



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:06 AM UTC

PDB ID : 1A4S / pdb_00001a4s
Title : BETAINE ALDEHYDE DEHYDROGENASE FROM COD LIVER
Authors : Johansson, K.; El Ahmad, M.; Hjelmqvist, L.; Ramaswamy, S.; Jornvall, H.; Eklund, H.
Deposited on : 1998-02-03
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

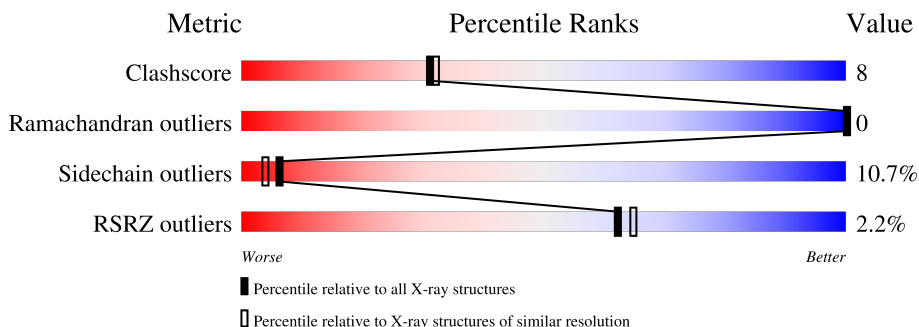
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	503	2% 73% 21% 5%
1	B	503	3% 73% 20% 6%
1	C	503	2% 76% 17% 6%
1	D	503	2% 76% 18% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15925 atoms, of which 0 are hydrogens and 0 are deuteriums.

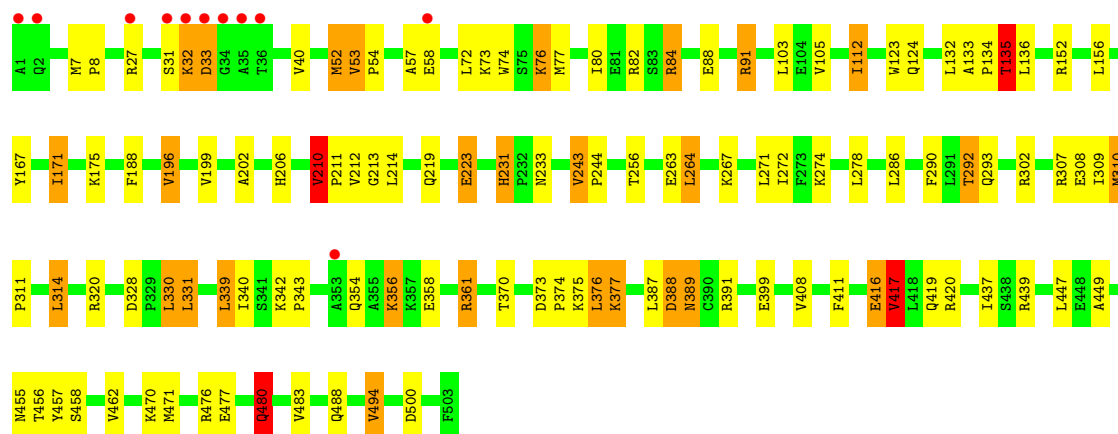
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BETAINE ALDEHYDE DEHYDROGENASE.

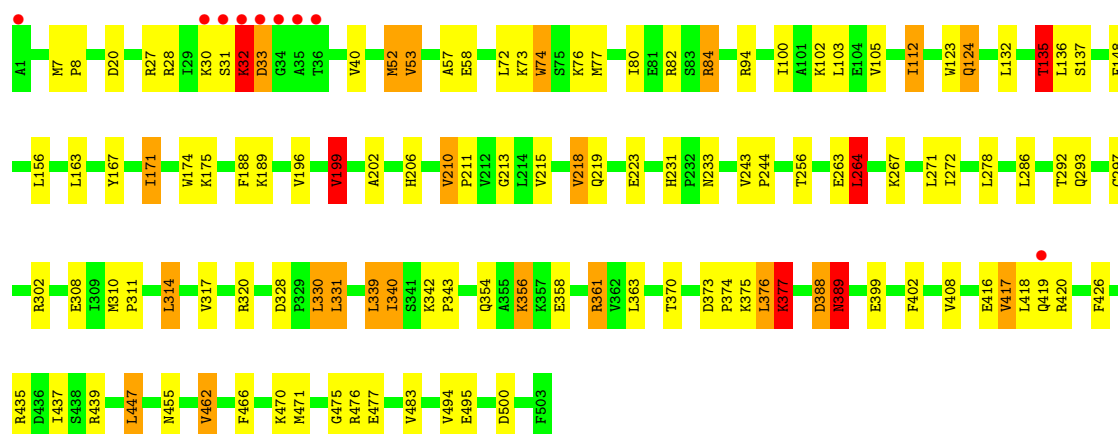
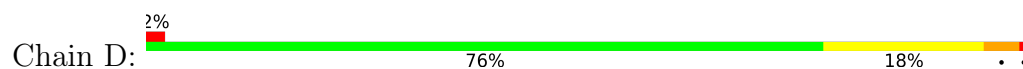
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	0	0
			3808	2408	651	719	30			
1	B	503	Total	C	N	O	S	0	0	0
			3808	2408	651	719	30			
1	C	503	Total	C	N	O	S	0	0	0
			3808	2408	651	719	30			
1	D	503	Total	C	N	O	S	0	0	0
			3808	2408	651	719	30			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	114	Total	O	0	0
			114	114		
2	B	211	Total	O	0	0
			211	211		
2	C	170	Total	O	0	0
			170	170		
2	D	198	Total	O	0	0
			198	198		



● Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.17Å 86.22Å 88.33Å 105.20° 115.13° 100.02°	Depositor
Resolution (Å)	8.00 – 2.10 8.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	75.2 (8.00-2.10) 73.9 (8.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.63 (at 2.09Å)	Xtriage
Refinement program	CNS 0.3	Depositor
R, R_{free}	0.223 , 0.253 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.51 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15925	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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	0.76	1/3882 (0.0%)	1.69	58/5265 (1.1%)
1	B	0.78	0/3882	1.77	63/5265 (1.2%)
1	C	0.72	0/3882	1.60	44/5265 (0.8%)
1	D	0.74	0/3882	1.63	44/5265 (0.8%)
All	All	0.75	1/15528 (0.0%)	1.67	209/21060 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	5
1	C	0	4
1	D	0	4
All	All	0	19

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	431	GLY	N-CA	5.07	1.50	1.45

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455	ASN	OD1-CG-ND2	-32.29	90.31	122.60
1	B	320	ARG	NE-CZ-NH2	28.49	144.84	119.20
1	B	320	ARG	NH1-CZ-NH2	-28.25	82.58	119.30
1	D	455	ASN	OD1-CG-ND2	-17.35	105.25	122.60
1	C	82	ARG	CD-NE-CZ	13.98	143.97	124.40
1	A	455	ASN	CB-CG-ND2	13.96	137.34	116.40
1	B	455	ASN	OD1-CG-ND2	-13.22	109.38	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	455	ASN	OD1-CG-ND2	-12.77	109.83	122.60
1	C	320	ARG	NH1-CZ-NH2	-12.15	103.51	119.30
1	A	417	VAL	CB-CA-C	-12.12	95.78	112.14
1	D	320	ARG	NH1-CZ-NH2	-12.09	103.59	119.30
1	A	82	ARG	CD-NE-CZ	12.06	141.28	124.40
1	D	82	ARG	CD-NE-CZ	11.88	141.03	124.40
1	A	417	VAL	N-CA-CB	11.52	126.21	110.54
1	D	320	ARG	NE-CZ-NH2	11.46	129.52	119.20
1	B	320	ARG	NE-CZ-NH1	11.05	132.55	121.50
1	C	417	VAL	CB-CA-C	-11.03	97.26	112.14
1	D	417	VAL	CB-CA-C	-10.47	98.00	112.14
1	B	417	VAL	CB-CA-C	-10.37	98.15	112.14
1	A	320	ARG	NH1-CZ-NH2	-10.18	106.07	119.30
1	C	320	ARG	NE-CZ-NH2	10.17	128.35	119.20
1	B	210	VAL	N-CA-CB	-10.16	99.52	109.99
1	B	82	ARG	CD-NE-CZ	10.05	138.47	124.40
1	C	417	VAL	N-CA-CB	9.98	124.11	110.54
1	A	210	VAL	N-CA-CB	-9.25	100.46	109.99
1	C	84	ARG	NE-CZ-NH2	9.13	127.42	119.20
1	B	417	VAL	N-CA-CB	9.09	122.90	110.54
1	D	417	VAL	N-CA-CB	8.89	122.63	110.54
1	C	196	VAL	N-CA-C	8.69	119.25	110.82
1	D	135	THR	N-CA-CB	-8.49	98.05	110.53
1	B	135	THR	N-CA-CB	-8.45	98.11	110.53
1	C	188	PHE	CA-CB-CG	8.44	122.24	113.80
1	D	210	VAL	N-CA-CB	-8.39	101.34	109.99
1	C	210	VAL	N-CA-CB	-8.27	101.47	109.99
1	B	112	ILE	N-CA-CB	8.25	122.96	110.58
1	A	188	PHE	CA-CB-CG	8.23	122.03	113.80
1	A	320	ARG	NE-CZ-NH1	8.12	129.62	121.50
1	B	388	ASP	CA-CB-CG	-7.98	104.62	112.60
1	B	174	TRP	CA-C-O	-7.71	111.39	120.10
1	C	91	ARG	NE-CZ-NH2	-7.58	112.38	119.20
1	C	264	LEU	CA-C-N	-7.58	113.05	122.75
1	C	264	LEU	C-N-CA	-7.58	113.05	122.75
1	D	388	ASP	CA-CB-CG	-7.54	105.06	112.60
1	C	135	THR	N-CA-CB	-7.42	98.87	110.44
1	C	33	ASP	CA-CB-CG	7.38	119.98	112.60
1	D	435	ARG	NE-CZ-NH2	-7.24	112.68	119.20
1	B	112	ILE	CA-C-O	-7.24	113.18	120.85
1	C	152	ARG	CD-NE-CZ	7.15	134.41	124.40
1	B	112	ILE	CB-CA-C	-7.14	102.37	112.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	THR	N-CA-CB	-7.08	100.12	110.53
1	D	389	ASN	OD1-CG-ND2	6.95	129.55	122.60
1	B	462	VAL	CB-CA-C	-6.95	101.01	112.26
1	D	455	ASN	CB-CG-ND2	6.85	126.68	116.40
1	A	290	PHE	N-CA-C	6.85	121.71	112.88
1	C	388	ASP	CA-CB-CG	-6.84	105.76	112.60
1	C	91	ARG	CD-NE-CZ	6.82	133.95	124.40
1	D	188	PHE	CA-CB-CG	6.76	120.56	113.80
1	A	426	PHE	CA-CB-CG	6.75	120.56	113.80
1	B	389	ASN	OD1-CG-ND2	6.70	129.30	122.60
1	D	462	VAL	CB-CA-C	-6.69	101.79	112.16
1	B	420	ARG	NE-CZ-NH2	-6.67	113.19	119.20
1	C	356	LYS	CA-CB-CG	6.65	127.39	114.10
1	C	320	ARG	NE-CZ-NH1	6.62	128.12	121.50
1	C	449	ALA	CA-C-O	-6.61	114.16	121.23
1	D	94	ARG	CD-NE-CZ	6.59	133.62	124.40
1	C	500	ASP	CA-CB-CG	-6.57	106.03	112.60
1	A	388	ASP	CA-CB-CG	-6.55	106.05	112.60
1	C	439	ARG	NE-CZ-NH2	-6.55	113.30	119.20
1	C	243	VAL	CA-C-O	6.53	123.06	118.69
1	B	264	LEU	CA-C-N	-6.50	114.43	122.75
1	B	264	LEU	C-N-CA	-6.50	114.43	122.75
1	D	476	ARG	CA-C-N	6.49	132.74	122.62
1	D	476	ARG	C-N-CA	6.49	132.74	122.62
1	D	112	ILE	N-CA-CB	6.48	122.50	110.77
1	D	420	ARG	NE-CZ-NH2	-6.46	113.39	119.20
1	B	475	GLY	N-CA-C	-6.44	105.08	112.29
1	B	188	PHE	CA-CB-CG	6.42	120.22	113.80
1	B	223	GLU	CB-CG-CD	6.40	123.48	112.60
1	A	243	VAL	O-C-N	6.28	124.44	120.42
1	A	494	VAL	N-CA-C	6.25	116.86	107.80
1	C	290	PHE	N-CA-C	6.24	121.74	112.94
1	B	84	ARG	NE-CZ-NH2	6.16	124.74	119.20
1	B	208	ALA	CA-C-O	-6.15	111.81	119.38
1	D	470	LYS	CB-CA-C	-6.11	109.52	116.54
1	D	500	ASP	CA-CB-CG	-6.11	106.50	112.60
1	A	264	LEU	CA-C-N	-6.09	114.96	122.75
1	A	264	LEU	C-N-CA	-6.09	114.96	122.75
1	B	124	GLN	OE1-CD-NE2	-6.08	116.52	122.60
1	B	351	PHE	CA-C-O	-6.08	114.44	120.82
1	A	152	ARG	CD-NE-CZ	6.07	132.90	124.40
1	C	437	ILE	N-CA-C	6.07	116.25	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	GLN	CA-C-O	6.05	126.97	120.55
1	B	130	ALA	CA-C-N	6.05	126.80	120.03
1	B	130	ALA	C-N-CA	6.05	126.80	120.03
1	C	223	GLU	CB-CG-CD	6.01	122.82	112.60
1	A	148	PHE	CA-C-O	-5.97	114.88	121.33
1	B	356	LYS	CA-CB-CG	5.89	125.88	114.10
1	A	110	LYS	CA-C-O	-5.88	115.18	121.94
1	B	437	ILE	N-CA-C	5.88	116.06	110.42
1	A	304	PHE	CA-C-O	-5.88	114.07	120.36
1	A	425	THR	CA-C-O	5.87	125.84	119.15
1	B	57	ALA	CA-C-N	5.86	128.13	120.28
1	B	57	ALA	C-N-CA	5.86	128.13	120.28
1	B	210	VAL	CB-CA-C	5.84	116.72	111.00
1	C	112	ILE	N-CA-CB	5.83	121.33	110.77
1	D	426	PHE	CA-CB-CG	5.83	119.63	113.80
1	C	112	ILE	CB-CA-C	-5.79	102.88	112.26
1	B	481	ALA	CA-C-O	5.78	126.63	120.10
1	A	455	ASN	CB-CG-OD1	5.77	132.34	120.80
1	B	187	VAL	N-CA-CB	5.76	119.13	111.64
1	B	356	LYS	N-CA-CB	5.76	119.21	110.28
1	A	223	GLU	CB-CG-CD	5.75	122.37	112.60
1	C	387	LEU	CA-C-O	5.74	126.79	120.71
1	A	53	VAL	CA-C-N	5.70	125.65	119.78
1	A	53	VAL	C-N-CA	5.70	125.65	119.78
1	D	112	ILE	CB-CA-C	-5.68	103.05	112.26
1	A	320	ARG	NE-CZ-NH2	5.67	124.31	119.20
1	B	96	ARG	CA-C-O	5.67	126.53	119.78
1	A	500	ASP	CA-CB-CG	-5.66	106.94	112.60
1	B	355	ALA	CA-C-O	-5.65	114.56	120.55
1	A	112	ILE	CB-CA-C	-5.59	103.20	112.26
1	B	97	ARG	CD-NE-CZ	5.59	132.22	124.40
1	B	298	THR	N-CA-C	5.58	119.93	113.18
1	C	292	THR	O-C-N	-5.57	115.64	122.55
1	A	328	ASP	CA-C-N	5.56	125.18	119.56
1	A	328	ASP	C-N-CA	5.56	125.18	119.56
1	D	218	VAL	N-CA-CB	5.56	119.08	111.41
1	B	290	PHE	N-CA-C	5.56	120.05	112.88
1	D	82	ARG	NE-CZ-NH2	-5.56	114.20	119.20
1	D	435	ARG	NH1-CZ-NH2	5.53	126.49	119.30
1	C	470	LYS	CB-CA-C	-5.52	110.19	116.54
1	A	242	SER	CA-C-N	5.52	124.74	120.33
1	A	242	SER	C-N-CA	5.52	124.74	120.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	215	VAL	O-C-N	-5.51	117.36	123.20
1	A	356	LYS	CA-CB-CG	5.51	125.12	114.10
1	A	82	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	B	243	VAL	CA-C-O	5.46	122.35	118.69
1	D	264	LEU	CA-C-N	-5.46	115.76	122.75
1	D	264	LEU	C-N-CA	-5.46	115.76	122.75
1	B	410	PRO	CA-C-O	-5.46	115.36	122.12
1	B	138	GLY	N-CA-C	-5.42	106.28	112.79
1	A	304	PHE	CA-C-N	-5.42	116.04	123.14
1	A	304	PHE	C-N-CA	-5.42	116.04	123.14
1	A	326	VAL	CA-C-O	-5.42	114.73	120.53
1	D	439	ARG	CA-C-O	-5.42	115.13	120.82
1	A	124	GLN	OE1-CD-NE2	-5.41	117.19	122.60
1	C	57	ALA	CA-C-N	5.41	127.52	120.28
1	C	57	ALA	C-N-CA	5.41	127.52	120.28
1	D	320	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	D	74	TRP	CA-C-O	5.38	126.15	119.97
1	B	135	THR	CA-C-O	5.37	125.05	119.14
1	D	33	ASP	CA-CB-CG	5.37	117.97	112.60
1	D	174	TRP	CA-C-O	-5.37	114.18	120.20
1	D	377	LYS	N-CA-C	5.37	117.83	111.33
1	C	416	GLU	CA-C-O	-5.36	115.37	121.00
1	B	242	SER	CA-C-N	5.34	124.60	120.33
1	B	242	SER	C-N-CA	5.34	124.60	120.33
1	B	435	ARG	NE-CZ-NH1	5.34	126.84	121.50
1	C	231	HIS	CA-C-O	5.32	125.12	119.80
1	D	356	LYS	N-CA-CB	5.31	118.51	110.28
1	C	494	VAL	N-CA-C	5.30	115.49	107.80
1	B	177	ALA	O-C-N	5.30	124.57	120.38
1	B	388	ASP	CB-CA-C	-5.29	100.30	110.24
1	A	295	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	C	488	GLN	OE1-CD-NE2	-5.28	117.32	122.60
1	B	435	ARG	NE-CZ-NH2	-5.26	114.47	119.20
1	A	218	VAL	N-CA-CB	5.25	118.66	111.41
1	B	377	LYS	N-CA-C	5.25	117.69	111.33
1	C	420	ARG	CD-NE-CZ	5.24	131.74	124.40
1	C	480	GLN	OE1-CD-NE2	5.23	127.83	122.60
1	B	53	VAL	CA-C-N	5.23	125.13	119.85
1	B	53	VAL	C-N-CA	5.23	125.13	119.85
1	B	78	ALA	CA-C-N	5.23	125.89	119.99
1	B	78	ALA	C-N-CA	5.23	125.89	119.99
1	A	135	THR	CA-CB-CG2	5.21	119.35	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ILE	N-CA-CB	5.19	120.17	110.77
1	A	494	VAL	CA-C-O	5.19	126.09	120.53
1	B	57	ALA	CA-C-O	5.19	126.45	120.90
1	B	307	ARG	CD-NE-CZ	5.18	131.65	124.40
1	A	79	GLY	CA-C-O	5.16	125.86	120.80
1	A	150	TYR	CA-C-O	-5.16	115.21	120.99
1	B	16	VAL	CA-C-O	-5.16	114.89	120.67
1	B	42	GLU	CA-C-N	5.16	124.77	119.05
1	B	42	GLU	C-N-CA	5.16	124.77	119.05
1	A	390	CYS	CA-C-O	-5.15	115.37	121.66
1	A	22	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	C	307	ARG	CD-NE-CZ	5.14	131.59	124.40
1	B	440	ALA	CA-C-O	-5.13	115.43	120.82
1	D	389	ASN	CA-CB-CG	-5.12	107.47	112.60
1	A	57	ALA	CA-C-N	5.12	127.14	120.28
1	A	57	ALA	C-N-CA	5.12	127.14	120.28
1	A	101	ALA	CA-C-O	5.12	126.20	120.82
1	A	462	VAL	CB-CA-C	-5.12	102.00	111.79
1	D	297	CYS	CA-C-O	-5.10	115.14	120.55
1	A	387	LEU	CA-C-O	5.10	126.11	120.71
1	C	439	ARG	CD-NE-CZ	5.09	131.52	124.40
1	A	313	PHE	CA-C-N	5.07	127.08	120.28
1	A	313	PHE	C-N-CA	5.07	127.08	120.28
1	D	340	ILE	N-CA-C	5.07	115.84	110.72
1	A	388	ASP	CA-C-O	-5.06	115.71	121.58
1	D	475	GLY	N-CA-C	-5.04	106.34	112.68
1	D	100	ILE	CA-C-O	-5.03	115.72	120.95
1	A	48	VAL	CA-C-O	-5.02	115.12	120.59
1	D	148	PHE	CA-C-O	-5.01	115.37	120.99
1	D	57	ALA	CA-C-N	5.01	127.00	120.28
1	D	57	ALA	C-N-CA	5.01	127.00	120.28
1	B	116	GLU	CA-C-O	-5.00	115.25	120.55
1	C	476	ARG	CA-C-N	5.00	130.42	122.62
1	C	476	ARG	C-N-CA	5.00	130.42	122.62

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	TYR	Mainchain
1	A	308	GLU	Mainchain
1	A	370	THR	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	424	THR	Mainchain
1	A	480	GLN	Mainchain
1	A	89	ALA	Mainchain
1	B	242	SER	Mainchain
1	B	265	GLY	Mainchain
1	B	308	GLU	Mainchain
1	B	40	VAL	Mainchain
1	B	480	GLN	Mainchain
1	C	308	GLU	Mainchain
1	C	370	THR	Mainchain
1	C	391	ARG	Mainchain
1	C	480	GLN	Mainchain
1	D	199	VAL	Mainchain
1	D	308	GLU	Mainchain
1	D	32	LYS	Mainchain
1	D	370	THR	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3808	0	3826	70	0
1	B	3808	0	3826	65	0
1	C	3808	0	3826	62	0
1	D	3808	0	3826	63	0
2	A	114	0	0	3	0
2	B	211	0	0	10	0
2	C	170	0	0	5	0
2	D	198	0	0	4	0
All	All	15925	0	15304	250	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 8.

All (250) 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:C:74:TRP:HA	1:C:77:MET:HE3	1.56	0.88
1:B:74:TRP:HA	1:B:77:MET:HE3	1.57	0.86
1:B:206:HIS:HE1	1:B:213:GLY:H	1.21	0.85
1:D:206:HIS:HE1	1:D:213:GLY:H	1.21	0.84
1:A:74:TRP:HA	1:A:77:MET:HE3	1.61	0.82
1:B:315:GLU:HG3	2:B:665:HOH:O	1.79	0.81
1:D:231:HIS:HD2	1:D:233:ASN:H	1.29	0.80
1:A:206:HIS:HE1	1:A:213:GLY:H	1.28	0.79
1:D:74:TRP:HA	1:D:77:MET:HE3	1.64	0.79
1:A:58:GLU:HB3	2:A:596:HOH:O	1.82	0.77
1:C:231:HIS:HD2	1:C:233:ASN:H	1.34	0.76
1:A:243:VAL:HB	1:A:244:PRO:HD3	1.66	0.76
1:D:73:LYS:HE3	1:D:77:MET:HE2	1.68	0.76
1:C:206:HIS:HE1	1:C:213:GLY:H	1.31	0.75
1:B:231:HIS:HD2	1:B:233:ASN:H	1.34	0.74
1:B:243:VAL:HB	1:B:244:PRO:HD3	1.69	0.74
1:C:243:VAL:HB	1:C:244:PRO:HD3	1.69	0.73
1:B:171:ILE:HD11	1:B:175:LYS:HE2	1.70	0.73
1:C:293:GLN:HB3	1:C:339:LEU:HD22	1.71	0.73
1:A:32:LYS:O	1:A:33:ASP:HB3	1.89	0.72
1:D:171:ILE:HD11	1:D:175:LYS:HE2	1.69	0.72
1:A:171:ILE:HD11	1:A:175:LYS:HE2	1.70	0.72
1:D:243:VAL:HB	1:D:244:PRO:HD3	1.73	0.71
1:B:73:LYS:HE3	1:B:77:MET:HE2	1.73	0.70
1:A:231:HIS:HD2	1:A:233:ASN:H	1.40	0.69
1:D:342:LYS:HB3	1:D:343:PRO:HD3	1.72	0.69
1:B:293:GLN:HB3	1:B:339:LEU:HD22	1.75	0.68
1:D:293:GLN:HB3	1:D:339:LEU:HD22	1.76	0.68
1:B:263:GLU:HB3	2:B:517:HOH:O	1.92	0.68
1:A:73:LYS:HE3	1:A:77:MET:HE2	1.74	0.67
1:C:77:MET:HE1	1:C:211:PRO:HG3	1.75	0.67
1:C:27:ARG:NH2	2:C:535:HOH:O	2.26	0.67
1:C:231:HIS:CD2	1:C:233:ASN:H	2.13	0.67
1:C:171:ILE:HD11	1:C:175:LYS:HE2	1.75	0.67
1:B:32:LYS:O	1:B:33:ASP:HB3	1.95	0.67
1:B:52:MET:CE	1:B:219:GLN:HB3	2.25	0.67
1:B:77:MET:HE1	1:B:211:PRO:HG3	1.77	0.66
1:C:73:LYS:HE3	1:C:77:MET:HE2	1.77	0.66
1:A:342:LYS:HB3	1:A:343:PRO:HD3	1.77	0.66
1:A:293:GLN:HB3	1:A:339:LEU:HD22	1.78	0.65
1:B:231:HIS:CD2	1:B:233:ASN:H	2.15	0.65
1:C:263:GLU:HB3	2:C:554:HOH:O	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:O	1:A:135:THR:HB	1.97	0.65
1:B:206:HIS:CE1	1:B:213:GLY:H	2.11	0.64
1:D:231:HIS:CD2	1:D:233:ASN:H	2.12	0.64
1:C:342:LYS:HB3	1:C:343:PRO:HD3	1.79	0.64
1:A:73:LYS:HG3	1:A:77:MET:CE	2.29	0.63
1:B:73:LYS:HG3	1:B:77:MET:CE	2.27	0.63
1:D:263:GLU:HB3	2:D:591:HOH:O	1.99	0.63
1:A:283:ARG:HB3	1:B:501:SER:HB2	1.81	0.63
1:D:361:ARG:HB3	1:D:388:ASP:HB3	1.81	0.62
1:A:77:MET:HE1	1:A:211:PRO:HG3	1.81	0.62
1:B:342:LYS:HB3	1:B:343:PRO:HD3	1.81	0.62
1:B:58:GLU:CD	1:B:58:GLU:H	2.08	0.61
1:B:77:MET:HE1	1:B:211:PRO:CG	2.30	0.61
1:C:58:GLU:H	1:C:58:GLU:CD	2.08	0.61
1:C:73:LYS:HG3	1:C:77:MET:CE	2.31	0.60
1:C:132:LEU:O	1:C:135:THR:HB	2.01	0.60
1:D:73:LYS:HG3	1:D:77:MET:CE	2.31	0.60
1:C:52:MET:CE	1:C:219:GLN:HB3	2.32	0.60
1:D:52:MET:CE	1:D:219:GLN:HB3	2.31	0.60
1:A:231:HIS:CD2	1:A:233:ASN:H	2.19	0.60
1:C:77:MET:HE1	1:C:211:PRO:CG	2.32	0.59
1:B:52:MET:HE3	1:B:219:GLN:HB3	1.85	0.59
1:D:58:GLU:CD	1:D:58:GLU:H	2.11	0.58
1:C:373:ASP:HB3	1:C:376:LEU:HD22	1.83	0.58
1:A:256:THR:HG23	1:B:471:MET:HE2	1.85	0.58
1:A:373:ASP:HB3	1:A:376:LEU:HD22	1.85	0.58
1:A:58:GLU:CD	1:A:58:GLU:H	2.11	0.58
1:C:32:LYS:O	1:C:33:ASP:HB3	2.03	0.58
1:D:373:ASP:HB3	1:D:376:LEU:HD22	1.85	0.58
1:D:132:LEU:O	1:D:135:THR:HB	2.04	0.57
1:B:361:ARG:NH2	2:B:696:HOH:O	2.37	0.57
1:C:167:TYR:O	1:C:171:ILE:HG22	2.04	0.57
1:A:310:MET:HE1	1:A:408:VAL:CG1	2.35	0.57
1:B:361:ARG:HB3	1:B:388:ASP:HB3	1.85	0.57
1:D:77:MET:HE1	1:D:211:PRO:HG3	1.85	0.57
1:D:31:SER:HB3	1:D:53:VAL:HG11	1.87	0.57
1:D:206:HIS:CE1	1:D:213:GLY:H	2.12	0.57
1:D:52:MET:HE3	1:D:219:GLN:HB3	1.85	0.56
1:B:31:SER:HB3	1:B:53:VAL:HG11	1.87	0.56
1:C:416:GLU:O	1:C:419:GLN:HG3	2.06	0.55
1:B:52:MET:HE1	1:B:219:GLN:HB3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:MET:HE3	1:C:219:GLN:HB3	1.88	0.55
1:B:52:MET:HE1	1:B:219:GLN:CB	2.37	0.55
1:C:133:ALA:HB3	1:C:134:PRO:HD3	1.89	0.55
1:C:310:MET:HE1	1:C:408:VAL:CG1	2.38	0.54
1:D:310:MET:HE1	1:D:408:VAL:CG1	2.38	0.54
1:A:361:ARG:HB3	1:A:388:ASP:HB3	1.90	0.54
1:B:167:TYR:O	1:B:171:ILE:HG22	2.08	0.54
1:B:373:ASP:HB3	1:B:376:LEU:HD22	1.90	0.53
1:D:52:MET:HE2	1:D:53:VAL:N	2.23	0.53
1:D:52:MET:HE1	1:D:219:GLN:CB	2.38	0.53
1:D:77:MET:HE1	1:D:211:PRO:CG	2.38	0.53
1:A:500:ASP:HB2	2:A:603:HOH:O	2.09	0.53
1:D:27:ARG:NH1	2:D:647:HOH:O	2.42	0.53
1:B:328:ASP:HB3	1:B:331:LEU:HD22	1.90	0.53
1:C:52:MET:HE1	1:C:219:GLN:CB	2.38	0.53
1:C:361:ARG:HB3	1:C:388:ASP:HB3	1.90	0.53
1:A:52:MET:HE1	1:A:219:GLN:HB2	1.92	0.53
1:C:256:THR:HG23	1:D:471:MET:HE2	1.91	0.53
1:C:374:PRO:HA	1:C:377:LYS:HE2	1.90	0.53
1:A:31:SER:HB3	1:A:53:VAL:HG11	1.91	0.52
1:A:133:ALA:HB3	1:A:134:PRO:HD3	1.92	0.52
1:B:73:LYS:HG3	1:B:77:MET:HE2	1.90	0.52
1:B:123:TRP:CZ3	1:B:124:GLN:HG2	2.45	0.52
1:B:347:LYS:HD3	2:B:552:HOH:O	2.09	0.52
1:C:354:GLN:O	1:C:358:GLU:HG3	2.10	0.52
1:A:206:HIS:CE1	1:A:213:GLY:H	2.19	0.51
1:A:374:PRO:HA	1:A:377:LYS:HE2	1.92	0.51
1:C:212:VAL:HG23	2:C:649:HOH:O	2.10	0.51
1:A:77:MET:HE1	1:A:211:PRO:CG	2.40	0.51
1:B:105:VAL:HG11	1:B:330:LEU:HD13	1.92	0.51
1:D:167:TYR:O	1:D:171:ILE:HG22	2.11	0.51
1:A:328:ASP:HB3	1:A:331:LEU:HD22	1.92	0.51
1:A:52:MET:HE1	1:A:219:GLN:CB	2.40	0.50
1:C:31:SER:HB3	1:C:53:VAL:HG11	1.92	0.50
1:B:132:LEU:O	1:B:135:THR:HB	2.12	0.50
1:A:110:LYS:NZ	1:A:118:ASP:OD2	2.36	0.50
1:D:310:MET:HE2	1:D:314:LEU:HD22	1.94	0.50
1:A:33:ASP:OD2	1:A:35:ALA:HB2	2.12	0.50
1:A:52:MET:HE2	1:A:53:VAL:N	2.27	0.49
1:B:310:MET:HE1	1:B:408:VAL:CG1	2.42	0.49
1:A:123:TRP:CZ3	1:A:124:GLN:HG2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:THR:O	1:A:292:THR:HG22	2.13	0.49
1:D:328:ASP:HB3	1:D:331:LEU:HD22	1.93	0.49
1:B:57:ALA:HA	1:B:227:LEU:HD22	1.95	0.49
1:B:361:ARG:NH1	2:B:696:HOH:O	2.46	0.49
1:A:52:MET:CE	1:A:219:GLN:HB3	2.42	0.48
1:C:328:ASP:HB3	1:C:331:LEU:HD22	1.96	0.48
1:C:471:MET:HE2	1:D:256:THR:HG23	1.96	0.48
1:D:52:MET:HE1	1:D:219:GLN:HB2	1.95	0.48
1:B:310:MET:HE2	1:B:314:LEU:HD13	1.95	0.48
1:A:437:ILE:HA	1:D:437:ILE:HB	1.95	0.48
1:D:32:LYS:O	1:D:33:ASP:HB3	2.12	0.48
1:D:105:VAL:HG11	1:D:330:LEU:HD13	1.95	0.48
1:C:73:LYS:HG3	1:C:77:MET:HE2	1.96	0.47
1:A:73:LYS:HG3	1:A:77:MET:HE2	1.95	0.47
1:C:105:VAL:HG11	1:C:330:LEU:HD13	1.95	0.47
1:D:310:MET:HE1	1:D:408:VAL:HG11	1.95	0.47
1:C:52:MET:HE1	1:C:219:GLN:HB2	1.95	0.47
1:C:310:MET:HE1	1:C:408:VAL:HG11	1.97	0.47
1:D:416:GLU:O	1:D:419:GLN:HG3	2.15	0.47
1:B:361:ARG:CZ	2:B:696:HOH:O	2.63	0.47
1:C:53:VAL:HG22	2:C:591:HOH:O	2.14	0.47
1:C:292:THR:HG22	1:C:292:THR:O	2.15	0.47
1:D:310:MET:HB3	1:D:311:PRO:HD3	1.95	0.47
1:C:310:MET:HB3	1:C:311:PRO:HD3	1.97	0.47
1:A:354:GLN:O	1:A:358:GLU:HG3	2.15	0.47
1:A:416:GLU:O	1:A:419:GLN:HG3	2.15	0.47
1:C:310:MET:HE2	1:C:314:LEU:HD22	1.97	0.47
1:B:310:MET:HE2	1:B:314:LEU:HD22	1.97	0.46
1:A:105:VAL:HG13	1:A:110:LYS:O	2.15	0.46
1:A:310:MET:HE1	1:A:408:VAL:HG11	1.97	0.46
1:B:369:LEU:HD21	2:B:583:HOH:O	2.15	0.46
1:C:374:PRO:HA	1:C:377:LYS:HD3	1.98	0.46
1:B:274:LYS:HA	1:B:309:ILE:HD13	1.98	0.46
1:A:267:LYS:HD2	1:A:302:ARG:HG3	1.97	0.46
1:B:52:MET:HE2	1:B:53:VAL:N	2.31	0.46
1:B:354:GLN:O	1:B:358:GLU:HG3	2.16	0.46
1:B:418:LEU:HD23	1:B:447:LEU:HD13	1.97	0.46
1:D:361:ARG:HB2	1:D:389:ASN:HB2	1.97	0.46
1:B:416:GLU:O	1:B:419:GLN:HG3	2.15	0.46
1:D:123:TRP:CZ3	1:D:124:GLN:HG2	2.50	0.46
1:D:374:PRO:HA	1:D:377:LYS:HE2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:MET:HE1	1:B:408:VAL:HG11	1.98	0.45
1:D:267:LYS:HD2	1:D:302:ARG:HG3	1.96	0.45
1:D:310:MET:HE2	1:D:314:LEU:HD13	1.96	0.45
1:A:52:MET:HE3	1:A:219:GLN:HB3	1.97	0.45
1:C:7:MET:N	1:C:8:PRO:CD	2.79	0.45
1:D:52:MET:CE	1:D:219:GLN:CB	2.94	0.45
1:D:354:GLN:O	1:D:358:GLU:HG3	2.17	0.45
1:A:167:TYR:O	1:A:171:ILE:HG22	2.17	0.45
1:A:437:ILE:HB	1:D:437:ILE:HA	1.98	0.45
1:C:52:MET:CE	1:C:219:GLN:CB	2.95	0.45
1:C:52:MET:HE2	1:C:53:VAL:N	2.32	0.45
1:A:140:HIS:O	1:D:137:SER:HB2	2.16	0.45
1:A:53:VAL:HA	1:A:54:PRO:HD2	1.85	0.45
1:A:112:ILE:HG13	1:A:329:PRO:O	2.17	0.45
1:B:361:ARG:HB2	1:B:389:ASN:HB2	1.99	0.45
1:C:480:GLN:HG3	2:C:637:HOH:O	2.16	0.45
1:D:374:PRO:HA	1:D:377:LYS:HD3	2.00	0.45
1:A:310:MET:HE2	1:A:314:LEU:HD22	2.00	0.44
1:A:374:PRO:HA	1:A:377:LYS:HD3	1.98	0.44
1:B:476:ARG:HH11	1:B:476:ARG:HD3	1.65	0.44
1:A:310:MET:HB3	1:A:311:PRO:HD3	1.98	0.44
1:B:457:TYR:O	1:B:458:SER:HB2	2.18	0.44
1:C:210:VAL:HG13	1:C:214:LEU:HB3	1.98	0.44
1:B:310:MET:HB3	1:B:311:PRO:HD3	1.99	0.44
1:B:466:PHE:HA	2:B:525:HOH:O	2.18	0.44
1:D:243:VAL:HA	1:D:264:LEU:HG	2.00	0.44
1:D:28:ARG:NH2	1:D:199:VAL:HG22	2.32	0.44
1:D:418:LEU:HD23	1:D:447:LEU:HD13	1.99	0.44
1:A:141:ILE:HG12	1:D:137:SER:HB3	1.98	0.44
1:A:84:ARG:HH11	1:A:84:ARG:HD3	1.61	0.44
1:C:202:ALA:O	1:C:206:HIS:HD2	2.01	0.44
1:A:177:ALA:N	1:A:178:PRO:HD2	2.33	0.43
1:C:53:VAL:HA	1:C:54:PRO:HD2	1.93	0.43
1:A:7:MET:N	1:A:8:PRO:CD	2.80	0.43
1:D:20:ASP:OD2	1:D:30:LYS:HG3	2.19	0.43
1:B:163:LEU:HD22	1:B:171:ILE:HD13	2.00	0.43
1:B:267:LYS:HD2	1:B:302:ARG:HG3	2.00	0.43
1:C:52:MET:HE1	1:C:219:GLN:HB3	1.99	0.43
1:D:84:ARG:HH11	1:D:84:ARG:HD3	1.66	0.43
1:B:434:THR:H	1:B:455:ASN:HD21	1.67	0.43
1:A:361:ARG:HB2	1:A:389:ASN:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:LYS:CE	1:C:77:MET:HE2	2.48	0.43
1:A:73:LYS:CE	1:A:77:MET:HE2	2.46	0.43
1:B:480:GLN:HG3	2:B:655:HOH:O	2.17	0.43
1:B:7:MET:N	1:B:8:PRO:CD	2.82	0.43
1:B:28:ARG:NH2	1:B:199:VAL:HG22	2.34	0.43
1:B:76:LYS:HA	1:B:76:LYS:HD2	1.89	0.43
1:C:76:LYS:HA	1:C:76:LYS:HD2	1.89	0.43
1:C:267:LYS:HD2	1:C:302:ARG:HG3	2.00	0.43
1:A:112:ILE:O	1:A:116:GLU:HG3	2.19	0.42
1:A:76:LYS:HA	1:A:76:LYS:HD2	1.91	0.42
1:C:274:LYS:HA	1:C:309:ILE:HD13	2.02	0.42
1:D:163:LEU:HD22	1:D:171:ILE:HD13	2.01	0.42
1:A:263:GLU:HB3	2:A:574:HOH:O	2.18	0.42
1:C:342:LYS:N	1:C:343:PRO:CD	2.82	0.42
1:B:189:LYS:HA	1:B:218:VAL:O	2.20	0.42
1:D:202:ALA:O	1:D:206:HIS:HD2	2.03	0.42
1:C:361:ARG:HB2	1:C:389:ASN:HB2	2.01	0.42
1:B:143:LEU:HB3	1:B:144:PRO:HD2	2.01	0.41
1:A:28:ARG:NH2	1:A:199:VAL:HG22	2.34	0.41
1:A:112:ILE:HG13	1:A:112:ILE:H	1.66	0.41
1:A:210:VAL:HA	1:A:211:PRO:HD3	1.99	0.41
1:A:491:THR:O	1:B:451:THR:HA	2.20	0.41
1:B:52:MET:CE	1:B:219:GLN:CB	2.96	0.41
1:C:123:TRP:CZ3	1:C:124:GLN:HG2	2.55	0.41
1:C:411:PHE:CG	1:C:417:VAL:HG13	2.55	0.41
1:D:73:LYS:HG3	1:D:77:MET:HE2	2.01	0.41
1:D:189:LYS:HA	1:D:218:VAL:O	2.20	0.41
1:D:466:PHE:HA	2:D:589:HOH:O	2.20	0.41
1:A:2:GLN:H	1:A:2:GLN:CD	2.28	0.41
1:D:292:THR:HG22	1:D:292:THR:O	2.20	0.41
1:B:361:ARG:HD3	2:B:667:HOH:O	2.20	0.41
1:C:456:THR:HB	1:D:495:GLU:HB2	2.02	0.41
1:A:279:GLU:O	1:A:283:ARG:HG3	2.20	0.41
1:C:243:VAL:N	1:C:244:PRO:CD	2.83	0.41
1:D:30:LYS:HB2	2:D:648:HOH:O	2.21	0.41
1:A:88:GLU:OE1	1:A:91:ARG:NH2	2.53	0.41
1:B:52:MET:HE1	1:B:219:GLN:HB2	2.04	0.40
1:A:177:ALA:HB3	1:A:178:PRO:HD3	2.04	0.40
1:C:457:TYR:O	1:C:458:SER:HB2	2.21	0.40
1:D:7:MET:N	1:D:8:PRO:CD	2.84	0.40
1:A:342:LYS:N	1:A:343:PRO:CD	2.84	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:HG	1:A:388:ASP:HB2	2.03	0.40
1:C:88:GLU:OE1	1:C:91:ARG:NH2	2.52	0.40
1:D:363:LEU:HG	1:D:388:ASP:HB2	2.04	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	501/503 (100%)	489 (98%)	12 (2%)	0	100	100
1	B	465/503 (92%)	451 (97%)	14 (3%)	0	100	100
1	C	501/503 (100%)	486 (97%)	15 (3%)	0	100	100
1	D	501/503 (100%)	485 (97%)	16 (3%)	0	100	100
All	All	1968/2012 (98%)	1911 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/410 (100%)	366 (89%)	44 (11%)	6	4
1	B	410/410 (100%)	365 (89%)	45 (11%)	6	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	410/410 (100%)	368 (90%)	42 (10%)	7	4
1	D	410/410 (100%)	365 (89%)	45 (11%)	6	3
All	All	1640/1640 (100%)	1464 (89%)	176 (11%)	6	4

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	40	VAL
1	A	52	MET
1	A	53	VAL
1	A	72	LEU
1	A	76	LYS
1	A	80	ILE
1	A	84	ARG
1	A	103	LEU
1	A	112	ILE
1	A	124	GLN
1	A	135	THR
1	A	136	LEU
1	A	156	LEU
1	A	171	ILE
1	A	196	VAL
1	A	199	VAL
1	A	210	VAL
1	A	223	GLU
1	A	257	VAL
1	A	264	LEU
1	A	271	LEU
1	A	272	ILE
1	A	278	LEU
1	A	286	LEU
1	A	310	MET
1	A	314	LEU
1	A	330	LEU
1	A	331	LEU
1	A	339	LEU
1	A	340	ILE
1	A	356	LYS
1	A	361	ARG
1	A	375	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	377	LYS
1	A	389	ASN
1	A	399	GLU
1	A	402	PHE
1	A	417	VAL
1	A	447	LEU
1	A	462	VAL
1	A	477	GLU
1	A	483	VAL
1	A	494	VAL
1	B	32	LYS
1	B	40	VAL
1	B	52	MET
1	B	53	VAL
1	B	72	LEU
1	B	76	LYS
1	B	80	ILE
1	B	84	ARG
1	B	102	LYS
1	B	103	LEU
1	B	112	ILE
1	B	124	GLN
1	B	135	THR
1	B	136	LEU
1	B	156	LEU
1	B	171	ILE
1	B	196	VAL
1	B	199	VAL
1	B	210	VAL
1	B	223	GLU
1	B	264	LEU
1	B	271	LEU
1	B	272	ILE
1	B	278	LEU
1	B	286	LEU
1	B	310	MET
1	B	314	LEU
1	B	330	LEU
1	B	331	LEU
1	B	339	LEU
1	B	340	ILE
1	B	356	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	361	ARG
1	B	375	LYS
1	B	376	LEU
1	B	377	LYS
1	B	389	ASN
1	B	399	GLU
1	B	402	PHE
1	B	417	VAL
1	B	447	LEU
1	B	462	VAL
1	B	477	GLU
1	B	483	VAL
1	B	494	VAL
1	C	32	LYS
1	C	40	VAL
1	C	52	MET
1	C	53	VAL
1	C	72	LEU
1	C	76	LYS
1	C	80	ILE
1	C	84	ARG
1	C	103	LEU
1	C	112	ILE
1	C	135	THR
1	C	136	LEU
1	C	156	LEU
1	C	171	ILE
1	C	196	VAL
1	C	199	VAL
1	C	210	VAL
1	C	223	GLU
1	C	264	LEU
1	C	271	LEU
1	C	272	ILE
1	C	278	LEU
1	C	286	LEU
1	C	310	MET
1	C	314	LEU
1	C	330	LEU
1	C	331	LEU
1	C	339	LEU
1	C	340	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	356	LYS
1	C	361	ARG
1	C	375	LYS
1	C	376	LEU
1	C	377	LYS
1	C	389	ASN
1	C	399	GLU
1	C	417	VAL
1	C	447	LEU
1	C	462	VAL
1	C	477	GLU
1	C	483	VAL
1	C	494	VAL
1	D	32	LYS
1	D	40	VAL
1	D	52	MET
1	D	53	VAL
1	D	72	LEU
1	D	76	LYS
1	D	80	ILE
1	D	84	ARG
1	D	102	LYS
1	D	103	LEU
1	D	112	ILE
1	D	124	GLN
1	D	135	THR
1	D	136	LEU
1	D	156	LEU
1	D	171	ILE
1	D	196	VAL
1	D	199	VAL
1	D	210	VAL
1	D	223	GLU
1	D	264	LEU
1	D	271	LEU
1	D	272	ILE
1	D	278	LEU
1	D	286	LEU
1	D	314	LEU
1	D	317	VAL
1	D	330	LEU
1	D	331	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	339	LEU
1	D	340	ILE
1	D	356	LYS
1	D	361	ARG
1	D	375	LYS
1	D	376	LEU
1	D	377	LYS
1	D	389	ASN
1	D	399	GLU
1	D	402	PHE
1	D	417	VAL
1	D	447	LEU
1	D	462	VAL
1	D	477	GLU
1	D	483	VAL
1	D	494	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	139	GLN
1	A	206	HIS
1	A	230	HIS
1	A	231	HIS
1	A	299	ASN
1	A	378	ASN
1	A	423	ASN
1	A	480	GLN
1	A	488	GLN
1	B	139	GLN
1	B	206	HIS
1	B	230	HIS
1	B	231	HIS
1	B	259	HIS
1	B	299	ASN
1	B	378	ASN
1	B	419	GLN
1	B	423	ASN
1	B	455	ASN
1	B	480	GLN
1	C	124	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	139	GLN
1	C	206	HIS
1	C	230	HIS
1	C	231	HIS
1	C	299	ASN
1	C	378	ASN
1	C	419	GLN
1	C	423	ASN
1	C	455	ASN
1	D	206	HIS
1	D	230	HIS
1	D	231	HIS
1	D	299	ASN
1	D	378	ASN
1	D	455	ASN
1	D	480	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 ⓘ

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	503/503 (100%)	-0.06	8 (1%) 70 73	5, 15, 30, 107	0
1	B	503/503 (100%)	-0.15	17 (3%) 48 50	5, 15, 30, 107	0
1	C	503/503 (100%)	-0.25	11 (2%) 62 65	5, 15, 30, 107	0
1	D	503/503 (100%)	-0.22	9 (1%) 67 70	5, 15, 30, 107	0
All	All	2012/2012 (100%)	-0.17	45 (2%) 62 65	5, 15, 31, 107	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	34	GLY	15.5
1	C	34	GLY	11.6
1	D	33	ASP	11.1
1	D	34	GLY	9.5
1	D	31	SER	8.1
1	D	32	LYS	6.6
1	B	35	ALA	6.3
1	B	33	ASP	6.2
1	A	34	GLY	5.9
1	C	33	ASP	5.4
1	C	36	THR	5.4
1	D	35	ALA	5.2
1	B	32	LYS	5.1
1	C	32	LYS	4.5
1	D	36	THR	3.7
1	A	33	ASP	3.6
1	B	36	THR	3.5
1	C	35	ALA	3.4
1	B	27	ARG	3.3
1	D	30	LYS	2.9
1	B	31	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	2	GLN	2.8
1	B	248	LYS	2.7
1	B	9	SER	2.7
1	C	27	ARG	2.6
1	B	333	GLU	2.5
1	C	1	ALA	2.5
1	C	31	SER	2.5
1	C	2	GLN	2.5
1	A	1	ALA	2.5
1	A	44	ALA	2.3
1	C	353	ALA	2.3
1	B	58	GLU	2.3
1	D	1	ALA	2.3
1	B	500	ASP	2.3
1	C	58	GLU	2.2
1	A	374	PRO	2.2
1	D	419	GLN	2.2
1	A	32	LYS	2.2
1	A	354	GLN	2.1
1	B	388	ASP	2.1
1	B	124	GLN	2.1
1	B	503	PHE	2.1
1	B	391	ARG	2.0
1	A	54	PRO	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.