



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 06:00 PM UTC

PDB ID : 2AVF / pdb_00002avf
Title : Crystal Structure of C-terminal Desundecapeptide Nitrite Reductase from *Achromobacter cycloclastes*
Authors : Li, H.T.; Chang, T.; Chang, W.C.; Chen, C.J.; Liu, M.Y.; Gui, L.L.; Zhang, J.P.; An, X.M.; Chang, W.R.
Deposited on : 2005-08-30
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

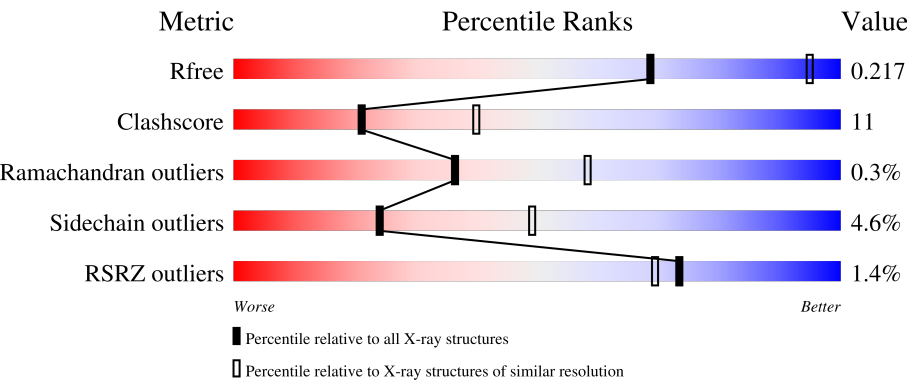
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	329	2% 67% 25% • 5%
1	B	329	% 66% 28% • •
1	C	329	% 73% 20% • •
1	D	329	2% 71% 22% • •
1	E	329	2% 73% 20% • •

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Mol	Chain	Length	Quality of chain
1	F	329	71% 25% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15115 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 Copper-containing nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2429	1550	419	452	8			
1	B	316	Total	C	N	O	S	0	0	0
			2450	1565	422	455	8			
1	C	316	Total	C	N	O	S	0	0	0
			2442	1557	421	456	8			
1	D	320	Total	C	N	O	S	0	0	0
			2468	1575	425	460	8			
1	E	315	Total	C	N	O	S	0	0	0
			2433	1552	420	453	8			
1	F	323	Total	C	N	O	S	0	0	0
			2499	1595	430	466	8			

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cu	0	0
			2	2		
2	B	2	Total	Cu	0	0
			2	2		
2	C	2	Total	Cu	0	0
			2	2		
2	D	2	Total	Cu	0	0
			2	2		
2	E	2	Total	Cu	0	0
			2	2		
2	F	2	Total	Cu	0	0
			2	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Cl 2 2	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	F	2	Total Cl 2 2	0	0

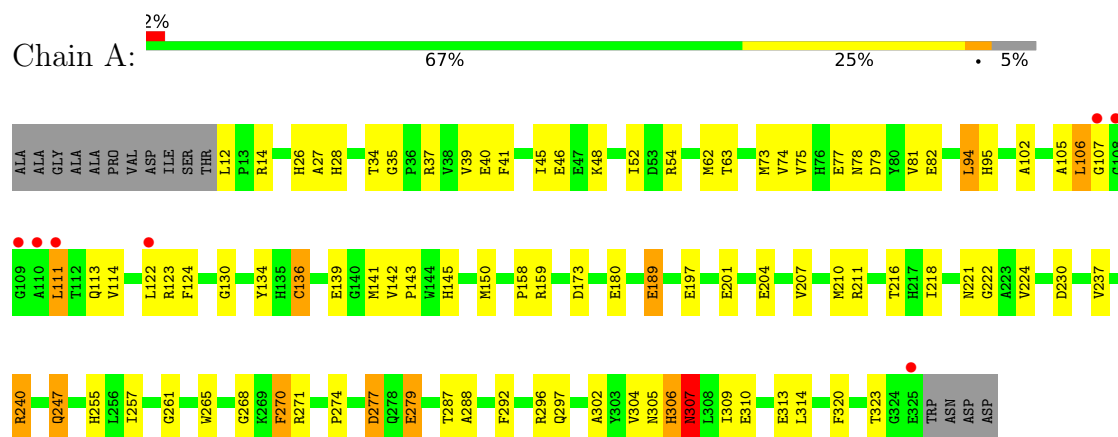
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	72	Total O 72 72	0	0
4	B	54	Total O 54 54	0	0
4	C	71	Total O 71 71	0	0
4	D	55	Total O 55 55	0	0
4	E	47	Total O 47 47	0	0
4	F	77	Total O 77 77	0	0

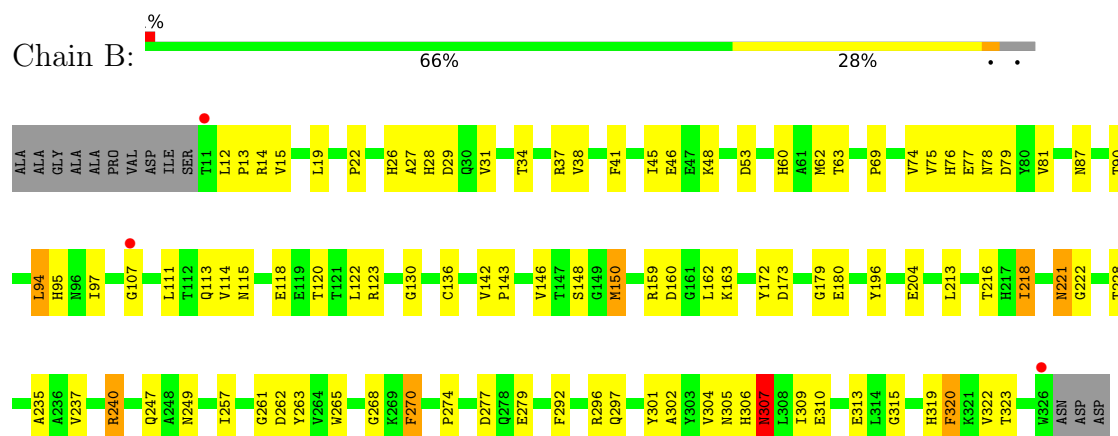
3 Residue-property plots [i](#)

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.

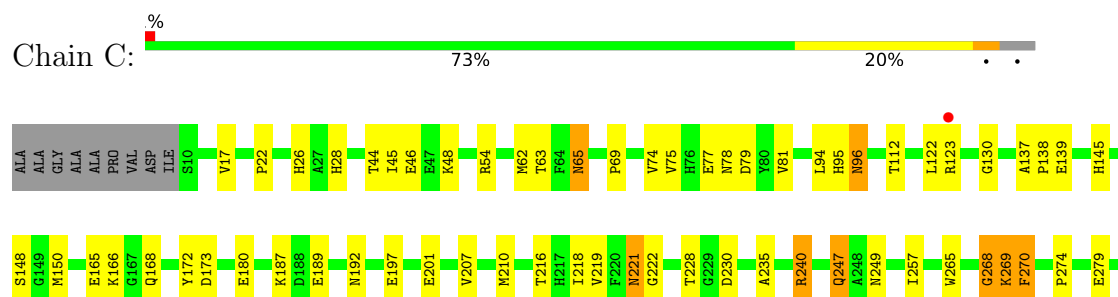
• Molecule 1: Copper-containing nitrite reductase



• Molecule 1: Copper-containing nitrite reductase

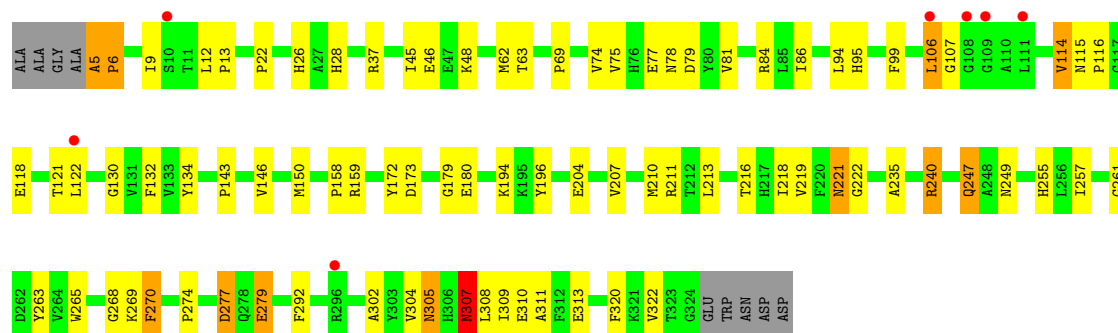


• Molecule 1: Copper-containing nitrite reductase

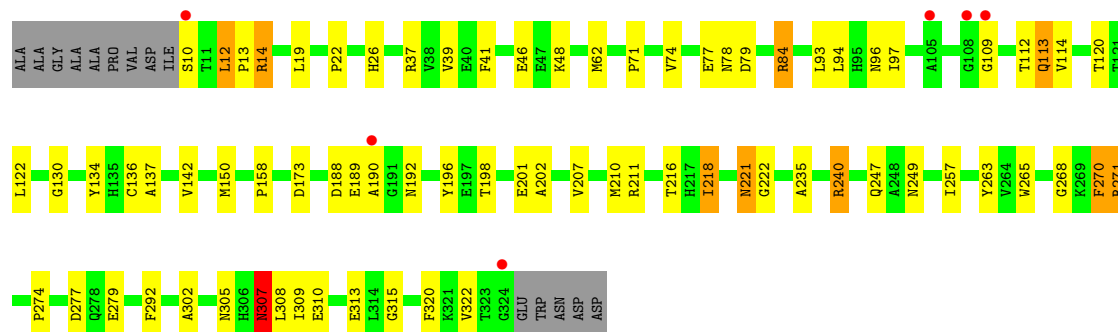
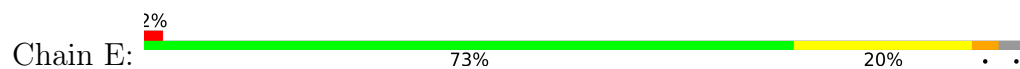




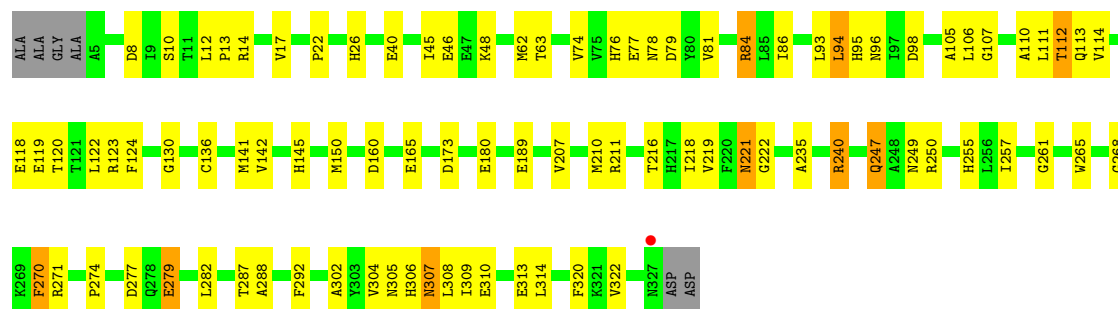
• Molecule 1: Copper-containing nitrite reductase



• Molecule 1: Copper-containing nitrite reductase



• Molecule 1: Copper-containing nitrite reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.78Å 111.07Å 122.88Å 90.00° 101.67° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.2 (20.00-2.60) 95.5 (20.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.59Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.182 , 0.217 0.182 , 0.217	Depositor DCC
R_{free} test set	2806 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15115	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: CL, CU

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	0.43	0/2496	1.00	18/3402 (0.5%)
1	B	0.41	0/2519	1.00	15/3435 (0.4%)
1	C	0.43	0/2509	1.00	15/3420 (0.4%)
1	D	0.41	0/2536	1.03	17/3459 (0.5%)
1	E	0.42	0/2500	0.99	19/3408 (0.6%)
1	F	0.42	0/2569	1.00	14/3505 (0.4%)
All	All	0.42	0/15129	1.00	98/20629 (0.5%)

There are no bond length outliers.

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	5	ALA	CA-C-N	14.11	137.47	119.84
1	D	5	ALA	C-N-CA	14.11	137.47	119.84
1	A	307	ASN	N-CA-C	-9.84	89.45	107.75
1	D	305	ASN	N-CA-C	-9.40	94.82	109.76
1	D	307	ASN	N-CA-C	-9.23	89.66	107.57
1	B	305	ASN	N-CA-C	-8.85	94.89	108.96
1	C	305	ASN	N-CA-C	-8.76	95.04	108.96
1	E	305	ASN	N-CA-C	-8.60	95.29	108.96
1	F	307	ASN	N-CA-C	-8.44	91.20	107.57
1	F	305	ASN	N-CA-C	-8.33	96.50	109.25
1	C	307	ASN	N-CA-C	-8.22	91.63	107.57
1	A	305	ASN	N-CA-C	-7.95	96.32	108.96
1	A	270	PHE	N-CA-C	7.84	122.10	112.54
1	B	307	ASN	N-CA-C	-7.76	92.52	107.57
1	E	307	ASN	N-CA-C	-7.73	91.79	107.41
1	D	270	PHE	N-CA-C	7.34	121.15	111.75
1	B	270	PHE	N-CA-C	7.31	121.64	112.87
1	C	306	HIS	N-CA-C	7.22	121.51	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	216	THR	N-CA-C	-7.21	104.61	113.41
1	D	222	GLY	N-CA-C	7.15	124.84	115.40
1	A	79	ASP	N-CA-C	-7.01	101.48	110.53
1	C	268	GLY	N-CA-C	6.99	125.02	114.61
1	F	222	GLY	N-CA-C	6.99	123.00	114.69
1	D	268	GLY	N-CA-C	6.92	124.92	114.61
1	C	270	PHE	N-CA-C	6.87	121.11	112.87
1	A	222	GLY	N-CA-C	6.85	124.12	115.21
1	C	304	VAL	N-CA-C	6.84	118.79	108.80
1	B	315	GLY	N-CA-C	6.77	124.81	115.27
1	B	222	GLY	N-CA-C	6.74	123.10	115.08
1	A	216	THR	N-CA-C	-6.57	105.08	113.23
1	E	216	THR	N-CA-C	-6.54	105.43	113.41
1	C	222	GLY	N-CA-C	6.54	124.03	115.40
1	A	268	GLY	N-CA-C	6.53	124.33	114.61
1	E	79	ASP	N-CA-C	-6.38	102.30	110.53
1	E	12	LEU	CA-C-N	6.37	126.28	119.85
1	E	12	LEU	C-N-CA	6.37	126.28	119.85
1	D	216	THR	N-CA-C	-6.36	105.65	113.41
1	B	279	GLU	N-CA-C	-6.34	103.63	112.45
1	F	279	GLU	N-CA-C	-6.27	103.73	112.45
1	B	216	THR	N-CA-C	-6.24	105.80	113.41
1	C	283	ILE	CA-C-N	6.11	126.08	119.78
1	C	283	ILE	C-N-CA	6.11	126.08	119.78
1	E	279	GLU	N-CA-C	-6.10	103.97	112.45
1	A	304	VAL	N-CA-C	6.09	117.69	108.80
1	B	63	THR	N-CA-C	6.05	118.90	109.52
1	A	261	GLY	N-CA-C	-6.01	98.95	113.18
1	D	279	GLU	N-CA-C	-5.98	104.14	112.45
1	C	63	THR	N-CA-C	5.86	118.32	109.41
1	C	216	THR	N-CA-C	-5.86	105.96	113.23
1	E	222	GLY	N-CA-C	5.86	122.93	114.67
1	B	304	VAL	N-CA-C	5.85	117.13	108.65
1	C	79	ASP	N-CA-C	-5.82	103.03	110.53
1	B	218	ILE	N-CA-C	-5.77	99.18	107.78
1	B	79	ASP	N-CA-C	-5.75	103.12	110.53
1	F	270	PHE	N-CA-C	5.72	119.87	113.01
1	E	268	GLY	N-CA-C	5.71	126.70	113.18
1	E	270	PHE	N-CA-C	5.69	119.84	113.01
1	E	315	GLY	N-CA-C	5.69	123.94	115.64
1	F	277	ASP	N-CA-C	5.67	119.39	111.90
1	F	261	GLY	N-CA-C	-5.63	99.83	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	79	ASP	N-CA-C	-5.53	103.39	110.53
1	A	279	GLU	N-CA-C	-5.52	104.77	112.45
1	D	134	TYR	N-CA-C	-5.51	100.04	109.24
1	E	97	ILE	N-CA-C	5.50	116.67	109.58
1	E	277	ASP	N-CA-C	5.47	118.98	111.54
1	E	271	ARG	N-CA-C	-5.47	106.45	113.01
1	F	304	VAL	N-CA-C	5.43	117.92	108.95
1	E	114	VAL	N-CA-C	5.42	115.92	108.12
1	A	277	ASP	N-CA-C	5.41	118.90	111.54
1	E	158	PRO	N-CA-C	-5.40	102.79	111.38
1	D	79	ASP	N-CA-C	-5.38	102.78	110.59
1	F	268	GLY	N-CA-C	5.35	125.86	113.18
1	C	279	GLU	N-CA-C	-5.33	105.04	112.45
1	C	219	VAL	N-CA-C	5.33	117.74	108.95
1	A	12	LEU	CA-C-N	5.32	125.22	119.85
1	A	12	LEU	C-N-CA	5.32	125.22	119.85
1	A	134	TYR	N-CA-C	-5.30	100.38	109.24
1	D	219	VAL	N-CA-C	5.24	117.60	108.95
1	B	306	HIS	N-CA-C	5.21	119.20	113.21
1	B	148	SER	N-CA-C	-5.19	106.34	113.30
1	A	52	ILE	N-CA-C	5.19	119.09	113.43
1	F	219	VAL	N-CA-C	5.18	117.50	108.95
1	A	306	HIS	N-CA-C	5.18	121.83	110.80
1	D	277	ASP	N-CA-C	5.17	118.58	111.54
1	E	218	ILE	N-CA-C	-5.17	100.08	107.78
1	A	63	THR	N-CA-C	5.17	117.53	109.52
1	F	306	HIS	N-CA-C	5.17	121.81	110.80
1	D	158	PRO	N-CA-C	-5.16	103.18	111.38
1	C	148	SER	N-CA-C	-5.14	106.41	113.30
1	B	268	GLY	N-CA-C	5.13	125.34	113.18
1	D	261	GLY	N-CA-C	-5.11	101.07	113.18
1	E	134	TYR	N-CA-C	-5.11	101.43	109.50
1	E	93	LEU	N-CA-C	5.09	117.97	110.59
1	D	304	VAL	N-CA-C	5.08	117.33	108.90
1	B	261	GLY	N-CA-C	-5.06	101.20	113.18
1	A	158	PRO	N-CA-C	-5.04	103.19	111.21
1	D	63	THR	N-CA-C	5.01	117.02	109.41
1	F	63	THR	N-CA-C	5.00	117.01	109.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2429	0	2363	57	0
1	B	2450	0	2380	58	0
1	C	2442	0	2375	53	0
1	D	2468	0	2405	54	0
1	E	2433	0	2369	53	0
1	F	2499	0	2427	58	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	F	2	0	0	0	0
4	A	72	0	0	2	0
4	B	54	0	0	1	0
4	C	71	0	0	1	0
4	D	55	0	0	1	0
4	E	47	0	0	0	0
4	F	77	0	0	1	0
All	All	15115	0	14319	319	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 11.

All (319) 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:E:14:ARG:HG2	1:E:14:ARG:HH11	1.13	1.13
1:A:106:LEU:HD13	1:A:122:LEU:HD21	1.46	0.97
1:F:106:LEU:HD22	1:F:122:LEU:HD11	1.44	0.95
1:E:112:THR:HG23	1:E:122:LEU:HD13	1.60	0.82
1:C:96:ASN:HD21	1:C:137:ALA:H	1.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ARG:HG2	1:B:38:VAL:HB	1.64	0.79
1:F:26:HIS:HE1	1:F:74:VAL:H	1.31	0.76
1:E:257:ILE:HD12	1:E:302:ALA:HB3	1.67	0.76
1:F:141:MET:HE3	1:F:145:HIS:HE2	1.50	0.76
1:D:26:HIS:HE1	1:D:74:VAL:H	1.34	0.76
1:A:271:ARG:HD2	1:B:277:ASP:OD2	1.86	0.75
1:C:112:THR:HG23	1:C:122:LEU:HD13	1.70	0.74
1:B:37:ARG:HG2	1:B:37:ARG:HH11	1.53	0.73
1:E:14:ARG:HH11	1:E:14:ARG:CG	1.96	0.72
1:C:112:THR:HG21	1:C:122:LEU:HD22	1.70	0.72
1:D:257:ILE:HD12	1:D:302:ALA:HB3	1.69	0.72
1:B:257:ILE:HD12	1:B:302:ALA:HB3	1.70	0.71
1:B:14:ARG:HG3	1:B:14:ARG:HH11	1.56	0.71
1:E:112:THR:HG21	1:E:122:LEU:HD22	1.73	0.70
1:E:14:ARG:HG2	1:E:14:ARG:NH1	1.94	0.70
1:A:26:HIS:HE1	1:A:74:VAL:H	1.39	0.70
1:F:112:THR:HG21	1:F:122:LEU:CD1	2.22	0.69
1:B:204:GLU:HB2	4:B:618:HOH:O	1.93	0.69
1:F:8:ASP:OD1	1:F:10:SER:HB3	1.93	0.68
1:A:257:ILE:HD12	1:A:302:ALA:HB3	1.74	0.68
1:E:84:ARG:HG2	1:E:84:ARG:HH11	1.58	0.68
1:A:94:LEU:HD12	1:A:94:LEU:C	2.20	0.67
1:A:111:LEU:HD12	1:A:113:GLN:HG3	1.76	0.66
1:C:218:ILE:HD12	1:C:310:GLU:HG2	1.79	0.65
1:D:180:GLU:HB3	1:D:247:GLN:HG2	1.79	0.65
1:D:173:ASP:OD2	1:D:240:ARG:HD3	1.96	0.65
1:E:46:GLU:OE2	1:E:48:LYS:HD3	1.97	0.64
1:C:96:ASN:ND2	1:C:137:ALA:H	1.95	0.64
1:C:26:HIS:HE1	1:C:74:VAL:H	1.44	0.63
1:E:22:PRO:HB2	1:E:221:ASN:HD21	1.62	0.63
1:A:62:MET:O	1:A:150:MET:HG3	1.98	0.63
1:A:197:GLU:HB2	1:A:201:GLU:OE2	1.99	0.62
1:A:41:PHE:CD2	1:A:73:MET:HE3	2.34	0.61
1:D:307:ASN:HD22	1:D:310:GLU:H	1.47	0.61
1:E:235:ALA:O	1:E:322:VAL:HA	1.99	0.61
1:B:37:ARG:HG2	1:B:37:ARG:NH1	2.15	0.61
1:E:307:ASN:HD22	1:E:307:ASN:C	2.07	0.61
1:F:46:GLU:OE2	1:F:48:LYS:HD3	2.00	0.61
1:C:46:GLU:OE2	1:C:48:LYS:HD3	2.01	0.60
1:B:77:GLU:O	1:B:78:ASN:HB2	1.99	0.60
1:F:26:HIS:CE1	1:F:74:VAL:H	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:PRO:HG2	4:A:519:HOH:O	2.01	0.60
1:C:28:HIS:HE1	1:C:172:TYR:OH	1.84	0.60
1:B:309:ILE:O	1:B:313:GLU:HB2	2.01	0.60
1:C:307:ASN:C	1:C:307:ASN:HD22	2.08	0.60
1:F:96:ASN:OD1	1:F:110:ALA:HA	2.01	0.60
1:D:13:PRO:HB2	1:D:37:ARG:HD3	1.84	0.60
1:D:28:HIS:HE1	1:D:172:TYR:OH	1.85	0.60
1:F:111:LEU:O	1:F:112:THR:HG23	2.01	0.59
1:F:77:GLU:O	1:F:78:ASN:HB2	2.02	0.59
1:D:106:LEU:CD1	1:D:106:LEU:N	2.66	0.59
1:D:106:LEU:N	1:D:106:LEU:HD12	2.17	0.59
1:C:26:HIS:CE1	1:C:74:VAL:H	2.21	0.59
1:D:207:VAL:O	1:D:211:ARG:HG3	2.02	0.59
1:F:173:ASP:OD2	1:F:240:ARG:HD3	2.03	0.59
1:E:96:ASN:HD21	1:E:109:GLY:C	2.11	0.58
1:F:106:LEU:HD13	1:F:122:LEU:HG	1.85	0.58
1:A:62:MET:C	1:A:150:MET:HG3	2.28	0.58
1:B:173:ASP:OD2	1:B:240:ARG:HD3	2.03	0.58
1:D:194:LYS:HE3	1:D:196:TYR:OH	2.03	0.58
1:F:96:ASN:HB2	1:F:113:GLN:HG2	1.85	0.58
1:B:46:GLU:OE2	1:B:48:LYS:HD3	2.03	0.58
1:F:112:THR:HG21	1:F:122:LEU:HD11	1.84	0.58
1:F:45:ILE:HG21	1:F:95:HIS:CD2	2.39	0.58
1:C:257:ILE:HD12	1:C:302:ALA:HB3	1.85	0.57
1:D:26:HIS:CE1	1:D:74:VAL:H	2.21	0.57
1:C:62:MET:O	1:C:150:MET:HG3	2.05	0.57
1:A:105:ALA:O	1:A:107:GLY:N	2.38	0.57
1:D:22:PRO:HB2	1:D:221:ASN:HD21	1.68	0.57
1:D:235:ALA:O	1:D:322:VAL:HA	2.05	0.56
1:E:62:MET:O	1:E:150:MET:HG3	2.05	0.56
1:D:309:ILE:O	1:D:313:GLU:HB2	2.05	0.56
1:F:141:MET:HE3	1:F:145:HIS:NE2	2.20	0.56
1:A:218:ILE:HD12	1:A:310:GLU:HG2	1.86	0.56
1:F:106:LEU:HD12	1:F:124:PHE:HB3	1.86	0.56
1:B:94:LEU:C	1:B:94:LEU:HD23	2.30	0.56
1:C:22:PRO:HB2	1:C:221:ASN:HD21	1.71	0.56
1:C:301:TYR:O	1:C:320:PHE:HB2	2.05	0.56
1:B:142:VAL:HB	1:B:143:PRO:HD3	1.88	0.56
1:B:62:MET:O	1:B:150:MET:HG3	2.06	0.56
1:C:268:GLY:C	1:C:269:LYS:HE3	2.31	0.56
1:A:207:VAL:O	1:A:211:ARG:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:GLU:OE2	1:D:48:LYS:HD3	2.06	0.55
1:E:198:THR:OG1	1:E:201:GLU:HB2	2.06	0.55
1:D:277:ASP:OD2	1:F:271:ARG:HD2	2.06	0.55
1:A:307:ASN:C	1:A:307:ASN:HD22	2.14	0.55
1:B:75:VAL:HG11	1:B:81:VAL:HG22	1.88	0.55
1:B:107:GLY:O	1:B:111:LEU:HD12	2.06	0.55
1:B:180:GLU:HB3	1:B:247:GLN:HG2	1.89	0.55
1:F:22:PRO:HB2	1:F:221:ASN:HD21	1.71	0.55
1:F:84:ARG:CZ	1:F:86:ILE:HD11	2.37	0.55
1:F:257:ILE:HD12	1:F:302:ALA:HB3	1.90	0.54
1:A:130:GLY:HA2	1:A:270:PHE:CD2	2.42	0.54
1:A:307:ASN:HA	1:C:249:ASN:O	2.07	0.54
1:D:114:VAL:HG23	1:D:118:GLU:HB2	1.89	0.54
1:E:112:THR:HA	1:E:120:THR:HG21	1.89	0.54
1:F:114:VAL:HG21	1:F:120:THR:HG22	1.90	0.54
1:A:26:HIS:CE1	1:A:74:VAL:H	2.23	0.54
1:C:45:ILE:HG21	1:C:95:HIS:CD2	2.42	0.54
1:E:77:GLU:O	1:E:78:ASN:HB2	2.07	0.54
1:E:173:ASP:OD2	1:E:240:ARG:HD3	2.07	0.54
1:A:46:GLU:OE2	1:A:48:LYS:HD3	2.06	0.54
1:C:130:GLY:HA2	1:C:270:PHE:CD2	2.42	0.54
1:C:165:GLU:OE2	1:C:166:LYS:HG3	2.09	0.53
1:D:9:ILE:O	1:D:9:ILE:HG22	2.08	0.53
1:B:228:THR:HB	1:B:319:HIS:CD2	2.43	0.53
1:C:77:GLU:O	1:C:78:ASN:HB2	2.08	0.53
1:C:240:ARG:HB3	1:C:292:PHE:CZ	2.43	0.53
1:C:166:LYS:CB	1:C:168:GLN:NE2	2.72	0.53
1:F:310:GLU:HA	1:F:314:LEU:HB2	1.89	0.53
1:B:14:ARG:HG3	1:B:14:ARG:NH1	2.22	0.53
1:E:207:VAL:O	1:E:211:ARG:HG3	2.09	0.53
1:B:22:PRO:HB2	1:B:221:ASN:HD21	1.74	0.52
1:F:240:ARG:HB3	1:F:292:PHE:CZ	2.44	0.52
1:B:28:HIS:HE1	1:B:172:TYR:OH	1.93	0.52
1:F:93:LEU:HD22	1:F:141:MET:HE1	1.90	0.52
1:C:44:THR:H	1:C:65:ASN:ND2	2.06	0.52
1:B:26:HIS:HD2	1:B:27:ALA:O	1.92	0.52
1:A:111:LEU:CD1	1:A:113:GLN:HG3	2.39	0.52
1:A:207:VAL:HA	1:A:210:MET:HE3	1.91	0.52
1:B:162:LEU:O	1:B:163:LYS:HD3	2.09	0.52
1:B:19:LEU:HD21	1:B:41:PHE:CD1	2.45	0.52
1:F:309:ILE:O	1:F:313:GLU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ASP:OD2	1:C:240:ARG:HD3	2.11	0.51
1:F:235:ALA:O	1:F:322:VAL:HA	2.11	0.51
1:A:77:GLU:O	1:A:78:ASN:HB2	2.09	0.51
1:A:106:LEU:CD1	1:A:122:LEU:HD21	2.29	0.51
1:F:62:MET:O	1:F:150:MET:HG3	2.10	0.51
1:F:106:LEU:HD22	1:F:122:LEU:CD1	2.31	0.51
1:D:143:PRO:HG2	4:D:648:HOH:O	2.09	0.51
1:B:130:GLY:HA2	1:B:270:PHE:CD2	2.45	0.51
1:F:287:THR:HG22	1:F:288:ALA:N	2.26	0.51
1:F:130:GLY:HA2	1:F:270:PHE:CD2	2.45	0.51
1:C:187:LYS:HA	1:C:192:ASN:O	2.11	0.50
1:E:19:LEU:HD13	1:E:71:PRO:CG	2.40	0.50
1:B:87:ASN:HB3	1:B:114:VAL:HG12	1.93	0.50
1:B:307:ASN:C	1:B:307:ASN:HD22	2.20	0.50
1:F:84:ARG:HD3	1:F:119:GLU:OE1	2.11	0.50
1:A:211:ARG:NH2	4:A:539:HOH:O	2.45	0.50
1:B:26:HIS:HE1	1:B:74:VAL:H	1.60	0.50
1:C:112:THR:CG2	1:C:122:LEU:HD13	2.38	0.50
1:C:138:PRO:HG2	1:C:145:HIS:CE1	2.47	0.50
1:E:265:TRP:CE2	1:E:274:PRO:HB3	2.46	0.50
1:F:62:MET:C	1:F:150:MET:HG3	2.37	0.50
1:C:166:LYS:HB2	1:C:168:GLN:NE2	2.27	0.50
1:D:218:ILE:HD12	1:D:310:GLU:HG2	1.94	0.50
1:B:13:PRO:HG2	1:B:37:ARG:NH1	2.26	0.49
1:E:112:THR:CG2	1:E:122:LEU:HD13	2.35	0.49
1:B:262:ASP:OD2	1:B:296:ARG:NH2	2.46	0.49
1:D:62:MET:C	1:D:150:MET:HG3	2.37	0.49
1:D:130:GLY:HA2	1:D:270:PHE:CD2	2.48	0.49
1:E:84:ARG:HH11	1:E:84:ARG:CG	2.26	0.49
1:F:94:LEU:C	1:F:94:LEU:HD23	2.37	0.49
1:C:228:THR:HG21	4:C:646:HOH:O	2.13	0.49
1:B:45:ILE:HG21	1:B:95:HIS:CD2	2.47	0.49
1:E:190:ALA:HB3	1:E:192:ASN:ND2	2.28	0.49
1:B:249:ASN:O	1:C:307:ASN:HA	2.13	0.49
1:C:94:LEU:C	1:C:94:LEU:HD23	2.38	0.48
1:D:62:MET:O	1:D:150:MET:HG3	2.13	0.48
1:A:54:ARG:HH21	1:A:224:VAL:HG12	1.79	0.48
1:A:173:ASP:OD2	1:A:240:ARG:HD3	2.13	0.48
1:F:26:HIS:HE1	1:F:74:VAL:N	2.06	0.48
1:F:105:ALA:C	1:F:107:GLY:H	2.21	0.48
1:A:94:LEU:HD12	1:A:95:HIS:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:VAL:O	1:D:114:VAL:HG13	2.13	0.48
1:A:265:TRP:CE2	1:A:274:PRO:HB3	2.49	0.48
1:C:207:VAL:HA	1:C:210:MET:HE3	1.96	0.48
1:C:235:ALA:O	1:C:322:VAL:HA	2.13	0.48
1:D:99:PHE:HD1	1:D:106:LEU:HD23	1.79	0.48
1:E:14:ARG:CG	1:E:14:ARG:NH1	2.63	0.48
1:E:62:MET:C	1:E:150:MET:HG3	2.39	0.48
1:E:240:ARG:HB3	1:E:292:PHE:CZ	2.49	0.48
1:F:207:VAL:O	1:F:211:ARG:HG3	2.14	0.48
1:C:94:LEU:HD23	1:C:95:HIS:N	2.28	0.48
1:B:263:TYR:HB2	1:B:292:PHE:HB3	1.94	0.47
1:A:106:LEU:HD13	1:A:122:LEU:CD2	2.30	0.47
1:A:39:VAL:HG21	1:A:75:VAL:HG12	1.95	0.47
1:B:114:VAL:HG13	1:B:118:GLU:HB2	1.96	0.47
1:D:77:GLU:O	1:D:78:ASN:HB2	2.14	0.47
1:F:114:VAL:HG13	1:F:118:GLU:HB2	1.96	0.47
1:A:240:ARG:HB3	1:A:292:PHE:CZ	2.49	0.47
1:D:305:ASN:O	1:D:311:ALA:HB2	2.15	0.47
1:E:196:TYR:CG	1:E:202:ALA:HB2	2.49	0.47
1:B:81:VAL:O	1:B:123:ARG:HA	2.15	0.47
1:C:96:ASN:C	1:C:96:ASN:HD22	2.23	0.47
1:B:26:HIS:O	1:B:28:HIS:HD2	1.98	0.47
1:B:31:VAL:HG13	1:B:160:ASP:HA	1.97	0.47
1:E:19:LEU:HD21	1:E:41:PHE:HD2	1.80	0.47
1:A:114:VAL:HG23	1:A:114:VAL:O	2.14	0.47
1:B:97:ILE:CG2	1:B:122:LEU:HD21	2.45	0.47
1:C:62:MET:C	1:C:150:MET:HG3	2.40	0.47
1:B:69:PRO:HG3	1:B:179:GLY:HA3	1.96	0.46
1:F:265:TRP:CE2	1:F:274:PRO:HB3	2.50	0.46
1:B:301:TYR:O	1:B:320:PHE:HB2	2.15	0.46
1:A:102:ALA:HB2	1:A:124:PHE:CG	2.51	0.46
1:A:287:THR:HG22	1:A:288:ALA:N	2.31	0.46
1:F:180:GLU:HB3	1:F:247:GLN:HG2	1.96	0.46
1:F:218:ILE:HD12	1:F:310:GLU:HB3	1.96	0.46
1:E:249:ASN:O	1:F:307:ASN:HA	2.15	0.46
1:C:218:ILE:CD1	1:C:310:GLU:HG2	2.46	0.46
1:D:240:ARG:HB3	1:D:292:PHE:CZ	2.50	0.46
1:E:142:VAL:CG1	1:F:308:LEU:HD13	2.45	0.46
1:D:13:PRO:HB2	1:D:37:ARG:CD	2.45	0.46
1:E:137:ALA:HA	1:E:142:VAL:HG22	1.98	0.46
1:B:60:HIS:HE2	1:B:196:TYR:C	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:THR:HB	1:B:319:HIS:HD2	1.79	0.45
1:A:142:VAL:HB	1:A:143:PRO:CD	2.46	0.45
1:A:180:GLU:HB3	1:A:247:GLN:HG2	1.98	0.45
1:D:263:TYR:HB2	1:D:292:PHE:HB3	1.97	0.45
1:D:249:ASN:O	1:E:307:ASN:HA	2.15	0.45
1:A:141:MET:HE3	1:A:145:HIS:NE2	2.32	0.45
1:C:166:LYS:HB3	1:C:168:GLN:NE2	2.31	0.45
1:D:75:VAL:HG11	1:D:81:VAL:HG22	1.99	0.45
1:D:265:TRP:CE2	1:D:274:PRO:HB3	2.52	0.45
1:E:19:LEU:HD13	1:E:71:PRO:HG3	1.98	0.45
1:F:76:HIS:HD2	4:F:625:HOH:O	2.00	0.45
1:D:5:ALA:HA	1:D:6:PRO:HD3	1.52	0.45
1:D:45:ILE:HG21	1:D:95:HIS:CD2	2.51	0.45
1:A:309:ILE:O	1:A:313:GLU:HB2	2.17	0.45
1:B:13:PRO:HG2	1:B:37:ARG:HH12	1.82	0.45
1:B:237:VAL:HG23	1:B:323:THR:O	2.17	0.45
1:A:237:VAL:HG23	1:A:323:THR:O	2.17	0.44
1:D:99:PHE:H	1:D:106:LEU:HD21	1.81	0.44
1:C:265:TRP:CE2	1:C:274:PRO:HB3	2.53	0.44
1:C:268:GLY:O	1:C:269:LYS:HE3	2.17	0.44
1:E:309:ILE:O	1:E:313:GLU:HB2	2.17	0.44
1:F:307:ASN:CG	1:F:310:GLU:HG3	2.42	0.44
1:A:189:GLU:HA	1:A:189:GLU:OE1	2.17	0.44
1:E:196:TYR:CD2	1:E:202:ALA:HB2	2.52	0.44
1:D:207:VAL:HA	1:D:210:MET:HE3	1.99	0.44
1:E:94:LEU:C	1:E:94:LEU:HD23	2.42	0.44
1:A:14:ARG:NH1	1:A:40:GLU:OE2	2.51	0.44
1:A:277:ASP:O	1:C:269:LYS:HD2	2.17	0.44
1:F:81:VAL:O	1:F:123:ARG:HA	2.17	0.44
1:F:207:VAL:HA	1:F:210:MET:HE3	2.00	0.44
1:B:53:ASP:OD1	1:B:53:ASP:C	2.61	0.44
1:E:263:TYR:HB2	1:E:292:PHE:HB3	1.99	0.44
1:F:255:HIS:ND1	1:F:279:GLU:O	2.51	0.44
1:A:111:LEU:HD12	1:A:113:GLN:H	1.83	0.44
1:B:235:ALA:O	1:B:322:VAL:HA	2.18	0.44
1:C:197:GLU:HB2	1:C:201:GLU:OE1	2.17	0.44
1:A:296:ARG:C	1:A:297:GLN:HG2	2.43	0.43
1:D:255:HIS:ND1	1:D:279:GLU:O	2.51	0.43
1:E:188:ASP:OD1	1:E:188:ASP:C	2.61	0.43
1:F:12:LEU:HA	1:F:13:PRO:HD3	1.83	0.43
1:E:130:GLY:HA2	1:E:270:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ASP:O	1:B:76:HIS:CE1	2.70	0.43
1:D:84:ARG:CZ	1:D:86:ILE:HD11	2.49	0.43
1:A:34:THR:O	1:A:159:ARG:NH2	2.52	0.43
1:D:307:ASN:HA	1:F:249:ASN:O	2.19	0.43
1:E:26:HIS:HE1	1:E:74:VAL:H	1.66	0.43
1:B:142:VAL:HG12	1:C:308:LEU:HD13	2.00	0.43
1:A:106:LEU:HD23	1:A:124:PHE:HB3	1.99	0.43
1:C:180:GLU:HB3	1:C:247:GLN:HG2	1.99	0.43
1:A:35:GLY:O	1:A:37:ARG:HG3	2.18	0.43
1:B:113:GLN:HE21	1:B:115:ASN:HD21	1.64	0.43
1:D:26:HIS:HE1	1:D:74:VAL:N	2.10	0.43
1:A:81:VAL:O	1:A:123:ARG:HA	2.18	0.43
1:A:306:HIS:O	1:A:306:HIS:ND1	2.52	0.42
1:E:112:THR:CA	1:E:120:THR:HG21	2.49	0.42
1:A:45:ILE:HG21	1:A:95:HIS:CD2	2.54	0.42
1:A:255:HIS:ND1	1:A:279:GLU:O	2.48	0.42
1:A:136:CYS:HB2	1:A:150:MET:HB3	2.02	0.42
1:C:45:ILE:HD13	1:C:95:HIS:HB2	2.02	0.42
1:E:113:GLN:HE21	1:E:113:GLN:HB2	1.57	0.42
1:C:65:ASN:HD22	1:C:65:ASN:HA	1.61	0.42
1:B:146:VAL:HG21	1:C:308:LEU:CD1	2.49	0.42
1:B:265:TRP:CE2	1:B:274:PRO:HB3	2.55	0.42
1:C:96:ASN:ND2	1:C:96:ASN:C	2.76	0.42
1:D:106:LEU:HD23	1:D:122:LEU:HD21	2.02	0.42
1:D:146:VAL:HG21	1:E:308:LEU:HD12	2.01	0.42
1:D:204:GLU:OE1	1:D:204:GLU:HA	2.19	0.42
1:E:189:GLU:OE1	1:E:189:GLU:HA	2.20	0.42
1:C:75:VAL:HG11	1:C:81:VAL:HG22	2.01	0.42
1:F:105:ALA:C	1:F:107:GLY:N	2.76	0.42
1:E:12:LEU:HA	1:E:13:PRO:HD3	1.80	0.42
1:E:112:THR:CG2	1:E:122:LEU:HD22	2.46	0.42
1:E:218:ILE:HD12	1:E:310:GLU:HG2	2.02	0.42
1:F:173:ASP:OD1	1:F:240:ARG:NH1	2.52	0.42
1:A:106:LEU:CD2	1:A:124:PHE:HB3	2.50	0.42
1:F:98:ASP:OD1	1:F:98:ASP:C	2.63	0.42
1:D:114:VAL:HG23	1:D:118:GLU:CB	2.50	0.41
1:B:12:LEU:O	1:B:14:ARG:NH1	2.53	0.41
1:D:99:PHE:HD1	1:D:106:LEU:CD2	2.33	0.41
1:D:12:LEU:HA	1:D:13:PRO:HD3	1.93	0.41
1:A:106:LEU:HB3	1:A:122:LEU:HD11	2.02	0.41
1:B:95:HIS:CG	1:B:150:MET:HE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:VAL:O	1:C:123:ARG:HA	2.20	0.41
1:C:307:ASN:C	1:C:307:ASN:ND2	2.78	0.41
1:D:115:ASN:HB3	1:D:116:PRO:CD	2.50	0.41
1:D:77:GLU:O	1:D:159:ARG:NH1	2.51	0.41
1:E:19:LEU:HD21	1:E:41:PHE:CD2	2.55	0.41
1:F:250:ARG:NH2	1:F:310:GLU:OE2	2.48	0.41
1:A:26:HIS:HD2	1:A:27:ALA:O	2.03	0.41
1:E:39:VAL:HG12	1:E:41:PHE:CE1	2.55	0.41
1:A:82:GLU:HA	1:A:122:LEU:O	2.20	0.41
1:B:34:THR:HB	1:B:37:ARG:NH2	2.36	0.41
1:B:218:ILE:HD12	1:B:310:GLU:HG2	2.01	0.41
1:D:132:PHE:CE2	1:D:269:LYS:HE3	2.55	0.41
1:D:257:ILE:HD12	1:D:302:ALA:CB	2.44	0.41
1:B:296:ARG:C	1:B:297:GLN:HG2	2.46	0.41
1:A:28:HIS:CD2	1:A:74:VAL:HG11	2.56	0.40
1:B:62:MET:C	1:B:150:MET:HG3	2.46	0.40
1:C:69:PRO:HD2	1:C:221:ASN:HD22	1.86	0.40
1:D:308:LEU:HD13	1:F:142:VAL:HG12	2.03	0.40
1:D:69:PRO:HG3	1:D:179:GLY:HA3	2.03	0.40
1:E:207:VAL:HA	1:E:210:MET:HE3	2.02	0.40
1:F:14:ARG:NH1	1:F:40:GLU:OE2	2.54	0.40
1:B:114:VAL:HG21	1:B:120:THR:HG22	2.02	0.40
1:C:138:PRO:HG2	1:C:145:HIS:ND1	2.37	0.40
1:E:84:ARG:CG	1:E:84:ARG:NH1	2.82	0.40
1:E:142:VAL:HG12	1:F:308:LEU:HD13	2.03	0.40
1:F:165:GLU:OE1	1:F:165:GLU:N	2.55	0.40
1:E:84:ARG:HG2	1:E:84:ARG:NH1	2.31	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/329 (95%)	297 (95%)	14 (4%)	1 (0%)	36	58
1	B	314/329 (95%)	301 (96%)	13 (4%)	0	100	100
1	C	314/329 (95%)	307 (98%)	7 (2%)	0	100	100
1	D	318/329 (97%)	305 (96%)	10 (3%)	3 (1%)	14	30
1	E	313/329 (95%)	297 (95%)	16 (5%)	0	100	100
1	F	321/329 (98%)	302 (94%)	18 (6%)	1 (0%)	36	58
All	All	1892/1974 (96%)	1809 (96%)	78 (4%)	5 (0%)	36	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	LEU
1	D	6	PRO
1	D	114	VAL
1	F	112	THR
1	D	107	GLY

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	253/263 (96%)	240 (95%)	13 (5%)	21	45
1	B	255/263 (97%)	244 (96%)	11 (4%)	26	51
1	C	255/263 (97%)	240 (94%)	15 (6%)	18	38
1	D	258/263 (98%)	249 (96%)	9 (4%)	32	59
1	E	254/263 (97%)	242 (95%)	12 (5%)	23	48
1	F	261/263 (99%)	250 (96%)	11 (4%)	26	52
All	All	1536/1578 (97%)	1465 (95%)	71 (5%)	24	49

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LEU
1	A	111	LEU
1	A	136	CYS
1	A	139	GLU
1	A	189	GLU
1	A	204	GLU
1	A	221	ASN
1	A	230	ASP
1	A	240	ARG
1	A	247	GLN
1	A	307	ASN
1	A	314	LEU
1	A	320	PHE
1	B	15	VAL
1	B	90	THR
1	B	94	LEU
1	B	136	CYS
1	B	150	MET
1	B	159	ARG
1	B	213	LEU
1	B	221	ASN
1	B	240	ARG
1	B	307	ASN
1	B	320	PHE
1	C	17	VAL
1	C	54	ARG
1	C	65	ASN
1	C	96	ASN
1	C	139	GLU
1	C	189	GLU
1	C	221	ASN
1	C	230	ASP
1	C	240	ARG
1	C	247	GLN
1	C	269	LYS
1	C	307	ASN
1	C	314	LEU
1	C	320	PHE
1	C	321	LYS
1	D	94	LEU
1	D	106	LEU
1	D	121	THR
1	D	213	LEU

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Mol	Chain	Res	Type
1	D	221	ASN
1	D	240	ARG
1	D	247	GLN
1	D	307	ASN
1	D	320	PHE
1	E	10	SER
1	E	14	ARG
1	E	37	ARG
1	E	84	ARG
1	E	113	GLN
1	E	136	CYS
1	E	221	ASN
1	E	240	ARG
1	E	247	GLN
1	E	271	ARG
1	E	307	ASN
1	E	320	PHE
1	F	17	VAL
1	F	84	ARG
1	F	94	LEU
1	F	136	CYS
1	F	160	ASP
1	F	189	GLU
1	F	221	ASN
1	F	240	ARG
1	F	247	GLN
1	F	282	LEU
1	F	320	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	78	ASN
1	A	96	ASN
1	A	221	ASN
1	A	307	ASN
1	B	26	HIS
1	B	28	HIS
1	B	78	ASN
1	B	113	GLN
1	B	221	ASN

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Mol	Chain	Res	Type
1	B	307	ASN
1	B	319	HIS
1	C	26	HIS
1	C	28	HIS
1	C	65	ASN
1	C	78	ASN
1	C	96	ASN
1	C	168	GLN
1	C	221	ASN
1	C	307	ASN
1	D	26	HIS
1	D	28	HIS
1	D	76	HIS
1	D	78	ASN
1	D	221	ASN
1	D	249	ASN
1	D	260	HIS
1	D	307	ASN
1	E	26	HIS
1	E	78	ASN
1	E	96	ASN
1	E	113	GLN
1	E	168	GLN
1	E	221	ASN
1	E	297	GLN
1	E	307	ASN
1	F	26	HIS
1	F	76	HIS
1	F	78	ASN
1	F	96	ASN
1	F	113	GLN
1	F	221	ASN
1	F	327	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	314/329 (95%)	-0.48	7 (2%) 62 57	11, 26, 51, 79	0
1	B	316/329 (96%)	-0.36	3 (0%) 81 78	15, 31, 56, 75	0
1	C	316/329 (96%)	-0.46	3 (0%) 81 78	13, 27, 55, 66	0
1	D	320/329 (97%)	-0.24	7 (2%) 62 57	16, 31, 63, 74	0
1	E	315/329 (95%)	-0.27	6 (1%) 66 61	15, 31, 58, 68	0
1	F	323/329 (98%)	-0.41	1 (0%) 90 88	12, 26, 58, 71	0
All	All	1904/1974 (96%)	-0.37	27 (1%) 73 69	11, 29, 57, 79	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	110	ALA	4.0
1	D	108	GLY	4.0
1	B	326	TRP	3.7
1	D	106	LEU	2.7
1	D	111	LEU	2.6
1	E	109	GLY	2.6
1	A	111	LEU	2.5
1	A	109	GLY	2.5
1	C	296	ARG	2.5
1	C	123	ARG	2.5
1	D	109	GLY	2.5
1	E	105	ALA	2.5
1	A	325	GLU	2.4
1	B	107	GLY	2.3
1	E	190	ALA	2.3
1	F	327	ASN	2.3
1	E	10	SER	2.3
1	A	122	LEU	2.3
1	D	122	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	296	ARG	2.2
1	B	11	THR	2.1
1	A	108	GLY	2.1
1	C	325	GLU	2.1
1	D	10	SER	2.1
1	E	108	GLY	2.1
1	A	107	GLY	2.0
1	E	324	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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(Å ²)	Q<0.9
2	CU	D	501	1/1	0.98	0.02	37,37,37,37	0
2	CU	B	501	1/1	0.99	0.01	25,25,25,25	0
2	CU	F	501	1/1	0.99	0.01	26,26,26,26	0
3	CL	B	601	1/1	0.99	0.02	26,26,26,26	0
3	CL	B	602	1/1	0.99	0.04	29,29,29,29	0
3	CL	C	603	1/1	0.99	0.03	26,26,26,26	0
3	CL	F	605	1/1	0.99	0.04	22,22,22,22	0
2	CU	A	501	1/1	1.00	0.03	19,19,19,19	0
2	CU	E	502	1/1	1.00	0.02	16,16,16,16	0
2	CU	E	501	1/1	1.00	0.01	29,29,29,29	0
2	CU	F	502	1/1	1.00	0.01	12,12,12,12	0
2	CU	B	502	1/1	1.00	0.02	14,14,14,14	0
2	CU	A	502	1/1	1.00	0.01	16,16,16,16	0
2	CU	C	502	1/1	1.00	0.01	16,16,16,16	0
2	CU	C	501	1/1	1.00	0.03	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	D	604	1/1	1.00	0.02	31,31,31,31	0
2	CU	D	502	1/1	1.00	0.03	17,17,17,17	0
3	CL	F	606	1/1	1.00	0.03	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.