



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:57 PM UTC

PDB ID : 1EEA / pdb_00001eea
Title : Acetylcholinesterase
Authors : Raves, M.L.; Giles, K.; Schrag, J.D.; Schmid, M.F.; Phillips Jr., G.N.; Wah, C.; Howard, A.J.; Silman, I.; Sussman, J.L.
Deposited on : 1999-01-26
Resolution : 4.50 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

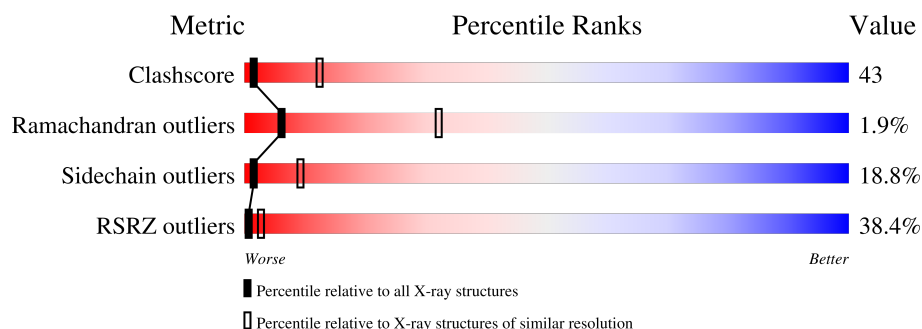
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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	534	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4115 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.

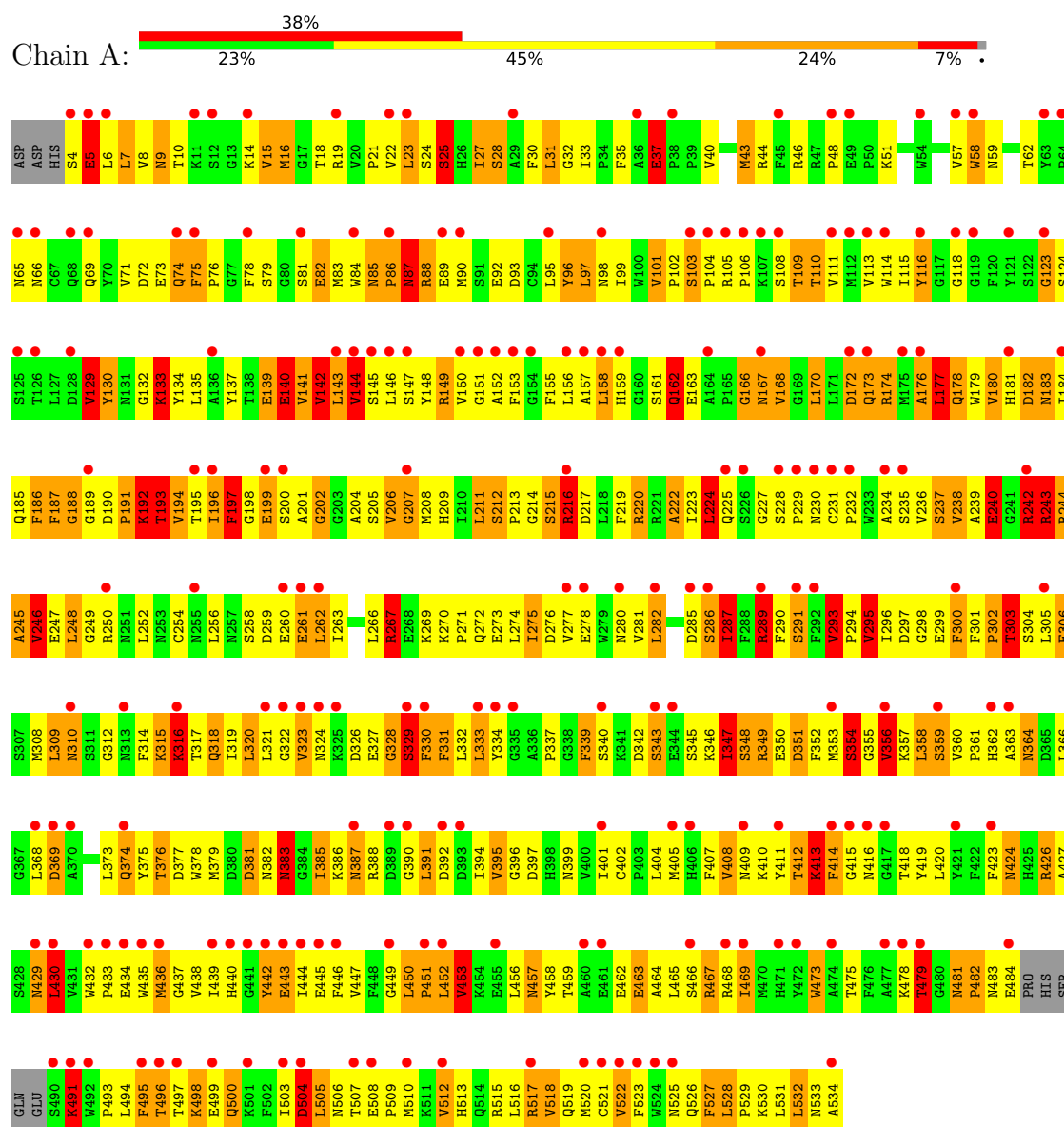
- Molecule 1 is a protein called PROTEIN (ACETYLCHOLINESTERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	526	4115	2663	694	737	21	0	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PROTEIN (ACETYLCHOLINESTERASE)



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	140.86Å 201.46Å 235.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 4.50 117.89 – 4.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-4.50) 82.1 (117.89-4.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 4.43Å)	Xtriage
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available) 0.341 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	107.7	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	4115	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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 [i](#)

5.1 Standard geometry [i](#)

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	1.53	25/4234 (0.6%)	2.55	338/5751 (5.9%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	SER	N-CA	9.52	1.55	1.46
1	A	293	VAL	N-CA	7.03	1.55	1.46
1	A	167	ASN	N-CA	-6.90	1.37	1.46
1	A	197	PHE	N-CA	6.84	1.53	1.45
1	A	290	PHE	N-CA	6.71	1.54	1.45
1	A	285	ASP	N-CA	6.34	1.53	1.46
1	A	285	ASP	CA-CB	-6.03	1.45	1.53
1	A	16	MET	N-CA	5.98	1.53	1.46
1	A	504	ASP	CA-CB	-5.95	1.44	1.53
1	A	436	MET	CA-CB	-5.75	1.43	1.53
1	A	479	THR	CA-CB	5.70	1.62	1.54
1	A	295	VAL	C-N	-5.62	1.28	1.33
1	A	242	ARG	CD-NE	5.62	1.54	1.46
1	A	391	LEU	N-CA	5.56	1.53	1.46
1	A	159	HIS	C-O	5.51	1.30	1.24
1	A	194	VAL	CA-C	5.43	1.59	1.52
1	A	317	THR	C-O	5.43	1.29	1.24
1	A	166	GLY	N-CA	5.38	1.53	1.45
1	A	436	MET	N-CA	5.37	1.53	1.46
1	A	316	LYS	CA-CB	-5.25	1.45	1.53
1	A	227	GLY	N-CA	5.16	1.51	1.45
1	A	192	LYS	N-CA	5.12	1.52	1.46
1	A	97	LEU	N-CA	5.12	1.52	1.45
1	A	195	THR	CA-CB	5.10	1.60	1.53
1	A	228	SER	CA-CB	-5.06	1.46	1.54

All (338) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	VAL	N-CA-CB	-15.37	89.70	111.21
1	A	85	ASN	CA-CB-CG	14.82	127.42	112.60
1	A	166	GLY	CA-C-N	13.41	147.16	121.54
1	A	166	GLY	C-N-CA	13.41	147.16	121.54
1	A	216	ARG	CD-NE-CZ	12.32	141.65	124.40
1	A	267	ARG	CD-NE-CZ	12.17	141.44	124.40
1	A	285	ASP	CB-CA-C	11.70	129.37	110.19
1	A	323	VAL	N-CA-CB	-11.34	96.65	112.52
1	A	434	GLU	CA-CB-CG	11.03	136.15	114.10
1	A	504	ASP	CA-CB-CG	10.82	123.42	112.60
1	A	216	ARG	NE-CZ-NH1	10.73	132.23	121.50
1	A	339	PHE	CA-C-O	-10.71	108.92	120.80
1	A	415	GLY	CA-C-O	-10.61	111.67	122.28
1	A	31	LEU	CA-C-O	10.55	131.88	120.38
1	A	414	PHE	CA-CB-CG	10.54	124.34	113.80
1	A	278	GLU	CB-CG-CD	10.01	129.62	112.60
1	A	383	ASN	CA-C-N	9.94	132.66	120.13
1	A	383	ASN	C-N-CA	9.94	132.66	120.13
1	A	228	SER	CB-CA-C	9.89	123.37	109.92
1	A	172	ASP	CA-CB-CG	9.72	122.32	112.60
1	A	168	VAL	CB-CA-C	9.70	124.74	112.04
1	A	195	THR	CA-C-O	-9.66	110.02	120.36
1	A	65	ASN	OD1-CG-ND2	9.65	132.25	122.60
1	A	167	ASN	OD1-CG-ND2	-9.59	113.01	122.60
1	A	243	ARG	NE-CZ-NH2	9.58	127.82	119.20
1	A	162	GLN	OE1-CD-NE2	-9.45	113.15	122.60
1	A	194	VAL	O-C-N	9.34	133.35	123.26
1	A	356	VAL	CA-C-O	-9.30	110.61	120.57
1	A	285	ASP	CA-CB-CG	9.08	121.68	112.60
1	A	132	GLY	N-CA-C	8.96	124.35	114.40
1	A	243	ARG	NE-CZ-NH1	-8.95	112.55	121.50
1	A	285	ASP	N-CA-C	-8.82	94.14	108.52
1	A	289	ARG	CB-CA-C	8.77	124.99	109.65
1	A	463	GLU	CB-CG-CD	8.77	127.51	112.60
1	A	309	LEU	CA-C-O	8.66	129.98	120.63
1	A	87	ASN	OD1-CG-ND2	8.55	131.15	122.60
1	A	228	SER	CA-C-O	-8.44	111.57	119.76
1	A	105	ARG	O-C-N	8.44	128.30	121.38
1	A	142	VAL	CB-CA-C	8.35	121.07	110.96
1	A	86	PRO	CA-C-O	-8.35	112.22	121.32
1	A	242	ARG	CD-NE-CZ	-8.31	112.77	124.40
1	A	426	ARG	CD-NE-CZ	8.24	135.94	124.40
1	A	504	ASP	N-CA-CB	8.21	123.80	110.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	GLY	N-CA-C	-8.20	102.57	112.49
1	A	293	VAL	CB-CA-C	8.17	126.23	111.36
1	A	442	TYR	CB-CA-C	8.13	124.85	110.37
1	A	59	ASN	CA-C-O	-8.10	111.10	120.49
1	A	65	ASN	O-C-N	8.09	132.01	122.79
1	A	440	HIS	CA-CB-CG	8.07	121.87	113.80
1	A	391	LEU	CB-CA-C	7.96	126.62	110.38
1	A	240	GLU	CB-CG-CD	7.92	126.06	112.60
1	A	228	SER	N-CA-C	-7.87	97.95	108.11
1	A	162	GLN	CB-CG-CD	7.85	125.94	112.60
1	A	331	PHE	CA-CB-CG	-7.84	105.96	113.80
1	A	248	LEU	N-CA-C	-7.81	102.76	111.28
1	A	69	GLN	OE1-CD-NE2	7.78	130.38	122.60
1	A	484	GLU	CA-CB-CG	7.63	129.37	114.10
1	A	168	VAL	CA-CB-CG1	7.62	123.36	110.40
1	A	347	ILE	CB-CG1-CD1	7.56	129.67	113.80
1	A	207	GLY	CA-C-O	-7.56	113.39	120.80
1	A	174	ARG	CD-NE-CZ	-7.55	113.82	124.40
1	A	9	ASN	CA-CB-CG	7.53	120.13	112.60
1	A	339	PHE	O-C-N	7.47	131.94	123.19
1	A	89	GLU	CA-C-O	-7.46	112.99	121.19
1	A	170	LEU	CB-CA-C	7.43	124.15	110.11
1	A	101	VAL	N-CA-C	7.40	115.95	107.89
1	A	129	VAL	O-C-N	7.40	132.37	122.31
1	A	133	LYS	N-CA-C	7.38	119.40	111.36
1	A	230	ASN	CA-CB-CG	-7.36	105.24	112.60
1	A	479	THR	CA-CB-OG1	-7.35	98.57	109.60
1	A	16	MET	CB-CA-C	7.31	122.17	110.19
1	A	220	ARG	CA-CB-CG	7.29	128.68	114.10
1	A	504	ASP	N-CA-C	-7.29	98.73	110.32
1	A	358	LEU	CA-C-O	-7.23	113.25	120.70
1	A	482	PRO	CA-C-N	7.21	131.81	121.50
1	A	482	PRO	C-N-CA	7.21	131.81	121.50
1	A	413	LYS	N-CA-CB	7.19	121.43	110.28
1	A	176	ALA	O-C-N	7.16	129.71	122.12
1	A	25	SER	CA-C-N	7.16	133.80	122.21
1	A	25	SER	C-N-CA	7.16	133.80	122.21
1	A	217	ASP	CA-CB-CG	7.13	119.73	112.60
1	A	368	LEU	CB-CA-C	7.11	122.59	110.79
1	A	287	ILE	CB-CA-C	7.06	122.32	110.95
1	A	88	ARG	CA-C-O	-7.05	113.19	121.44
1	A	35	PHE	CA-CB-CG	7.04	120.84	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	GLU	O-C-N	7.03	129.57	122.12
1	A	396	GLY	CA-C-N	7.03	129.70	120.28
1	A	396	GLY	C-N-CA	7.03	129.70	120.28
1	A	186	PHE	CA-CB-CG	-7.02	106.78	113.80
1	A	224	LEU	O-C-N	7.01	131.48	123.27
1	A	391	LEU	N-CA-C	-7.01	103.40	112.23
1	A	16	MET	CA-CB-CG	6.98	128.06	114.10
1	A	387	ASN	CA-CB-CG	6.96	119.56	112.60
1	A	463	GLU	N-CA-C	-6.96	103.69	111.28
1	A	180	VAL	O-C-N	6.94	128.60	121.87
1	A	297	ASP	CA-C-O	-6.93	110.71	119.31
1	A	254	CYS	O-C-N	6.91	132.01	123.10
1	A	182	ASP	CA-C-O	-6.90	110.28	119.11
1	A	350	GLU	N-CA-CB	6.88	119.98	110.01
1	A	479	THR	CA-C-O	-6.87	111.62	118.97
1	A	280	ASN	CA-C-O	-6.86	110.97	119.28
1	A	522	VAL	CA-CB-CG1	6.85	122.05	110.40
1	A	155	PHE	N-CA-CB	-6.81	101.67	111.54
1	A	453	VAL	CB-CA-C	6.78	118.56	111.23
1	A	201	ALA	CA-C-O	6.77	127.24	119.18
1	A	317	THR	CA-C-O	-6.77	112.47	121.47
1	A	174	ARG	NE-CZ-NH1	-6.72	114.78	121.50
1	A	430	LEU	CA-C-O	-6.68	113.80	121.15
1	A	152	ALA	O-C-N	6.68	129.03	122.09
1	A	244	ARG	NE-CZ-NH2	-6.67	113.20	119.20
1	A	464	ALA	CA-C-N	6.67	129.51	120.38
1	A	464	ALA	C-N-CA	6.67	129.51	120.38
1	A	527	PHE	N-CA-C	6.67	118.23	110.97
1	A	322	GLY	CA-C-N	6.66	132.51	122.92
1	A	322	GLY	C-N-CA	6.66	132.51	122.92
1	A	328	GLY	N-CA-C	6.66	121.29	112.77
1	A	290	PHE	CB-CA-C	6.64	122.41	109.33
1	A	194	VAL	N-CA-CB	6.62	120.54	111.41
1	A	382	ASN	O-C-N	6.62	130.98	122.04
1	A	462	GLU	N-CA-C	-6.61	104.24	112.90
1	A	291	SER	N-CA-C	6.58	118.33	111.03
1	A	369	ASP	CA-C-O	-6.58	113.91	120.82
1	A	481	ASN	CB-CA-C	6.57	119.06	109.20
1	A	123	GLY	CA-C-O	6.57	127.44	121.66
1	A	199	GLU	N-CA-C	6.56	119.59	108.90
1	A	401	ILE	N-CA-C	6.55	116.71	110.42
1	A	217	ASP	N-CA-C	6.53	120.99	112.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	LEU	CB-CA-C	6.47	121.04	110.88
1	A	188	GLY	N-CA-C	-6.45	105.86	114.95
1	A	275	ILE	CA-C-N	6.44	129.23	120.54
1	A	275	ILE	C-N-CA	6.44	129.23	120.54
1	A	222	ALA	CA-C-N	6.40	131.89	122.99
1	A	222	ALA	C-N-CA	6.40	131.89	122.99
1	A	162	GLN	N-CA-CB	6.40	120.42	110.44
1	A	31	LEU	O-C-N	-6.38	115.77	123.29
1	A	173	GLN	O-C-N	6.37	128.72	122.09
1	A	442	TYR	CA-CB-CG	-6.36	102.45	113.90
1	A	424	ASN	CA-CB-CG	-6.33	106.28	112.60
1	A	512	VAL	N-CA-C	-6.32	99.29	108.71
1	A	238	VAL	CA-C-O	-6.31	113.65	120.47
1	A	270	LYS	CB-CA-C	6.31	119.43	109.27
1	A	366	LEU	N-CA-C	-6.31	104.40	111.28
1	A	413	LYS	CA-C-O	-6.29	112.74	119.97
1	A	287	ILE	N-CA-C	-6.27	99.36	108.89
1	A	297	ASP	N-CA-C	6.27	120.66	112.89
1	A	387	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	A	450	LEU	O-C-N	6.26	128.52	121.32
1	A	150	VAL	CA-C-O	-6.25	116.74	121.68
1	A	62	THR	CA-C-N	6.24	129.56	120.51
1	A	62	THR	C-N-CA	6.24	129.56	120.51
1	A	404	LEU	N-CA-C	-6.22	104.58	111.36
1	A	463	GLU	N-CA-CB	6.21	119.26	110.12
1	A	286	SER	CA-CB-OG	-6.21	98.68	111.10
1	A	96	TYR	CA-CB-CG	-6.20	102.73	113.90
1	A	315	LYS	CA-C-O	-6.20	114.20	120.96
1	A	364	ASN	CA-C-N	6.20	128.50	120.44
1	A	364	ASN	C-N-CA	6.20	128.50	120.44
1	A	239	ALA	O-C-N	6.19	128.44	122.07
1	A	237	SER	N-CA-C	-6.18	102.37	110.53
1	A	473	TRP	CA-C-O	-6.17	113.88	120.42
1	A	219	PHE	CA-CB-CG	-6.16	107.64	113.80
1	A	244	ARG	NE-CZ-NH1	6.15	127.65	121.50
1	A	354	SER	N-CA-CB	6.15	119.36	110.20
1	A	436	MET	CB-CA-C	6.13	122.79	109.99
1	A	532	LEU	CA-C-O	-6.11	112.40	119.61
1	A	364	ASN	N-CA-C	-6.09	101.95	110.35
1	A	193	THR	CA-CB-OG1	-6.08	100.48	109.60
1	A	129	VAL	CA-C-O	-6.07	111.57	119.53
1	A	79	SER	CA-CB-OG	-6.07	98.96	111.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	SER	O-C-N	6.06	126.92	121.35
1	A	95	LEU	N-CA-CB	-6.03	101.89	110.46
1	A	506	ASN	OD1-CG-ND2	6.03	128.63	122.60
1	A	170	LEU	N-CA-C	-6.03	104.07	112.45
1	A	37	GLU	N-CA-CB	-6.02	102.75	110.03
1	A	178	GLN	CA-C-O	-6.01	114.46	121.07
1	A	351	ASP	CA-CB-CG	-6.00	106.60	112.60
1	A	79	SER	CA-C-O	-5.98	114.21	120.55
1	A	327	GLU	CA-C-O	-5.97	112.75	119.79
1	A	495	PHE	N-CA-C	-5.96	101.02	109.96
1	A	148	TYR	CA-CB-CG	5.96	124.63	113.90
1	A	155	PHE	CA-CB-CG	5.92	119.72	113.80
1	A	303	THR	N-CA-CB	5.91	121.51	110.87
1	A	144	VAL	CA-CB-CG2	5.91	120.44	110.40
1	A	88	ARG	CA-CB-CG	5.90	125.90	114.10
1	A	302	PRO	N-CD-CG	-5.89	94.36	103.20
1	A	494	LEU	CA-CB-CG	5.89	136.92	116.30
1	A	505	LEU	CB-CA-C	5.88	121.10	111.23
1	A	206	VAL	CA-C-O	5.87	127.52	121.41
1	A	215	SER	N-CA-C	5.87	119.63	112.23
1	A	342	ASP	N-CA-C	5.87	119.50	112.93
1	A	440	HIS	O-C-N	5.87	130.39	122.59
1	A	310	ASN	OD1-CG-ND2	5.86	128.46	122.60
1	A	348	SER	CA-C-O	-5.86	114.73	121.47
1	A	153	PHE	O-C-N	5.84	128.31	122.12
1	A	231	CYS	CA-C-O	-5.84	113.94	120.25
1	A	200	SER	CA-C-O	-5.83	112.17	120.51
1	A	436	MET	CA-CB-CG	5.82	125.74	114.10
1	A	170	LEU	N-CA-CB	-5.82	101.59	110.26
1	A	426	ARG	CA-CB-CG	5.80	125.70	114.10
1	A	141	VAL	CA-C-N	-5.78	115.14	122.37
1	A	141	VAL	C-N-CA	-5.78	115.14	122.37
1	A	155	PHE	CB-CA-C	5.78	120.20	111.18
1	A	459	THR	CA-CB-OG1	-5.78	100.94	109.60
1	A	359	SER	CA-C-O	-5.77	114.30	120.42
1	A	97	LEU	CA-CB-CG	5.77	136.50	116.30
1	A	405	MET	CA-C-O	-5.76	113.34	119.97
1	A	473	TRP	O-C-N	5.76	128.72	122.15
1	A	31	LEU	N-CA-C	5.76	118.34	109.07
1	A	261	GLU	O-C-N	5.76	128.31	122.09
1	A	392	ASP	N-CA-C	-5.75	105.01	111.28
1	A	303	THR	CB-CA-C	-5.75	99.56	113.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	LEU	CA-C-N	5.74	132.51	121.54
1	A	158	LEU	C-N-CA	5.74	132.51	121.54
1	A	37	GLU	CB-CA-C	5.74	117.13	108.86
1	A	58	TRP	CA-C-O	-5.73	113.85	120.49
1	A	521	CYS	CA-C-N	-5.71	111.15	120.64
1	A	521	CYS	C-N-CA	-5.71	111.15	120.64
1	A	116	TYR	N-CA-C	5.70	118.54	110.50
1	A	245	ALA	O-C-N	5.70	128.25	122.09
1	A	491	LYS	N-CA-C	5.67	118.58	110.24
1	A	358	LEU	O-C-N	5.65	128.19	122.09
1	A	447	VAL	CA-C-O	-5.63	114.51	120.64
1	A	395	VAL	CA-C-O	-5.61	115.22	121.05
1	A	484	GLU	CA-C-O	-5.61	111.27	120.80
1	A	97	LEU	CA-C-O	-5.59	114.57	121.06
1	A	147	SER	O-C-N	5.58	130.59	123.11
1	A	191	PRO	O-C-N	5.57	130.34	122.37
1	A	299	GLU	N-CA-C	-5.57	102.56	111.02
1	A	217	ASP	CA-C-N	5.55	133.04	121.94
1	A	217	ASP	C-N-CA	5.55	133.04	121.94
1	A	273	GLU	OE1-CD-OE2	5.55	136.21	122.90
1	A	185	GLN	O-C-N	5.54	129.08	122.27
1	A	161	SER	N-CA-C	5.53	119.08	110.17
1	A	526	GLN	CA-CB-CG	5.52	125.14	114.10
1	A	507	THR	CA-CB-OG1	-5.51	101.34	109.60
1	A	187	PHE	O-C-N	5.51	128.40	122.34
1	A	246	VAL	O-C-N	5.50	127.49	121.83
1	A	157	ALA	N-CA-C	5.49	118.50	107.41
1	A	479	THR	OG1-CB-CG2	5.49	120.28	109.30
1	A	267	ARG	NE-CZ-NH1	5.48	126.98	121.50
1	A	306	GLU	O-C-N	5.46	128.38	122.15
1	A	369	ASP	O-C-N	5.46	127.70	122.07
1	A	151	GLY	O-C-N	-5.46	117.43	123.05
1	A	248	LEU	CA-C-N	5.46	126.14	120.03
1	A	248	LEU	C-N-CA	5.46	126.14	120.03
1	A	97	LEU	CB-CA-C	5.45	121.66	109.56
1	A	525	ASN	CB-CA-C	5.44	119.50	110.90
1	A	93	ASP	CA-CB-CG	5.42	118.03	112.60
1	A	92	GLU	N-CA-CB	5.42	118.69	110.28
1	A	437	GLY	CA-C-N	-5.42	116.23	122.95
1	A	437	GLY	C-N-CA	-5.42	116.23	122.95
1	A	201	ALA	N-CA-C	-5.42	106.67	113.28
1	A	457	ASN	N-CA-C	5.42	119.31	111.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	SER	N-CA-C	5.41	117.26	111.36
1	A	198	GLY	CA-C-O	5.41	126.86	121.29
1	A	522	VAL	N-CA-C	-5.38	104.50	112.04
1	A	402	CYS	CA-C-O	-5.38	112.78	120.16
1	A	145	SER	O-C-N	5.38	129.56	123.27
1	A	468	ARG	NE-CZ-NH1	-5.38	116.12	121.50
1	A	196	ILE	CA-C-O	-5.38	114.15	120.76
1	A	495	PHE	CB-CA-C	5.37	118.49	109.89
1	A	149	ARG	CD-NE-CZ	5.37	131.91	124.40
1	A	450	LEU	CA-C-O	-5.37	112.80	120.16
1	A	343	SER	CA-C-O	-5.36	115.54	121.33
1	A	65	ASN	N-CA-C	-5.36	103.46	110.53
1	A	133	LYS	CA-C-O	-5.36	114.74	120.42
1	A	199	GLU	CB-CA-C	-5.36	99.91	109.71
1	A	183	ASN	OD1-CG-ND2	5.35	127.95	122.60
1	A	161	SER	CA-C-O	-5.35	114.97	121.28
1	A	142	VAL	CA-C-N	-5.35	115.34	122.72
1	A	142	VAL	C-N-CA	-5.35	115.34	122.72
1	A	10	THR	CA-C-O	-5.35	115.21	121.46
1	A	387	ASN	N-CA-C	-5.33	105.58	111.71
1	A	228	SER	O-C-N	5.33	125.98	121.83
1	A	202	GLY	CA-C-N	5.32	125.85	120.00
1	A	202	GLY	C-N-CA	5.32	125.85	120.00
1	A	479	THR	N-CA-C	5.32	120.78	113.97
1	A	481	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	143	LEU	CB-CA-C	5.31	118.51	109.75
1	A	463	GLU	CG-CD-OE1	5.30	130.60	118.40
1	A	260	GLU	O-C-N	5.30	127.74	122.12
1	A	259	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	216	ARG	NE-CZ-NH2	-5.29	114.43	119.20
1	A	300	PHE	CA-CB-CG	5.29	119.09	113.80
1	A	517	ARG	CA-CB-CG	5.29	124.69	114.10
1	A	295	VAL	N-CA-CB	-5.29	102.39	110.86
1	A	88	ARG	N-CA-C	-5.29	101.32	109.52
1	A	5	GLU	CA-C-N	5.28	131.05	121.92
1	A	5	GLU	C-N-CA	5.28	131.05	121.92
1	A	75	PHE	CB-CA-C	5.27	117.97	110.96
1	A	201	ALA	CB-CA-C	5.26	119.83	109.72
1	A	108	SER	CA-C-O	-5.26	114.78	120.09
1	A	500	GLN	N-CA-C	5.26	118.88	111.52
1	A	276	ASP	CA-C-O	-5.25	115.28	120.90
1	A	31	LEU	N-CA-CB	-5.24	102.34	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ARG	CB-CG-CD	5.24	123.34	111.30
1	A	139	GLU	N-CA-C	5.24	119.65	113.16
1	A	81	SER	CA-C-O	5.23	125.32	119.41
1	A	84	TRP	CA-C-O	-5.22	113.24	119.35
1	A	167	ASN	CB-CG-ND2	5.22	124.24	116.40
1	A	467	ARG	CD-NE-CZ	5.22	131.71	124.40
1	A	43	MET	CA-CB-CG	-5.22	103.66	114.10
1	A	37	GLU	CA-C-O	-5.20	115.92	120.60
1	A	376	THR	CA-C-N	5.20	128.21	120.31
1	A	376	THR	C-N-CA	5.20	128.21	120.31
1	A	457	ASN	OD1-CG-ND2	5.20	127.80	122.60
1	A	289	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	A	168	VAL	N-CA-CB	-5.19	103.98	110.47
1	A	374	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	A	289	ARG	NE-CZ-NH1	5.17	126.67	121.50
1	A	413	LYS	N-CA-C	-5.17	105.82	111.82
1	A	173	GLN	N-CA-CB	5.17	117.64	109.94
1	A	458	TYR	N-CA-C	-5.17	102.37	110.17
1	A	356	VAL	CA-C-N	5.15	128.15	120.31
1	A	356	VAL	C-N-CA	5.15	128.15	120.31
1	A	415	GLY	O-C-N	5.14	127.77	122.88
1	A	518	VAL	N-CA-C	5.14	115.35	110.42
1	A	147	SER	N-CA-CB	5.13	119.51	111.20
1	A	114	TRP	CA-C-O	-5.12	115.21	121.05
1	A	222	ALA	N-CA-CB	-5.12	102.01	111.53
1	A	354	SER	N-CA-C	-5.11	105.41	111.69
1	A	407	PHE	CA-C-O	-5.10	115.46	120.82
1	A	83	MET	CB-CG-SD	-5.10	97.40	112.70
1	A	443	GLU	N-CA-CB	5.09	117.84	110.26
1	A	180	VAL	CA-C-N	5.08	127.35	120.65
1	A	180	VAL	C-N-CA	5.08	127.35	120.65
1	A	242	ARG	CA-CB-CG	-5.07	103.96	114.10
1	A	231	CYS	O-C-N	5.07	127.11	121.43
1	A	185	GLN	N-CA-C	-5.06	105.95	111.82
1	A	109	THR	CA-CB-OG1	-5.06	102.01	109.60
1	A	426	ARG	NE-CZ-NH1	-5.05	116.45	121.50
1	A	249	GLY	O-C-N	5.05	127.06	122.17
1	A	179	TRP	O-C-N	-5.04	116.77	122.12
1	A	244	ARG	CD-NE-CZ	5.04	131.46	124.40
1	A	374	GLN	N-CA-C	5.04	116.85	111.36
1	A	232	PRO	O-C-N	5.03	128.71	122.22
1	A	130	TYR	N-CA-C	-5.03	106.39	112.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	10	THR	N-CA-C	-5.00	101.94	109.85

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	4115	0	3958	349	17
All	All	4115	0	3958	349	17

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 43.

All (349) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:SER:HB2	1:A:137:TYR:HE2	1.15	1.11
1:A:433:PRO:HD2	1:A:436:MET:HE3	1.24	1.09
1:A:7:LEU:HD23	1:A:16:MET:HE2	1.39	1.04
1:A:349:ARG:HG3	1:A:349:ARG:HH11	1.25	0.98
1:A:339:PHE:HZ	1:A:391:LEU:HD23	1.33	0.94
1:A:25:SER:HB2	1:A:137:TYR:CE2	2.05	0.92
1:A:240:GLU:OE1	1:A:243:ARG:HD3	1.70	0.92
1:A:453:VAL:CG2	1:A:456:LEU:HG	1.98	0.92
1:A:225:GLN:HE22	1:A:473:TRP:HE1	1.19	0.91
1:A:479:THR:HG22	1:A:481:ASN:H	1.35	0.90
1:A:243:ARG:HH12	1:A:244:ARG:HG2	1.34	0.90
1:A:208:MET:HE1	1:A:294:PRO:HG2	1.52	0.89
1:A:87:ASN:HD22	1:A:87:ASN:H	1.22	0.87
1:A:27:ILE:HD12	1:A:137:TYR:HB2	1.54	0.86
1:A:410:LYS:O	1:A:413:LYS:HE2	1.75	0.86
1:A:9:ASN:ND2	1:A:14:LYS:HZ3	1.75	0.85
1:A:449:GLY:HA2	1:A:466:SER:OG	1.77	0.85
1:A:190:ASP:OD1	1:A:192:LYS:HG2	1.77	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ILE:CD1	1:A:137:TYR:HB2	2.07	0.84
1:A:303:THR:HG22	1:A:304:SER:H	1.40	0.84
1:A:349:ARG:HG3	1:A:349:ARG:NH1	1.85	0.84
1:A:508:GLU:HB3	1:A:509:PRO:HD2	1.59	0.84
1:A:208:MET:HG2	1:A:229:PRO:HB3	1.61	0.81
1:A:433:PRO:HD2	1:A:436:MET:CE	2.09	0.80
1:A:73:GLU:O	1:A:76:PRO:HD3	1.83	0.79
1:A:433:PRO:CD	1:A:436:MET:HE3	2.11	0.78
1:A:339:PHE:CZ	1:A:391:LEU:HD23	2.19	0.78
1:A:296:ILE:HD12	1:A:305:LEU:HD13	1.64	0.78
1:A:408:VAL:O	1:A:412:THR:HG23	1.84	0.78
1:A:360:VAL:HG12	1:A:363:ALA:HB2	1.64	0.78
1:A:170:LEU:HD21	1:A:208:MET:HE3	1.66	0.77
1:A:176:ALA:O	1:A:180:VAL:HG23	1.85	0.77
1:A:345:SER:O	1:A:347:ILE:HD13	1.83	0.77
1:A:413:LYS:HE3	1:A:414:PHE:CE1	2.21	0.76
1:A:48:PRO:HG3	1:A:172:ASP:OD1	1.85	0.76
1:A:243:ARG:NH1	1:A:244:ARG:HG2	1.99	0.76
1:A:178:GLN:O	1:A:181:HIS:HB3	1.86	0.76
1:A:306:GLU:O	1:A:310:ASN:HB2	1.86	0.75
1:A:432:TRP:CE3	1:A:436:MET:HE1	2.22	0.75
1:A:289:ARG:NH2	1:A:399:ASN:OD1	2.19	0.74
1:A:452:LEU:HD12	1:A:463:GLU:HG2	1.69	0.74
1:A:496:THR:CG2	1:A:498:LYS:HB3	2.17	0.74
1:A:87:ASN:HD22	1:A:87:ASN:N	1.81	0.74
1:A:258:SER:OG	1:A:261:GLU:HG2	1.88	0.74
1:A:282:LEU:HD13	1:A:291:SER:OG	1.88	0.74
1:A:193:THR:HG23	1:A:220:ARG:NH1	2.03	0.73
1:A:312:GLY:O	1:A:316:LYS:HE2	1.86	0.73
1:A:71:VAL:HG21	1:A:90:MET:HE1	1.71	0.73
1:A:86:PRO:HG2	1:A:90:MET:HE2	1.69	0.73
1:A:87:ASN:H	1:A:87:ASN:ND2	1.87	0.73
1:A:321:LEU:O	1:A:420:LEU:HA	1.89	0.72
1:A:208:MET:HE1	1:A:294:PRO:CG	2.20	0.72
1:A:146:LEU:HD12	1:A:146:LEU:C	2.15	0.72
1:A:469:ILE:HD11	1:A:505:LEU:HG	1.72	0.72
1:A:211:LEU:HD11	1:A:309:LEU:HD12	1.73	0.71
1:A:134:TYR:CE2	1:A:453:VAL:HG12	2.25	0.71
1:A:427:ALA:HB1	1:A:429:ASN:ND2	2.06	0.70
1:A:320:LEU:HD23	1:A:320:LEU:C	2.17	0.70
1:A:453:VAL:HG22	1:A:456:LEU:HG	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LYS:HD3	1:A:385:ILE:HD11	1.72	0.69
1:A:170:LEU:HD11	1:A:208:MET:CE	2.22	0.69
1:A:216:ARG:CG	1:A:315:LYS:HB2	2.23	0.69
1:A:40:VAL:O	1:A:43:MET:HB2	1.92	0.68
1:A:216:ARG:HG3	1:A:315:LYS:HB2	1.76	0.68
1:A:339:PHE:HA	1:A:345:SER:HB3	1.76	0.68
1:A:9:ASN:HD21	1:A:14:LYS:HZ3	1.42	0.67
1:A:349:ARG:NE	1:A:381:ASP:O	2.27	0.67
1:A:192:LYS:O	1:A:220:ARG:NH1	2.26	0.67
1:A:452:LEU:HD12	1:A:463:GLU:CG	2.24	0.67
1:A:170:LEU:HD11	1:A:208:MET:HE3	1.77	0.67
1:A:261:GLU:OE1	1:A:261:GLU:HA	1.95	0.66
1:A:19:ARG:HG3	1:A:19:ARG:HH11	1.60	0.66
1:A:216:ARG:O	1:A:315:LYS:HD2	1.95	0.66
1:A:450:LEU:C	1:A:452:LEU:H	2.04	0.66
1:A:475:THR:O	1:A:479:THR:HB	1.96	0.66
1:A:19:ARG:HG3	1:A:19:ARG:NH1	2.11	0.66
1:A:46:ARG:HD2	1:A:162:GLN:NE2	2.11	0.66
1:A:359:SER:C	1:A:361:PRO:HD3	2.21	0.66
1:A:110:THR:OG1	1:A:478:LYS:HB3	1.96	0.65
1:A:429:ASN:ND2	1:A:429:ASN:H	1.94	0.64
1:A:225:GLN:NE2	1:A:473:TRP:HE1	1.93	0.64
1:A:347:ILE:HG23	1:A:351:ASP:HB3	1.79	0.64
1:A:346:LYS:HD3	1:A:385:ILE:CD1	2.28	0.64
1:A:349:ARG:HH11	1:A:349:ARG:CG	2.06	0.64
1:A:166:GLY:O	1:A:168:VAL:HG23	1.98	0.64
1:A:106:PRO:CG	1:A:109:THR:HG21	2.28	0.63
1:A:193:THR:HG22	1:A:220:ARG:HG2	1.78	0.63
1:A:71:VAL:CG2	1:A:90:MET:HE1	2.28	0.63
1:A:347:ILE:HG23	1:A:351:ASP:CB	2.29	0.63
1:A:246:VAL:HG23	1:A:256:LEU:HD13	1.81	0.63
1:A:355:GLY:HA3	1:A:391:LEU:HD11	1.81	0.62
1:A:72:ASP:OD2	1:A:334:TYR:HE2	1.83	0.62
1:A:413:LYS:HE3	1:A:414:PHE:HE1	1.65	0.62
1:A:236:VAL:O	1:A:295:VAL:HA	1.99	0.61
1:A:247:GLU:CD	1:A:250:ARG:HE	2.07	0.61
1:A:6:LEU:HD12	1:A:28:SER:OG	2.01	0.61
1:A:177:LEU:HD11	1:A:196:ILE:HG22	1.83	0.61
1:A:303:THR:CG2	1:A:304:SER:H	2.02	0.61
1:A:324:ASN:ND2	1:A:423:PHE:HB3	2.16	0.61
1:A:212:SER:HB2	1:A:300:PHE:O	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PRO:HB2	1:A:435:TRP:CD1	2.36	0.61
1:A:170:LEU:HD21	1:A:208:MET:CE	2.31	0.60
1:A:397:ASP:OD1	1:A:517:ARG:NH1	2.34	0.60
1:A:204:ALA:O	1:A:208:MET:HG3	2.02	0.60
1:A:345:SER:O	1:A:388:ARG:HG3	2.02	0.60
1:A:240:GLU:OE2	1:A:244:ARG:NE	2.34	0.59
1:A:85:ASN:HB3	1:A:86:PRO:HD2	1.83	0.59
1:A:243:ARG:HH12	1:A:244:ARG:CG	2.13	0.59
1:A:7:LEU:HD13	1:A:7:LEU:C	2.27	0.59
1:A:353:MET:O	1:A:357:LYS:HE3	2.03	0.59
1:A:408:VAL:CG1	1:A:409:ASN:N	2.66	0.58
1:A:86:PRO:CG	1:A:90:MET:HE2	2.33	0.58
1:A:223:ILE:HA	1:A:320:LEU:O	2.02	0.58
1:A:316:LYS:HB3	1:A:414:PHE:O	2.03	0.58
1:A:184:ILE:HA	1:A:187:PHE:HD2	1.67	0.58
1:A:339:PHE:HA	1:A:345:SER:CB	2.33	0.58
1:A:354:SER:HA	1:A:357:LYS:HE3	1.85	0.58
1:A:504:ASP:OD2	1:A:513:HIS:HE1	1.86	0.58
1:A:395:VAL:O	1:A:399:ASN:HB2	2.03	0.58
1:A:106:PRO:HG2	1:A:109:THR:HG21	1.86	0.58
1:A:333:LEU:HD12	1:A:436:MET:HE1	1.86	0.57
1:A:74:GLN:C	1:A:76:PRO:HD3	2.29	0.57
1:A:189:GLY:O	1:A:191:PRO:HD3	2.04	0.57
1:A:235:SER:HA	1:A:294:PRO:O	2.04	0.57
1:A:449:GLY:O	1:A:452:LEU:HB2	2.05	0.57
1:A:22:VAL:O	1:A:23:LEU:C	2.48	0.56
1:A:32:GLY:HA2	1:A:96:TYR:HB3	1.88	0.56
1:A:46:ARG:CD	1:A:162:GLN:NE2	2.69	0.56
1:A:324:ASN:HD22	1:A:423:PHE:HB3	1.69	0.56
1:A:496:THR:HG22	1:A:498:LYS:HB3	1.87	0.56
1:A:418:THR:HB	1:A:495:PHE:HB3	1.87	0.56
1:A:427:ALA:HB1	1:A:429:ASN:HD21	1.70	0.56
1:A:349:ARG:HH21	1:A:376:THR:HG23	1.71	0.56
1:A:360:VAL:CG1	1:A:363:ALA:HB2	2.32	0.56
1:A:450:LEU:N	1:A:451:PRO:CD	2.69	0.56
1:A:78:PHE:HE2	1:A:432:TRP:CZ3	2.23	0.56
1:A:27:ILE:HD11	1:A:137:TYR:HB2	1.87	0.55
1:A:498:LYS:HG3	1:A:499:GLU:CG	2.36	0.55
1:A:192:LYS:O	1:A:193:THR:HG23	2.07	0.55
1:A:258:SER:O	1:A:261:GLU:HB2	2.06	0.55
1:A:37:GLU:HG2	1:A:51:LYS:HA	1.86	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASN:O	1:A:144:VAL:HA	2.07	0.55
1:A:349:ARG:CD	1:A:381:ASP:O	2.55	0.55
1:A:528:LEU:HB3	1:A:529:PRO:HD3	1.89	0.55
1:A:302:PRO:HD2	1:A:308:MET:CE	2.36	0.55
1:A:432:TRP:CE3	1:A:436:MET:CE	2.89	0.55
1:A:520:MET:O	1:A:523:PHE:HB3	2.07	0.54
1:A:310:ASN:OD1	1:A:410:LYS:NZ	2.38	0.54
1:A:286:SER:HB3	1:A:361:PRO:HG3	1.89	0.54
1:A:208:MET:HB3	1:A:301:PHE:CZ	2.43	0.54
1:A:211:LEU:HD11	1:A:309:LEU:CD1	2.38	0.54
1:A:408:VAL:HG22	1:A:418:THR:HG21	1.89	0.54
1:A:9:ASN:ND2	1:A:14:LYS:NZ	2.52	0.53
1:A:72:ASP:OD2	1:A:334:TYR:CE2	2.61	0.53
1:A:479:THR:HG22	1:A:481:ASN:N	2.13	0.53
1:A:247:GLU:HB3	1:A:281:VAL:HG12	1.89	0.53
1:A:296:ILE:CD1	1:A:305:LEU:HD13	2.35	0.53
1:A:450:LEU:C	1:A:452:LEU:N	2.66	0.53
1:A:110:THR:OG1	1:A:478:LYS:CB	2.56	0.52
1:A:321:LEU:HD21	1:A:408:VAL:HG23	1.91	0.52
1:A:7:LEU:C	1:A:7:LEU:CD1	2.82	0.52
1:A:424:ASN:OD1	1:A:424:ASN:N	2.41	0.52
1:A:286:SER:CB	1:A:361:PRO:HG3	2.39	0.52
1:A:8:VAL:HG11	1:A:187:PHE:CE1	2.44	0.52
1:A:9:ASN:HD21	1:A:14:LYS:NZ	2.08	0.52
1:A:242:ARG:O	1:A:245:ALA:HB3	2.09	0.52
1:A:15:VAL:HG22	1:A:58:TRP:HB3	1.92	0.52
1:A:412:THR:HG21	1:A:495:PHE:HD2	1.75	0.52
1:A:446:PHE:CE2	1:A:465:LEU:HD23	2.45	0.52
1:A:503:ILE:HG22	1:A:512:VAL:HG22	1.91	0.51
1:A:287:ILE:HD11	1:A:331:PHE:C	2.36	0.51
1:A:66:ASN:ND2	1:A:88:ARG:H	2.09	0.51
1:A:109:THR:HG22	1:A:188:GLY:O	2.11	0.51
1:A:208:MET:HB3	1:A:301:PHE:CE1	2.45	0.51
1:A:252:LEU:HD13	1:A:269:LYS:HG3	1.92	0.51
1:A:312:GLY:HA2	1:A:314:PHE:CE2	2.45	0.51
1:A:496:THR:HG22	1:A:499:GLU:H	1.76	0.51
1:A:44:ARG:O	1:A:267:ARG:NH1	2.37	0.51
1:A:377:ASP:OD1	1:A:377:ASP:O	2.27	0.51
1:A:139:GLU:O	1:A:140:GLU:C	2.53	0.50
1:A:106:PRO:HG2	1:A:109:THR:CG2	2.41	0.50
1:A:216:ARG:HG2	1:A:315:LYS:HB2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ILE:O	1:A:319:ILE:HG13	2.11	0.50
1:A:177:LEU:HD11	1:A:196:ILE:CG2	2.40	0.50
1:A:173:GLN:OE1	1:A:209:HIS:HE1	1.95	0.50
1:A:22:VAL:HG23	1:A:133:LYS:HG3	1.93	0.50
1:A:135:LEU:HB3	1:A:143:LEU:CD1	2.42	0.50
1:A:211:LEU:O	1:A:308:MET:HE1	2.12	0.49
1:A:333:LEU:C	1:A:333:LEU:CD2	2.84	0.49
1:A:129:VAL:HG12	1:A:450:LEU:HD22	1.94	0.49
1:A:204:ALA:O	1:A:208:MET:CG	2.60	0.49
1:A:238:VAL:HA	1:A:295:VAL:HG22	1.94	0.49
1:A:450:LEU:O	1:A:452:LEU:N	2.46	0.49
1:A:7:LEU:CD2	1:A:16:MET:HE2	2.27	0.49
1:A:111:VAL:HG13	1:A:142:VAL:HG12	1.94	0.49
1:A:4:SER:O	1:A:6:LEU:N	2.46	0.49
1:A:314:PHE:CE1	1:A:411:TYR:CE1	3.01	0.49
1:A:287:ILE:HG22	1:A:358:LEU:C	2.38	0.48
1:A:5:GLU:OE1	1:A:5:GLU:HA	2.14	0.48
1:A:456:LEU:O	1:A:457:ASN:HB2	2.14	0.48
1:A:527:PHE:CZ	1:A:531:LEU:HD12	2.48	0.48
1:A:515:ARG:HB3	1:A:518:VAL:HB	1.96	0.48
1:A:46:ARG:NE	1:A:162:GLN:NE2	2.60	0.48
1:A:243:ARG:NH1	1:A:244:ARG:CG	2.72	0.48
1:A:333:LEU:HD12	1:A:436:MET:CE	2.44	0.48
1:A:207:GLY:HA3	1:A:229:PRO:HD3	1.95	0.48
1:A:234:ALA:O	1:A:294:PRO:HD2	2.14	0.48
1:A:346:LYS:CD	1:A:385:ILE:CD1	2.92	0.48
1:A:349:ARG:HD3	1:A:381:ASP:O	2.12	0.48
1:A:376:THR:HG22	1:A:378:TRP:H	1.79	0.48
1:A:413:LYS:CE	1:A:414:PHE:CE1	2.94	0.48
1:A:46:ARG:NH2	1:A:162:GLN:OE1	2.47	0.47
1:A:330:PHE:HE2	1:A:442:TYR:HE1	1.61	0.47
1:A:332:LEU:O	1:A:333:LEU:C	2.56	0.47
1:A:432:TRP:HB3	1:A:436:MET:HE3	1.95	0.47
1:A:491:LYS:HE2	1:A:491:LYS:N	2.29	0.47
1:A:182:ASP:C	1:A:183:ASN:ND2	2.73	0.47
1:A:451:PRO:HG2	1:A:466:SER:HB2	1.97	0.47
1:A:158:LEU:HD12	1:A:263:ILE:HD11	1.97	0.47
1:A:170:LEU:HG	1:A:300:PHE:CZ	2.50	0.47
1:A:346:LYS:HG2	1:A:385:ILE:HD13	1.96	0.47
1:A:359:SER:C	1:A:361:PRO:CD	2.87	0.47
1:A:246:VAL:HG23	1:A:256:LEU:CD1	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ASN:ND2	1:A:429:ASN:N	2.60	0.47
1:A:213:PRO:HA	1:A:216:ARG:HD3	1.96	0.47
1:A:503:ILE:CG2	1:A:512:VAL:HG22	2.45	0.47
1:A:7:LEU:HD21	1:A:57:VAL:HG22	1.98	0.46
1:A:263:ILE:O	1:A:267:ARG:HG3	2.16	0.46
1:A:452:LEU:CD1	1:A:463:GLU:HG2	2.43	0.46
1:A:46:ARG:CZ	1:A:162:GLN:OE1	2.64	0.46
1:A:130:TYR:HE1	1:A:444:ILE:HD13	1.80	0.46
1:A:339:PHE:CZ	1:A:391:LEU:CD2	2.96	0.46
1:A:433:PRO:HG2	1:A:436:MET:HE2	1.98	0.46
1:A:87:ASN:N	1:A:87:ASN:ND2	2.45	0.46
1:A:223:ILE:HD13	1:A:473:TRP:CD1	2.50	0.46
1:A:223:ILE:HG23	1:A:320:LEU:HD22	1.98	0.46
1:A:163:GLU:HB3	1:A:267:ARG:HH22	1.80	0.46
1:A:491:LYS:O	1:A:493:PRO:HD3	2.15	0.46
1:A:73:GLU:O	1:A:76:PRO:CD	2.58	0.46
1:A:223:ILE:HG23	1:A:320:LEU:CD2	2.46	0.46
1:A:364:ASN:N	1:A:364:ASN:OD1	2.47	0.46
1:A:533:ASN:O	1:A:534:ALA:C	2.59	0.46
1:A:348:SER:OG	1:A:351:ASP:HB2	2.15	0.45
1:A:360:VAL:N	1:A:361:PRO:HD3	2.32	0.45
1:A:413:LYS:CE	1:A:414:PHE:HE1	2.29	0.45
1:A:82:GLU:HA	1:A:85:ASN:HD22	1.81	0.45
1:A:177:LEU:HD21	1:A:196:ILE:HG21	1.97	0.45
1:A:199:GLU:HA	1:A:225:GLN:O	2.15	0.45
1:A:321:LEU:HD21	1:A:408:VAL:CG2	2.46	0.45
1:A:6:LEU:CD1	1:A:28:SER:OG	2.64	0.45
1:A:298:GLY:HA2	1:A:301:PHE:O	2.15	0.45
1:A:430:LEU:HD23	1:A:430:LEU:HA	1.79	0.45
1:A:116:TYR:CE1	1:A:123:GLY:HA3	2.51	0.45
1:A:236:VAL:HG13	1:A:293:VAL:HG12	1.98	0.45
1:A:443:GLU:O	1:A:444:ILE:C	2.59	0.45
1:A:22:VAL:HG13	1:A:137:TYR:CD2	2.51	0.45
1:A:33:ILE:HD12	1:A:99:ILE:HD12	1.98	0.45
1:A:72:ASP:N	1:A:85:ASN:OD1	2.48	0.45
1:A:135:LEU:HD23	1:A:143:LEU:HD11	1.98	0.45
1:A:149:ARG:NH2	1:A:168:VAL:HG13	2.32	0.45
1:A:174:ARG:NH2	1:A:214:GLY:HA3	2.32	0.45
1:A:375:TYR:CZ	1:A:520:MET:SD	3.10	0.45
1:A:333:LEU:HD23	1:A:333:LEU:O	2.17	0.45
1:A:346:LYS:CD	1:A:385:ILE:HD13	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:GLU:O	1:A:467:ARG:HG3	2.17	0.45
1:A:360:VAL:N	1:A:361:PRO:CD	2.80	0.45
1:A:158:LEU:HD11	1:A:262:LEU:HD13	1.98	0.44
1:A:349:ARG:HA	1:A:349:ARG:HD2	1.81	0.44
1:A:432:TRP:HE3	1:A:436:MET:CE	2.30	0.44
1:A:453:VAL:HG22	1:A:456:LEU:CG	2.44	0.44
1:A:134:TYR:CE2	1:A:453:VAL:CG1	2.97	0.44
1:A:149:ARG:HH22	1:A:168:VAL:HG13	1.82	0.44
1:A:236:VAL:HG13	1:A:293:VAL:CG1	2.48	0.44
1:A:491:LYS:HE2	1:A:491:LYS:H	1.81	0.44
1:A:66:ASN:O	1:A:90:MET:HA	2.18	0.44
1:A:343:SER:C	1:A:345:SER:H	2.25	0.44
1:A:412:THR:HG22	1:A:418:THR:OG1	2.17	0.44
1:A:450:LEU:N	1:A:451:PRO:HD2	2.33	0.44
1:A:383:ASN:C	1:A:383:ASN:HD22	2.24	0.43
1:A:453:VAL:CG2	1:A:456:LEU:CG	2.83	0.43
1:A:272:GLN:NE2	1:A:275:ILE:HB	2.33	0.43
1:A:103:SER:HA	1:A:104:PRO:C	2.43	0.43
1:A:197:PHE:HD1	1:A:197:PHE:H	1.65	0.43
1:A:326:ASP:HB2	1:A:438:VAL:O	2.19	0.43
1:A:330:PHE:CD2	1:A:439:ILE:CG2	3.01	0.43
1:A:504:ASP:OD2	1:A:513:HIS:CE1	2.68	0.43
1:A:101:VAL:HA	1:A:102:PRO:HD3	1.85	0.43
1:A:113:VAL:HG13	1:A:144:VAL:HG22	2.01	0.43
1:A:44:ARG:NH1	1:A:266:LEU:O	2.52	0.43
1:A:224:LEU:HD12	1:A:224:LEU:N	2.34	0.43
1:A:258:SER:OG	1:A:261:GLU:CG	2.62	0.43
1:A:318:GLN:HE22	1:A:416:ASN:HD22	1.67	0.43
1:A:115:ILE:O	1:A:202:GLY:HA3	2.19	0.42
1:A:196:ILE:O	1:A:196:ILE:HG13	2.19	0.42
1:A:240:GLU:O	1:A:244:ARG:HG3	2.19	0.42
1:A:337:PRO:HG2	1:A:337:PRO:O	2.19	0.42
1:A:206:VAL:O	1:A:207:GLY:C	2.57	0.42
1:A:360:VAL:HG12	1:A:363:ALA:CB	2.43	0.42
1:A:433:PRO:HG2	1:A:436:MET:CE	2.48	0.42
1:A:383:ASN:OD1	1:A:386:LYS:HG3	2.19	0.42
1:A:510:MET:HE3	1:A:512:VAL:HG23	2.01	0.42
1:A:352:PHE:O	1:A:356:VAL:HG13	2.19	0.42
1:A:429:ASN:O	1:A:430:LEU:C	2.62	0.42
1:A:170:LEU:HD11	1:A:208:MET:HE2	2.01	0.42
1:A:209:HIS:HD2	1:A:215:SER:OG	2.03	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:PHE:CE1	1:A:411:TYR:CD1	3.08	0.42
1:A:139:GLU:O	1:A:140:GLU:O	2.37	0.42
1:A:78:PHE:HE2	1:A:432:TRP:CE3	2.38	0.42
1:A:349:ARG:HD3	1:A:387:ASN:HD21	1.84	0.42
1:A:21:PRO:O	1:A:133:LYS:HE2	2.20	0.42
1:A:75:PHE:O	1:A:76:PRO:C	2.61	0.42
1:A:178:GLN:O	1:A:181:HIS:CB	2.63	0.42
1:A:528:LEU:HD22	1:A:532:LEU:HG	2.01	0.42
1:A:22:VAL:CG1	1:A:137:TYR:CD2	3.03	0.41
1:A:129:VAL:HG12	1:A:450:LEU:CD2	2.50	0.41
1:A:236:VAL:HG23	1:A:237:SER:O	2.20	0.41
1:A:298:GLY:CA	1:A:301:PHE:O	2.68	0.41
1:A:430:LEU:HD21	1:A:442:TYR:CD2	2.55	0.41
1:A:498:LYS:HG3	1:A:499:GLU:N	2.34	0.41
1:A:355:GLY:O	1:A:358:LEU:HB2	2.20	0.41
1:A:481:ASN:OD1	1:A:483:ASN:HB2	2.19	0.41
1:A:222:ALA:HB3	1:A:319:ILE:HG22	2.02	0.41
1:A:271:PRO:O	1:A:275:ILE:HG13	2.21	0.41
1:A:378:TRP:HA	1:A:378:TRP:CE3	2.56	0.41
1:A:419:TYR:CE2	1:A:482:PRO:HD2	2.55	0.41
1:A:242:ARG:HH11	1:A:242:ARG:HD2	1.54	0.41
1:A:250:ARG:HG3	1:A:256:LEU:HD11	2.02	0.41
1:A:96:TYR:CD1	1:A:96:TYR:N	2.89	0.41
1:A:318:GLN:NE2	1:A:416:ASN:HD22	2.18	0.41
1:A:383:ASN:C	1:A:383:ASN:ND2	2.79	0.41
1:A:408:VAL:HG12	1:A:409:ASN:N	2.36	0.41
1:A:173:GLN:OE1	1:A:205:SER:HB3	2.20	0.41
1:A:433:PRO:CD	1:A:436:MET:CE	2.85	0.41
1:A:443:GLU:HG2	1:A:444:ILE:N	2.35	0.41
1:A:7:LEU:HD13	1:A:8:VAL:N	2.36	0.41
1:A:27:ILE:CG2	1:A:28:SER:N	2.84	0.41
1:A:149:ARG:NH2	1:A:168:VAL:CG1	2.84	0.41
1:A:248:LEU:HD12	1:A:277:VAL:HG23	2.03	0.41
1:A:328:GLY:O	1:A:329:SER:C	2.64	0.41
1:A:329:SER:HB3	1:A:436:MET:HB3	2.02	0.41
1:A:390:GLY:O	1:A:394:ILE:HG13	2.21	0.41
1:A:439:ILE:O	1:A:442:TYR:HB2	2.21	0.41
1:A:410:LYS:HD2	1:A:410:LYS:HA	1.84	0.41
1:A:135:LEU:HB3	1:A:143:LEU:HD12	2.03	0.40
1:A:354:SER:HA	1:A:357:LYS:CE	2.51	0.40
1:A:453:VAL:HG23	1:A:456:LEU:HG	1.97	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ARG:C	1:A:252:LEU:H	2.29	0.40
1:A:30:PHE:HB3	1:A:33:ILE:HD11	2.02	0.40
1:A:246:VAL:CG2	1:A:256:LEU:HD13	2.51	0.40

All (17) 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:379:MET:SD	1:A:515:ARG:CG[2_555]	0.62	1.58
1:A:379:MET:SD	1:A:515:ARG:CD[2_555]	1.08	1.12
1:A:14:LYS:CE	1:A:186:PHE:CE1[14_555]	1.17	1.03
1:A:379:MET:CG	1:A:515:ARG:CD[2_555]	1.51	0.69
1:A:14:LYS:CE	1:A:186:PHE:CZ[14_555]	1.53	0.67
1:A:369:ASP:OD2	1:A:530:LYS:NZ[2_555]	1.62	0.58
1:A:14:LYS:NZ	1:A:186:PHE:CE1[14_555]	1.63	0.57
1:A:379:MET:CB	1:A:515:ARG:NE[2_555]	1.76	0.44
1:A:379:MET:CB	1:A:515:ARG:CD[2_555]	1.87	0.33
1:A:373:LEU:CD2	1:A:527:PHE:CB[2_555]	1.91	0.29
1:A:19:ARG:NE	1:A:19:ARG:NE[8_555]	1.93	0.27
1:A:379:MET:SD	1:A:515:ARG:CB[2_555]	1.94	0.26
1:A:379:MET:CE	1:A:500:GLN:NE2[2_555]	2.00	0.20
1:A:379:MET:SD	1:A:515:ARG:NE[2_555]	2.06	0.14
1:A:14:LYS:NZ	1:A:186:PHE:CD1[14_555]	2.11	0.09
1:A:379:MET:CE	1:A:515:ARG:CG[2_555]	2.17	0.03
1:A:379:MET:CE	1:A:500:GLN:CD[2_555]	2.17	0.03

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	522/534 (98%)	455 (87%)	57 (11%)	10 (2%)	6 32

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	5	GLU
1	A	25	SER
1	A	381	ASP
1	A	216	ARG
1	A	329	SER
1	A	451	PRO
1	A	140	GLU
1	A	498	LYS
1	A	118	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	432/467 (92%)	351 (81%)	81 (19%)	1 9

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	7	LEU
1	A	15	VAL
1	A	18	THR
1	A	23	LEU
1	A	24	SER
1	A	27	ILE
1	A	28	SER
1	A	31	LEU
1	A	37	GLU
1	A	74	GLN
1	A	82	GLU
1	A	87	ASN
1	A	97	LEU
1	A	103	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	110	THR
1	A	124	SER
1	A	129	VAL
1	A	133	LYS
1	A	140	GLU
1	A	141	VAL
1	A	142	VAL
1	A	144	VAL
1	A	156	LEU
1	A	162	GLN
1	A	177	LEU
1	A	192	LYS
1	A	193	THR
1	A	194	VAL
1	A	197	PHE
1	A	211	LEU
1	A	216	ARG
1	A	224	LEU
1	A	240	GLU
1	A	242	ARG
1	A	243	ARG
1	A	246	VAL
1	A	262	LEU
1	A	267	ARG
1	A	274	LEU
1	A	282	LEU
1	A	287	ILE
1	A	289	ARG
1	A	293	VAL
1	A	295	VAL
1	A	303	THR
1	A	316	LYS
1	A	318	GLN
1	A	320	LEU
1	A	323	VAL
1	A	329	SER
1	A	330	PHE
1	A	333	LEU
1	A	340	SER
1	A	347	ILE
1	A	349	ARG
1	A	354	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	356	VAL
1	A	362	HIS
1	A	374	GLN
1	A	383	ASN
1	A	385	ILE
1	A	408	VAL
1	A	412	THR
1	A	413	LYS
1	A	426	ARG
1	A	429	ASN
1	A	430	LEU
1	A	445	GLU
1	A	452	LEU
1	A	453	VAL
1	A	469	ILE
1	A	479	THR
1	A	491	LYS
1	A	496	THR
1	A	497	THR
1	A	504	ASP
1	A	516	LEU
1	A	519	GLN
1	A	522	VAL
1	A	528	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	59	ASN
1	A	66	ASN
1	A	87	ASN
1	A	209	HIS
1	A	225	GLN
1	A	272	GLN
1	A	324	ASN
1	A	416	ASN
1	A	429	ASN
1	A	500	GLN
1	A	513	HIS
1	A	514	GLN

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	526/534 (98%)	1.85	202 (38%) 1 3	20, 20, 20, 20	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLU	8.5
1	A	484	GLU	8.0
1	A	231	CYS	8.0
1	A	105	ARG	6.6
1	A	415	GLY	6.4
1	A	512	VAL	6.2
1	A	277	VAL	6.0
1	A	446	PHE	6.0
1	A	69	GLN	5.8
1	A	66	ASN	5.7
1	A	285	ASP	5.6
1	A	58	TRP	5.6
1	A	278	GLU	5.6
1	A	106	PRO	5.3
1	A	147	SER	5.2
1	A	145	SER	5.2
1	A	286	SER	5.1
1	A	255	ASN	5.1
1	A	136	ALA	5.0
1	A	154	GLY	5.0
1	A	19	ARG	4.8
1	A	226	SER	4.7
1	A	153	PHE	4.7
1	A	4	SER	4.7
1	A	414	PHE	4.6
1	A	434	GLU	4.6
1	A	48	PRO	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	175	MET	4.5
1	A	300	PHE	4.4
1	A	232	PRO	4.4
1	A	322	GLY	4.2
1	A	54	TRP	4.2
1	A	324	ASN	4.2
1	A	125	SER	4.0
1	A	432	TRP	4.0
1	A	497	THR	4.0
1	A	200	SER	4.0
1	A	229	PRO	4.0
1	A	49	GLU	3.9
1	A	374	GLN	3.9
1	A	393	ASP	3.9
1	A	524	TRP	3.9
1	A	439	ILE	3.9
1	A	282	LEU	3.9
1	A	90	MET	3.9
1	A	504	ASP	3.9
1	A	451	PRO	3.8
1	A	417	GLY	3.8
1	A	507	THR	3.8
1	A	195	THR	3.8
1	A	520	MET	3.7
1	A	478	LYS	3.7
1	A	234	ALA	3.7
1	A	184	ILE	3.6
1	A	146	LEU	3.6
1	A	441	GLY	3.6
1	A	490	SER	3.5
1	A	189	GLY	3.5
1	A	144	VAL	3.5
1	A	440	HIS	3.4
1	A	157	ALA	3.4
1	A	65	ASN	3.4
1	A	525	ASN	3.4
1	A	461	GLU	3.3
1	A	452	LEU	3.3
1	A	150	VAL	3.3
1	A	104	PRO	3.3
1	A	98	ASN	3.2
1	A	305	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	390	GLY	3.2
1	A	445	GLU	3.2
1	A	323	VAL	3.2
1	A	334	TYR	3.1
1	A	363	ALA	3.1
1	A	443	GLU	3.1
1	A	436	MET	3.1
1	A	75	PHE	3.1
1	A	126	THR	3.1
1	A	68	GLN	3.1
1	A	479	THR	3.0
1	A	113	VAL	3.0
1	A	460	ALA	3.0
1	A	114	TRP	3.0
1	A	38	PRO	3.0
1	A	112	MET	3.0
1	A	164	ALA	3.0
1	A	151	GLY	3.0
1	A	409	ASN	3.0
1	A	6	LEU	2.9
1	A	118	GLY	2.9
1	A	291	SER	2.9
1	A	330	PHE	2.9
1	A	158	LEU	2.9
1	A	496	THR	2.9
1	A	173	GLN	2.9
1	A	416	ASN	2.9
1	A	325	LYS	2.9
1	A	389	ASP	2.8
1	A	534	ALA	2.8
1	A	468	ARG	2.8
1	A	230	ASN	2.7
1	A	503	ILE	2.7
1	A	474	ALA	2.7
1	A	495	PHE	2.7
1	A	369	ASP	2.7
1	A	333	LEU	2.7
1	A	477	ALA	2.7
1	A	228	SER	2.7
1	A	152	ALA	2.7
1	A	387	ASN	2.7
1	A	523	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	406	HIS	2.7
1	A	86	PRO	2.7
1	A	196	ILE	2.6
1	A	444	ILE	2.6
1	A	362	HIS	2.6
1	A	501	LYS	2.6
1	A	260	GLU	2.6
1	A	45	PHE	2.6
1	A	225	GLN	2.6
1	A	370	ALA	2.6
1	A	491	LYS	2.6
1	A	321	LEU	2.6
1	A	199	GLU	2.6
1	A	89	GLU	2.6
1	A	64	PRO	2.6
1	A	289	ARG	2.6
1	A	405	MET	2.6
1	A	167	ASN	2.6
1	A	262	LEU	2.5
1	A	466	SER	2.5
1	A	344	GLU	2.5
1	A	121	TYR	2.5
1	A	119	GLY	2.5
1	A	81	SER	2.5
1	A	411	TYR	2.5
1	A	492	TRP	2.5
1	A	111	VAL	2.5
1	A	449	GLY	2.5
1	A	343	SER	2.5
1	A	74	GLN	2.5
1	A	143	LEU	2.5
1	A	455	GLU	2.5
1	A	435	TRP	2.5
1	A	261	GLU	2.4
1	A	103	SER	2.4
1	A	313	ASN	2.4
1	A	353	MET	2.4
1	A	108	SER	2.4
1	A	292	PHE	2.4
1	A	316	LYS	2.4
1	A	128	ASP	2.4
1	A	392	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	310	ASN	2.3
1	A	522	VAL	2.3
1	A	12	SER	2.3
1	A	329	SER	2.3
1	A	442	TYR	2.3
1	A	356	VAL	2.3
1	A	36	ALA	2.3
1	A	368	LEU	2.3
1	A	107	LYS	2.3
1	A	280	ASN	2.3
1	A	116	TYR	2.3
1	A	423	PHE	2.2
1	A	499	GLU	2.2
1	A	78	PHE	2.2
1	A	429	ASN	2.2
1	A	22	VAL	2.2
1	A	359	SER	2.2
1	A	63	TYR	2.2
1	A	156	LEU	2.2
1	A	207	GLY	2.2
1	A	335	GLY	2.2
1	A	401	ILE	2.2
1	A	433	PRO	2.2
1	A	159	HIS	2.2
1	A	11	LYS	2.2
1	A	508	GLU	2.1
1	A	123	GLY	2.1
1	A	521	CYS	2.1
1	A	172	ASP	2.1
1	A	340	SER	2.1
1	A	14	LYS	2.1
1	A	510	MET	2.1
1	A	421	TYR	2.1
1	A	472	TYR	2.1
1	A	95	LEU	2.1
1	A	430	LEU	2.1
1	A	216	ARG	2.1
1	A	29	ALA	2.1
1	A	23	LEU	2.1
1	A	57	VAL	2.1
1	A	250	ARG	2.0
1	A	517	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	469	ILE	2.0
1	A	84	TRP	2.0
1	A	242	ARG	2.0
1	A	235	SER	2.0
1	A	176	ALA	2.0
1	A	181	HIS	2.0
1	A	471	HIS	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.