



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:50 AM UTC

PDB ID : 5GT6 / pdb_00005gt6
Title : Apo structure of Aldehyde Dehydrogenase from Bacillus cereus
Authors : Ngo, H.P.T.; Hong, S.H.; Ho, T.H.; Oh, D.K.; Kang, L.W.
Deposited on : 2016-08-18
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

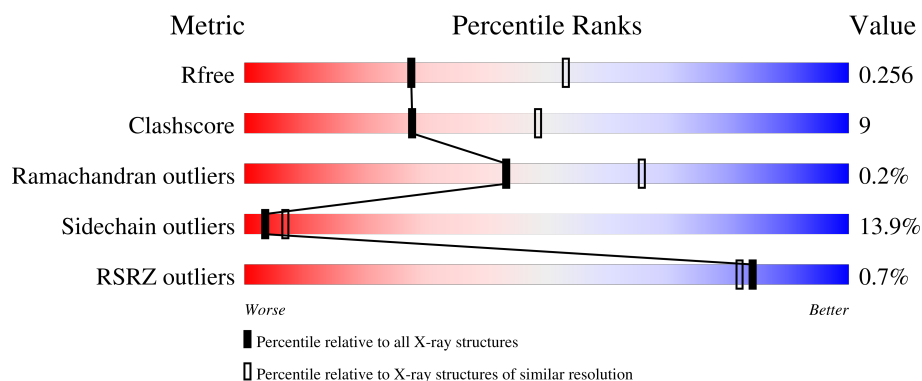
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	508	
1	B	508	
1	C	508	
1	D	508	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15213 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	491	Total	C	N	O	S	0	0	0
			3791	2414	630	733	14			
1	B	489	Total	C	N	O	S	0	0	0
			3776	2406	627	729	14			
1	C	487	Total	C	N	O	S	0	0	0
			3759	2395	625	725	14			
1	D	491	Total	C	N	O	S	0	0	0
			3791	2414	630	733	14			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP A0A150BLG9
A	-12	GLY	-	expression tag	UNP A0A150BLG9
A	-11	SER	-	expression tag	UNP A0A150BLG9
A	-10	SER	-	expression tag	UNP A0A150BLG9
A	-9	HIS	-	expression tag	UNP A0A150BLG9
A	-8	HIS	-	expression tag	UNP A0A150BLG9
A	-7	HIS	-	expression tag	UNP A0A150BLG9
A	-6	HIS	-	expression tag	UNP A0A150BLG9
A	-5	HIS	-	expression tag	UNP A0A150BLG9
A	-4	HIS	-	expression tag	UNP A0A150BLG9
A	-3	SER	-	expression tag	UNP A0A150BLG9
A	-2	GLN	-	expression tag	UNP A0A150BLG9
A	-1	ASP	-	expression tag	UNP A0A150BLG9
A	0	PRO	-	expression tag	UNP A0A150BLG9
B	-13	MET	-	expression tag	UNP A0A150BLG9
B	-12	GLY	-	expression tag	UNP A0A150BLG9
B	-11	SER	-	expression tag	UNP A0A150BLG9
B	-10	SER	-	expression tag	UNP A0A150BLG9
B	-9	HIS	-	expression tag	UNP A0A150BLG9
B	-8	HIS	-	expression tag	UNP A0A150BLG9
B	-7	HIS	-	expression tag	UNP A0A150BLG9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP A0A150BLG9
B	-5	HIS	-	expression tag	UNP A0A150BLG9
B	-4	HIS	-	expression tag	UNP A0A150BLG9
B	-3	SER	-	expression tag	UNP A0A150BLG9
B	-2	GLN	-	expression tag	UNP A0A150BLG9
B	-1	ASP	-	expression tag	UNP A0A150BLG9
B	0	PRO	-	expression tag	UNP A0A150BLG9
C	-13	MET	-	expression tag	UNP A0A150BLG9
C	-12	GLY	-	expression tag	UNP A0A150BLG9
C	-11	SER	-	expression tag	UNP A0A150BLG9
C	-10	SER	-	expression tag	UNP A0A150BLG9
C	-9	HIS	-	expression tag	UNP A0A150BLG9
C	-8	HIS	-	expression tag	UNP A0A150BLG9
C	-7	HIS	-	expression tag	UNP A0A150BLG9
C	-6	HIS	-	expression tag	UNP A0A150BLG9
C	-5	HIS	-	expression tag	UNP A0A150BLG9
C	-4	HIS	-	expression tag	UNP A0A150BLG9
C	-3	SER	-	expression tag	UNP A0A150BLG9
C	-2	GLN	-	expression tag	UNP A0A150BLG9
C	-1	ASP	-	expression tag	UNP A0A150BLG9
C	0	PRO	-	expression tag	UNP A0A150BLG9
D	-13	MET	-	expression tag	UNP A0A150BLG9
D	-12	GLY	-	expression tag	UNP A0A150BLG9
D	-11	SER	-	expression tag	UNP A0A150BLG9
D	-10	SER	-	expression tag	UNP A0A150BLG9
D	-9	HIS	-	expression tag	UNP A0A150BLG9
D	-8	HIS	-	expression tag	UNP A0A150BLG9
D	-7	HIS	-	expression tag	UNP A0A150BLG9
D	-6	HIS	-	expression tag	UNP A0A150BLG9
D	-5	HIS	-	expression tag	UNP A0A150BLG9
D	-4	HIS	-	expression tag	UNP A0A150BLG9
D	-3	SER	-	expression tag	UNP A0A150BLG9
D	-2	GLN	-	expression tag	UNP A0A150BLG9
D	-1	ASP	-	expression tag	UNP A0A150BLG9
D	0	PRO	-	expression tag	UNP A0A150BLG9

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Na 1	0	0
2	D	1	Total 1	Na 1	0	0

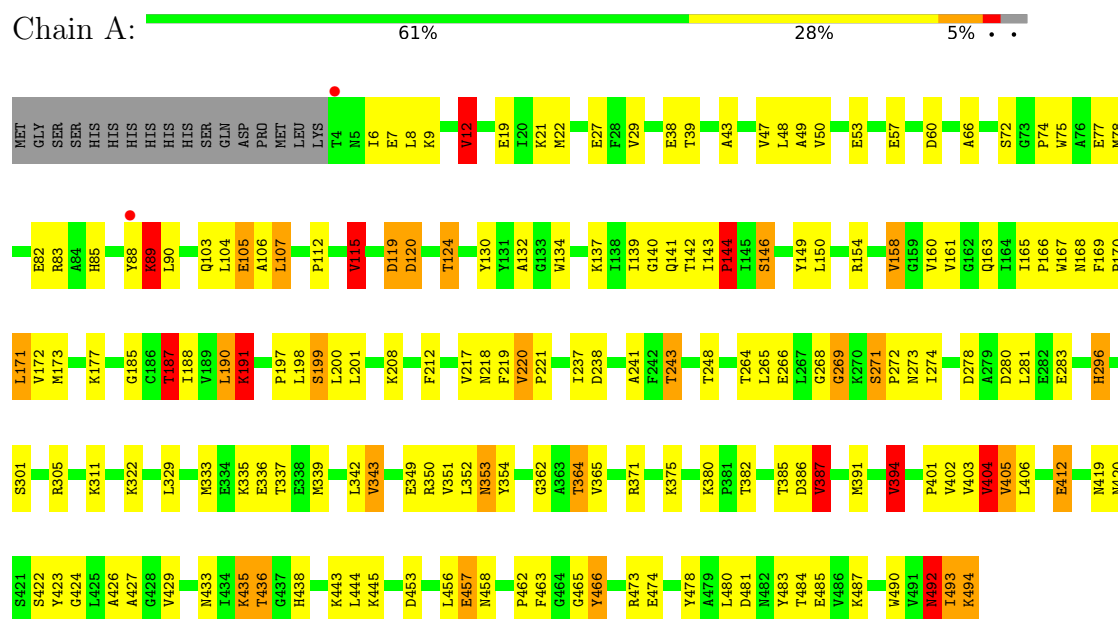
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total 26	O 26	0	0
3	B	23	Total 23	O 23	0	0
3	C	26	Total 26	O 26	0	0
3	D	17	Total 17	O 17	0	0

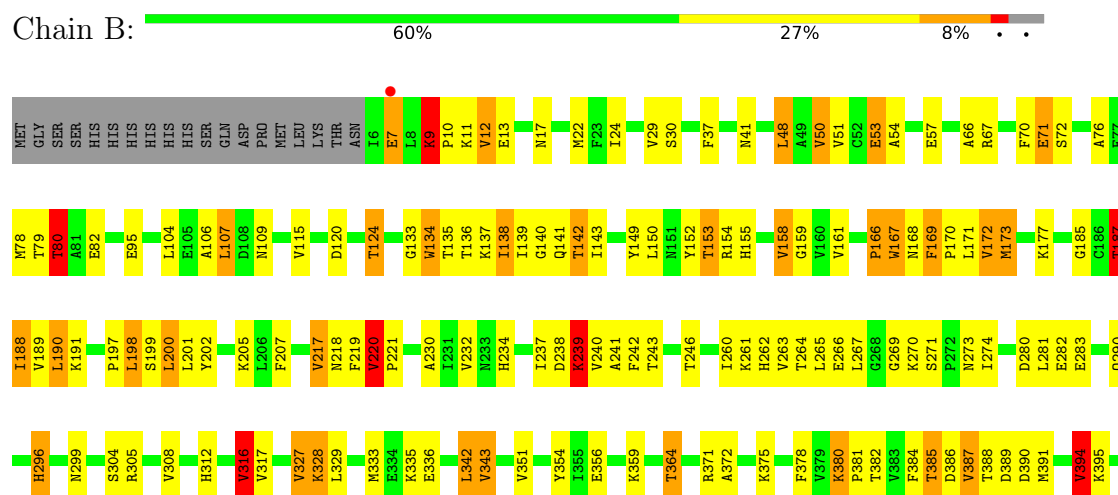
3 Residue-property plots [i](#)

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

• Molecule 1: Betaine-aldehyde dehydrogenase

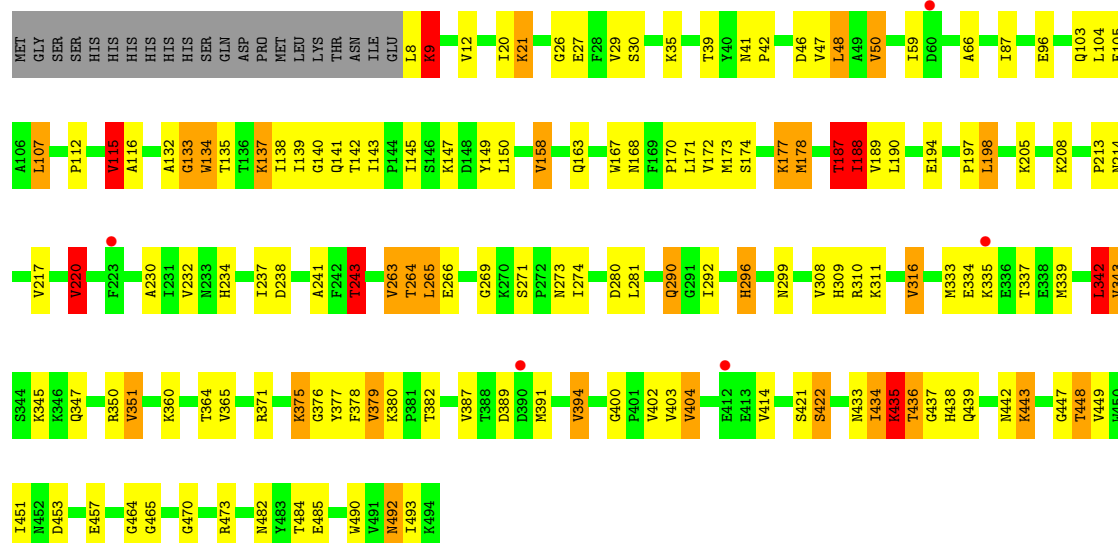


• Molecule 1: Betaine-aldehyde dehydrogenase

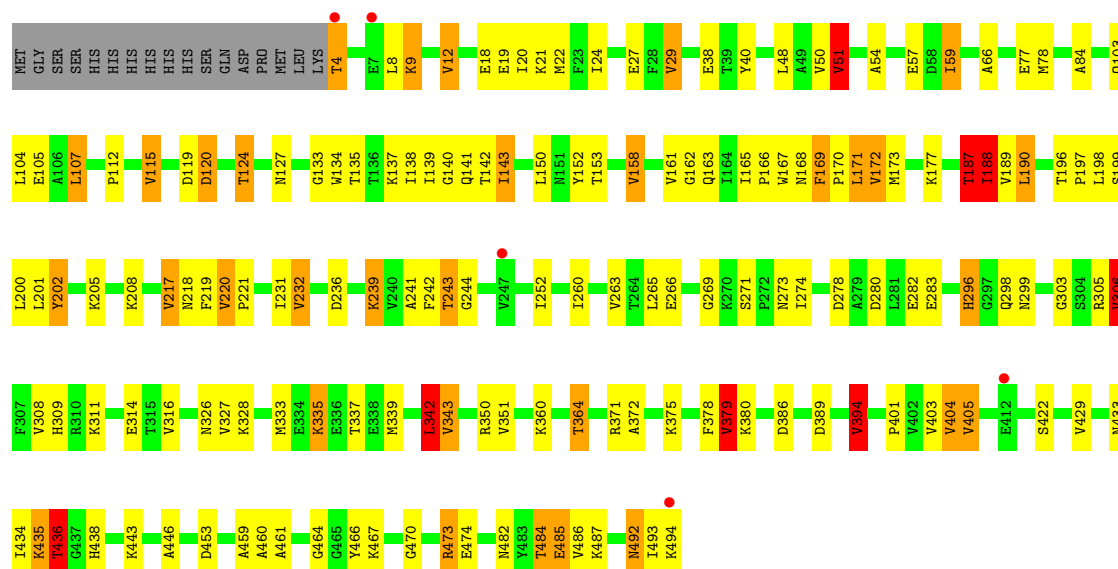




• Molecule 1: Betaine-aldehyde dehydrogenase



• Molecule 1: Betaine-aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.53Å 93.28Å 145.47Å 90.00° 98.05° 90.00°	Depositor
Resolution (Å)	49.57 – 2.60 49.57 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.57-2.60) 99.0 (49.57-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	38.30 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.182 , 0.251 0.194 , 0.256	Depositor DCC
R_{free} test set	3423 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 25.4	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	0.92	EDS
Total number of atoms	15213	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
NA

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	1.72	86/3870 (2.2%)	1.39	49/5250 (0.9%)
1	B	1.62	77/3855 (2.0%)	1.34	36/5229 (0.7%)
1	C	1.60	61/3838 (1.6%)	1.35	39/5206 (0.7%)
1	D	1.56	59/3870 (1.5%)	1.30	32/5250 (0.6%)
All	All	1.63	283/15433 (1.8%)	1.35	156/20935 (0.7%)

All (283) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	265	LEU	C-O	-8.64	1.14	1.24
1	A	490	TRP	C-O	-8.39	1.14	1.24
1	A	154	ARG	C-O	-8.04	1.14	1.24
1	A	403	VAL	C-O	-7.94	1.15	1.24
1	A	188	ILE	C-O	-7.73	1.16	1.24
1	C	188	ILE	C-O	-7.67	1.16	1.24
1	B	415	ILE	C-O	-7.62	1.15	1.24
1	B	273	ASN	C-O	-7.49	1.15	1.24
1	A	453	ASP	C-O	-7.47	1.15	1.23
1	A	269	GLY	C-O	-7.44	1.16	1.23
1	A	50	VAL	C-O	-7.42	1.16	1.24
1	C	241	ALA	C-O	-7.39	1.15	1.23
1	A	485	GLU	C-O	-7.37	1.15	1.24
1	A	141	GLN	C-O	-7.36	1.15	1.23
1	B	305	ARG	C-O	-7.35	1.15	1.24
1	D	453	ASP	C-O	-7.25	1.16	1.24
1	A	165	ILE	C-O	-7.19	1.17	1.24
1	C	177	LYS	C-O	-7.11	1.15	1.24
1	C	378	PHE	C-O	-7.10	1.15	1.23
1	B	50	VAL	C-O	-7.09	1.16	1.24
1	A	150	LEU	C-O	-7.08	1.15	1.24
1	A	143	ILE	C-O	-7.07	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	187	THR	C-O	-7.07	1.15	1.24
1	B	449	VAL	C-O	-7.05	1.16	1.24
1	D	138	ILE	C-O	-7.05	1.15	1.24
1	A	305	ARG	C-O	-7.00	1.15	1.24
1	A	463	PHE	C-O	-6.96	1.15	1.23
1	A	429	VAL	C-O	-6.94	1.16	1.24
1	C	453	ASP	C-O	-6.93	1.16	1.23
1	D	220	VAL	C-O	-6.91	1.15	1.24
1	D	243	THR	C-O	-6.87	1.16	1.24
1	B	299	ASN	C-O	-6.87	1.15	1.23
1	C	198	LEU	C-O	-6.86	1.16	1.24
1	D	269	GLY	C-O	-6.86	1.16	1.23
1	B	140	GLY	C-O	-6.86	1.17	1.23
1	C	133	GLY	C-O	-6.81	1.15	1.24
1	D	474	GLU	C-O	-6.77	1.15	1.23
1	C	402	VAL	C-O	-6.73	1.16	1.24
1	B	493	ILE	C-O	-6.72	1.16	1.24
1	D	197	PRO	C-O	-6.69	1.16	1.24
1	A	197	PRO	C-O	-6.69	1.16	1.24
1	B	426	ALA	C-O	-6.69	1.16	1.23
1	B	263	VAL	C-O	-6.63	1.17	1.24
1	C	197	PRO	C-O	-6.63	1.16	1.24
1	A	198	LEU	C-O	-6.62	1.16	1.24
1	B	80	THR	C-O	-6.59	1.16	1.24
1	C	269	GLY	C-O	-6.57	1.16	1.23
1	B	149	TYR	C-O	-6.57	1.15	1.23
1	C	145	ILE	N-CA	-6.56	1.40	1.46
1	A	458	ASN	C-O	-6.56	1.15	1.23
1	A	272	PRO	C-O	-6.55	1.17	1.23
1	B	243	THR	C-O	-6.55	1.16	1.23
1	B	265	LEU	C-O	-6.50	1.16	1.24
1	A	427	ALA	C-O	-6.50	1.15	1.23
1	D	188	ILE	C-O	-6.50	1.17	1.24
1	D	165	ILE	C-O	-6.50	1.17	1.24
1	D	460	ALA	C-O	-6.49	1.15	1.24
1	A	219	PHE	C-O	-6.48	1.16	1.24
1	B	197	PRO	C-O	-6.47	1.16	1.24
1	B	435	LYS	C-O	-6.46	1.16	1.24
1	D	474	GLU	CA-C	-6.44	1.44	1.52
1	D	274	ILE	C-O	-6.43	1.17	1.24
1	B	169	PHE	C-O	-6.38	1.16	1.24
1	D	29	VAL	C-O	-6.36	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	SER	C-O	-6.36	1.15	1.24
1	B	155	HIS	C-O	-6.35	1.15	1.23
1	D	218	ASN	C-O	-6.33	1.16	1.23
1	B	189	VAL	C-O	-6.31	1.16	1.24
1	A	406	LEU	C-O	-6.29	1.17	1.24
1	C	50	VAL	C-O	-6.26	1.17	1.24
1	C	134	TRP	C-O	-6.26	1.16	1.24
1	A	6	ILE	C-O	-6.25	1.17	1.24
1	D	461	ALA	C-O	-6.22	1.17	1.24
1	B	242	PHE	C-O	-6.19	1.16	1.23
1	A	119	ASP	CA-C	-6.17	1.48	1.52
1	D	485	GLU	C-O	-6.14	1.17	1.23
1	B	53	GLU	C-O	-6.10	1.16	1.24
1	C	189	VAL	C-O	-6.10	1.17	1.24
1	B	270	LYS	C-O	-6.09	1.16	1.23
1	B	405	VAL	C-O	-6.09	1.17	1.24
1	C	30	SER	CA-C	-6.09	1.44	1.53
1	C	449	VAL	C-O	-6.07	1.17	1.24
1	C	142	THR	C-O	-6.06	1.17	1.24
1	B	447	GLY	C-O	-6.06	1.16	1.23
1	B	141	GLN	C-O	-6.05	1.16	1.23
1	A	274	ILE	C-O	-6.01	1.17	1.24
1	A	273	ASN	C-O	-6.00	1.17	1.24
1	B	433	ASN	C-O	-6.00	1.16	1.24
1	A	39	THR	C-O	-5.99	1.16	1.23
1	C	422	SER	C-O	-5.99	1.16	1.24
1	D	379	VAL	C-O	-5.97	1.18	1.24
1	A	241	ALA	C-O	-5.96	1.17	1.23
1	A	185	GLY	C-O	-5.96	1.16	1.24
1	C	243	THR	C-O	-5.96	1.16	1.23
1	A	412	GLU	C-O	-5.95	1.17	1.24
1	A	481	ASP	C-O	-5.95	1.16	1.24
1	A	350	ARG	C-O	-5.94	1.17	1.24
1	D	305	ARG	C-O	-5.94	1.17	1.23
1	D	119	ASP	C-O	-5.91	1.16	1.24
1	D	466	TYR	C-O	-5.90	1.16	1.23
1	A	456	LEU	C-O	-5.87	1.17	1.24
1	A	171	LEU	C-O	-5.87	1.17	1.24
1	D	133	GLY	C-O	-5.86	1.17	1.24
1	D	394	VAL	C-O	-5.86	1.17	1.24
1	B	274	ILE	C-O	-5.86	1.17	1.24
1	C	490	TRP	C-O	-5.85	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	VAL	C-O	-5.84	1.17	1.24
1	D	143	ILE	C-O	-5.84	1.17	1.24
1	B	394	VAL	C-O	-5.83	1.17	1.24
1	A	237	ILE	C-O	-5.82	1.17	1.24
1	D	189	VAL	C-O	-5.82	1.17	1.24
1	A	337	THR	C-O	-5.82	1.17	1.24
1	D	303	GLY	C-O	-5.80	1.16	1.23
1	D	142	THR	C-O	-5.78	1.17	1.24
1	D	486	VAL	C-O	-5.78	1.17	1.24
1	D	162	GLY	C-O	-5.77	1.16	1.23
1	C	30	SER	C-O	-5.76	1.16	1.23
1	B	241	ALA	C-O	-5.75	1.17	1.23
1	A	354	TYR	C-O	-5.75	1.16	1.24
1	A	187	THR	C-O	-5.75	1.16	1.23
1	A	483	TYR	C-O	-5.75	1.16	1.24
1	B	382	THR	C-O	-5.75	1.16	1.24
1	C	442	ASN	C-O	-5.73	1.17	1.24
1	B	492	ASN	C-O	-5.73	1.17	1.23
1	D	51	VAL	C-O	-5.72	1.18	1.24
1	B	458	ASN	C-O	-5.72	1.16	1.23
1	A	119	ASP	C-O	-5.71	1.16	1.23
1	A	385	THR	C-O	-5.71	1.16	1.23
1	C	451	ILE	C-O	-5.71	1.18	1.24
1	B	51	VAL	C-O	-5.70	1.18	1.24
1	B	200	LEU	C-O	-5.70	1.17	1.24
1	A	404	VAL	C-O	-5.69	1.18	1.24
1	B	198	LEU	C-O	-5.68	1.17	1.24
1	D	51	VAL	N-CA	-5.68	1.39	1.46
1	C	457	GLU	C-O	-5.68	1.16	1.23
1	B	218	ASN	C-O	-5.68	1.17	1.24
1	A	149	TYR	C-O	-5.66	1.16	1.23
1	C	400	GLY	C-O	-5.66	1.16	1.24
1	D	378	PHE	C-O	-5.66	1.16	1.23
1	D	19	GLU	C-O	-5.66	1.17	1.23
1	A	190	LEU	C-O	-5.65	1.17	1.24
1	B	464	GLY	C-O	-5.65	1.16	1.23
1	A	115	VAL	C-O	-5.64	1.17	1.24
1	B	457	GLU	C-O	-5.63	1.16	1.23
1	B	10	PRO	C-O	-5.63	1.16	1.24
1	A	218	ASN	C-O	-5.62	1.17	1.23
1	C	168	ASN	C-O	-5.62	1.17	1.24
1	D	168	ASN	C-O	-5.62	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	334	GLU	C-O	-5.61	1.17	1.23
1	C	143	ILE	C-O	-5.59	1.18	1.24
1	C	437	GLY	C-O	-5.59	1.17	1.23
1	C	379	VAL	C-O	-5.59	1.18	1.24
1	D	141	GLN	C-O	-5.58	1.16	1.23
1	D	244	GLY	C-O	-5.58	1.16	1.24
1	C	309	HIS	C-O	-5.57	1.17	1.23
1	B	469	SER	C-O	-5.57	1.16	1.24
1	C	167	TRP	C-O	-5.56	1.16	1.24
1	B	264	THR	C-O	-5.56	1.17	1.24
1	D	140	GLY	C-O	-5.56	1.18	1.23
1	D	59	ILE	C-O	-5.55	1.16	1.24
1	B	188	ILE	C-O	-5.51	1.18	1.24
1	C	220	VAL	C-O	-5.51	1.17	1.24
1	A	90	LEU	C-O	-5.50	1.17	1.24
1	A	352	LEU	C-O	-5.47	1.17	1.24
1	D	40	TYR	C-O	-5.46	1.16	1.23
1	D	120	ASP	C-O	-5.46	1.17	1.24
1	B	76	ALA	C-O	-5.46	1.17	1.24
1	B	316	VAL	C-O	-5.46	1.17	1.24
1	A	493	ILE	C-O	-5.45	1.17	1.24
1	B	483	TYR	C-O	-5.45	1.16	1.24
1	D	298	GLN	C-O	-5.45	1.16	1.23
1	C	116	ALA	C-O	-5.45	1.17	1.24
1	D	163	GLN	C-O	-5.44	1.17	1.24
1	B	380	LYS	C-O	-5.44	1.17	1.24
1	D	446	ALA	CA-C	-5.44	1.46	1.52
1	A	120	ASP	C-O	-5.43	1.17	1.24
1	A	480	LEU	C-O	-5.42	1.17	1.24
1	B	406	LEU	C-O	-5.42	1.17	1.24
1	B	134	TRP	C-O	-5.42	1.16	1.24
1	A	106	ALA	C-O	-5.40	1.17	1.24
1	B	185	GLY	C-O	-5.40	1.16	1.24
1	D	350	ARG	C-O	-5.38	1.17	1.24
1	A	74	PRO	C-O	-5.38	1.17	1.24
1	A	264	THR	C-O	-5.38	1.17	1.24
1	B	240	VAL	C-O	-5.37	1.18	1.24
1	A	265	LEU	C-O	-5.37	1.17	1.23
1	B	456	LEU	C-O	-5.37	1.17	1.24
1	C	115	VAL	C-O	-5.36	1.18	1.24
1	A	143	ILE	CA-C	-5.36	1.48	1.53
1	B	143	ILE	C-O	-5.35	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	138	ILE	C-O	-5.35	1.17	1.24
1	B	328	LYS	C-O	-5.35	1.17	1.24
1	D	242	PHE	C-O	-5.35	1.17	1.23
1	C	280	ASP	C-O	-5.34	1.17	1.24
1	C	150	LEU	C-O	-5.34	1.18	1.24
1	D	241	ALA	C-O	-5.33	1.17	1.23
1	A	457	GLU	C-O	-5.33	1.17	1.23
1	B	170	PRO	C-O	-5.32	1.17	1.24
1	B	354	TYR	C-O	-5.32	1.17	1.24
1	C	290	GLN	C-O	-5.32	1.17	1.24
1	D	169	PHE	C-O	-5.32	1.18	1.24
1	C	237	ILE	C-O	-5.31	1.17	1.24
1	D	170	PRO	C-O	-5.31	1.17	1.24
1	B	154	ARG	C-O	-5.31	1.17	1.24
1	D	405	VAL	C-O	-5.31	1.18	1.24
1	A	12	VAL	C-O	-5.30	1.17	1.24
1	B	312	HIS	C-O	-5.29	1.16	1.24
1	A	144	PRO	C-O	-5.29	1.17	1.24
1	A	149	TYR	CA-C	-5.29	1.46	1.52
1	C	39	THR	C-O	-5.29	1.17	1.24
1	C	263	VAL	C-O	-5.29	1.18	1.24
1	D	161	VAL	C-O	-5.27	1.18	1.24
1	C	435	LYS	C-O	-5.27	1.18	1.24
1	B	468	GLN	C-O	-5.26	1.17	1.24
1	B	201	LEU	C-O	-5.26	1.17	1.24
1	C	174	SER	C-O	-5.26	1.17	1.24
1	A	6	ILE	CA-C	-5.25	1.46	1.52
1	A	382	THR	C-O	-5.25	1.17	1.24
1	A	492	ASN	C-O	-5.25	1.17	1.24
1	C	281	LEU	C-O	-5.25	1.17	1.24
1	C	41	ASN	C-O	-5.25	1.17	1.24
1	B	153	THR	C-O	-5.24	1.17	1.23
1	B	317	VAL	C-O	-5.23	1.18	1.24
1	B	207	PHE	C-O	-5.22	1.17	1.24
1	D	473	ARG	C-O	-5.22	1.17	1.23
1	B	142	THR	C-O	-5.22	1.18	1.24
1	A	165	ILE	CA-C	-5.22	1.48	1.52
1	B	106	ALA	C-O	-5.21	1.17	1.24
1	A	27	GLU	C-O	-5.21	1.17	1.23
1	B	95	GLU	C-O	-5.20	1.18	1.24
1	D	484	THR	C-O	-5.20	1.17	1.23
1	D	134	TRP	C-O	-5.20	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	VAL	C-O	-5.20	1.18	1.23
1	B	299	ASN	N-CA	-5.20	1.40	1.46
1	B	30	SER	C-O	-5.19	1.16	1.23
1	A	53	GLU	C-O	-5.18	1.17	1.24
1	C	149	TYR	C-O	-5.18	1.17	1.23
1	B	281	LEU	C-O	-5.17	1.18	1.24
1	B	239	LYS	C-O	-5.16	1.17	1.23
1	D	309	HIS	C-O	-5.15	1.17	1.23
1	A	238	ASP	C-O	-5.15	1.17	1.24
1	D	436	THR	C-O	-5.15	1.17	1.24
1	A	473	ARG	C-O	-5.15	1.17	1.23
1	A	394	VAL	C-O	-5.14	1.18	1.24
1	C	421	SER	C-O	-5.14	1.17	1.23
1	C	299	ASN	N-CA	-5.14	1.40	1.46
1	C	141	GLN	C-O	-5.14	1.17	1.23
1	C	46	ASP	C-O	-5.14	1.17	1.23
1	A	435	LYS	C-O	-5.13	1.18	1.24
1	A	422	SER	C-O	-5.13	1.17	1.24
1	B	238	ASP	C-O	-5.13	1.17	1.24
1	B	9	LYS	CA-C	-5.12	1.47	1.53
1	A	199	SER	C-O	-5.12	1.18	1.24
1	A	142	THR	C-O	-5.12	1.18	1.24
1	A	243	THR	C-O	-5.12	1.18	1.24
1	C	375	LYS	C-O	-5.12	1.17	1.23
1	C	382	THR	C-O	-5.12	1.17	1.24
1	A	89	LYS	C-O	-5.11	1.17	1.24
1	B	384	PHE	C-O	-5.11	1.17	1.23
1	C	20	ILE	C-O	-5.11	1.18	1.24
1	D	328	LYS	C-O	-5.11	1.17	1.23
1	B	378	PHE	C-O	-5.10	1.17	1.23
1	A	280	ASP	C-O	-5.10	1.17	1.23
1	A	420	ASN	C-O	-5.10	1.18	1.23
1	A	419	ASN	C-O	-5.09	1.17	1.24
1	C	213	PRO	C-O	-5.09	1.17	1.23
1	D	299	ASN	C-O	-5.09	1.18	1.23
1	D	171	LEU	C-O	-5.08	1.17	1.24
1	A	474	GLU	C-O	-5.06	1.17	1.23
1	C	273	ASN	C-O	-5.05	1.18	1.24
1	D	273	ASN	C-O	-5.05	1.18	1.24
1	B	150	LEU	C-O	-5.04	1.18	1.24
1	C	380	LYS	C-N	5.04	1.39	1.33
1	A	7	GLU	C-O	-5.03	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	492	ASN	C-O	-5.03	1.18	1.24
1	C	343	VAL	C-O	-5.02	1.18	1.24
1	A	278	ASP	C-O	-5.02	1.17	1.24
1	A	402	VAL	C-O	-5.02	1.18	1.24
1	C	376	GLY	C-O	-5.01	1.17	1.23
1	A	271	SER	CA-C	-5.01	1.47	1.53
1	D	202	TYR	C-O	-5.01	1.18	1.24
1	A	380	LYS	C-N	5.00	1.39	1.33
1	C	47	VAL	C-O	-5.00	1.18	1.24

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	198	LEU	N-CA-C	11.40	124.79	111.11
1	A	188	ILE	N-CA-C	11.13	124.51	108.48
1	A	198	LEU	N-CA-C	10.58	122.81	111.28
1	B	188	ILE	N-CA-C	10.27	123.27	108.48
1	A	168	ASN	N-CA-C	9.80	122.04	111.36
1	C	271	SER	N-CA-C	9.70	120.75	109.60
1	B	271	SER	N-CA-C	9.46	121.66	109.64
1	B	220	VAL	N-CA-C	9.31	117.37	108.15
1	D	198	LEU	N-CA-C	9.07	120.77	111.07
1	C	178	MET	N-CA-C	8.64	120.78	111.36
1	B	198	LEU	N-CA-C	8.63	120.30	111.07
1	C	188	ILE	N-CA-C	8.57	122.84	108.86
1	B	41	ASN	N-CA-C	-8.56	97.34	109.24
1	A	280	ASP	N-CA-C	-8.54	92.96	107.99
1	C	274	ILE	N-CA-C	8.42	120.28	107.99
1	D	188	ILE	N-CA-C	8.21	121.49	108.85
1	D	389	ASP	N-CA-C	8.14	121.07	111.71
1	D	120	ASP	N-CA-C	8.14	119.78	111.07
1	A	158	VAL	CB-CA-C	-8.13	101.39	112.04
1	D	139	ILE	N-CA-C	7.98	121.01	108.89
1	D	343	VAL	N-CA-C	7.80	120.80	111.05
1	A	422	SER	N-CA-C	-7.72	103.86	113.28
1	C	343	VAL	N-CA-C	7.65	120.61	111.05
1	D	280	ASP	N-CA-C	-7.63	96.85	108.67
1	C	158	VAL	CB-CA-C	-7.60	101.88	112.14
1	C	470	GLY	N-CA-C	7.56	122.06	110.88
1	D	274	ILE	N-CA-C	7.50	118.68	107.80
1	B	167	TRP	N-CA-C	7.46	122.38	113.28
1	A	274	ILE	N-CA-C	7.37	118.76	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	342	LEU	N-CA-C	-7.36	100.61	110.55
1	D	271	SER	N-CA-C	7.26	118.86	109.64
1	C	465	GLY	N-CA-C	7.25	124.83	111.12
1	B	170	PRO	N-CA-C	7.19	123.75	113.47
1	D	158	VAL	CB-CA-C	-7.08	100.79	112.26
1	B	158	VAL	CB-CA-C	-6.96	102.92	112.04
1	B	168	ASN	N-CA-C	6.94	120.98	112.23
1	B	342	LEU	N-CA-C	-6.92	101.39	110.53
1	D	141	GLN	N-CA-C	6.87	120.70	109.85
1	A	143	ILE	N-CA-C	6.86	115.55	107.73
1	B	158	VAL	N-CA-CB	6.84	119.02	110.47
1	A	167	TRP	N-CA-C	6.82	121.76	113.38
1	D	337	THR	N-CA-C	6.77	120.19	110.24
1	A	170	PRO	N-CA-C	6.75	124.71	113.78
1	A	6	ILE	N-CA-C	-6.75	99.98	108.89
1	C	150	LEU	N-CA-C	-6.74	97.43	108.41
1	D	167	TRP	N-CA-C	6.71	121.47	113.28
1	A	19	GLU	N-CA-C	-6.70	101.05	110.50
1	B	139	ILE	N-CA-C	6.67	119.66	109.12
1	A	268	GLY	N-CA-C	6.62	122.77	111.98
1	A	362	GLY	N-CA-C	6.59	122.67	114.37
1	A	342	LEU	N-CA-C	-6.58	101.67	110.55
1	D	466	TYR	N-CA-C	-6.52	100.81	110.46
1	C	143	ILE	N-CA-C	6.51	115.16	107.73
1	A	466	TYR	N-CA-C	-6.51	100.32	110.42
1	C	141	GLN	N-CA-C	6.47	120.07	109.85
1	B	466	TYR	N-CA-C	-6.45	101.24	110.59
1	D	196	THR	CA-C-N	-6.44	113.58	120.47
1	D	196	THR	C-N-CA	-6.44	113.58	120.47
1	C	174	SER	N-CA-C	-6.43	104.36	111.82
1	A	137	LYS	N-CA-C	6.40	121.01	112.30
1	A	7	GLU	N-CA-C	6.40	119.56	109.96
1	A	281	LEU	N-CA-C	6.37	118.22	111.28
1	B	187	THR	CB-CA-C	6.33	121.46	109.37
1	C	342	LEU	N-CA-C	-6.30	102.05	110.55
1	D	165	ILE	N-CA-C	6.29	114.83	107.84
1	B	343	VAL	N-CA-C	6.28	121.61	113.07
1	B	281	LEU	N-CA-C	6.26	117.77	111.07
1	A	382	THR	N-CA-C	6.25	119.09	108.90
1	B	382	THR	N-CA-C	6.24	119.58	109.40
1	D	187	THR	CB-CA-C	6.24	121.71	109.35
1	C	335	LYS	N-CA-C	6.24	118.88	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	VAL	N-CA-CB	6.19	118.20	110.47
1	B	280	ASP	CA-C-N	6.16	128.45	120.44
1	B	280	ASP	C-N-CA	6.16	128.45	120.44
1	D	196	THR	N-CA-C	6.16	119.22	108.75
1	B	141	GLN	N-CA-C	6.14	119.65	110.14
1	B	242	PHE	N-CA-C	6.13	119.48	109.06
1	C	170	PRO	N-CA-C	6.12	123.69	113.78
1	A	191	LYS	CA-C-N	-6.08	114.28	120.85
1	A	191	LYS	C-N-CA	-6.08	114.28	120.85
1	A	335	LYS	N-CA-C	6.07	118.86	111.82
1	D	405	VAL	CB-CA-C	6.04	119.83	110.83
1	C	382	THR	N-CA-C	6.00	118.69	108.90
1	A	343	VAL	N-CA-C	6.00	118.55	111.05
1	D	278	ASP	N-CA-C	6.00	119.56	112.72
1	C	139	ILE	N-CA-C	6.00	118.26	108.97
1	A	187	THR	CB-CA-C	5.97	121.10	109.33
1	A	337	THR	N-CA-C	5.95	118.83	109.96
1	C	264	THR	CB-CA-C	5.95	120.46	109.70
1	C	337	THR	N-CA-C	5.94	118.88	109.96
1	C	238	ASP	N-CA-C	5.94	120.26	112.89
1	C	50	VAL	CB-CA-C	5.91	119.79	110.81
1	D	29	VAL	N-CA-C	5.91	117.42	108.80
1	B	354	TYR	N-CA-C	-5.88	104.99	111.82
1	A	465	GLY	N-CA-C	5.87	123.65	112.51
1	B	143	ILE	N-CA-C	5.86	113.87	107.60
1	D	170	PRO	N-CA-C	5.83	123.23	113.78
1	A	47	VAL	N-CA-C	-5.79	101.34	109.21
1	B	238	ASP	N-CA-C	5.78	119.51	112.23
1	B	274	ILE	N-CA-C	5.73	116.19	108.17
1	C	142	THR	N-CA-CB	5.72	119.58	110.65
1	C	187	THR	CB-CA-C	5.70	120.57	109.33
1	A	405	VAL	CB-CA-C	5.69	119.27	110.96
1	B	389	ASP	N-CA-C	5.69	119.48	112.54
1	B	72	SER	N-CA-C	-5.68	101.11	109.18
1	B	405	VAL	N-CA-C	5.67	116.03	107.75
1	C	280	ASP	N-CA-C	-5.64	99.92	108.67
1	A	493	ILE	CA-C-N	5.64	131.85	121.70
1	A	493	ILE	C-N-CA	5.64	131.85	121.70
1	B	335	LYS	N-CA-C	5.58	119.19	112.38
1	B	467	LYS	N-CA-C	5.58	116.79	108.31
1	D	40	TYR	N-CA-C	5.58	118.34	110.14
1	A	142	THR	N-CA-CB	5.56	119.33	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	ALA	N-CA-C	5.55	117.28	108.79
1	C	422	SER	N-CA-C	-5.51	106.40	113.23
1	B	142	THR	N-CA-C	-5.48	99.48	108.41
1	A	406	LEU	N-CA-C	5.48	119.14	108.85
1	A	139	ILE	N-CA-C	5.47	117.46	108.97
1	C	434	ILE	N-CA-C	5.45	116.08	110.36
1	C	378	PHE	N-CA-C	5.42	119.07	109.96
1	C	168	ASN	N-CA-C	5.42	118.10	111.82
1	A	278	ASP	N-CA-C	5.40	118.98	112.93
1	B	280	ASP	N-CA-C	-5.38	98.97	108.23
1	C	9	LYS	N-CA-C	5.36	115.77	109.60
1	B	29	VAL	N-CA-C	5.33	117.75	108.90
1	A	405	VAL	N-CA-C	5.30	115.48	107.80
1	A	139	ILE	CA-C-N	5.29	127.14	122.43
1	A	139	ILE	C-N-CA	5.29	127.14	122.43
1	C	310	ARG	N-CA-C	5.25	117.42	111.11
1	B	11	LYS	N-CA-C	5.25	118.78	112.38
1	A	29	VAL	N-CA-C	5.24	117.60	108.90
1	D	38	GLU	N-CA-C	5.21	117.98	109.59
1	C	243	THR	CB-CA-C	5.20	119.65	109.35
1	B	202	TYR	N-CA-C	-5.16	105.34	111.69
1	D	306	VAL	N-CA-CB	5.16	117.25	111.21
1	A	141	GLN	N-CA-C	5.15	118.14	109.95
1	C	443	LYS	N-CA-C	5.14	118.81	112.54
1	A	271	SER	N-CA-C	5.14	115.89	109.57
1	D	150	LEU	N-CA-C	-5.12	100.17	108.52
1	D	422	SER	N-CA-C	-5.12	106.88	113.23
1	C	42	PRO	N-CA-C	5.11	120.32	114.03
1	A	72	SER	N-CA-C	5.11	116.61	108.79
1	D	236	ASP	N-CA-C	5.11	119.15	113.02
1	C	140	GLY	N-CA-C	-5.08	105.61	112.57
1	B	50	VAL	CB-CA-C	5.08	118.14	110.63
1	A	265	LEU	N-CA-C	5.08	117.72	109.24
1	D	470	GLY	N-CA-C	5.06	117.44	110.56
1	A	212	PHE	CA-C-N	-5.04	114.52	119.92
1	A	212	PHE	C-N-CA	-5.04	114.52	119.92
1	A	237	ILE	CB-CA-C	5.03	117.15	110.91
1	C	220	VAL	N-CA-CB	-5.03	104.17	111.21
1	C	50	VAL	N-CA-C	-5.02	101.25	108.53
1	A	21	LYS	N-CA-C	5.02	117.95	110.52
1	C	137	LYS	N-CA-C	5.02	119.13	112.30
1	C	142	THR	CB-CA-C	5.02	118.49	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	467	LYS	N-CA-C	5.01	115.93	108.31

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	3791	0	3740	74	1
1	B	3776	0	3727	84	0
1	C	3759	0	3710	69	1
1	D	3791	0	3739	70	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	26	0	0	1	0
3	B	23	0	0	0	0
3	C	26	0	0	1	0
3	D	17	0	0	0	0
All	All	15213	0	14916	270	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (270) 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:54:ALA:CB	1:B:220:VAL:HG12	1.73	1.18
1:A:494:LYS:HD3	1:C:439:GLN:HE22	1.10	1.11
1:B:54:ALA:HB2	1:B:220:VAL:HG12	1.42	1.00
1:B:7:GLU:N	1:B:7:GLU:OE2	1.94	0.99
1:B:54:ALA:CB	1:B:220:VAL:CG1	2.40	0.98
1:A:494:LYS:HD3	1:C:439:GLN:NE2	1.81	0.95
1:B:237:ILE:O	1:B:261:LYS:NZ	2.02	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ALA:HB2	1:B:220:VAL:CG1	2.01	0.90
1:A:433:ASN:HB3	1:A:436:THR:HG23	1.57	0.87
1:A:492:ASN:HD22	1:A:494:LYS:H	1.22	0.87
1:C:433:ASN:HB3	1:C:436:THR:HG23	1.56	0.86
1:D:266:GLU:OE1	1:D:464:GLY:HA2	1.78	0.83
1:A:492:ASN:ND2	1:A:494:LYS:H	1.77	0.82
1:B:492:ASN:ND2	1:B:494:LYS:H	1.77	0.82
1:A:9:LYS:HB3	1:A:12:VAL:HG13	1.62	0.81
1:A:433:ASN:HD22	1:A:436:THR:H	1.29	0.79
1:A:166:PRO:HG2	1:A:173:MET:HE3	1.66	0.78
1:A:105:GLU:OE1	1:A:199:SER:OG	2.03	0.77
1:B:66:ALA:HB1	1:B:187:THR:CG2	2.15	0.76
1:B:66:ALA:O	1:B:187:THR:HG21	1.85	0.76
1:D:9:LYS:H	1:D:103:GLN:HE22	1.36	0.74
1:C:188:ILE:HD11	1:C:190:LEU:HB2	1.70	0.73
1:D:66:ALA:HB1	1:D:187:THR:HG23	1.68	0.73
1:D:342:LEU:HD22	1:D:379:VAL:HG13	1.71	0.72
1:D:492:ASN:ND2	1:D:494:LYS:H	1.87	0.72
1:A:66:ALA:O	1:A:187:THR:HG21	1.89	0.71
1:B:364:THR:HG21	1:B:386:ASP:OD2	1.89	0.71
1:C:177:LYS:NZ	1:C:243:THR:HG22	2.06	0.71
1:D:120:ASP:O	1:D:124:THR:HG23	1.89	0.71
1:D:54:ALA:CB	1:D:220:VAL:CG1	2.69	0.70
1:C:66:ALA:O	1:C:187:THR:HG21	1.91	0.70
1:B:364:THR:CG2	1:B:386:ASP:OD2	2.39	0.69
1:C:243:THR:HB	1:C:266:GLU:HB2	1.74	0.69
1:A:492:ASN:HD21	1:A:494:LYS:HA	1.58	0.69
1:B:54:ALA:HB3	1:B:220:VAL:HG12	1.68	0.69
1:B:435:LYS:HG3	1:D:493:ILE:HA	1.75	0.68
1:C:387:VAL:HG11	1:C:404:VAL:HG13	1.75	0.68
1:B:433:ASN:HB3	1:B:436:THR:HG23	1.77	0.67
1:D:124:THR:HG22	1:D:172:VAL:HB	1.76	0.67
1:C:177:LYS:HZ1	1:C:243:THR:HG22	1.60	0.67
1:A:387:VAL:HG13	1:A:394:VAL:HG11	1.77	0.67
1:B:80:THR:CG2	1:B:136:THR:HG22	2.24	0.67
1:B:246:THR:HA	1:B:267:LEU:HD13	1.77	0.67
1:A:462:PRO:HG3	1:A:478:TYR:CD2	2.30	0.66
1:C:448:THR:HG23	3:C:617:HOH:O	1.96	0.66
1:A:9:LYS:H	1:A:103:GLN:HE22	1.45	0.64
1:C:59:ILE:CD1	1:C:220:VAL:HG11	2.27	0.64
1:D:188:ILE:CD1	1:D:190:LEU:HB2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:GLN:OE1	1:C:188:ILE:HD13	1.98	0.64
1:C:188:ILE:CD1	1:C:190:LEU:HB2	2.27	0.64
1:B:80:THR:HG23	1:B:136:THR:HG22	1.80	0.63
1:B:387:VAL:HG11	1:B:404:VAL:CG1	2.29	0.63
1:A:120:ASP:O	1:A:124:THR:HG23	1.99	0.63
1:B:37:PHE:HD2	1:B:53:GLU:HG3	1.64	0.63
1:B:107:LEU:HD13	1:B:333:MET:HG3	1.79	0.63
1:B:54:ALA:HB1	1:B:220:VAL:CG1	2.27	0.62
1:B:493:ILE:O	1:B:494:LYS:HB2	1.99	0.62
1:D:107:LEU:HD13	1:D:333:MET:HG3	1.80	0.62
1:B:492:ASN:C	1:B:492:ASN:HD22	2.07	0.62
1:D:54:ALA:CB	1:D:220:VAL:HG12	2.30	0.62
1:D:66:ALA:O	1:D:187:THR:HG21	2.00	0.62
1:B:433:ASN:HD22	1:B:436:THR:H	1.48	0.61
1:D:22:MET:HE1	1:D:220:VAL:HG13	1.83	0.61
1:D:492:ASN:C	1:D:492:ASN:HD22	2.08	0.60
1:D:243:THR:HG23	1:D:266:GLU:HB3	1.83	0.60
1:A:435:LYS:HG2	1:C:493:ILE:HA	1.84	0.60
1:C:59:ILE:HD13	1:C:220:VAL:HG11	1.83	0.60
1:A:112:PRO:HB2	1:A:115:VAL:HG13	1.84	0.60
1:D:342:LEU:HD22	1:D:379:VAL:CG1	2.31	0.59
1:B:493:ILE:HA	1:D:435:LYS:HG3	1.84	0.59
1:D:177:LYS:NZ	1:D:243:THR:OG1	2.34	0.59
1:D:433:ASN:HD22	1:D:436:THR:H	1.50	0.59
1:D:127:ASN:OD1	1:D:459:ALA:HB2	2.03	0.59
1:C:387:VAL:HG23	1:C:391:MET:SD	2.43	0.58
1:D:66:ALA:HB1	1:D:187:THR:CG2	2.33	0.58
1:B:177:LYS:NZ	1:B:474:GLU:OE1	2.35	0.58
1:C:66:ALA:HB1	1:C:187:THR:CG2	2.34	0.58
1:A:492:ASN:ND2	1:A:494:LYS:N	2.50	0.58
1:C:264:THR:HG21	1:C:482:ASN:CG	2.28	0.58
1:C:308:VAL:HG11	1:C:316:VAL:CG1	2.34	0.58
1:C:27:GLU:OE2	1:C:27:GLU:HA	2.04	0.57
1:A:75:TRP:CH2	1:A:83:ARG:HD2	2.39	0.57
1:C:243:THR:HA	1:C:266:GLU:O	2.04	0.57
1:B:37:PHE:CD2	1:B:53:GLU:HG3	2.40	0.57
1:A:22:MET:HG2	1:A:221:PRO:HD2	1.87	0.57
1:B:22:MET:HE3	1:B:24:ILE:HD11	1.87	0.56
1:C:264:THR:HG21	1:C:482:ASN:ND2	2.20	0.56
1:C:387:VAL:HG22	1:C:394:VAL:HG11	1.87	0.56
1:B:435:LYS:NZ	1:D:492:ASN:ND2	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LEU:HD12	1:A:200:LEU:HD21	1.87	0.55
1:B:70:PHE:CE1	1:B:159:GLY:HA2	2.42	0.55
1:D:394:VAL:HB	1:D:404:VAL:HG11	1.89	0.55
1:A:339:MET:HE1	1:A:401:PRO:HG3	1.89	0.55
1:C:26:GLY:HA3	1:C:214:ASN:ND2	2.22	0.55
1:C:447:GLY:HA3	1:C:464:GLY:O	2.07	0.55
1:A:466:TYR:CE1	1:D:485:GLU:HG3	2.42	0.54
1:A:243:THR:HG23	1:A:266:GLU:HB2	1.90	0.54
1:A:433:ASN:ND2	1:A:436:THR:H	2.03	0.54
1:C:188:ILE:HD11	1:C:190:LEU:CB	2.36	0.54
1:A:66:ALA:HB1	1:A:187:THR:CG2	2.38	0.54
1:B:239:LYS:NZ	1:B:262:HIS:HD2	2.06	0.54
1:B:80:THR:HG23	1:B:136:THR:CG2	2.37	0.53
1:B:67:ARG:O	1:B:71:GLU:HG3	2.07	0.53
1:A:107:LEU:HD13	1:A:333:MET:HG3	1.88	0.53
1:B:22:MET:HG2	1:B:221:PRO:HD2	1.90	0.53
1:D:217:VAL:HG13	1:D:219:PHE:CZ	2.44	0.53
1:B:266:GLU:OE2	1:B:474:GLU:HG3	2.09	0.53
1:B:66:ALA:HB1	1:B:187:THR:HG23	1.90	0.53
1:D:4:THR:HB	1:D:335:LYS:HD3	1.91	0.52
1:B:387:VAL:HG13	1:B:394:VAL:HG11	1.90	0.52
1:C:387:VAL:HG22	1:C:394:VAL:CG1	2.39	0.52
1:A:191:LYS:HG2	1:A:220:VAL:O	2.10	0.52
1:C:112:PRO:HB2	1:C:115:VAL:HG13	1.92	0.52
1:C:66:ALA:HB1	1:C:187:THR:HG23	1.92	0.51
1:A:493:ILE:HA	1:C:435:LYS:HG3	1.92	0.51
1:B:387:VAL:HG21	1:B:404:VAL:HG13	1.91	0.51
1:C:389:ASP:HA	1:C:394:VAL:HG21	1.91	0.51
1:B:166:PRO:HD2	1:B:173:MET:HG2	1.93	0.51
1:B:356:GLU:OE1	1:B:359:LYS:NZ	2.44	0.51
1:B:492:ASN:HD22	1:B:494:LYS:H	1.56	0.51
1:D:9:LYS:HB3	1:D:12:VAL:HG13	1.91	0.51
1:D:22:MET:HE2	1:D:24:ILE:HD11	1.91	0.51
1:A:462:PRO:HG3	1:A:478:TYR:CE2	2.45	0.51
1:D:200:LEU:O	1:D:200:LEU:HG	2.10	0.50
1:D:364:THR:CG2	1:D:386:ASP:OD2	2.60	0.50
1:A:130:TYR:O	1:C:137:LYS:NZ	2.38	0.50
1:A:492:ASN:HD22	1:A:492:ASN:C	2.19	0.50
1:D:54:ALA:CB	1:D:220:VAL:HG13	2.42	0.50
1:A:339:MET:CE	1:A:401:PRO:HG3	2.42	0.49
1:B:260:ILE:O	1:B:260:ILE:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLN:O	1:A:107:LEU:HB2	2.11	0.49
1:C:308:VAL:HG11	1:C:316:VAL:HG13	1.94	0.49
1:B:152:TYR:OH	1:C:438:HIS:HD2	1.96	0.49
1:C:107:LEU:HD13	1:C:333:MET:HG3	1.95	0.49
1:D:54:ALA:HB1	1:D:220:VAL:CG1	2.41	0.49
1:D:464:GLY:HA3	1:D:473:ARG:HD3	1.94	0.49
1:D:492:ASN:HD22	1:D:494:LYS:H	1.59	0.49
1:B:66:ALA:HB1	1:B:187:THR:HG22	1.95	0.49
1:D:433:ASN:ND2	1:D:436:THR:HG23	2.28	0.49
1:B:9:LYS:CB	1:B:12:VAL:HG13	2.43	0.48
1:B:435:LYS:HZ3	1:D:492:ASN:ND2	2.11	0.48
1:B:22:MET:CE	1:B:24:ILE:HD11	2.42	0.48
1:C:433:ASN:HD22	1:C:436:THR:H	1.61	0.48
1:B:239:LYS:HZ2	1:B:262:HIS:HD2	1.61	0.48
1:D:59:ILE:HD12	1:D:231:ILE:HG13	1.95	0.48
1:A:166:PRO:CG	1:A:173:MET:HE3	2.42	0.48
1:B:54:ALA:HB1	1:B:220:VAL:HG11	1.96	0.48
1:D:20:ILE:HB	1:D:51:VAL:HG13	1.96	0.48
1:C:21:LYS:HG2	1:C:29:VAL:C	2.38	0.48
1:B:66:ALA:C	1:B:187:THR:HG21	2.38	0.47
1:C:21:LYS:HG2	1:C:29:VAL:O	2.14	0.47
1:B:9:LYS:HB2	1:B:12:VAL:HG13	1.96	0.47
1:B:169:PHE:O	1:B:173:MET:HB2	2.15	0.47
1:C:296:HIS:N	1:C:296:HIS:CD2	2.82	0.47
1:A:349:GLU:O	1:A:353:ASN:HB2	2.14	0.47
1:A:438:HIS:HD2	1:D:152:TYR:OH	1.98	0.47
1:B:48:LEU:HD13	1:B:198:LEU:CD1	2.45	0.47
1:C:220:VAL:O	1:C:220:VAL:HG13	2.14	0.47
1:C:9:LYS:H	1:C:103:GLN:HE22	1.62	0.47
1:A:88:TYR:CD2	1:A:132:ALA:HB1	2.50	0.47
1:A:296:HIS:N	1:A:296:HIS:CD2	2.83	0.47
1:B:464:GLY:HA3	1:B:473:ARG:HD3	1.97	0.47
1:C:292:ILE:HG21	1:C:403:VAL:HB	1.96	0.47
1:B:120:ASP:O	1:B:124:THR:HG23	2.14	0.46
1:B:124:THR:HG22	1:B:172:VAL:HA	1.97	0.46
1:B:134:TRP:CD1	1:D:137:LYS:HE3	2.51	0.46
1:A:438:HIS:CE1	1:B:438:HIS:HE1	2.33	0.46
1:D:201:LEU:HD11	1:D:221:PRO:HG3	1.97	0.46
1:D:22:MET:CE	1:D:220:VAL:HG13	2.44	0.46
1:A:364:THR:HG23	1:A:386:ASP:HB2	1.96	0.46
1:A:120:ASP:O	1:A:124:THR:CG2	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:THR:HG21	1:D:386:ASP:OD2	2.16	0.46
1:C:308:VAL:HG11	1:C:316:VAL:HG11	1.98	0.46
1:A:444:LEU:O	1:D:487:LYS:NZ	2.44	0.46
1:B:458:ASN:O	1:B:459:ALA:C	2.58	0.45
1:C:48:LEU:HD11	1:C:107:LEU:HB3	1.97	0.45
1:B:133:GLY:O	1:B:137:LYS:HD2	2.16	0.45
1:C:178:MET:HE2	1:C:190:LEU:CD2	2.45	0.45
1:A:394:VAL:HB	1:A:404:VAL:HG11	1.98	0.45
1:D:54:ALA:HB3	1:D:220:VAL:HG12	1.99	0.45
1:D:306:VAL:HG12	1:D:403:VAL:CG2	2.46	0.45
1:A:85:HIS:CE1	1:A:89:LYS:HD2	2.52	0.45
1:A:492:ASN:ND2	1:A:494:LYS:HA	2.30	0.45
1:D:112:PRO:HB2	1:D:115:VAL:HG13	1.99	0.45
1:A:492:ASN:O	1:C:435:LYS:HD2	2.16	0.45
1:D:339:MET:HE1	1:D:401:PRO:HG3	1.97	0.45
1:A:22:MET:HE3	1:A:220:VAL:HG12	1.98	0.45
1:D:239:LYS:HD2	1:D:482:ASN:O	2.16	0.45
1:A:160:VAL:HG22	1:A:187:THR:HG22	1.99	0.45
1:A:190:LEU:HD12	1:A:200:LEU:CD2	2.46	0.45
1:C:387:VAL:CG2	1:C:394:VAL:CG1	2.95	0.45
1:B:190:LEU:HD13	1:B:191:LYS:N	2.33	0.44
1:D:120:ASP:O	1:D:124:THR:CG2	2.64	0.44
1:D:21:LYS:HG2	1:D:29:VAL:C	2.42	0.44
1:D:84:ALA:HB2	1:D:135:THR:OG1	2.16	0.44
1:C:66:ALA:C	1:C:187:THR:HG21	2.43	0.44
1:B:138:ILE:HG22	1:B:138:ILE:O	2.16	0.44
1:B:372:ALA:HB2	1:B:380:LYS:HG3	1.98	0.44
1:C:133:GLY:O	1:C:137:LYS:HD2	2.17	0.44
1:C:230:ALA:O	1:C:234:HIS:HB2	2.18	0.44
1:A:66:ALA:C	1:A:187:THR:HG21	2.42	0.44
1:A:269:GLY:HA2	1:A:423:TYR:CG	2.53	0.44
1:B:391:MET:HB2	1:B:394:VAL:HG13	1.99	0.44
1:B:296:HIS:CD2	1:B:296:HIS:N	2.85	0.44
1:A:140:GLY:HA3	1:B:142:THR:OG1	2.17	0.44
1:C:433:ASN:HD22	1:C:436:THR:CG2	2.31	0.44
1:A:438:HIS:HE1	1:B:438:HIS:HE1	1.64	0.43
1:D:296:HIS:N	1:D:296:HIS:CD2	2.87	0.43
1:C:134:TRP:O	1:C:138:ILE:HG13	2.18	0.43
1:C:296:HIS:CD2	1:C:339:MET:HG3	2.54	0.43
1:C:434:ILE:HA	1:D:434:ILE:HB	2.00	0.43
1:A:391:MET:HB2	1:A:394:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ASN:HD21	1:A:494:LYS:CA	2.28	0.43
1:D:153:THR:HA	1:D:487:LYS:O	2.19	0.43
1:A:466:TYR:CZ	1:D:485:GLU:HG3	2.54	0.43
1:A:43:ALA:HB2	3:A:609:HOH:O	2.18	0.43
1:B:308:VAL:HG21	1:B:316:VAL:CG2	2.48	0.43
1:C:433:ASN:ND2	1:C:436:THR:CG2	2.82	0.43
1:B:269:GLY:HA2	1:B:423:TYR:HB3	2.01	0.43
1:B:466:TYR:CE1	1:C:485:GLU:HG3	2.53	0.43
1:C:438:HIS:HE1	1:D:438:HIS:HE1	1.67	0.43
1:A:269:GLY:HA2	1:A:423:TYR:CD1	2.54	0.42
1:C:342:LEU:HB2	1:C:377:TYR:O	2.19	0.42
1:A:364:THR:HG23	1:A:386:ASP:OD2	2.18	0.42
1:B:217:VAL:HG13	1:B:219:PHE:CZ	2.54	0.42
1:B:7:GLU:N	1:B:7:GLU:CD	2.72	0.42
1:A:134:TRP:CD1	1:C:137:LYS:HE2	2.54	0.42
1:A:201:LEU:HD11	1:A:221:PRO:HG3	2.02	0.42
1:A:364:THR:CG2	1:A:386:ASP:OD2	2.68	0.42
1:B:327:VAL:CG1	1:B:381:PRO:HG2	2.49	0.42
1:B:153:THR:HA	1:B:487:LYS:O	2.20	0.42
1:C:48:LEU:HD13	1:C:198:LEU:CD1	2.50	0.42
1:C:263:VAL:HG12	1:C:265:LEU:HG	2.02	0.42
1:D:263:VAL:HG12	1:D:265:LEU:HG	2.01	0.42
1:D:372:ALA:HB2	1:D:380:LYS:HG3	2.01	0.42
1:B:134:TRP:NE1	1:D:137:LYS:HE3	2.34	0.41
1:A:435:LYS:CG	1:C:493:ILE:HA	2.49	0.41
1:D:166:PRO:HD2	1:D:173:MET:SD	2.61	0.41
1:D:232:VAL:HG21	1:D:252:ILE:HG12	2.02	0.41
1:D:492:ASN:ND2	1:D:494:LYS:N	2.64	0.41
1:A:163:GLN:HB2	1:A:190:LEU:HD23	2.03	0.41
1:C:342:LEU:HD22	1:C:379:VAL:HG23	2.02	0.41
1:D:54:ALA:HB2	1:D:220:VAL:HG13	2.01	0.41
1:A:163:GLN:CD	1:A:177:LYS:HB3	2.45	0.41
1:A:166:PRO:HD3	1:A:243:THR:O	2.20	0.41
1:D:492:ASN:ND2	1:D:492:ASN:C	2.72	0.41
1:A:107:LEU:HD13	1:A:333:MET:CG	2.51	0.41
1:C:87:ILE:HG22	1:C:132:ALA:HB2	2.03	0.41
1:C:464:GLY:HA3	1:C:473:ARG:HD3	2.03	0.41
1:A:144:PRO:HG2	1:A:144:PRO:O	2.21	0.41
1:A:146:SER:HB2	1:B:79:THR:HG22	2.03	0.41
1:B:387:VAL:HG11	1:B:404:VAL:HG13	2.03	0.41
1:D:260:ILE:O	1:D:260:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:MET:HG2	1:A:82:GLU:CB	2.52	0.40
1:A:271:SER:HB3	1:A:426:ALA:O	2.22	0.40
1:B:167:TRP:CE3	1:B:343:VAL:HG11	2.56	0.40
1:B:364:THR:HG23	1:B:385:THR:HG22	2.02	0.40
1:C:220:VAL:O	1:C:220:VAL:CG1	2.68	0.40
1:D:202:TYR:CD1	1:D:202:TYR:C	2.99	0.40
1:A:169:PHE:O	1:A:173:MET:HB2	2.20	0.40
1:B:492:ASN:ND2	1:D:435:LYS:NZ	2.70	0.40
1:C:48:LEU:HD13	1:C:198:LEU:HD12	2.03	0.40
1:A:115:VAL:O	1:A:119:ASP:HB2	2.21	0.40
1:B:78:MET:HG3	1:B:82:GLU:HB2	2.03	0.40
1:B:167:TRP:CD2	1:B:343:VAL:HG11	2.57	0.40
1:B:230:ALA:O	1:B:234:HIS:HB2	2.21	0.40
1:C:347:GLN:O	1:C:351:VAL:HG13	2.21	0.40
1:D:169:PHE:HB3	1:D:172:VAL:HG13	2.02	0.40
1:B:107:LEU:HD13	1:B:333:MET:CG	2.50	0.40
1:C:433:ASN:ND2	1:C:436:THR:HG22	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:OE1	1:C:35:LYS:NZ[1_655]	2.13	0.07

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	489/508 (96%)	473 (97%)	15 (3%)	1 (0%)	43	66
1	B	487/508 (96%)	466 (96%)	20 (4%)	1 (0%)	43	66
1	C	485/508 (96%)	473 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	489/508 (96%)	467 (96%)	21 (4%)	1 (0%)	43	66
All	All	1950/2032 (96%)	1879 (96%)	68 (4%)	3 (0%)	43	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	78	MET
1	A	424	GLY
1	B	166	PRO

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	398/414 (96%)	347 (87%)	51 (13%)	4	8
1	B	396/414 (96%)	333 (84%)	63 (16%)	2	4
1	C	394/414 (95%)	344 (87%)	50 (13%)	4	9
1	D	398/414 (96%)	341 (86%)	57 (14%)	3	6
All	All	1586/1656 (96%)	1365 (86%)	221 (14%)	3	7

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	12	VAL
1	A	48	LEU
1	A	57	GLU
1	A	60	ASP
1	A	77	GLU
1	A	89	LYS
1	A	104	LEU
1	A	105	GLU
1	A	107	LEU
1	A	115	VAL

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Mol	Chain	Res	Type
1	A	124	THR
1	A	144	PRO
1	A	146	SER
1	A	158	VAL
1	A	161	VAL
1	A	171	LEU
1	A	172	VAL
1	A	187	THR
1	A	191	LYS
1	A	208	LYS
1	A	217	VAL
1	A	220	VAL
1	A	248	THR
1	A	283	GLU
1	A	296	HIS
1	A	301	SER
1	A	311	LYS
1	A	322	LYS
1	A	329	LEU
1	A	336	GLU
1	A	343	VAL
1	A	351	VAL
1	A	353	ASN
1	A	364	THR
1	A	365	VAL
1	A	371	ARG
1	A	375	LYS
1	A	387	VAL
1	A	394	VAL
1	A	404	VAL
1	A	405	VAL
1	A	412	GLU
1	A	436	THR
1	A	443	LYS
1	A	445	LYS
1	A	457	GLU
1	A	484	THR
1	A	487	LYS
1	A	492	ASN
1	A	494	LYS
1	B	7	GLU
1	B	9	LYS

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Mol	Chain	Res	Type
1	B	12	VAL
1	B	13	GLU
1	B	17	ASN
1	B	48	LEU
1	B	50	VAL
1	B	57	GLU
1	B	71	GLU
1	B	80	THR
1	B	104	LEU
1	B	107	LEU
1	B	109	ASN
1	B	115	VAL
1	B	124	THR
1	B	135	THR
1	B	158	VAL
1	B	161	VAL
1	B	171	LEU
1	B	172	VAL
1	B	173	MET
1	B	187	THR
1	B	188	ILE
1	B	190	LEU
1	B	199	SER
1	B	200	LEU
1	B	205	LYS
1	B	217	VAL
1	B	220	VAL
1	B	232	VAL
1	B	239	LYS
1	B	282	GLU
1	B	283	GLU
1	B	290	GLN
1	B	296	HIS
1	B	316	VAL
1	B	327	VAL
1	B	328	LYS
1	B	329	LEU
1	B	336	GLU
1	B	342	LEU
1	B	351	VAL
1	B	364	THR
1	B	371	ARG

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Mol	Chain	Res	Type
1	B	375	LYS
1	B	385	THR
1	B	387	VAL
1	B	388	THR
1	B	390	ASP
1	B	394	VAL
1	B	395	LYS
1	B	399	PHE
1	B	405	VAL
1	B	406	LEU
1	B	416	GLU
1	B	429	VAL
1	B	435	LYS
1	B	436	THR
1	B	443	LYS
1	B	445	LYS
1	B	469	SER
1	B	484	THR
1	B	492	ASN
1	C	8	LEU
1	C	9	LYS
1	C	12	VAL
1	C	21	LYS
1	C	48	LEU
1	C	50	VAL
1	C	96	GLU
1	C	104	LEU
1	C	105	GLU
1	C	107	LEU
1	C	115	VAL
1	C	135	THR
1	C	147	LYS
1	C	158	VAL
1	C	171	LEU
1	C	172	VAL
1	C	173	MET
1	C	187	THR
1	C	188	ILE
1	C	194	GLU
1	C	205	LYS
1	C	208	LYS
1	C	217	VAL

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Mol	Chain	Res	Type
1	C	220	VAL
1	C	232	VAL
1	C	243	THR
1	C	290	GLN
1	C	296	HIS
1	C	311	LYS
1	C	316	VAL
1	C	342	LEU
1	C	343	VAL
1	C	345	LYS
1	C	350	ARG
1	C	351	VAL
1	C	360	LYS
1	C	364	THR
1	C	365	VAL
1	C	371	ARG
1	C	375	LYS
1	C	394	VAL
1	C	404	VAL
1	C	414	VAL
1	C	422	SER
1	C	435	LYS
1	C	436	THR
1	C	443	LYS
1	C	448	THR
1	C	484	THR
1	C	492	ASN
1	D	4	THR
1	D	8	LEU
1	D	9	LYS
1	D	12	VAL
1	D	18	GLU
1	D	27	GLU
1	D	48	LEU
1	D	50	VAL
1	D	51	VAL
1	D	57	GLU
1	D	77	GLU
1	D	104	LEU
1	D	105	GLU
1	D	107	LEU
1	D	115	VAL

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Mol	Chain	Res	Type
1	D	124	THR
1	D	143	ILE
1	D	158	VAL
1	D	171	LEU
1	D	172	VAL
1	D	187	THR
1	D	188	ILE
1	D	190	LEU
1	D	199	SER
1	D	205	LYS
1	D	208	LYS
1	D	217	VAL
1	D	232	VAL
1	D	239	LYS
1	D	282	GLU
1	D	283	GLU
1	D	296	HIS
1	D	306	VAL
1	D	308	VAL
1	D	311	LYS
1	D	314	GLU
1	D	316	VAL
1	D	326	ASN
1	D	327	VAL
1	D	335	LYS
1	D	342	LEU
1	D	343	VAL
1	D	351	VAL
1	D	360	LYS
1	D	364	THR
1	D	371	ARG
1	D	375	LYS
1	D	379	VAL
1	D	394	VAL
1	D	404	VAL
1	D	405	VAL
1	D	429	VAL
1	D	435	LYS
1	D	436	THR
1	D	443	LYS
1	D	484	THR
1	D	492	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	85	HIS
1	A	103	GLN
1	A	114	GLN
1	A	214	ASN
1	A	262	HIS
1	A	325	ASN
1	A	326	ASN
1	A	357	GLN
1	A	432	GLN
1	A	433	ASN
1	A	438	HIS
1	A	442	ASN
1	A	468	GLN
1	A	482	ASN
1	A	492	ASN
1	B	85	HIS
1	B	114	GLN
1	B	141	GLN
1	B	235	HIS
1	B	262	HIS
1	B	298	GLN
1	B	299	ASN
1	B	312	HIS
1	B	325	ASN
1	B	326	ASN
1	B	432	GLN
1	B	433	ASN
1	B	438	HIS
1	B	492	ASN
1	C	85	HIS
1	C	103	GLN
1	C	114	GLN
1	C	214	ASN
1	C	233	ASN
1	C	255	GLN
1	C	262	HIS
1	C	290	GLN
1	C	326	ASN
1	C	432	GLN
1	C	433	ASN

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Mol	Chain	Res	Type
1	C	438	HIS
1	C	439	GLN
1	C	482	ASN
1	C	492	ASN
1	D	103	GLN
1	D	114	GLN
1	D	151	ASN
1	D	214	ASN
1	D	233	ASN
1	D	255	GLN
1	D	262	HIS
1	D	325	ASN
1	D	347	GLN
1	D	432	GLN
1	D	433	ASN
1	D	438	HIS
1	D	492	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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	491/508 (96%)	-0.29	2 (0%) 88 86	11, 18, 34, 46	0
1	B	489/508 (96%)	-0.26	2 (0%) 88 86	10, 19, 33, 63	0
1	C	487/508 (95%)	-0.26	5 (1%) 79 76	10, 19, 33, 46	0
1	D	491/508 (96%)	-0.19	5 (1%) 79 76	11, 21, 36, 57	0
All	All	1958/2032 (96%)	-0.25	14 (0%) 84 82	10, 19, 34, 63	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	GLU	3.6
1	A	88	TYR	3.6
1	D	4	THR	3.5
1	B	494	LYS	3.3
1	D	7	GLU	2.9
1	A	4	THR	2.9
1	D	247	VAL	2.6
1	D	412	GLU	2.5
1	D	494	LYS	2.3
1	C	390	ASP	2.2
1	C	412	GLU	2.2
1	C	60	ASP	2.1
1	C	335	LYS	2.1
1	C	223	PHE	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	D	501	1/1	0.85	0.08	20,20,20,20	0
2	NA	B	501	1/1	0.87	0.15	19,19,19,19	0
2	NA	A	501	1/1	0.87	0.09	16,16,16,16	0
2	NA	C	501	1/1	0.94	0.07	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.