



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:48 AM UTC

PDB ID : 3TKK / pdb_00003tkk
Title : Crystal Structure Analysis of a recombinant predicted acetamidase/ formamidase from the thermophile thermoanaerobacter tengcongensis
Authors : Qian, M.; Huang, Q.; Wu, G.; Lai, L.; Tang, Y.; Pei, J.; Kusunoki, M.
Deposited on : 2011-08-26
Resolution : 1.99 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
Mogul : 2022.3.0, CSD as543be (2022)
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

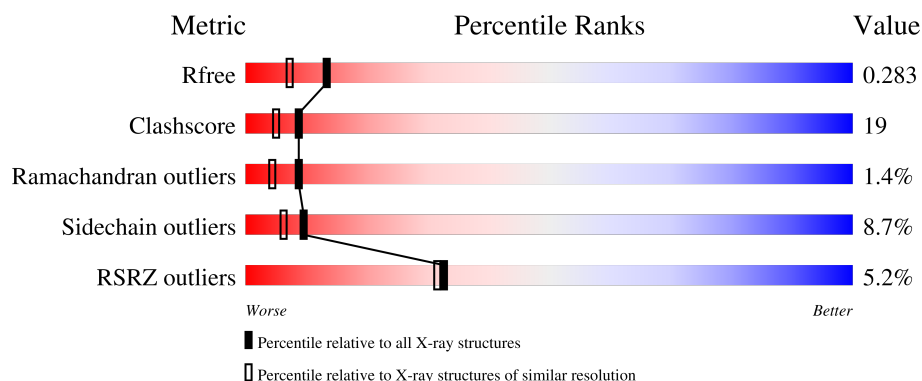
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	301	4% 60% 34% 5%
1	B	301	5% 71% 23% 5%
1	C	301	5% 66% 28% 5%
1	D	301	6% 64% 28% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9872 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 Predicted acetamidase/formamidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2257	1436	369	442	10			
1	B	301	Total	C	N	O	S	0	0	0
			2257	1436	369	442	10			
1	C	301	Total	C	N	O	S	0	0	0
			2257	1436	369	442	10			
1	D	301	Total	C	N	O	S	0	0	0
			2257	1436	369	442	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8R8S5
A	-1	HIS	-	expression tag	UNP Q8R8S5
B	-2	SER	-	expression tag	UNP Q8R8S5
B	-1	HIS	-	expression tag	UNP Q8R8S5
C	-2	SER	-	expression tag	UNP Q8R8S5
C	-1	HIS	-	expression tag	UNP Q8R8S5
D	-2	SER	-	expression tag	UNP Q8R8S5
D	-1	HIS	-	expression tag	UNP Q8R8S5

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

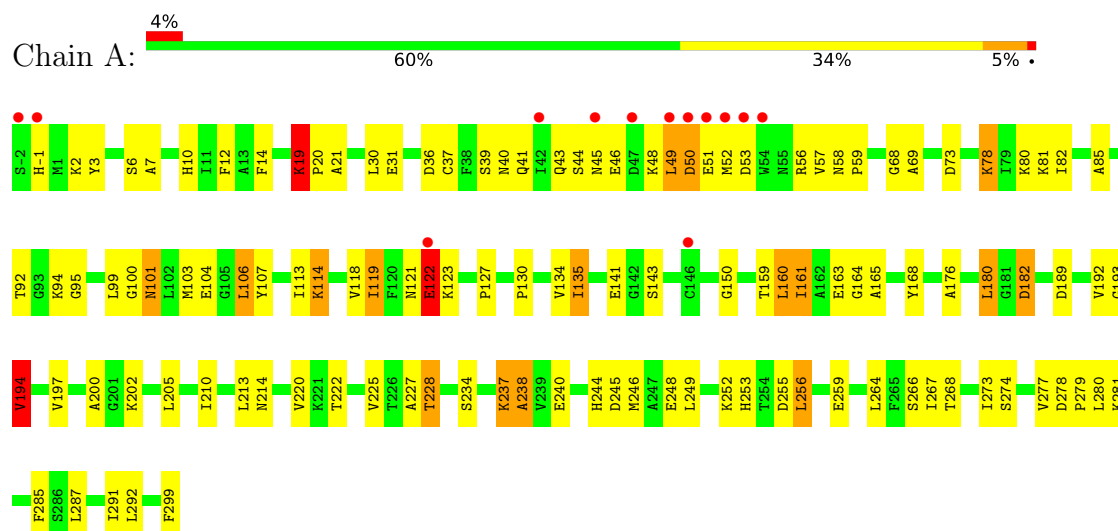
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	292	Total 292	O 292	0	0
4	B	153	Total 153	O 153	0	0
4	C	254	Total 254	O 254	0	0
4	D	136	Total 136	O 136	0	0

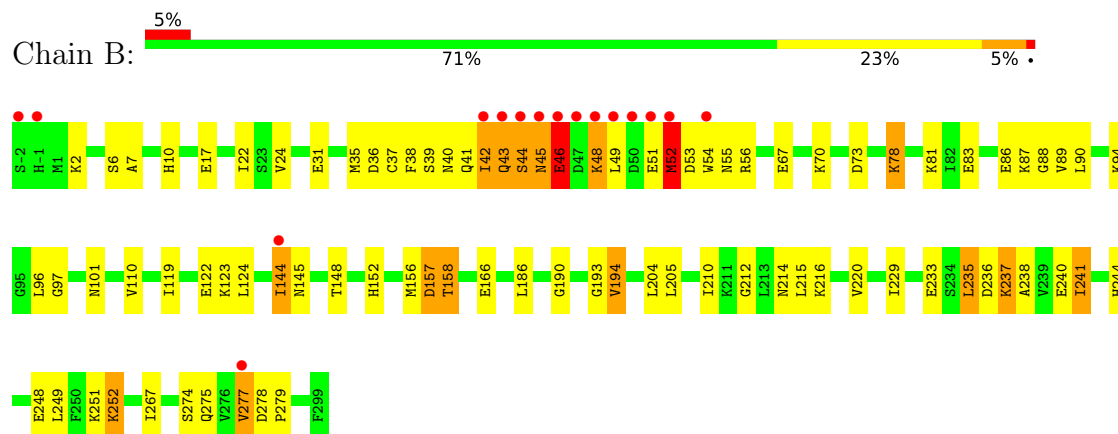
3 Residue-property plots [i](#)

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.

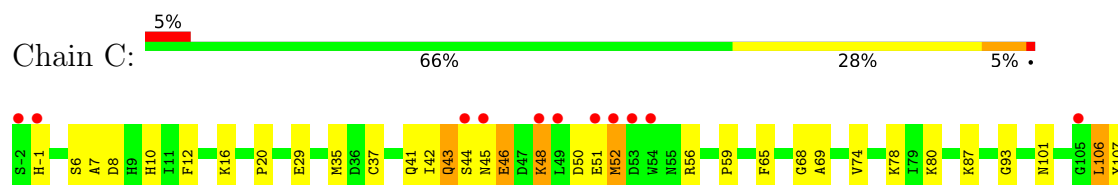
• Molecule 1: Predicted acetamidase/formamidase

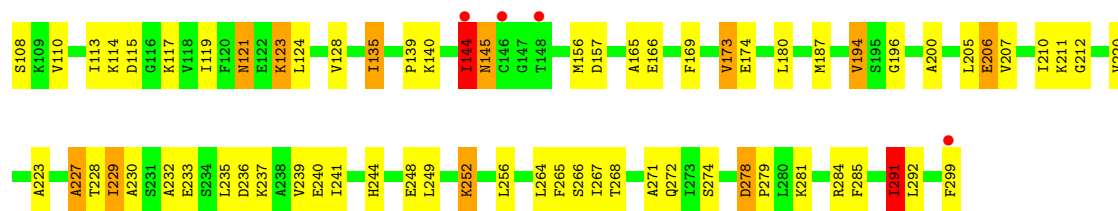


• Molecule 1: Predicted acetamidase/formamidase

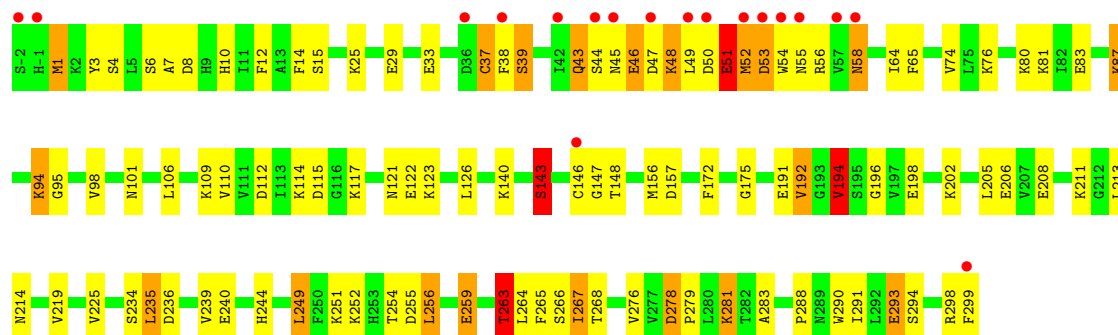


• Molecule 1: Predicted acetamidase/formamidase





● Molecule 1: Predicted acetamidase/formamidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.23Å 152.88Å 100.25Å 90.00° 99.49° 90.00°	Depositor
Resolution (Å)	50.00 – 1.99 50.00 – 1.99	Depositor EDS
% Data completeness (in resolution range)	94.7 (50.00-1.99) 94.7 (50.00-1.99)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.174 , 0.237 0.240 , 0.283	Depositor DCC
R_{free} test set	3985 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.692	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9872	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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: CA, CSD, ZN

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	1.83	38/2285 (1.7%)	1.56	19/3088 (0.6%)
1	B	1.26	6/2285 (0.3%)	1.30	6/3088 (0.2%)
1	C	1.58	21/2285 (0.9%)	1.42	11/3088 (0.4%)
1	D	1.22	5/2285 (0.2%)	1.27	11/3088 (0.4%)
All	All	1.49	70/9140 (0.8%)	1.39	47/12352 (0.4%)

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	1

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	ASN	C-O	9.00	1.28	1.23
1	C	144	ILE	CA-CB	8.81	1.65	1.54
1	A	69	ALA	CA-CB	8.68	1.66	1.53
1	C	267	ILE	N-CA	-8.65	1.37	1.46
1	A	281	LYS	N-CA	8.61	1.56	1.45
1	C	267	ILE	CA-CB	8.12	1.64	1.54
1	D	192	VAL	CB-CG1	-7.35	1.28	1.52
1	A	225	VAL	C-O	7.16	1.31	1.23
1	A	274	SER	CA-C	-7.09	1.45	1.53
1	A	135	ILE	CG1-CD1	6.92	1.78	1.51
1	A	118	VAL	N-CA	-6.84	1.39	1.46
1	B	252	LYS	C-O	-6.75	1.15	1.24
1	A	192	VAL	N-CA	6.70	1.54	1.46
1	C	206	GLU	C-O	6.69	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	268	THR	C-O	-6.66	1.15	1.24
1	A	274	SER	C-N	6.65	1.41	1.33
1	D	194	VAL	N-CA	6.54	1.54	1.46
1	A	277	VAL	CA-CB	6.41	1.63	1.54
1	A	161	ILE	CG1-CD1	6.38	1.76	1.51
1	C	165	ALA	CA-CB	-6.37	1.43	1.53
1	A	234	SER	CA-C	-6.25	1.45	1.52
1	C	232	ALA	N-CA	6.20	1.53	1.46
1	A	59	PRO	C-O	-6.20	1.16	1.23
1	A	168	TYR	CA-C	-6.18	1.45	1.52
1	A	160	LEU	CA-C	6.18	1.61	1.52
1	A	165	ALA	CA-CB	-6.16	1.43	1.53
1	A	182	ASP	CA-C	-6.16	1.45	1.53
1	A	273	ILE	C-O	6.14	1.31	1.24
1	C	227	ALA	N-CA	6.13	1.53	1.46
1	C	135	ILE	CA-CB	-6.12	1.46	1.54
1	B	88	GLY	N-CA	6.05	1.51	1.45
1	A	238	ALA	CA-CB	5.99	1.62	1.53
1	A	85	ALA	CA-CB	-5.96	1.43	1.53
1	C	271	ALA	CA-CB	5.89	1.62	1.53
1	A	92	THR	C-O	-5.78	1.18	1.24
1	A	189	ASP	C-O	5.75	1.30	1.23
1	B	52	MET	C-N	-5.74	1.24	1.33
1	B	238	ALA	CA-CB	5.72	1.62	1.53
1	A	280	LEU	C-O	5.68	1.31	1.23
1	A	192	VAL	CA-CB	5.65	1.60	1.54
1	C	200	ALA	CA-CB	5.65	1.62	1.53
1	C	229	ILE	CA-CB	5.64	1.62	1.54
1	C	228	THR	N-CA	-5.63	1.38	1.45
1	A	220	VAL	CA-C	-5.59	1.46	1.52
1	A	176	ALA	CA-CB	5.59	1.62	1.53
1	B	267	ILE	CA-CB	5.51	1.61	1.54
1	A	267	ILE	C-O	5.50	1.30	1.24
1	A	159	THR	CA-CB	5.42	1.62	1.53
1	A	163	GLU	N-CA	-5.39	1.39	1.46
1	B	96	LEU	N-CA	5.39	1.52	1.46
1	A	150	GLY	N-CA	5.37	1.51	1.44
1	C	223	ALA	CA-CB	5.35	1.62	1.53
1	C	-1	HIS	C-N	5.34	1.40	1.33
1	A	197	VAL	CA-C	5.31	1.59	1.52
1	C	173	VAL	C-O	-5.27	1.18	1.23
1	D	283	ALA	C-O	5.27	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	128	VAL	CA-CB	-5.24	1.49	1.54
1	C	69	ALA	CA-CB	5.23	1.60	1.53
1	C	74	VAL	C-O	5.23	1.29	1.24
1	C	239	VAL	CA-CB	5.23	1.60	1.54
1	C	230	ALA	C-O	5.17	1.30	1.23
1	A	159	THR	CB-CG2	5.12	1.69	1.52
1	D	225	VAL	C-O	5.12	1.29	1.23
1	A	100	GLY	C-O	5.09	1.31	1.23
1	A	130	PRO	N-CA	5.08	1.53	1.47
1	A	180	LEU	N-CA	5.07	1.52	1.45
1	D	58	ASN	C-O	5.05	1.26	1.23
1	A	122	GLU	C-O	-5.04	1.18	1.24
1	A	14	PHE	N-CA	5.03	1.52	1.46
1	A	134	VAL	CA-CB	-5.02	1.47	1.54

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	GLY	N-CA-C	-8.72	104.31	114.69
1	C	278	ASP	CA-C-N	-8.29	111.19	119.56
1	C	278	ASP	C-N-CA	-8.29	111.19	119.56
1	D	278	ASP	CA-C-N	-8.28	110.41	119.19
1	D	278	ASP	C-N-CA	-8.28	110.41	119.19
1	A	58	ASN	CB-CA-C	-7.24	103.91	110.71
1	C	169	PHE	CA-C-N	-7.02	112.76	119.85
1	C	169	PHE	C-N-CA	-7.02	112.76	119.85
1	C	210	ILE	CB-CA-C	-6.69	100.86	110.83
1	D	293	GLU	N-CA-C	-6.64	104.12	111.82
1	A	228	THR	N-CA-C	-6.49	100.88	110.48
1	A	245	ASP	N-CA-C	-6.28	104.52	111.36
1	C	196	GLY	N-CA-C	-6.18	103.76	112.60
1	A	99	LEU	N-CA-C	-6.02	105.86	112.72
1	A	237	LYS	CA-C-N	-5.98	112.27	120.28
1	A	237	LYS	C-N-CA	-5.98	112.27	120.28
1	A	101	ASN	N-CA-C	-5.93	106.02	113.20
1	A	200	ALA	N-CA-C	-5.93	101.99	110.59
1	A	19	LYS	CA-C-N	5.78	125.72	119.76
1	A	19	LYS	C-N-CA	5.78	125.72	119.76
1	B	190	GLY	N-CA-C	-5.78	106.74	114.25
1	B	277	VAL	CB-CA-C	-5.78	104.60	111.65
1	C	265	PHE	N-CA-C	-5.72	105.13	111.36
1	A	222	THR	N-CA-C	-5.67	100.80	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	143	SER	N-CA-C	-5.67	100.44	109.23
1	D	265	PHE	N-CA-C	-5.66	105.25	111.82
1	D	196	GLY	N-CA-C	-5.63	104.54	112.60
1	A	21	ALA	N-CA-C	-5.62	105.15	112.23
1	D	58	ASN	CB-CA-C	-5.61	105.44	110.71
1	C	291	ILE	N-CA-C	5.58	115.78	110.42
1	A	73	ASP	CA-C-N	-5.55	115.23	122.94
1	A	73	ASP	C-N-CA	-5.55	115.23	122.94
1	C	241	ILE	N-CA-C	-5.47	105.19	110.72
1	A	95	GLY	CA-C-N	-5.45	115.48	123.00
1	A	95	GLY	C-N-CA	-5.45	115.48	123.00
1	D	147	GLY	N-CA-C	5.37	120.58	114.67
1	B	157	ASP	CA-C-N	-5.30	115.53	123.00
1	B	157	ASP	C-N-CA	-5.30	115.53	123.00
1	D	263	THR	N-CA-CB	-5.28	102.42	110.07
1	B	48	LYS	N-CA-C	5.25	117.68	107.71
1	B	241	ILE	N-CA-C	-5.22	105.62	110.53
1	A	210	ILE	CB-CA-C	-5.22	103.74	110.84
1	D	64	ILE	CB-CA-C	-5.21	103.85	110.98
1	D	148	THR	N-CA-C	5.19	116.93	109.04
1	C	68	GLY	N-CA-C	-5.12	108.60	114.69
1	C	93	GLY	N-CA-C	5.09	117.61	110.38
1	A	68	GLY	N-CA-C	-5.08	108.64	114.69

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	LEU	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	2257	0	2295	75	1
1	B	2257	0	2293	93	0
1	C	2257	0	2294	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2257	0	2293	112	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	292	0	0	14	1
4	B	153	0	0	9	0
4	C	254	0	0	14	0
4	D	136	0	0	11	0
All	All	9872	0	9175	340	1

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 19.

All (340) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ASN:HB3	1:B:110:VAL:CG2	1.22	1.57
1:A:135:ILE:CD1	1:A:135:ILE:CG1	1.78	1.56
1:A:161:ILE:CD1	1:A:161:ILE:CG1	1.76	1.56
1:B:45:ASN:CB	1:B:110:VAL:HG23	1.54	1.33
1:B:45:ASN:CB	1:B:110:VAL:CG2	2.05	1.33
1:B:216:LYS:HD2	4:B:506:HOH:O	1.45	1.12
1:A:31:GLU:OE1	1:A:202:LYS:HE2	1.49	1.11
1:B:45:ASN:HB2	1:B:110:VAL:HG23	1.31	1.09
1:B:45:ASN:HB3	1:B:110:VAL:HG21	1.10	1.09
1:B:43:GLN:HG3	1:B:87:LYS:NZ	1.68	1.06
1:B:43:GLN:O	1:B:110:VAL:HG21	1.53	1.06
1:C:51:GLU:HB2	4:C:786:HOH:O	1.57	1.05
1:A:143:SER:O	4:A:455:HOH:O	1.76	1.02
1:D:58:ASN:HB3	1:D:146:CYS:SG	2.02	1.00
1:B:44:SER:O	1:B:45:ASN:ND2	1.96	0.98
1:D:254:THR:HG22	1:D:256:LEU:H	1.27	0.98
1:D:15:SER:HB2	1:D:143:SER:HB2	1.46	0.97
1:D:44:SER:HB2	1:D:48:LYS:HG2	1.46	0.97
1:D:45:ASN:HA	4:D:651:HOH:O	1.63	0.96
1:A:49:LEU:HD12	1:A:50:ASP:H	1.28	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:ASN:HB2	1:D:110:VAL:HG23	1.48	0.95
1:C:29:GLU:OE2	1:C:80:LYS:NZ	2.00	0.94
1:A:31:GLU:OE1	1:A:202:LYS:CE	2.17	0.93
1:B:45:ASN:HB3	1:B:110:VAL:CB	2.01	0.91
1:A:114:LYS:HE3	4:A:398:HOH:O	1.71	0.91
1:B:43:GLN:HG3	1:B:87:LYS:HZ3	1.28	0.90
1:C:144:ILE:HD12	1:C:144:ILE:H	1.37	0.90
1:A:7:ALA:O	1:A:10:HIS:HD2	1.54	0.90
1:A:41:GLN:HE22	1:A:53:ASP:H	1.14	0.90
1:C:212:GLY:O	1:D:46:GLU:HG3	1.72	0.89
1:C:121:ASN:C	1:C:121:ASN:HD22	1.79	0.88
1:A:31:GLU:HB3	1:A:202:LYS:HE3	1.55	0.88
1:C:220:VAL:HG23	1:C:229:ILE:HD11	1.56	0.87
1:B:53:ASP:O	1:B:55:ASN:N	2.08	0.86
1:A:44:SER:O	1:A:48:LYS:HB2	1.74	0.86
1:D:299:PHE:OXT	4:D:658:HOH:O	1.92	0.86
1:D:44:SER:O	1:D:45:ASN:HB3	1.76	0.85
1:D:12:PHE:O	1:D:146:CYS:HB2	1.75	0.85
1:A:43:GLN:H	1:A:48:LYS:HD3	1.41	0.84
1:D:50:ASP:HB3	1:D:106:LEU:HD13	1.59	0.84
1:D:58:ASN:CB	1:D:146:CYS:SG	2.65	0.83
1:A:256:LEU:HD21	4:C:466:HOH:O	1.79	0.82
1:B:53:ASP:O	1:B:53:ASP:OD1	1.98	0.81
1:D:276:VAL:HB	1:D:281:LYS:HE3	1.60	0.81
1:B:278:ASP:HB3	1:B:279:PRO:HD2	1.60	0.81
1:D:45:ASN:HB2	1:D:110:VAL:CG2	2.10	0.81
1:D:249:LEU:HD21	1:D:299:PHE:HZ	1.46	0.80
1:B:248:GLU:OE2	1:B:252:LYS:HE3	1.81	0.80
1:C:121:ASN:ND2	1:C:123:LYS:H	1.80	0.80
1:B:43:GLN:HG3	1:B:87:LYS:HZ1	1.47	0.79
1:C:121:ASN:ND2	1:C:124:LEU:H	1.79	0.79
1:C:45:ASN:OD1	4:C:603:HOH:O	2.00	0.79
1:A:255:ASP:OD2	4:A:414:HOH:O	2.01	0.79
1:D:299:PHE:HB2	4:D:799:HOH:O	1.83	0.79
1:C:211:LYS:O	4:C:706:HOH:O	2.02	0.78
1:B:43:GLN:CG	1:B:87:LYS:NZ	2.46	0.77
1:D:249:LEU:HD21	1:D:299:PHE:CZ	2.19	0.77
1:D:50:ASP:O	1:D:51:GLU:HB3	1.84	0.76
1:B:235:LEU:HB2	1:D:236:ASP:OD1	1.86	0.76
1:A:104:GLU:OE2	4:A:392:HOH:O	2.03	0.75
1:B:237:LYS:HE2	1:B:241:ILE:HG13	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:CD1	1:A:135:ILE:CB	2.66	0.74
1:B:45:ASN:CB	1:B:110:VAL:HG21	1.96	0.74
1:C:139:PRO:HG3	1:C:144:ILE:HD11	1.69	0.74
1:C:117:LYS:NZ	4:C:627:HOH:O	2.14	0.73
1:C:220:VAL:CG2	1:C:229:ILE:HD11	2.19	0.73
1:B:278:ASP:HB3	1:B:279:PRO:CD	2.19	0.73
1:D:44:SER:HB2	1:D:48:LYS:CG	2.18	0.73
1:C:139:PRO:CG	1:C:144:ILE:HD11	2.20	0.72
1:C:44:SER:HB2	1:C:48:LYS:HE2	1.72	0.71
1:D:254:THR:CG2	1:D:256:LEU:HB2	2.19	0.71
1:A:279:PRO:O	4:A:334:HOH:O	2.07	0.71
1:A:41:GLN:NE2	1:A:53:ASP:H	1.86	0.71
1:C:220:VAL:HG23	1:C:229:ILE:CD1	2.20	0.71
1:D:254:THR:HG22	1:D:256:LEU:N	2.04	0.70
1:C:7:ALA:O	1:C:10:HIS:HD2	1.74	0.70
1:D:264:LEU:O	1:D:268:THR:HG22	1.90	0.70
1:B:2:LYS:HE2	1:B:31:GLU:HG3	1.73	0.69
1:C:144:ILE:HD12	1:C:144:ILE:N	2.02	0.69
1:D:46:GLU:HA	1:D:46:GLU:OE1	1.90	0.69
1:B:45:ASN:CG	1:B:46:GLU:N	2.51	0.69
1:B:42:ILE:HD13	1:B:48:LYS:O	1.91	0.69
1:C:121:ASN:C	1:C:121:ASN:ND2	2.51	0.68
1:B:43:GLN:CG	1:B:87:LYS:HZ1	2.05	0.68
1:C:121:ASN:OD1	4:C:466:HOH:O	2.12	0.68
1:C:248:GLU:OE2	1:C:252:LYS:HD2	1.92	0.68
1:B:24:VAL:O	1:B:67:GLU:HG3	1.94	0.68
1:D:239:VAL:CG2	4:D:597:HOH:O	2.41	0.68
1:B:123:LYS:NZ	1:D:294:SER:O	2.27	0.68
1:B:237:LYS:HE3	1:B:237:LYS:O	1.95	0.67
1:B:78:LYS:HG3	1:B:166:GLU:HG2	1.76	0.67
1:C:41:GLN:NE2	1:C:52:MET:HE3	2.10	0.66
1:B:237:LYS:HE3	1:B:237:LYS:HA	1.77	0.66
1:D:214:ASN:HB3	4:D:481:HOH:O	1.95	0.66
1:A:49:LEU:HD12	1:A:50:ASP:N	2.07	0.65
1:D:44:SER:O	1:D:45:ASN:CB	2.43	0.65
1:A:122:GLU:H	1:A:122:GLU:CD	2.04	0.65
1:D:254:THR:HG21	1:D:256:LEU:HB2	1.76	0.65
1:C:121:ASN:HD21	1:C:124:LEU:H	1.41	0.65
1:C:44:SER:O	1:C:46:GLU:N	2.26	0.64
1:D:276:VAL:CB	1:D:281:LYS:HE3	2.28	0.64
1:C:43:GLN:OE1	4:C:819:HOH:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ASP:OD2	4:D:329:HOH:O	2.14	0.64
1:A:248:GLU:OE2	1:A:252:LYS:HD2	1.98	0.64
1:B:237:LYS:HE3	1:B:237:LYS:CA	2.28	0.63
1:A:12:PHE:CE1	1:A:56:ARG:HA	2.33	0.63
1:D:240:GLU:O	1:D:244:HIS:HD2	1.81	0.63
1:C:278:ASP:HB3	1:C:279:PRO:HD2	1.80	0.63
1:D:1:MET:HG2	1:D:3:TYR:CZ	2.34	0.62
1:D:140:LYS:HG2	1:D:172:PHE:HB3	1.81	0.62
1:D:94:LYS:HE2	1:D:95:GLY:N	2.15	0.62
1:A:205:LEU:HD12	1:A:205:LEU:C	2.25	0.61
1:A:41:GLN:HE22	1:A:53:ASP:N	1.93	0.61
1:D:48:LYS:CE	4:D:666:HOH:O	2.49	0.61
1:C:240:GLU:O	1:C:244:HIS:HD2	1.83	0.61
1:C:78:LYS:HD3	1:C:166:GLU:HG2	1.82	0.60
1:C:212:GLY:O	1:D:46:GLU:C	2.44	0.60
1:D:7:ALA:H	1:D:33:GLU:CG	2.14	0.60
1:A:113:ILE:C	1:A:114:LYS:HG2	2.26	0.60
1:B:56:ARG:HG2	1:B:56:ARG:HH11	1.67	0.60
1:D:259:GLU:O	1:D:263:THR:HB	2.00	0.60
1:C:44:SER:C	1:C:46:GLU:H	2.10	0.60
1:B:122:GLU:CD	1:B:122:GLU:H	2.09	0.60
1:D:15:SER:HB2	1:D:143:SER:CB	2.29	0.59
1:A:278:ASP:HB3	1:A:279:PRO:CD	2.32	0.59
1:D:278:ASP:HB3	1:D:279:PRO:CD	2.33	0.59
1:B:144:ILE:HG12	1:B:152:HIS:CE1	2.37	0.59
1:C:212:GLY:C	1:D:46:GLU:HG3	2.28	0.58
1:C:10:HIS:HE1	4:C:417:HOH:O	1.87	0.58
1:D:47:ASP:O	1:D:49:LEU:N	2.29	0.58
1:C:236:ASP:O	1:C:240:GLU:HG3	2.04	0.57
1:A:141:GLU:HB2	4:A:337:HOH:O	2.04	0.57
1:B:43:GLN:H	1:B:48:LYS:HE3	1.69	0.57
1:B:240:GLU:O	1:B:244:HIS:HD2	1.86	0.57
1:D:276:VAL:CA	1:D:281:LYS:HE3	2.35	0.57
1:A:-1:HIS:N	4:A:543:HOH:O	2.37	0.57
1:B:97:GLY:HA2	1:B:277:VAL:HG12	1.87	0.57
1:A:7:ALA:O	1:A:10:HIS:CD2	2.46	0.56
1:C:205:LEU:HD12	1:C:205:LEU:C	2.30	0.56
1:D:278:ASP:HB3	1:D:279:PRO:HD2	1.85	0.56
1:A:43:GLN:HB2	1:A:48:LYS:HZ2	1.70	0.56
1:B:216:LYS:CD	4:B:506:HOH:O	2.24	0.56
1:C:121:ASN:ND2	1:C:123:LYS:N	2.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:GLN:CD	1:B:52:MET:HB3	2.30	0.56
1:C:42:ILE:O	1:C:42:ILE:HG22	2.06	0.56
1:A:240:GLU:O	1:A:244:HIS:HD2	1.89	0.55
1:A:36:ASP:H	1:A:40:ASN:ND2	2.04	0.55
1:B:2:LYS:HE2	1:B:31:GLU:CG	2.36	0.55
1:C:46:GLU:C	1:C:48:LYS:H	2.15	0.55
1:D:7:ALA:N	1:D:33:GLU:HG2	2.22	0.55
1:D:290:TRP:HA	1:D:293:GLU:HG3	1.87	0.55
1:D:205:LEU:C	1:D:205:LEU:HD12	2.31	0.55
1:B:157:ASP:HB2	1:B:275:GLN:HG2	1.89	0.55
1:D:7:ALA:H	1:D:33:GLU:HG2	1.72	0.55
1:D:7:ALA:HB2	1:D:33:GLU:HG3	1.89	0.55
1:B:67:GLU:OE1	4:B:363:HOH:O	2.18	0.55
1:B:36:ASP:H	1:B:40:ASN:HD21	1.55	0.54
1:B:119:ILE:HD12	1:B:119:ILE:H	1.71	0.54
1:D:44:SER:C	1:D:46:GLU:H	2.14	0.54
1:A:78:LYS:HB2	1:A:78:LYS:NZ	2.23	0.54
1:A:6:SER:HB3	4:A:360:HOH:O	2.07	0.54
1:A:51:GLU:HG3	1:A:51:GLU:O	2.06	0.54
1:C:121:ASN:HD21	1:C:124:LEU:N	2.04	0.54
1:D:37:CSD:HB3	1:D:198:GLU:OE1	2.07	0.54
1:D:122:GLU:CD	1:D:122:GLU:H	2.15	0.54
1:D:239:VAL:HG23	1:D:240:GLU:N	2.21	0.54
1:D:251:LYS:O	4:D:556:HOH:O	2.18	0.54
1:C:248:GLU:OE2	1:C:252:LYS:CD	2.55	0.54
1:A:119:ILE:N	1:A:119:ILE:HD13	2.23	0.53
1:C:272:GLN:HE21	1:C:284:ARG:HE	1.55	0.53
1:D:7:ALA:O	1:D:10:HIS:HD2	1.91	0.53
1:A:213:LEU:HD22	1:A:299:PHE:HB3	1.91	0.53
1:B:36:ASP:H	1:B:40:ASN:ND2	2.07	0.53
1:D:94:LYS:HE2	1:D:95:GLY:H	1.73	0.52
1:A:122:GLU:CD	1:A:122:GLU:N	2.66	0.52
1:A:264:LEU:O	1:A:268:THR:HG22	2.08	0.52
1:C:135:ILE:HG23	1:C:135:ILE:O	2.07	0.52
1:A:237:LYS:O	1:A:238:ALA:C	2.50	0.52
1:C:237:LYS:HD2	1:C:237:LYS:O	2.09	0.52
1:D:157:ASP:OD2	1:D:191:GLU:OE1	2.28	0.52
1:B:144:ILE:HD13	1:B:148:THR:O	2.10	0.52
1:A:46:GLU:CD	1:B:212:GLY:HA2	2.35	0.51
1:D:117:LYS:HA	1:D:126:LEU:O	2.11	0.51
1:A:278:ASP:HB3	1:A:279:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:PHE:O	1:D:56:ARG:O	2.29	0.51
1:A:244:HIS:HE1	1:C:101:ASN:OD1	1.93	0.51
1:D:156:MET:O	1:D:157:ASP:C	2.54	0.51
1:C:206:GLU:HG2	1:C:207:VAL:N	2.25	0.51
1:D:50:ASP:O	1:D:51:GLU:CB	2.58	0.51
1:B:46:GLU:C	1:B:48:LYS:H	2.19	0.50
1:B:70:LYS:HB2	1:B:73:ASP:OD2	2.11	0.50
1:D:38:PHE:O	1:D:39:SER:HB2	2.10	0.50
1:B:7:ALA:O	1:B:10:HIS:HD2	1.95	0.50
1:D:29:GLU:OE2	1:D:80:LYS:NZ	2.33	0.50
1:A:193:GLY:O	1:A:194:VAL:HB	2.11	0.50
1:B:42:ILE:HG23	1:B:89:VAL:HG21	1.94	0.50
1:B:49:LEU:HB2	1:B:51:GLU:HG2	1.94	0.50
1:C:44:SER:HB2	1:C:48:LYS:HG2	1.94	0.50
1:D:46:GLU:HB2	4:D:649:HOH:O	2.10	0.50
1:A:78:LYS:HD2	1:A:80:LYS:HE2	1.93	0.49
1:B:101:ASN:OD1	1:D:244:HIS:HE1	1.95	0.49
1:C:272:GLN:NE2	1:C:284:ARG:HE	2.09	0.49
1:D:276:VAL:HB	1:D:281:LYS:CE	2.37	0.49
1:B:45:ASN:HB3	1:B:110:VAL:HB	1.90	0.49
1:D:43:GLN:OE1	1:D:43:GLN:N	2.45	0.49
1:C:278:ASP:HB3	1:C:279:PRO:CD	2.43	0.49
1:D:52:MET:O	1:D:53:ASP:HB2	2.12	0.49
1:B:42:ILE:HG23	4:B:356:HOH:O	2.12	0.49
1:B:144:ILE:O	1:B:144:ILE:HD12	2.11	0.49
1:D:239:VAL:HG21	4:D:597:HOH:O	2.07	0.49
1:B:220:VAL:CG1	1:B:229:ILE:HD11	2.42	0.49
1:D:38:PHE:O	1:D:39:SER:CB	2.61	0.49
1:D:87:LYS:O	1:D:87:LYS:HG2	2.13	0.49
1:D:45:ASN:CG	1:D:110:VAL:H	2.21	0.49
1:D:54:TRP:C	1:D:56:ARG:H	2.22	0.48
1:C:20:PRO:HB3	1:C:65:PHE:HB2	1.95	0.48
1:C:299:PHE:HD1	4:C:335:HOH:O	1.95	0.48
1:D:45:ASN:OD1	1:D:109:LYS:HA	2.13	0.48
1:B:237:LYS:HE3	1:B:237:LYS:C	2.38	0.48
1:D:219:VAL:HG11	1:D:299:PHE:CE1	2.49	0.48
1:D:254:THR:HG22	1:D:256:LEU:HB2	1.94	0.48
1:C:50:ASP:HB2	1:C:106:LEU:HD12	1.94	0.48
1:D:98:VAL:HB	1:D:192:VAL:HG13	1.96	0.48
1:A:-1:HIS:HE1	4:A:634:HOH:O	1.95	0.48
1:D:1:MET:HE3	1:D:1:MET:HB2	1.80	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ASN:CG	1:B:110:VAL:HB	2.38	0.47
1:C:113:ILE:O	1:C:114:LYS:HD3	2.14	0.47
1:D:58:ASN:HB2	1:D:146:CYS:SG	2.51	0.47
1:B:158:THR:HG22	1:B:274:SER:CB	2.44	0.47
1:A:43:GLN:CB	1:A:48:LYS:HZ2	2.27	0.47
1:A:161:ILE:CD1	1:A:161:ILE:CB	2.79	0.47
1:B:90:LEU:HD13	1:D:263:THR:HG23	1.97	0.47
1:D:254:THR:HG22	1:D:255:ASP:N	2.29	0.47
1:D:121:ASN:ND2	4:D:529:HOH:O	2.45	0.47
1:B:193:GLY:H	1:D:266:SER:HB2	1.78	0.47
1:C:87:LYS:CE	4:C:373:HOH:O	2.60	0.47
1:A:114:LYS:CE	4:A:398:HOH:O	2.46	0.46
1:B:237:LYS:O	1:B:237:LYS:CE	2.63	0.46
1:B:251:LYS:O	1:B:251:LYS:HG2	2.13	0.46
1:C:6:SER:HB2	1:C:8:ASP:OD1	2.16	0.46
1:A:113:ILE:O	1:A:114:LYS:HG2	2.14	0.46
1:C:157:ASP:O	1:C:187:MET:HE1	2.15	0.46
1:C:240:GLU:O	1:C:244:HIS:CD2	2.67	0.46
1:A:253:HIS:HE1	4:A:408:HOH:O	1.99	0.46
1:C:12:PHE:CE1	1:C:56:ARG:HA	2.50	0.46
1:B:220:VAL:HG12	1:B:229:ILE:HD11	1.98	0.46
1:A:94:LYS:HG3	1:A:103:MET:O	2.16	0.46
1:B:122:GLU:CD	1:B:122:GLU:N	2.74	0.46
1:C:139:PRO:HG2	1:C:144:ILE:HD11	1.96	0.46
1:C:174:GLU:HG2	4:C:741:HOH:O	2.15	0.46
1:C:43:GLN:HE21	1:C:43:GLN:HB3	1.52	0.46
1:B:94:LYS:NZ	4:B:646:HOH:O	2.48	0.46
1:A:36:ASP:H	1:A:40:ASN:HD21	1.62	0.45
1:B:244:HIS:HE1	1:D:101:ASN:OD1	1.98	0.45
1:C:43:GLN:C	1:C:45:ASN:N	2.74	0.45
1:B:193:GLY:H	1:D:266:SER:CB	2.29	0.45
1:A:182:ASP:CG	1:A:182:ASP:O	2.58	0.45
1:B:119:ILE:HD12	1:B:119:ILE:N	2.31	0.45
1:B:233:GLU:HG3	4:B:430:HOH:O	2.16	0.45
1:C:240:GLU:OE2	4:C:362:HOH:O	2.21	0.45
1:A:46:GLU:HG2	1:B:214:ASN:ND2	2.31	0.45
1:D:65:PHE:CE1	1:D:175:GLY:HA3	2.52	0.45
1:D:44:SER:CB	1:D:48:LYS:HG2	2.33	0.45
1:A:51:GLU:O	1:A:51:GLU:CG	2.65	0.44
1:D:7:ALA:O	1:D:10:HIS:CD2	2.69	0.44
1:A:94:LYS:HE2	1:A:104:GLU:OE1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:GLY:O	1:D:46:GLU:O	2.36	0.44
1:A:214:ASN:ND2	4:A:769:HOH:O	2.41	0.44
1:C:156:MET:O	1:C:157:ASP:C	2.60	0.44
1:D:49:LEU:O	1:D:50:ASP:C	2.60	0.44
1:A:82:ILE:HD13	1:A:82:ILE:HG21	1.75	0.44
1:A:180:LEU:HD23	1:A:180:LEU:N	2.32	0.44
1:B:144:ILE:HD11	1:B:152:HIS:NE2	2.32	0.44
1:B:7:ALA:HB1	1:B:35:MET:HG3	1.99	0.44
1:A:228:THR:HB	4:A:304:HOH:O	2.18	0.44
1:A:101:ASN:OD1	1:C:244:HIS:HE1	2.00	0.44
1:A:39:SER:O	1:A:40:ASN:HB2	2.18	0.43
1:C:114:LYS:HD3	1:C:114:LYS:HA	1.73	0.43
1:C:248:GLU:HG3	1:C:252:LYS:HD3	1.99	0.43
1:B:41:GLN:OE1	1:B:52:MET:HB3	2.18	0.43
1:D:1:MET:HG2	1:D:3:TYR:CE2	2.53	0.43
1:B:158:THR:HG22	1:B:274:SER:HB3	2.00	0.43
1:D:293:GLU:C	1:D:293:GLU:CD	2.86	0.43
1:A:31:GLU:CB	1:A:202:LYS:HE3	2.38	0.43
1:B:186:LEU:HG	1:D:267:ILE:O	2.19	0.43
1:B:216:LYS:HB3	4:B:432:HOH:O	2.18	0.43
1:C:35:MET:HB2	1:C:59:PRO:HG2	2.00	0.43
1:D:6:SER:HA	1:D:33:GLU:HG2	2.01	0.43
1:A:2:LYS:HE2	1:A:31:GLU:OE2	2.19	0.43
1:C:206:GLU:OE1	4:C:336:HOH:O	2.21	0.43
1:B:156:MET:O	1:B:158:THR:HG22	2.18	0.43
1:D:14:PHE:O	1:D:143:SER:HA	2.18	0.43
1:A:246:MET:HE3	1:A:287:LEU:HD12	1.99	0.43
1:B:53:ASP:C	1:B:55:ASN:N	2.77	0.42
1:B:81:LYS:HB2	1:B:204:LEU:HB3	2.00	0.42
1:C:7:ALA:O	1:C:10:HIS:CD2	2.63	0.42
1:D:12:PHE:CE1	1:D:56:ARG:HA	2.54	0.42
1:D:1:MET:HG2	1:D:3:TYR:OH	2.20	0.42
1:D:44:SER:C	1:D:46:GLU:N	2.78	0.42
1:D:81:LYS:HE3	1:D:81:LYS:HB2	1.56	0.42
1:D:83:GLU:OE2	1:D:202:LYS:HE3	2.20	0.42
1:C:45:ASN:HA	1:C:110:VAL:HG23	2.02	0.42
1:D:288:PRO:HD2	1:D:291:ILE:HG13	2.02	0.42
1:D:76:LYS:HE2	1:D:208:GLU:OE2	2.20	0.42
1:A:-1:HIS:CE1	4:A:634:HOH:O	2.72	0.42
1:A:227:ALA:HA	1:A:285:PHE:O	2.20	0.42
1:B:45:ASN:CB	1:B:110:VAL:HB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:MET:HE2	1:B:39:SER:C	2.45	0.42
1:B:144:ILE:HD12	1:B:145:ASN:O	2.19	0.42
1:B:193:GLY:HA2	4:B:319:HOH:O	2.20	0.42
1:B:215:LEU:HD23	1:B:215:LEU:HA	1.91	0.42
1:C:46:GLU:C	1:C:48:LYS:N	2.77	0.42
1:D:7:ALA:H	1:D:33:GLU:CD	2.28	0.42
1:B:236:ASP:OD2	1:D:234:SER:HB2	2.19	0.41
1:C:123:LYS:NZ	1:C:123:LYS:HB2	2.35	0.41
1:A:43:GLN:H	1:A:48:LYS:CD	2.20	0.41
1:C:227:ALA:HA	1:C:285:PHE:O	2.20	0.41
1:B:237:LYS:NZ	1:B:240:GLU:OE1	2.52	0.41
1:D:74:VAL:HG21	1:D:213:LEU:HD23	2.01	0.41
1:A:121:ASN:HB2	1:A:122:GLU:OE1	2.20	0.41
1:B:236:ASP:OD1	1:D:235:LEU:HB2	2.20	0.41
1:D:37:CSD:O	1:D:58:ASN:N	2.47	0.41
1:C:264:LEU:HD21	1:C:291:ILE:CG2	2.50	0.41
1:D:259:GLU:CD	1:D:259:GLU:H	2.29	0.41
1:A:119:ILE:N	1:A:119:ILE:CD1	2.84	0.41
1:B:38:PHE:O	1:B:41:GLN:HG3	2.21	0.41
1:D:240:GLU:O	1:D:244:HIS:CD2	2.68	0.41
1:C:274:SER:HA	4:C:304:HOH:O	2.21	0.41
1:C:123:LYS:NZ	1:C:123:LYS:CB	2.84	0.40
1:B:278:ASP:O	1:B:279:PRO:C	2.63	0.40
1:C:114:LYS:HB2	1:C:119:ILE:HD11	2.03	0.40
1:D:254:THR:CG2	1:D:255:ASP:N	2.83	0.40
1:A:19:LYS:HA	1:A:20:PRO:HD3	1.91	0.40
1:B:67:GLU:HB3	4:B:363:HOH:O	2.20	0.40
1:C:235:LEU:HA	1:C:235:LEU:HD23	1.81	0.40
1:D:114:LYS:O	1:D:115:ASP:C	2.64	0.40
1:A:3:TYR:O	1:A:30:LEU:HA	2.21	0.40
1:A:106:LEU:HD13	1:A:107:TYR:H	1.86	0.40
1:A:193:GLY:O	1:A:194:VAL:CB	2.69	0.40
1:B:205:LEU:C	1:B:205:LEU:HD12	2.47	0.40

All (1) 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:114:LYS:NZ	4:A:455:HOH:O[1_455]	1.55	0.65

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	298/301 (99%)	276 (93%)	19 (6%)	3 (1%)	12	8
1	B	298/301 (99%)	273 (92%)	21 (7%)	4 (1%)	9	5
1	C	298/301 (99%)	277 (93%)	17 (6%)	4 (1%)	9	5
1	D	298/301 (99%)	276 (93%)	16 (5%)	6 (2%)	6	2
All	All	1192/1204 (99%)	1102 (92%)	73 (6%)	17 (1%)	9	4

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	VAL
1	B	44	SER
1	B	194	VAL
1	C	52	MET
1	C	194	VAL
1	D	39	SER
1	D	48	LYS
1	D	51	GLU
1	D	53	ASP
1	D	194	VAL
1	A	50	ASP
1	B	46	GLU
1	B	54	TRP
1	C	46	GLU
1	C	145	ASN
1	A	45	ASN
1	D	55	ASN

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	245/245 (100%)	226 (92%)	19 (8%)	11	8
1	B	245/245 (100%)	226 (92%)	19 (8%)	11	8
1	C	245/245 (100%)	222 (91%)	23 (9%)	8	5
1	D	245/245 (100%)	221 (90%)	24 (10%)	7	5
All	All	980/980 (100%)	895 (91%)	85 (9%)	9	6

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	49	LEU
1	A	52	MET
1	A	57	VAL
1	A	78	LYS
1	A	81	LYS
1	A	106	LEU
1	A	114	LYS
1	A	119	ILE
1	A	122	GLU
1	A	123	LYS
1	A	127	PRO
1	A	194	VAL
1	A	249	LEU
1	A	256	LEU
1	A	259	GLU
1	A	266	SER
1	A	291	ILE
1	A	292	LEU
1	B	6	SER
1	B	17	GLU
1	B	22	ILE
1	B	42	ILE
1	B	43	GLN
1	B	45	ASN
1	B	46	GLU
1	B	52	MET
1	B	78	LYS

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Mol	Chain	Res	Type
1	B	83	GLU
1	B	86	GLU
1	B	124	LEU
1	B	144	ILE
1	B	158	THR
1	B	194	VAL
1	B	210	ILE
1	B	235	LEU
1	B	237	LYS
1	B	249	LEU
1	C	16	LYS
1	C	43	GLN
1	C	48	LYS
1	C	106	LEU
1	C	107	TYR
1	C	108	SER
1	C	115	ASP
1	C	121	ASN
1	C	123	LYS
1	C	140	LYS
1	C	144	ILE
1	C	145	ASN
1	C	173	VAL
1	C	180	LEU
1	C	194	VAL
1	C	233	GLU
1	C	249	LEU
1	C	252	LYS
1	C	256	LEU
1	C	266	SER
1	C	281	LYS
1	C	291	ILE
1	C	292	LEU
1	D	1	MET
1	D	4	SER
1	D	8	ASP
1	D	25	LYS
1	D	43	GLN
1	D	46	GLU
1	D	51	GLU
1	D	52	MET
1	D	87	LYS

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Mol	Chain	Res	Type
1	D	94	LYS
1	D	123	LYS
1	D	143	SER
1	D	194	VAL
1	D	206	GLU
1	D	211	LYS
1	D	235	LEU
1	D	249	LEU
1	D	252	LYS
1	D	256	LEU
1	D	259	GLU
1	D	263	THR
1	D	267	ILE
1	D	281	LYS
1	D	298	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	40	ASN
1	A	41	GLN
1	A	244	HIS
1	B	9	HIS
1	B	10	HIS
1	B	40	ASN
1	B	43	GLN
1	B	58	ASN
1	B	244	HIS
1	C	-1	HIS
1	C	10	HIS
1	C	43	GLN
1	C	45	ASN
1	C	101	ASN
1	C	121	ASN
1	C	145	ASN
1	C	214	ASN
1	C	244	HIS
1	C	272	GLN
1	D	10	HIS
1	D	58	ASN
1	D	145	ASN

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Mol	Chain	Res	Type
1	D	244	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	D	37	1,3	4,7,8	2.30	2 (50%)	1,8,10	6.65	1 (100%)
1	CSD	C	37	1,3	4,7,8	0.52	0	1,8,10	10.03	1 (100%)
1	CSD	A	37	1,3	4,7,8	2.37	2 (50%)	1,8,10	7.94	1 (100%)
1	CSD	B	37	1,3	4,7,8	1.03	0	1,8,10	5.94	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	D	37	1,3	-	0/2/6/8	-
1	CSD	C	37	1,3	-	1/2/6/8	-
1	CSD	A	37	1,3	-	2/2/6/8	-
1	CSD	B	37	1,3	-	2/2/6/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	37	CSD	CB-SG	3.72	1.99	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	CSD	CB-SG	3.20	1.97	1.79
1	A	37	CSD	OD1-SG	2.63	1.50	1.47
1	D	37	CSD	OD1-SG	2.25	1.49	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	37	CSD	OD1-SG-CB	10.03	124.07	105.60
1	A	37	CSD	OD1-SG-CB	7.94	120.23	105.60
1	D	37	CSD	OD1-SG-CB	6.65	117.85	105.60
1	B	37	CSD	OD1-SG-CB	5.94	116.54	105.60

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	37	CSD	N-CA-CB-SG
1	A	37	CSD	CA-CB-SG-OD1
1	B	37	CSD	N-CA-CB-SG
1	B	37	CSD	CA-CB-SG-OD1
1	C	37	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	37	CSD	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	300/301 (99%)	0.20	13 (4%)	40 39	15, 27, 61, 95	0
1	B	300/301 (99%)	0.56	16 (5%)	32 31	21, 42, 68, 103	0
1	C	300/301 (99%)	0.30	15 (5%)	34 33	17, 31, 69, 118	0
1	D	300/301 (99%)	0.71	18 (6%)	27 26	24, 46, 80, 110	0
All	All	1200/1204 (99%)	0.44	62 (5%)	33 31	15, 38, 70, 118	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	44	SER	6.6
1	D	49	LEU	6.4
1	B	45	ASN	5.8
1	D	54	TRP	5.2
1	B	49	LEU	5.1
1	B	47	ASP	4.4
1	A	54	TRP	4.4
1	A	49	LEU	4.3
1	B	54	TRP	4.1
1	D	55	ASN	4.1
1	D	52	MET	4.1
1	B	-1	HIS	4.0
1	D	38	PHE	3.9
1	C	54	TRP	3.9
1	B	43	GLN	3.8
1	D	-2	SER	3.7
1	C	49	LEU	3.5
1	C	44	SER	3.5
1	A	-2	SER	3.5
1	B	46	GLU	3.5
1	B	52	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	52	MET	3.3
1	D	299	PHE	3.3
1	A	53	ASP	3.2
1	A	47	ASP	3.2
1	B	144	ILE	3.0
1	B	-2	SER	3.0
1	D	47	ASP	3.0
1	C	52	MET	3.0
1	D	58	ASN	2.9
1	D	57	VAL	2.9
1	D	146	CYS	2.9
1	C	-2	SER	2.9
1	D	53	ASP	2.8
1	D	-1	HIS	2.7
1	B	42	ILE	2.7
1	C	144	ILE	2.7
1	A	50	ASP	2.6
1	C	45	ASN	2.6
1	C	-1	HIS	2.5
1	D	45	ASN	2.5
1	B	51	GLU	2.5
1	B	50	ASP	2.4
1	C	53	ASP	2.4
1	A	146	CYS	2.4
1	A	51	GLU	2.4
1	C	146	CYS	2.4
1	C	51	GLU	2.3
1	D	44	SER	2.3
1	D	42	ILE	2.3
1	C	105	GLY	2.3
1	D	36	ASP	2.3
1	A	-1	HIS	2.3
1	D	50	ASP	2.2
1	B	48	LYS	2.2
1	A	122	GLU	2.1
1	A	45	ASN	2.1
1	A	42	ILE	2.1
1	C	148	THR	2.1
1	B	277	VAL	2.1
1	C	48	LYS	2.1
1	C	299	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSD	A	37	8/9	0.72	0.18	36,39,46,49	3
1	CSD	D	37	8/9	0.81	0.15	56,60,67,67	0
1	CSD	C	37	8/9	0.84	0.15	42,44,55,55	3
1	CSD	B	37	8/9	0.84	0.12	51,54,63,64	0

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	CA	B	304	1/1	0.96	0.22	5,5,5,5	0
2	CA	A	300	1/1	0.97	0.24	5,5,5,5	0
2	CA	C	306	1/1	0.98	0.16	4,4,4,4	0
2	CA	D	308	1/1	0.98	0.20	7,7,7,7	0
3	ZN	A	301	1/1	0.98	0.08	7,7,7,7	1
2	CA	A	302	1/1	0.99	0.08	6,6,6,6	0
3	ZN	B	303	1/1	0.99	0.25	8,8,8,8	0
3	ZN	C	305	1/1	0.99	0.14	2,2,2,2	1
3	ZN	D	307	1/1	0.99	0.28	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.