C	-9.41	100.90	111.82
1	A	1	ALA	CB-CA-C	-9.26	96.61	110.50
1	A	252	ILE	N-CA-C	-8.19	102.07	111.00
1	A	1	ALA	CA-C-N	7.81	134.36	121.39
1	A	1	ALA	C-N-CA	7.81	134.36	121.39
1	A	257	LEU	N-CA-C	-7.69	102.97	111.36
1	A	49	LEU	N-CA-C	-7.66	102.58	112.23
1	A	254	ALA	N-CA-C	-7.52	103.17	111.36
1	A	13	ASN	O-C-N	-7.49	114.46	121.35
1	A	276	PRO	CA-C-O	-7.48	112.51	122.08
1	A	206	MET	N-CA-C	-7.47	103.96	113.23
1	A	34	VAL	CG1-CB-CG2	-7.38	94.57	110.80
1	A	74	VAL	N-CA-C	-7.36	103.29	110.72
1	A	239	GLY	N-CA-C	-7.19	105.29	115.43
1	A	10	THR	OG1-CB-CG2	-7.17	94.96	109.30
1	A	167	LEU	N-CA-C	7.10	119.99	108.63
1	A	19	MET	O-C-N	-6.95	114.76	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ALA	CA-C-O	6.70	126.85	120.09
1	A	61	LYS	CA-C-N	6.60	128.14	121.35
1	A	61	LYS	C-N-CA	6.60	128.14	121.35
1	A	99	LEU	N-CA-C	-6.47	104.64	112.54
1	A	155	ALA	N-CA-C	-6.45	104.33	111.82
1	A	115	VAL	N-CA-C	-6.44	104.22	110.72
1	A	1	ALA	N-CA-CB	-6.43	100.76	110.40
1	A	283	SER	N-CA-C	6.37	119.48	110.50
1	A	116	ALA	N-CA-C	-6.33	104.48	111.82
1	A	53	GLU	N-CA-C	-6.15	104.57	111.28
1	A	21	LYS	O-C-N	-6.11	114.75	122.27
1	A	28	LYS	N-CA-C	-6.08	105.35	112.89
1	A	20	LYS	CA-C-O	-6.02	114.50	120.82
1	A	69	SER	O-C-N	-6.02	115.32	123.15
1	A	203	THR	N-CA-C	-5.96	104.70	111.14
1	A	62	GLY	O-C-N	-5.95	118.04	123.57
1	A	223	VAL	O-C-N	5.90	129.19	122.93
1	A	46	GLN	N-CA-C	-5.86	104.84	112.23
1	A	115	VAL	O-C-N	-5.84	115.81	121.83
1	A	147	SER	N-CA-C	-5.84	104.87	112.23
1	A	184	ALA	N-CA-C	-5.80	103.76	111.24
1	A	6	VAL	CA-C-N	5.79	129.83	122.37
1	A	6	VAL	C-N-CA	5.79	129.83	122.37
1	A	68	LEU	N-CA-C	5.78	117.58	111.28
1	A	39	SER	CB-CA-C	-5.73	99.84	108.61
1	A	58	LYS	CA-C-N	-5.73	115.36	123.03
1	A	58	LYS	C-N-CA	-5.73	115.36	123.03
1	A	13	ASN	CA-C-O	5.72	123.56	119.32
1	A	161	LYS	N-CA-C	-5.72	105.03	112.23
1	A	281	VAL	CG1-CB-CG2	-5.72	98.22	110.80
1	A	2	ALA	N-CA-C	5.67	118.87	110.48
1	A	47	SER	N-CA-CB	5.66	119.01	110.30
1	A	255	THR	N-CA-C	-5.65	105.26	111.82
1	A	239	GLY	CA-C-O	-5.63	112.58	119.06
1	A	51	LEU	CA-C-N	5.62	127.81	120.28
1	A	51	LEU	C-N-CA	5.62	127.81	120.28
1	A	178	ILE	N-CA-C	-5.62	105.37	110.82
1	A	230	PRO	N-CA-C	-5.60	106.86	113.86
1	A	240	GLN	N-CA-CB	5.58	118.70	110.33
1	A	221	VAL	N-CA-CB	5.50	116.53	110.53
1	A	8	LEU	N-CA-C	5.50	117.61	109.69
1	A	24	GLU	CA-C-N	5.49	128.09	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	GLU	C-N-CA	5.49	128.09	120.29
1	A	280	LEU	CD1-CG-CD2	-5.46	98.78	110.80
1	A	2	ALA	CA-C-O	-5.46	115.19	121.47
1	A	149	GLU	N-CA-C	-5.44	105.38	112.23
1	A	95	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	229	ILE	CB-CG1-CD1	-5.32	102.63	113.80
1	A	253	GLY	N-CA-C	-5.31	105.97	112.77
1	A	247	GLN	N-CA-CB	5.31	119.06	110.51
1	A	10	THR	CA-C-O	-5.29	115.33	121.26
1	A	30	LEU	N-CA-C	5.29	118.89	112.23
1	A	130	GLY	O-C-N	5.28	127.98	122.86
1	A	188	LEU	CA-C-O	5.22	125.81	119.38
1	A	269	VAL	CG1-CB-CG2	-5.17	99.44	110.80
1	A	61	LYS	N-CA-C	5.13	117.27	111.11
1	A	67	PRO	CB-CA-C	-5.13	105.11	111.11
1	A	23	ILE	N-CA-C	-5.13	105.41	111.00
1	A	279	LYS	N-CA-CB	5.11	118.60	110.16
1	A	80	ALA	CA-C-N	5.11	127.54	120.29
1	A	80	ALA	C-N-CA	5.11	127.54	120.29
1	A	71	VAL	CB-CA-C	-5.10	105.43	111.65
1	A	235	MET	N-CA-C	-5.08	105.82	111.36
1	A	192	PRO	N-CD-CG	-5.07	95.59	103.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	ALA	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ALA	Peptide,Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2133	0	2184	44	4
2	A	1	0	0	2	0
3	A	10	0	0	0	0
All	All	2144	0	2184	44	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (44) 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:146:ALA:CA	1:A:146:ALA:CB	1.76	1.61
1:A:161:LYS:CD	1:A:161:LYS:CE	1.75	1.60
1:A:234:LYS:CD	1:A:234:LYS:CE	1.80	1.57
1:A:166:LYS:CD	1:A:166:LYS:CE	1.75	1.56
1:A:1:ALA:N	1:A:1:ALA:CA	1.68	1.52
1:A:179:LYS:CE	1:A:179:LYS:NZ	1.68	1.52
1:A:274:LYS:CE	1:A:274:LYS:NZ	1.72	1.50
1:A:61:LYS:NZ	1:A:61:LYS:CE	1.76	1.49
1:A:206:MET:CE	1:A:206:MET:SD	2.11	1.38
1:A:1:ALA:C	1:A:1:ALA:O	1.73	1.31
1:A:1:ALA:CB	2:A:1289:NI:NI	1.21	1.15
1:A:1:ALA:CA	1:A:1:ALA:CB	2.43	0.97
1:A:1:ALA:HB2	2:A:1289:NI:NI	0.99	0.87
1:A:1:ALA:CA	1:A:1:ALA:O	2.24	0.86
1:A:1:ALA:N	1:A:1:ALA:HA	1.97	0.75
1:A:139:ILE:H	1:A:139:ILE:HD12	1.56	0.69
1:A:202:ASP:O	1:A:206:MET:HE2	1.98	0.64
1:A:234:LYS:CE	1:A:234:LYS:CG	2.75	0.62
1:A:186:ASN:O	1:A:190:ARG:HG2	2.01	0.61
1:A:137:ALA:O	1:A:197:ILE:HG22	2.02	0.60
1:A:161:LYS:CE	1:A:161:LYS:CG	2.77	0.58
1:A:229:ILE:HB	1:A:230:PRO:CD	2.35	0.57
1:A:1:ALA:C	1:A:1:ALA:CB	2.78	0.57
1:A:145:ASN:HD22	1:A:175:TRP:HZ2	1.53	0.56
1:A:202:ASP:OD2	1:A:232:ALA:HB3	2.06	0.55
1:A:75:MET:N	1:A:76:PRO:CD	2.70	0.55
1:A:184:ALA:HB3	1:A:211:ALA:HB2	1.90	0.53
1:A:183:VAL:O	1:A:187:VAL:HG23	2.09	0.53
1:A:166:LYS:CE	1:A:166:LYS:CG	2.81	0.52
1:A:184:ALA:HB1	1:A:211:ALA:HB3	1.93	0.51
1:A:177:ARG:HG2	1:A:207:GLY:CA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:THR:O	1:A:227:ASP:HB2	2.11	0.50
1:A:139:ILE:HD12	1:A:139:ILE:N	2.23	0.49
1:A:75:MET:HB2	1:A:76:PRO:HD3	1.95	0.48
1:A:274:LYS:NZ	1:A:274:LYS:CD	2.69	0.48
1:A:138:ILE:O	1:A:170:SER:HA	2.14	0.46
1:A:206:MET:CE	1:A:206:MET:CG	2.93	0.46
1:A:134:GLY:HA3	1:A:195:LYS:HD3	2.00	0.44
1:A:3:GLU:HG3	1:A:4:TYR:CD1	2.52	0.43
1:A:146:ALA:CB	1:A:146:ALA:N	2.67	0.43
1:A:184:ALA:CB	1:A:211:ALA:CB	2.96	0.43
1:A:71:VAL:HG12	1:A:98:ASN:HD22	1.84	0.43
1:A:202:ASP:OD2	1:A:232:ALA:CB	2.68	0.42
1:A:176:ASP:HB3	1:A:179:LYS:HB3	2.03	0.41

All (4) 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:A:1:ALA:CB	1:A:1:ALA:CB[6_566]	1.19	1.01
1:A:1:ALA:CA	1:A:1:ALA:CB[12_665]	1.33	0.87
1:A:1:ALA:C	1:A:1:ALA:CB[12_665]	2.00	0.20
1:A:1:ALA:N	1:A:1:ALA:CB[12_665]	2.10	0.10

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	286/288 (99%)	267 (93%)	16 (6%)	3 (1%)	12	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	TRP
1	A	227	ASP
1	A	91	ASP

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	222/222 (100%)	210 (95%)	12 (5%)	20 50

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	34	VAL
1	A	127	ASP
1	A	128	LYS
1	A	177	ARG
1	A	178	ILE
1	A	185	THR
1	A	195	LYS
1	A	197	ILE
1	A	202	ASP
1	A	241	MET
1	A	282	ASP

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	105	ASN
1	A	114	ASN
1	A	145	ASN
1	A	191	ASN
1	A	210	GLN
1	A	240	GLN
1	A	248	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 [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	288/288 (100%)	0.24	13 (4%)	38 20	6, 32, 68, 247	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	11.1
1	A	2	ALA	3.3
1	A	180	ALA	2.9
1	A	203	THR	2.8
1	A	173	ALA	2.8
1	A	214	ASN	2.6
1	A	183	VAL	2.6
1	A	174	ASP	2.4
1	A	146	ALA	2.3
1	A	185	THR	2.2
1	A	189	GLN	2.2
1	A	175	TRP	2.2
1	A	210	GLN	2.2

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

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($\text{\AA}^2$)	Q<0.9
2	NI	A	1289	1/1	0.82	0.25	22,22,22,22	1

6.5 Other polymers

There are no such residues in this entry.