



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:38 PM UTC

PDB ID : 1EAY / pdb_00001eay
Title : CHEY-BINDING (P2) DOMAIN OF CHEA IN COMPLEX WITH CHEY FROM ESCHERICHIA COLI
Authors : Mcevoy, M.M.; Hausrath, A.C.; Randolph, G.B.; Remington, S.J.; Dahlquist, F.W.
Deposited on : 1998-04-23
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

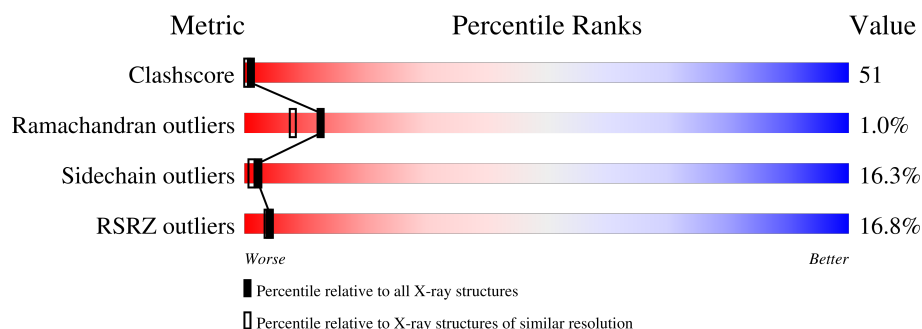
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
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	128	16% 17% 46% 34% .
1	B	128	17% 20% 48% 27% 5%
2	C	74	12% 20% 38% 24% 8% 9%
2	D	74	20% 24% 43% 24% . 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3058 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 CHEY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	128	Total	C	N	O	S	0	0	0
			953	612	154	181	6			
1	B	128	Total	C	N	O	S	0	0	0
			966	617	158	185	6			

- Molecule 2 is a protein called CHEA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	67	Total	C	N	O	S	0	0	0
			501	317	80	103	1			
2	D	69	Total	C	N	O	S	0	0	0
			514	325	82	106	1			

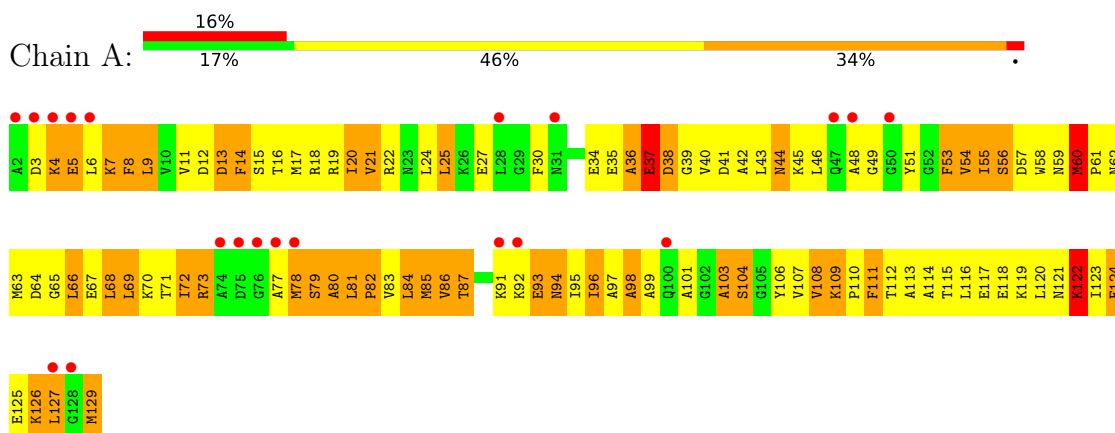
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total	O	0	0
			54	54		
3	B	32	Total	O	0	0
			32	32		
3	C	27	Total	O	0	0
			27	27		
3	D	11	Total	O	0	0
			11	11		

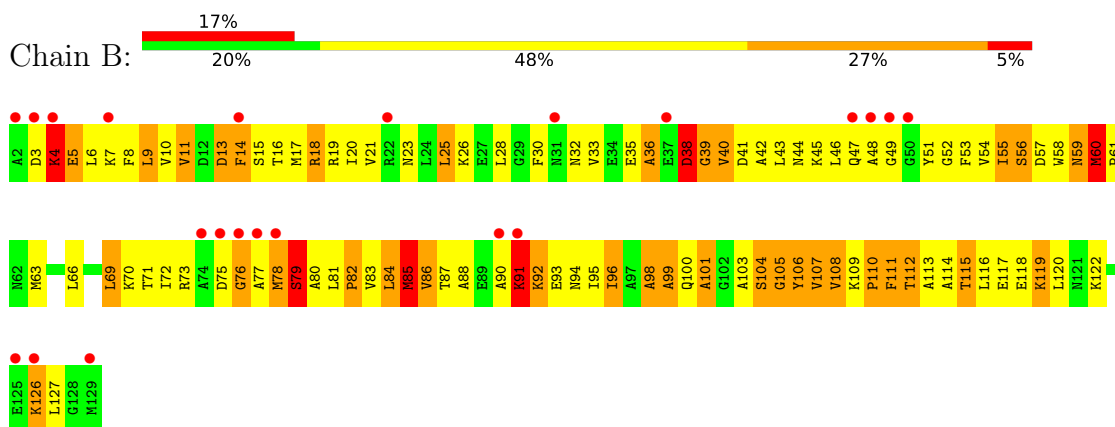
3 Residue-property plots [i](#)

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.

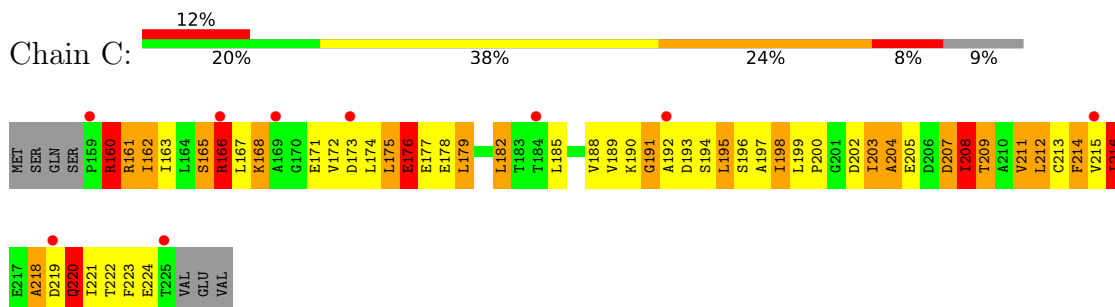
• Molecule 1: CHEY



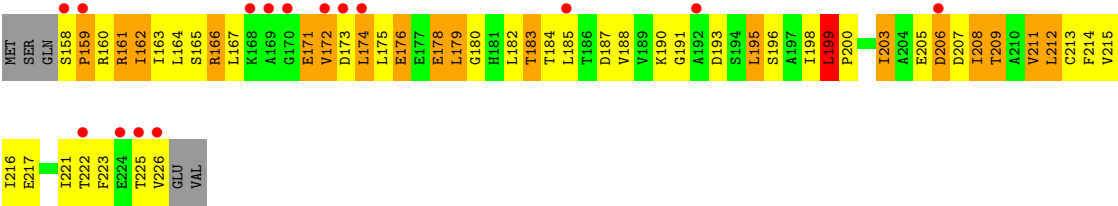
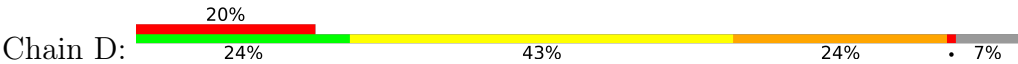
• Molecule 1: CHEY



• Molecule 2: CHEA



● Molecule 2: CHEA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.50Å 64.20Å 158.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	78.0 (20.00-2.00) 78.3 (20.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.51 (at 1.95Å)	Xtriage
Refinement program	TNT 5-F	Depositor
R, R_{free}	0.217 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	8.7	Xtriage
Anisotropy	1.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 183.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	3058	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.97	35/965 (3.6%)	2.15	43/1302 (3.3%)
1	B	1.85	19/978 (1.9%)	2.08	39/1318 (3.0%)
2	C	1.98	15/505 (3.0%)	2.12	24/687 (3.5%)
2	D	1.96	14/518 (2.7%)	2.13	29/706 (4.1%)
All	All	1.93	83/2966 (2.8%)	2.12	135/4013 (3.4%)

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	196	SER	CA-C	-8.22	1.42	1.52
2	C	194	SER	CA-C	-7.79	1.43	1.52
2	D	222	THR	CA-C	-7.58	1.43	1.52
1	A	112	THR	CA-C	-7.30	1.42	1.53
1	A	82	PRO	C-N	-7.18	1.24	1.33
1	A	8	PHE	N-CA	-7.11	1.37	1.46
2	D	160	ARG	N-CA	-7.08	1.37	1.46
1	A	85	MET	N-CA	-7.02	1.37	1.46
1	A	81	LEU	C-N	6.84	1.40	1.33
1	B	106	TYR	CA-C	6.82	1.61	1.52
1	A	71	THR	CA-C	-6.70	1.44	1.52
1	A	56	SER	CA-C	-6.62	1.44	1.52
1	B	86	VAL	CA-C	-6.62	1.44	1.52
1	B	36	ALA	CA-C	-6.50	1.44	1.52
1	A	57	ASP	N-CA	-6.46	1.37	1.45
1	A	14	PHE	N-CA	6.44	1.54	1.46
2	D	195	LEU	N-CA	-6.34	1.39	1.46
1	B	110	PRO	C-N	-6.33	1.24	1.33
1	A	56	SER	N-CA	-6.22	1.38	1.46
1	B	98	ALA	N-CA	-6.14	1.39	1.46
2	C	197	ALA	N-CA	-6.07	1.38	1.46
2	C	198	ILE	N-CA	-6.04	1.39	1.46
1	A	38	ASP	N-CA	6.03	1.53	1.46
1	B	56	SER	N-CA	-5.99	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	165	SER	N-CA	-5.98	1.39	1.45
2	C	208	ILE	CA-C	-5.92	1.45	1.52
1	A	84	LEU	CA-C	-5.91	1.45	1.53
2	D	212	LEU	CA-C	-5.90	1.44	1.52
2	D	196	SER	N-CA	-5.90	1.38	1.45
1	A	67	GLU	CA-C	-5.86	1.44	1.52
1	A	83	VAL	N-CA	-5.83	1.38	1.46
1	B	104	SER	CA-C	5.83	1.59	1.52
1	B	55	ILE	CA-C	-5.82	1.45	1.52
1	A	110	PRO	C-N	-5.74	1.25	1.33
2	C	195	LEU	C-N	-5.74	1.24	1.33
1	A	103	ALA	N-CA	5.71	1.53	1.45
1	A	54	VAL	N-CA	-5.63	1.39	1.46
1	A	53	PHE	CA-C	-5.62	1.46	1.52
2	D	187	ASP	CA-C	-5.60	1.46	1.53
2	D	162	ILE	N-CA	-5.60	1.39	1.46
1	A	36	ALA	CA-C	-5.60	1.45	1.52
1	B	84	LEU	C-N	-5.58	1.25	1.33
2	D	193	ASP	C-N	-5.58	1.26	1.33
2	C	162	ILE	C-N	-5.57	1.26	1.33
2	C	222	THR	CA-C	-5.57	1.45	1.52
1	B	57	ASP	C-N	-5.57	1.26	1.33
2	D	221	ILE	N-CA	-5.57	1.39	1.46
1	A	86	VAL	CA-C	-5.56	1.45	1.52
1	A	12	ASP	C-N	-5.50	1.25	1.33
1	A	87	THR	N-CA	-5.48	1.39	1.45
1	B	84	LEU	CA-CB	5.45	1.60	1.53
1	B	112	THR	C-N	-5.44	1.26	1.33
2	D	161	ARG	N-CA	-5.43	1.39	1.46
2	C	209	THR	N-CA	-5.42	1.40	1.46
1	B	106	TYR	N-CA	5.42	1.52	1.45
2	C	195	LEU	N-CA	-5.39	1.40	1.46
1	A	106	TYR	CA-C	5.38	1.59	1.52
1	B	14	PHE	N-CA	5.37	1.52	1.46
2	D	161	ARG	CA-C	-5.35	1.46	1.52
2	D	223	PHE	N-CA	-5.31	1.39	1.46
1	A	113	ALA	N-CA	-5.29	1.40	1.46
1	B	84	LEU	N-CA	5.28	1.52	1.46
2	D	223	PHE	CA-C	-5.26	1.46	1.52
1	A	20	ILE	CA-CB	-5.24	1.47	1.54
2	C	220	GLN	CA-C	-5.24	1.45	1.52
1	A	118	GLU	CA-C	5.24	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	195	LEU	C-N	-5.23	1.25	1.33
1	A	56	SER	C-N	-5.20	1.26	1.33
1	A	53	PHE	N-CA	-5.18	1.40	1.46
1	A	80	ALA	CA-C	5.18	1.59	1.52
1	A	124	PHE	N-CA	-5.18	1.40	1.46
1	A	37	GLU	C-N	5.14	1.40	1.33
2	C	163	ILE	N-CA	-5.12	1.40	1.46
1	A	71	THR	N-CA	-5.09	1.39	1.46
1	A	69	LEU	CA-C	5.08	1.59	1.52
1	B	107	VAL	N-CA	5.07	1.52	1.46
2	C	189	VAL	N-CA	-5.06	1.40	1.46
1	B	84	LEU	CA-C	-5.06	1.46	1.52
1	B	85	MET	N-CA	-5.06	1.39	1.46
2	C	204	ALA	CA-C	-5.06	1.46	1.52
1	A	73	ARG	CA-C	5.05	1.59	1.52
1	B	69	LEU	CA-C	5.04	1.59	1.52
1	A	99	ALA	CA-C	5.03	1.59	1.52

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ALA	N-CA-C	10.51	123.80	111.71
1	A	82	PRO	N-CA-CB	10.37	110.18	103.23
1	B	108	VAL	N-CA-C	9.60	121.71	107.80
1	B	80	ALA	N-CA-C	9.44	124.11	112.59
1	A	15	SER	N-CA-C	9.33	122.30	111.11
2	C	162	ILE	CA-C-N	-9.15	111.23	123.12
2	C	162	ILE	C-N-CA	-9.15	111.23	123.12
2	C	176	GLU	N-CA-C	-8.81	101.76	111.36
1	A	55	ILE	N-CA-CB	8.32	120.54	111.89
1	A	55	ILE	N-CA-C	-7.93	93.55	106.32
1	B	115	THR	N-CA-C	7.86	119.63	111.14
1	A	118	GLU	N-CA-C	7.77	119.75	111.28
1	A	68	LEU	N-CA-C	-7.71	102.57	110.97
1	A	60	MET	N-CA-C	7.64	115.10	108.22
1	B	44	ASN	N-CA-C	-7.56	103.04	111.28
2	C	216	ILE	N-CA-CB	-7.56	103.98	112.45
1	B	57	ASP	N-CA-C	-7.51	100.62	110.53
1	A	21	VAL	N-CA-C	-7.37	102.62	110.36
1	B	36	ALA	N-CA-C	-7.20	98.36	109.52
1	A	71	THR	N-CA-C	-7.18	102.86	111.69
2	C	212	LEU	N-CA-C	-7.14	103.50	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	196	SER	N-CA-C	-6.97	98.49	109.50
1	A	25	LEU	N-CA-C	-6.88	103.01	111.33
2	D	223	PHE	CA-CB-CG	-6.84	106.96	113.80
1	A	53	PHE	CA-C-N	-6.82	114.17	122.90
1	A	53	PHE	C-N-CA	-6.82	114.17	122.90
1	B	59	ASN	N-CA-C	6.71	119.88	109.07
1	B	96	ILE	N-CA-C	6.67	117.29	110.82
2	C	211	VAL	N-CA-C	6.65	118.63	111.58
1	A	73	ARG	N-CA-C	6.60	120.54	112.23
1	A	112	THR	N-CA-C	-6.57	101.06	110.59
2	D	179	LEU	CA-C-N	6.57	128.35	120.14
2	D	179	LEU	C-N-CA	6.57	128.35	120.14
1	A	80	ALA	N-CA-C	6.55	121.21	112.30
1	A	14	PHE	N-CA-C	6.52	119.35	108.20
1	B	23	ASN	N-CA-C	6.51	118.38	111.28
1	A	82	PRO	CB-CA-C	-6.51	105.48	111.40
1	A	7	LYS	N-CA-CB	6.49	120.02	110.35
1	A	84	LEU	CA-C-N	-6.41	112.33	121.50
1	A	84	LEU	C-N-CA	-6.41	112.33	121.50
2	C	193	ASP	CA-C-N	-6.40	111.85	122.21
2	C	193	ASP	C-N-CA	-6.40	111.85	122.21
2	D	193	ASP	CA-C-N	-6.36	112.19	122.36
2	D	193	ASP	C-N-CA	-6.36	112.19	122.36
1	B	94	ASN	N-CA-C	-6.33	104.31	111.14
1	A	72	ILE	N-CA-C	-6.32	104.35	110.42
2	D	159	PRO	N-CA-CB	6.32	109.33	103.39
2	D	212	LEU	N-CA-C	-6.30	104.46	111.71
2	D	208	ILE	CB-CA-C	-6.25	103.59	112.22
1	B	92	LYS	N-CA-C	6.23	121.58	111.37
1	B	91	LYS	N-CA-C	6.22	119.38	109.24
2	C	214	PHE	CB-CA-C	-6.22	97.69	110.38
1	A	67	GLU	N-CA-C	-6.21	104.62	111.82
2	D	161	ARG	CA-C-N	-6.21	114.96	122.90
2	D	161	ARG	C-N-CA	-6.21	114.96	122.90
1	A	38	ASP	N-CA-C	6.19	116.74	108.38
2	D	221	ILE	CA-C-N	-6.16	113.70	122.94
2	D	221	ILE	C-N-CA	-6.16	113.70	122.94
2	D	209	THR	N-CA-C	-6.14	103.74	111.11
2	D	196	SER	N-CA-C	-6.11	99.84	109.50
2	D	206	ASP	CA-CB-CG	6.11	118.71	112.60
1	B	55	ILE	N-CA-CB	6.10	121.30	111.23
1	B	110	PRO	CA-C-N	-6.09	112.57	122.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	110	PRO	C-N-CA	-6.09	112.57	122.81
2	D	199	LEU	CB-CA-C	-6.09	99.29	108.61
2	D	160	ARG	CA-C-N	-6.07	113.61	122.65
2	D	160	ARG	C-N-CA	-6.07	113.61	122.65
2	C	195	LEU	CA-C-O	6.00	127.82	120.25
1	A	124	PHE	N-CA-C	-5.99	103.92	111.11
1	B	119	LYS	N-CA-C	5.99	117.49	110.97
1	A	94	ASN	N-CA-C	-5.96	104.70	111.14
2	D	176	GLU	N-CA-C	-5.95	104.70	111.07
2	D	211	VAL	N-CA-C	5.91	117.45	111.00
1	A	86	VAL	N-CA-CB	5.90	117.15	110.72
1	A	108	VAL	N-CA-C	5.89	116.35	107.80
1	B	79	SER	N-CA-C	5.89	123.35	110.80
2	D	171	GLU	N-CA-C	-5.84	105.00	111.71
1	B	71	THR	N-CA-C	-5.80	104.95	111.28
1	A	19	ARG	N-CA-C	5.80	117.69	111.36
2	C	208	ILE	O-C-N	5.80	127.49	121.87
1	B	85	MET	CB-CA-C	5.78	119.07	109.53
1	B	101	ALA	N-CA-C	-5.78	106.08	113.01
2	D	162	ILE	CA-C-N	-5.76	115.52	122.90
2	D	162	ILE	C-N-CA	-5.76	115.52	122.90
1	B	99	ALA	N-CA-C	5.75	117.63	111.36
1	B	9	LEU	N-CA-C	-5.73	98.40	108.20
2	C	208	ILE	N-CA-C	-5.72	104.78	110.62
2	D	208	ILE	O-C-N	5.72	127.72	121.83
2	C	160	ARG	CA-C-N	-5.63	114.77	122.93
2	C	160	ARG	C-N-CA	-5.63	114.77	122.93
2	C	166	ARG	N-CA-C	5.60	118.84	111.28
1	A	67	GLU	O-C-N	5.59	129.14	122.27
1	B	40	VAL	N-CA-C	-5.59	104.92	110.62
1	B	13	ASP	CA-CB-CG	-5.57	107.03	112.60
1	B	105	GLY	CA-C-O	-5.56	116.08	121.75
1	A	98	ALA	N-CA-C	-5.55	105.13	111.07
1	A	66	LEU	N-CA-C	5.54	118.50	111.69
1	A	112	THR	CB-CA-C	-5.54	100.05	110.51
1	A	38	ASP	CA-C-N	5.52	126.08	120.00
1	A	38	ASP	C-N-CA	5.52	126.08	120.00
1	A	122	LYS	N-CA-C	5.49	117.34	111.36
1	A	9	LEU	N-CA-C	-5.47	98.36	107.99
1	A	84	LEU	N-CA-CB	5.38	119.26	110.39
1	B	60	MET	N-CA-C	5.37	115.04	108.11
1	A	92	LYS	N-CA-C	5.36	120.16	111.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	PRO	N-CA-CB	5.36	108.28	103.19
2	D	205	GLU	O-C-N	5.35	127.79	122.12
1	B	84	LEU	N-CA-CB	5.34	119.13	110.42
1	B	38	ASP	N-CA-C	5.33	116.24	108.14
2	C	218	ALA	N-CA-C	5.33	118.56	111.75
2	C	220	GLN	N-CA-C	-5.32	106.74	113.18
1	B	39	GLY	N-CA-C	5.28	118.88	112.49
1	A	126	LYS	N-CA-C	5.26	117.76	111.71
2	C	182	LEU	CB-CA-C	-5.26	100.17	110.11
2	C	207	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	96	ILE	CB-CA-C	-5.23	105.23	112.24
1	B	104	SER	N-CA-C	5.22	120.66	113.97
1	B	33	VAL	N-CA-C	5.22	115.63	108.12
1	B	55	ILE	CA-C-N	-5.19	114.92	122.65
1	B	55	ILE	C-N-CA	-5.19	114.92	122.65
2	C	179	LEU	N-CA-C	-5.16	105.77	111.71
1	A	97	ALA	N-CA-C	-5.16	105.66	111.28
1	B	25	LEU	N-CA-C	-5.15	105.16	111.75
1	B	18	ARG	CA-C-N	5.14	127.62	120.63
1	B	18	ARG	C-N-CA	5.14	127.62	120.63
1	B	55	ILE	N-CA-C	-5.12	98.68	109.34
2	D	163	ILE	N-CA-CB	5.11	117.19	111.21
2	D	191	GLY	N-CA-C	-5.10	104.40	112.66
1	B	41	ASP	N-CA-C	-5.09	105.63	111.07
2	C	191	GLY	CA-C-N	-5.07	113.48	120.28
2	C	191	GLY	C-N-CA	-5.07	113.48	120.28
2	D	174	LEU	N-CA-C	5.07	116.62	111.14
1	A	57	ASP	CA-CB-CG	-5.06	107.54	112.60
2	D	166	ARG	N-CA-C	5.03	116.79	110.91
2	C	168	LYS	N-CA-C	5.03	117.90	110.46

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	953	0	957	103	0
1	B	966	0	977	118	0
2	C	501	0	505	47	0
2	D	514	0	518	38	0
3	A	54	0	0	6	0
3	B	32	0	0	4	0
3	C	27	0	0	0	0
3	D	11	0	0	0	0
All	All	3058	0	2957	298	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 51.

All (298) 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:17:MET:HE2	1:B:21:VAL:HG23	1.49	0.95
1:A:54:VAL:HG12	1:A:56:SER:HB2	1.48	0.94
1:B:122:LYS:HE3	2:D:215:VAL:HG13	1.53	0.90
2:C:175:LEU:HD11	2:C:216:ILE:HD13	1.53	0.89
2:C:166:ARG:NH2	2:C:220:GLN:HA	1.88	0.87
2:D:179:LEU:HB2	2:D:185:LEU:HD11	1.57	0.87
1:A:84:LEU:HD13	1:A:123:ILE:HD11	1.59	0.85
2:D:179:LEU:CB	2:D:185:LEU:HD11	2.07	0.84
1:A:17:MET:HE3	1:A:21:VAL:CG2	2.09	0.82
1:B:14:PHE:CZ	1:B:16:THR:HB	2.14	0.82
2:C:215:VAL:HG12	2:C:216:ILE:HD12	1.62	0.81
1:A:59:ASN:O	1:A:60:MET:HG3	1.81	0.80
1:B:17:MET:HE2	1:B:21:VAL:CG2	2.11	0.80
1:A:54:VAL:CG1	1:A:56:SER:HB2	2.12	0.79
2:C:162:ILE:HB	2:C:199:LEU:HD22	1.65	0.79
1:A:109:LYS:HA	1:A:111:PHE:CD2	2.18	0.78
1:B:59:ASN:C	1:B:60:MET:HG3	2.11	0.76
2:C:166:ARG:NH1	2:C:220:GLN:HG3	2.01	0.76
1:B:59:ASN:O	1:B:60:MET:HG3	1.84	0.76
1:A:124:PHE:HD1	1:A:129:MET:HE2	1.52	0.74
1:B:17:MET:CE	1:B:21:VAL:HG23	2.18	0.74
1:B:6:LEU:HD21	1:B:53:PHE:HD2	1.53	0.74
1:B:66:LEU:HD12	1:B:69:LEU:HD23	1.68	0.74
1:B:18:ARG:HD2	1:B:35:GLU:OE1	1.88	0.73
1:B:10:VAL:O	1:B:35:GLU:HA	1.89	0.73
1:B:46:LEU:HD23	1:B:51:TYR:CD2	2.24	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:HB3	1:A:30:PHE:HB2	1.71	0.73
2:D:161:ARG:HB2	2:D:226:VAL:HG22	1.70	0.73
1:B:11:VAL:HG12	1:B:60:MET:SD	2.28	0.72
1:A:73:ARG:HD3	1:A:79:SER:O	1.88	0.72
1:A:72:ILE:HA	1:A:78:MET:HE3	1.69	0.72
1:A:14:PHE:CZ	1:A:16:THR:HB	2.25	0.71
1:A:72:ILE:HG23	1:A:78:MET:HB3	1.73	0.71
1:A:91:LYS:O	1:A:95:ILE:HG13	1.92	0.69
1:B:73:ARG:HD3	1:B:79:SER:O	1.92	0.69
1:B:4:LYS:HA	1:B:30:PHE:CD2	2.27	0.69
1:A:91:LYS:HG2	3:A:149:HOH:O	1.92	0.68
1:A:53:PHE:CE1	1:A:84:LEU:HB2	2.29	0.68
1:A:9:LEU:HB2	1:A:51:TYR:CD1	2.28	0.67
1:A:55:ILE:HG23	1:A:86:VAL:HG23	1.77	0.67
1:A:126:LYS:O	1:A:126:LYS:HG3	1.92	0.67
1:B:75:ASP:HB3	1:B:78:MET:HE2	1.77	0.66
2:D:173:ASP:O	2:D:176:GLU:HB3	1.94	0.66
2:D:198:ILE:HD12	2:D:198:ILE:N	2.10	0.66
1:A:59:ASN:C	1:A:60:MET:HG3	2.19	0.66
1:B:11:VAL:HG13	1:B:36:ALA:HB3	1.77	0.66
1:B:51:TYR:O	1:B:81:LEU:HD21	1.96	0.66
2:D:172:VAL:O	2:D:176:GLU:HB2	1.96	0.65
1:A:101:ALA:HB2	3:A:151:HOH:O	1.96	0.65
1:B:69:LEU:O	1:B:72:ILE:HB	1.96	0.65
1:B:70:LYS:HD2	3:B:152:HOH:O	1.96	0.65
1:B:75:ASP:O	1:B:77:ALA:N	2.30	0.64
1:B:4:LYS:HA	1:B:30:PHE:CE2	2.32	0.64
1:A:53:PHE:HE1	1:A:84:LEU:HB2	1.63	0.64
1:B:38:ASP:HB2	1:B:61:PRO:O	1.97	0.64
1:B:46:LEU:HD23	1:B:51:TYR:HD2	1.63	0.64
1:B:96:ILE:O	1:B:99:ALA:N	2.31	0.63
2:C:168:LYS:O	2:C:171:GLU:HB2	1.98	0.63
1:A:42:ALA:O	1:A:46:LEU:N	2.31	0.63
1:A:114:ALA:O	1:A:117:GLU:HB3	1.99	0.63
1:B:58:TRP:CZ3	1:B:85:MET:HE2	2.35	0.62
1:B:107:VAL:HG22	1:B:108:VAL:N	2.13	0.62
1:A:9:LEU:HG	1:A:11:VAL:HG22	1.81	0.62
1:A:18:ARG:NE	1:A:35:GLU:HB3	2.15	0.62
2:D:173:ASP:OD1	2:D:190:LYS:HE2	2.00	0.62
1:A:11:VAL:HG12	1:A:60:MET:SD	2.40	0.61
1:A:45:LYS:O	1:A:48:ALA:HB3	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:173:ASP:OD1	2:C:190:LYS:NZ	2.29	0.61
1:A:17:MET:HE3	1:A:21:VAL:HG23	1.81	0.61
1:A:14:PHE:O	1:A:18:ARG:HG3	2.00	0.60
1:B:9:LEU:HG	1:B:11:VAL:HG22	1.83	0.60
1:B:58:TRP:CE3	1:B:85:MET:HE2	2.36	0.60
1:B:109:LYS:HA	1:B:111:PHE:CD1	2.37	0.60
1:B:126:LYS:NZ	2:D:213:CYS:O	2.29	0.60
1:A:93:GLU:CD	1:A:93:GLU:H	2.09	0.60
1:B:43:LEU:HD12	1:B:63:MET:HE1	1.83	0.60
1:A:40:VAL:O	1:A:44:ASN:N	2.28	0.60
1:B:7:LYS:HD3	1:B:51:TYR:CD1	2.37	0.60
2:C:172:VAL:CG1	2:C:190:LYS:HG2	2.33	0.59
1:A:120:LEU:HB3	1:A:124:PHE:CE2	2.38	0.59
1:B:39:GLY:HA3	1:B:63:MET:HB3	1.83	0.59
1:A:107:VAL:HG22	1:A:108:VAL:N	2.17	0.59
1:B:39:GLY:N	1:B:63:MET:O	2.34	0.58
1:A:111:PHE:CD1	1:A:116:LEU:HB2	2.38	0.58
1:A:25:LEU:O	1:A:30:PHE:N	2.33	0.58
1:B:75:ASP:HB3	1:B:78:MET:CE	2.32	0.58
2:D:162:ILE:HB	2:D:199:LEU:HD22	1.86	0.58
1:A:82:PRO:HA	1:A:104:SER:OG	2.03	0.58
1:B:100:GLN:NE2	2:D:207:ASP:OD1	2.32	0.58
1:B:14:PHE:CE2	1:B:16:THR:HB	2.39	0.58
1:B:43:LEU:HD12	1:B:63:MET:CE	2.33	0.57
1:A:53:PHE:HE1	1:A:84:LEU:CB	2.17	0.57
1:A:38:ASP:O	1:A:42:ALA:N	2.30	0.57
2:C:213:CYS:HA	2:C:216:ILE:O	2.04	0.57
2:C:172:VAL:O	2:C:176:GLU:HB3	2.05	0.57
1:A:39:GLY:O	1:A:43:LEU:HB2	2.05	0.56
1:B:42:ALA:O	1:B:46:LEU:N	2.36	0.56
1:B:110:PRO:HA	3:B:135:HOH:O	2.04	0.56
1:A:9:LEU:HD11	1:A:36:ALA:HB2	1.86	0.56
1:B:17:MET:O	1:B:18:ARG:C	2.45	0.56
1:B:84:LEU:HD12	1:B:105:GLY:C	2.30	0.56
2:C:182:LEU:HD11	2:C:211:VAL:HB	1.86	0.56
2:D:188:VAL:HG13	2:D:195:LEU:HD11	1.87	0.56
1:B:17:MET:HE3	1:B:20:ILE:HB	1.87	0.56
1:A:98:ALA:HB1	1:A:103:ALA:HB3	1.87	0.56
2:C:165:SER:C	2:C:166:ARG:HG3	2.29	0.56
1:A:4:LYS:HA	1:A:30:PHE:CD2	2.41	0.56
1:B:93:GLU:CD	1:B:93:GLU:H	2.14	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LEU:CD1	1:B:63:MET:HE1	2.36	0.55
1:B:75:ASP:O	1:B:76:GLY:C	2.47	0.55
1:B:42:ALA:HA	1:B:45:LYS:HB2	1.88	0.55
1:A:64:ASP:O	1:A:68:LEU:HB2	2.07	0.55
1:A:49:GLY:HA2	3:A:145:HOH:O	2.07	0.54
1:B:39:GLY:O	1:B:43:LEU:N	2.34	0.54
1:A:65:GLY:O	1:A:68:LEU:HB3	2.08	0.54
1:A:37:GLU:HB2	3:A:178:HOH:O	2.07	0.54
2:C:218:ALA:HA	2:C:221:ILE:HD12	1.89	0.54
2:D:162:ILE:HD11	2:D:212:LEU:HD12	1.89	0.53
1:A:73:ARG:NH1	1:A:80:ALA:HA	2.23	0.53
1:A:126:LYS:NZ	2:C:213:CYS:O	2.34	0.53
2:C:188:VAL:HG13	2:C:195:LEU:HD11	1.89	0.53
1:A:7:LYS:HD3	1:A:51:TYR:CE1	2.44	0.53
2:D:179:LEU:HB3	2:D:185:LEU:HD11	1.89	0.53
1:B:91:LYS:O	1:B:95:ILE:HG13	2.08	0.53
1:B:4:LYS:HE3	1:B:30:PHE:CZ	2.45	0.52
1:A:124:PHE:HD1	1:A:129:MET:CE	2.21	0.52
1:B:16:THR:O	1:B:19:ARG:HB3	2.10	0.52
1:B:39:GLY:C	1:B:63:MET:HB3	2.35	0.52
1:B:8:PHE:HD2	1:B:55:ILE:HG13	1.75	0.52
1:B:39:GLY:CA	1:B:63:MET:HB3	2.40	0.52
2:C:166:ARG:CZ	2:C:220:GLN:HG3	2.39	0.52
2:C:202:ASP:OD1	2:C:203:ILE:HG22	2.10	0.52
1:A:24:LEU:O	1:A:25:LEU:C	2.52	0.52
1:A:109:LYS:HA	1:A:111:PHE:CE2	2.45	0.51
1:A:55:ILE:HG23	1:A:86:VAL:CG2	2.39	0.51
1:A:95:ILE:HG23	2:C:214:PHE:HE2	1.76	0.51
1:B:40:VAL:N	1:B:63:MET:HB3	2.26	0.51
1:B:13:ASP:OD1	1:B:13:ASP:N	2.34	0.51
2:C:182:LEU:HD11	2:C:211:VAL:CG1	2.41	0.51
1:A:27:GLU:O	1:A:27:GLU:HG3	2.09	0.51
1:B:55:ILE:CG2	1:B:86:VAL:HG23	2.41	0.51
2:C:174:LEU:O	2:C:178:GLU:N	2.44	0.51
1:B:84:LEU:HD12	1:B:106:TYR:HA	1.92	0.51
1:A:41:ASP:O	1:A:45:LYS:HB2	2.11	0.50
2:C:179:LEU:CB	2:C:185:LEU:HD11	2.41	0.50
1:B:3:ASP:C	1:B:5:GLU:H	2.19	0.50
2:D:174:LEU:HG	2:D:175:LEU:N	2.24	0.50
1:B:53:PHE:HE1	1:B:84:LEU:HB3	1.76	0.50
1:A:70:LYS:HE3	3:A:182:HOH:O	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ARG:HD2	1:B:35:GLU:CD	2.36	0.50
1:A:66:LEU:HA	1:A:69:LEU:HB3	1.93	0.50
1:B:55:ILE:HG23	1:B:86:VAL:HG23	1.93	0.49
2:D:159:PRO:HG2	2:D:226:VAL:HB	1.95	0.49
1:A:6:LEU:HD21	1:A:53:PHE:HB2	1.94	0.49
1:A:42:ALA:O	1:A:46:LEU:HG	2.11	0.49
1:B:43:LEU:HD12	1:B:63:MET:SD	2.51	0.49
1:B:52:GLY:O	1:B:82:PRO:HG2	2.13	0.49
1:B:90:ALA:HB2	1:B:108:VAL:HG21	1.94	0.49
1:A:17:MET:O	1:A:18:ARG:C	2.52	0.49
1:B:84:LEU:HD12	1:B:106:TYR:N	2.27	0.49
1:A:122:LYS:HA	1:A:125:GLU:HB2	1.94	0.49
1:B:106:TYR:O	1:B:119:LYS:NZ	2.30	0.49
2:C:174:LEU:HA	2:C:177:GLU:HB2	1.94	0.49
1:B:6:LEU:CD2	1:B:53:PHE:HD2	2.22	0.49
1:B:4:LYS:HE3	1:B:30:PHE:CE1	2.47	0.48
1:A:115:THR:O	1:A:116:LEU:C	2.53	0.48
1:B:25:LEU:HD22	1:B:30:PHE:HB2	1.95	0.48
2:C:204:ALA:O	2:C:205:GLU:C	2.56	0.48
1:A:94:ASN:ND2	3:A:149:HOH:O	2.33	0.48
2:C:179:LEU:HB3	2:C:185:LEU:HD11	1.95	0.48
1:B:88:ALA:HA	1:B:109:LYS:HE2	1.95	0.48
1:A:58:TRP:CE3	1:A:85:MET:HE2	2.49	0.48
1:B:101:ALA:HB2	3:B:154:HOH:O	2.13	0.48
1:B:107:VAL:CG2	1:B:108:VAL:N	2.77	0.48
1:A:6:LEU:HD21	1:A:53:PHE:CD2	2.48	0.48
1:A:109:LYS:HA	1:A:111:PHE:HD2	1.73	0.48
1:B:122:LYS:CE	2:D:215:VAL:HG13	2.34	0.48
1:B:115:THR:O	1:B:116:LEU:C	2.56	0.47
2:C:203:ILE:HG12	2:C:208:ILE:HG13	1.96	0.47
1:A:54:VAL:HG12	1:A:56:SER:CB	2.32	0.47
1:B:3:ASP:O	1:B:5:GLU:N	2.48	0.47
1:B:75:ASP:CB	1:B:78:MET:HE2	2.44	0.47
1:A:9:LEU:HD13	1:A:51:TYR:CE1	2.50	0.47
1:A:60:MET:HE3	1:A:60:MET:HB2	1.63	0.47
1:A:66:LEU:O	1:A:70:LYS:N	2.45	0.47
2:D:174:LEU:O	2:D:174:LEU:HD12	2.14	0.47
1:A:38:ASP:HB2	1:A:61:PRO:O	2.15	0.47
1:A:43:LEU:HD22	1:A:63:MET:SD	2.55	0.47
1:A:14:PHE:CD2	1:A:17:MET:HB2	2.50	0.47
1:B:84:LEU:HD12	1:B:106:TYR:CA	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ALA:CA	1:B:109:LYS:HE2	2.45	0.47
2:C:215:VAL:HG12	2:C:216:ILE:CD1	2.41	0.47
2:D:165:SER:C	2:D:166:ARG:HG3	2.39	0.47
1:B:7:LYS:HD3	1:B:51:TYR:CE1	2.51	0.46
1:B:6:LEU:HD21	1:B:53:PHE:CD2	2.43	0.46
1:B:109:LYS:HA	1:B:111:PHE:HD1	1.78	0.46
1:A:17:MET:HE3	1:A:21:VAL:HG22	1.93	0.46
1:B:32:ASN:C	1:B:32:ASN:HD22	2.23	0.46
2:C:166:ARG:HH22	2:C:220:GLN:HA	1.72	0.46
1:A:6:LEU:HD23	1:A:8:PHE:CZ	2.50	0.46
1:A:96:ILE:HD11	2:C:203:ILE:HD12	1.98	0.46
1:A:3:ASP:C	1:A:5:GLU:H	2.23	0.46
1:A:13:ASP:OD1	1:A:13:ASP:N	2.32	0.46
1:A:43:LEU:HD13	1:A:68:LEU:HD12	1.97	0.46
2:D:161:ARG:HB2	2:D:226:VAL:CG2	2.42	0.46
1:A:34:GLU:CG	1:A:35:GLU:N	2.78	0.46
1:A:84:LEU:HD13	1:A:123:ILE:CD1	2.40	0.46
1:A:108:VAL:O	1:A:111:PHE:HD2	1.99	0.46
1:B:53:PHE:HE1	1:B:84:LEU:CB	2.29	0.46
2:C:191:GLY:O	2:C:192:ALA:C	2.55	0.46
1:B:88:ALA:HA	1:B:109:LYS:HG3	1.98	0.45
1:B:6:LEU:CD2	1:B:53:PHE:CD2	3.00	0.45
1:B:119:LYS:O	1:B:120:LEU:C	2.52	0.45
1:A:40:VAL:CG2	1:A:62:ASN:HB3	2.46	0.45
1:A:121:ASN:O	1:A:124:PHE:HB2	2.17	0.45
2:D:212:LEU:O	2:D:215:VAL:N	2.37	0.45
1:B:17:MET:C	1:B:19:ARG:N	2.73	0.45
1:B:66:LEU:CD1	1:B:69:LEU:HD23	2.41	0.45
2:D:203:ILE:HG22	2:D:207:ASP:HB2	1.99	0.45
1:B:98:ALA:O	1:B:103:ALA:N	2.37	0.45
1:B:113:ALA:O	1:B:114:ALA:C	2.60	0.45
2:D:158:SER:N	2:D:225:THR:CG2	2.80	0.45
1:A:107:VAL:CG2	1:A:108:VAL:N	2.80	0.44
1:B:32:ASN:C	1:B:32:ASN:ND2	2.75	0.44
1:B:86:VAL:CG1	1:B:87:THR:N	2.80	0.44
2:D:165:SER:HB3	2:D:166:ARG:HG3	1.99	0.44
1:A:9:LEU:HG	1:A:11:VAL:CG2	2.48	0.44
2:C:195:LEU:HD12	2:C:195:LEU:HA	1.71	0.44
1:A:25:LEU:CD2	1:A:116:LEU:HD21	2.48	0.44
1:B:84:LEU:CD1	1:B:106:TYR:HA	2.48	0.44
1:A:127:LEU:HD12	1:A:127:LEU:HA	1.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PHE:CD1	1:A:129:MET:CE	2.99	0.44
1:B:3:ASP:O	1:B:6:LEU:N	2.40	0.44
1:B:72:ILE:HA	1:B:78:MET:HE3	2.00	0.44
1:B:7:LYS:HG2	1:B:7:LYS:O	2.17	0.44
1:B:43:LEU:CD1	1:B:63:MET:SD	3.06	0.43
1:B:86:VAL:HG12	1:B:87:THR:N	2.33	0.43
2:D:167:LEU:HD11	2:D:195:LEU:HB3	1.99	0.43
2:D:183:THR:OG1	2:D:200:PRO:HG2	2.18	0.43
1:B:19:ARG:O	1:B:20:ILE:C	2.58	0.43
1:A:55:ILE:CG2	1:A:86:VAL:CG2	2.97	0.43
1:A:39:GLY:HA3	1:A:63:MET:O	2.18	0.43
2:D:183:THR:HG23	2:D:184:THR:N	2.33	0.43
1:A:68:LEU:O	1:A:72:ILE:HG13	2.19	0.43
1:B:83:VAL:HG12	1:B:85:MET:SD	2.59	0.43
2:C:203:ILE:HG13	2:C:207:ASP:HB2	2.00	0.43
1:B:54:VAL:HG12	1:B:56:SER:HB2	1.99	0.43
1:B:108:VAL:O	1:B:111:PHE:HD1	2.02	0.43
2:C:171:GLU:O	2:C:175:LEU:HB2	2.18	0.42
2:C:175:LEU:HD23	2:C:175:LEU:HA	1.62	0.42
1:B:106:TYR:CD2	1:B:106:TYR:C	2.97	0.42
2:C:160:ARG:HA	2:C:224:GLU:O	2.19	0.42
2:C:167:LEU:CD1	2:C:195:LEU:HB2	2.49	0.42
1:B:17:MET:CE	1:B:20:ILE:HB	2.50	0.42
1:B:40:VAL:HG23	1:B:63:MET:HB2	2.01	0.42
1:A:115:THR:C	1:A:117:GLU:N	2.75	0.42
2:C:161:ARG:HG3	2:C:162:ILE:N	2.35	0.42
2:C:179:LEU:HG	2:C:212:LEU:HD21	2.00	0.42
2:C:188:VAL:O	2:C:188:VAL:HG12	2.19	0.42
2:C:182:LEU:HD11	2:C:211:VAL:HG11	2.01	0.42
2:D:212:LEU:C	2:D:214:PHE:N	2.73	0.42
1:B:60:MET:HE3	1:B:60:MET:HB2	1.73	0.42
1:B:75:ASP:C	1:B:77:ALA:N	2.77	0.42
1:A:81:LEU:HD12	1:A:81:LEU:HA	1.91	0.42
1:B:46:LEU:C	1:B:48:ALA:H	2.28	0.41
1:A:98:ALA:HB1	1:A:103:ALA:CB	2.48	0.41
2:C:219:ASP:C	2:C:221:ILE:H	2.22	0.41
2:D:164:LEU:HD22	2:D:216:ILE:HD11	2.02	0.41
2:D:167:LEU:CD1	2:D:195:LEU:HB3	2.50	0.41
1:B:112:THR:O	1:B:113:ALA:C	2.61	0.41
1:A:18:ARG:O	1:A:22:ARG:HB2	2.21	0.41
1:B:9:LEU:HG	1:B:11:VAL:CG2	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:CD1	1:B:106:TYR:CA	2.99	0.41
2:C:160:ARG:NE	2:C:223:PHE:HB3	2.34	0.41
2:D:211:VAL:O	2:D:214:PHE:HB2	2.21	0.41
1:B:49:GLY:HA3	3:B:148:HOH:O	2.20	0.41
2:D:182:LEU:HA	2:D:182:LEU:HD12	1.85	0.41
1:B:117:GLU:O	1:B:118:GLU:C	2.56	0.41
2:D:209:THR:O	2:D:213:CYS:SG	2.79	0.41
1:A:122:LYS:HE2	2:C:171:GLU:OE2	2.20	0.41
1:B:26:LYS:C	1:B:28:LEU:N	2.79	0.41
2:D:161:ARG:NH1	2:D:198:ILE:HD11	2.36	0.41
2:C:212:LEU:C	2:C:214:PHE:N	2.78	0.41
2:D:178:GLU:C	2:D:180:GLY:N	2.77	0.41
1:A:3:ASP:C	1:A:5:GLU:N	2.79	0.40
1:B:75:ASP:CB	1:B:78:MET:CE	2.99	0.40
2:C:182:LEU:HD11	2:C:211:VAL:CB	2.49	0.40
2:C:209:THR:O	2:C:213:CYS:SG	2.79	0.40
1:A:17:MET:CE	1:A:21:VAL:HG23	2.51	0.40
1:A:60:MET:HA	1:A:61:PRO:HD3	1.90	0.40
2:D:162:ILE:O	2:D:162:ILE:HG23	2.21	0.40
1:A:20:ILE:O	1:A:21:VAL:C	2.64	0.40
2:D:161:ARG:HG2	2:D:162:ILE:N	2.36	0.40
2:D:178:GLU:O	2:D:179:LEU:C	2.64	0.40
2:C:199:LEU:HA	2:C:200:PRO:HD2	1.92	0.40
1:A:93:GLU:CD	1:A:93:GLU:N	2.76	0.40
1:B:3:ASP:C	1:B:5:GLU:N	2.78	0.40
2:C:211:VAL:C	2:C:213:CYS:N	2.72	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	126/128 (98%)	119 (94%)	6 (5%)	1 (1%)	16	11
1	B	126/128 (98%)	112 (89%)	11 (9%)	3 (2%)	4	2
2	C	65/74 (88%)	61 (94%)	4 (6%)	0	100	100
2	D	67/74 (90%)	64 (96%)	3 (4%)	0	100	100
All	All	384/404 (95%)	356 (93%)	24 (6%)	4 (1%)	12	8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	LYS
1	B	79	SER
1	A	79	SER
1	B	76	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	95/102 (93%)	79 (83%)	16 (17%)	2	1
1	B	99/102 (97%)	84 (85%)	15 (15%)	3	1
2	C	55/64 (86%)	45 (82%)	10 (18%)	2	1
2	D	57/64 (89%)	48 (84%)	9 (16%)	2	1
All	All	306/332 (92%)	256 (84%)	50 (16%)	2	1

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	5	GLU
1	A	13	ASP
1	A	37	GLU
1	A	44	ASN
1	A	60	MET
1	A	78	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	87	THR
1	A	93	GLU
1	A	104	SER
1	A	109	LYS
1	A	111	PHE
1	A	119	LYS
1	A	122	LYS
1	A	127	LEU
1	A	129	MET
1	B	4	LYS
1	B	5	GLU
1	B	11	VAL
1	B	15	SER
1	B	38	ASP
1	B	47	GLN
1	B	60	MET
1	B	78	MET
1	B	85	MET
1	B	91	LYS
1	B	92	LYS
1	B	104	SER
1	B	111	PHE
1	B	126	LYS
1	B	127	LEU
2	C	160	ARG
2	C	161	ARG
2	C	166	ARG
2	C	175	LEU
2	C	176	GLU
2	C	198	ILE
2	C	203	ILE
2	C	208	ILE
2	C	216	ILE
2	C	220	GLN
2	D	171	GLU
2	D	172	VAL
2	D	178	GLU
2	D	183	THR
2	D	199	LEU
2	D	203	ILE
2	D	206	ASP
2	D	208	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	217	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	B	23	ASN
1	B	32	ASN
1	B	44	ASN
1	B	94	ASN
1	B	121	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	128/128 (100%)	1.07	20 (15%) 5 4	17, 33, 65, 83	0
1	B	128/128 (100%)	1.07	22 (17%) 4 3	20, 32, 70, 85	0
2	C	67/74 (90%)	0.98	9 (13%) 7 6	21, 36, 55, 75	0
2	D	69/74 (93%)	1.30	15 (21%) 2 2	23, 37, 64, 78	0
All	All	392/404 (97%)	1.09	66 (16%) 4 4	17, 35, 67, 85	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	6.9
2	D	226	VAL	6.3
2	D	169	ALA	5.8
1	B	49	GLY	5.7
1	A	2	ALA	5.1
1	A	3	ASP	4.7
1	A	128	GLY	4.3
1	B	50	GLY	4.2
2	D	158	SER	4.1
1	B	77	ALA	4.1
2	D	170	GLY	3.8
2	D	192	ALA	3.7
2	C	159	PRO	3.6
1	A	5	GLU	3.6
1	B	48	ALA	3.6
1	A	127	LEU	3.5
1	A	4	LYS	3.5
1	B	3	ASP	3.4
1	B	75	ASP	3.4
2	C	225	THR	3.3
1	B	4	LYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	159	PRO	3.2
2	D	168	LYS	3.2
1	B	76	GLY	3.2
1	A	48	ALA	3.0
1	A	47	GLN	2.9
2	D	185	LEU	2.9
1	A	50	GLY	2.9
1	B	47	GLN	2.8
1	A	77	ALA	2.7
1	B	78	MET	2.7
1	B	74	ALA	2.6
2	C	169	ALA	2.6
1	A	31	ASN	2.6
1	B	126	LYS	2.6
1	B	37	GLU	2.6
2	D	174	LEU	2.6
1	A	75	ASP	2.6
1	B	14	PHE	2.5
1	B	7	LYS	2.5
1	A	78	MET	2.4
2	C	184	THR	2.4
2	C	173	ASP	2.4
1	A	91	LYS	2.3
1	B	91	LYS	2.3
2	D	172	VAL	2.3
1	A	92	LYS	2.3
2	D	225	THR	2.3
1	A	76	GLY	2.3
1	A	6	LEU	2.3
2	C	219	ASP	2.2
2	D	224	GLU	2.2
1	B	31	ASN	2.2
1	B	125	GLU	2.2
1	A	28	LEU	2.2
1	B	129	MET	2.2
1	A	100	GLN	2.1
1	B	90	ALA	2.1
1	B	22	ARG	2.1
2	C	166	ARG	2.1
2	C	215	VAL	2.1
2	C	192	ALA	2.1
1	A	74	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	173	ASP	2.0
2	D	206	ASP	2.0
2	D	222	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.