



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:17 AM UTC

PDB ID : 4CUJ / pdb_00004cuJ
Title : Structure of Salmonella D-Lactate Dehydrogenase
Authors : Attarataya, J.; Zaccai, N.R.; Shoemark, D.K.; Brady, R.L.
Deposited on : 2014-03-19
Resolution : 1.88 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

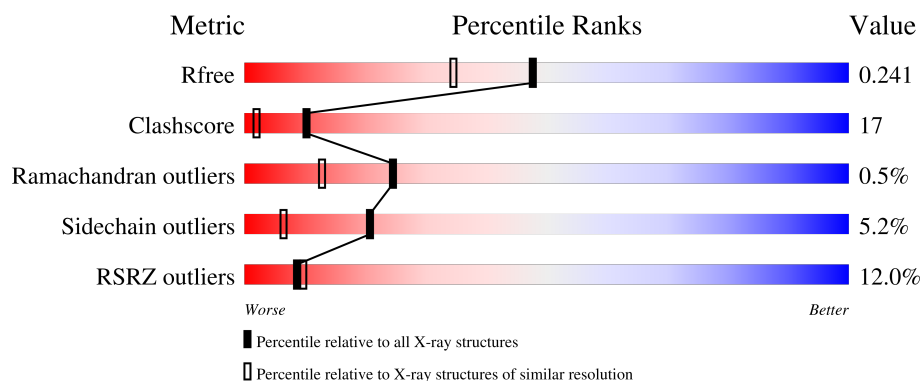
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	338	 6% 54% 39% . . .
1	B	338	 9% 59% 33% . . .
1	C	338	 7% 59% 33% 5% . . .
1	D	338	 24% 48% 37% 10% . . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10915 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 D-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2567	1630	438	484	15			
1	B	330	Total	C	N	O	S	0	0	0
			2567	1630	438	484	15			
1	C	329	Total	C	N	O	S	0	0	0
			2558	1624	436	483	15			
1	D	329	Total	C	N	O	S	0	0	0
			2558	1624	436	483	15			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	330	LYS	-	expression tag	UNP Q8Z780
A	331	SER	-	expression tag	UNP Q8Z780
A	332	SER	-	expression tag	UNP Q8Z780
A	333	HIS	-	expression tag	UNP Q8Z780
A	334	HIS	-	expression tag	UNP Q8Z780
A	335	HIS	-	expression tag	UNP Q8Z780
A	336	HIS	-	expression tag	UNP Q8Z780
A	337	HIS	-	expression tag	UNP Q8Z780
A	338	HIS	-	expression tag	UNP Q8Z780
A	273	VAL	ASN	conflict	UNP Q8Z780
B	330	LYS	-	expression tag	UNP Q8Z780
B	331	SER	-	expression tag	UNP Q8Z780
B	332	SER	-	expression tag	UNP Q8Z780
B	333	HIS	-	expression tag	UNP Q8Z780
B	334	HIS	-	expression tag	UNP Q8Z780
B	335	HIS	-	expression tag	UNP Q8Z780
B	336	HIS	-	expression tag	UNP Q8Z780
B	337	HIS	-	expression tag	UNP Q8Z780
B	338	HIS	-	expression tag	UNP Q8Z780
B	273	VAL	ASN	conflict	UNP Q8Z780
C	330	LYS	-	expression tag	UNP Q8Z780

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Chain	Residue	Modelled	Actual	Comment	Reference
C	331	SER	-	expression tag	UNP Q8Z780
C	332	SER	-	expression tag	UNP Q8Z780
C	333	HIS	-	expression tag	UNP Q8Z780
C	334	HIS	-	expression tag	UNP Q8Z780
C	335	HIS	-	expression tag	UNP Q8Z780
C	336	HIS	-	expression tag	UNP Q8Z780
C	337	HIS	-	expression tag	UNP Q8Z780
C	338	HIS	-	expression tag	UNP Q8Z780
C	273	VAL	ASN	conflict	UNP Q8Z780
D	330	LYS	-	expression tag	UNP Q8Z780
D	331	SER	-	expression tag	UNP Q8Z780
D	332	SER	-	expression tag	UNP Q8Z780
D	333	HIS	-	expression tag	UNP Q8Z780
D	334	HIS	-	expression tag	UNP Q8Z780
D	335	HIS	-	expression tag	UNP Q8Z780
D	336	HIS	-	expression tag	UNP Q8Z780
D	337	HIS	-	expression tag	UNP Q8Z780
D	338	HIS	-	expression tag	UNP Q8Z780
D	273	VAL	ASN	conflict	UNP Q8Z780

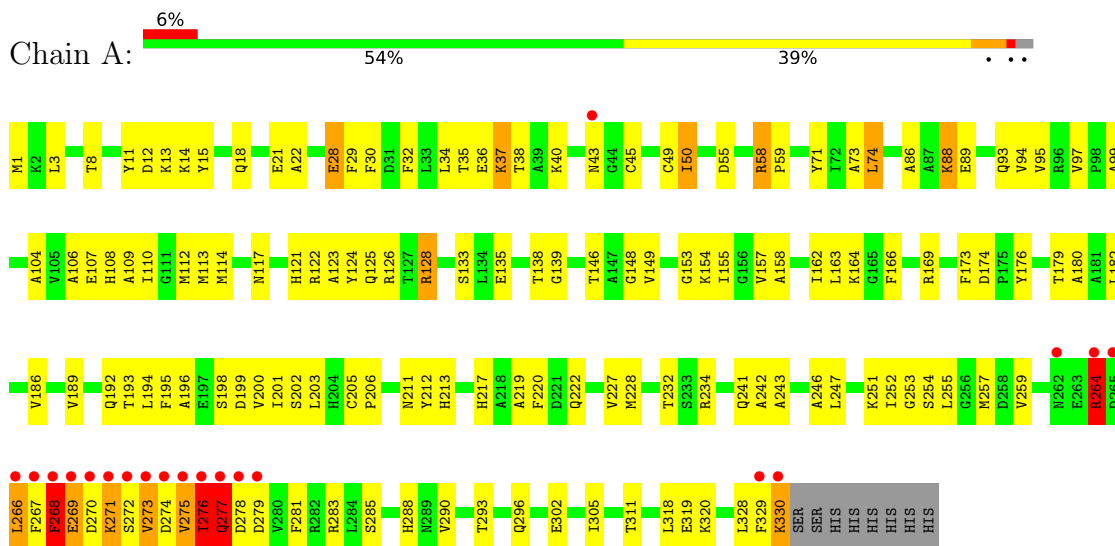
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	216	Total O 216 216	0	0
2	B	164	Total O 164 164	0	0
2	C	148	Total O 148 148	0	0
2	D	137	Total O 137 137	0	0

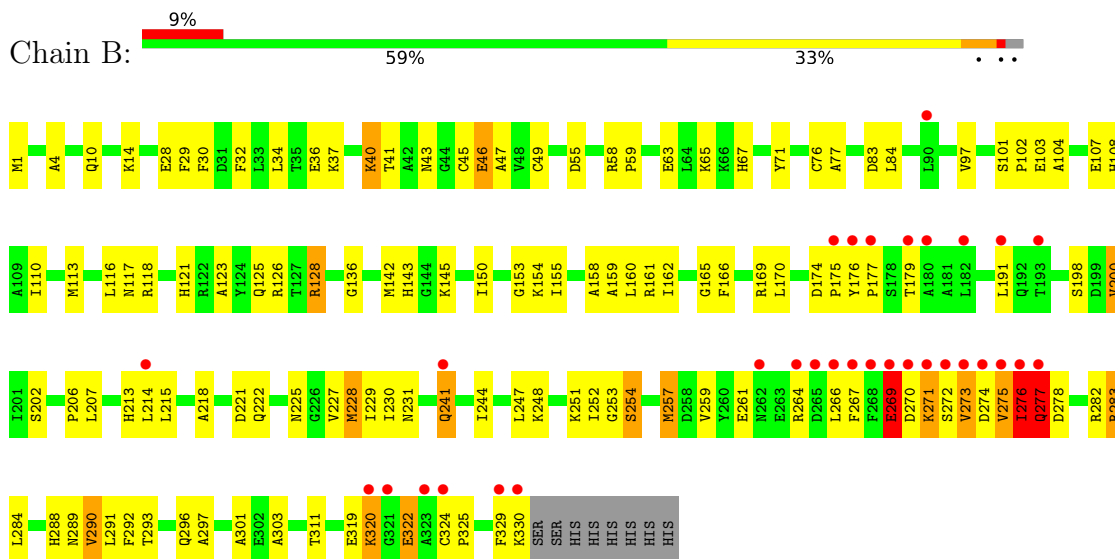
3 Residue-property plots

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: D-LACTATE DEHYDROGENASE

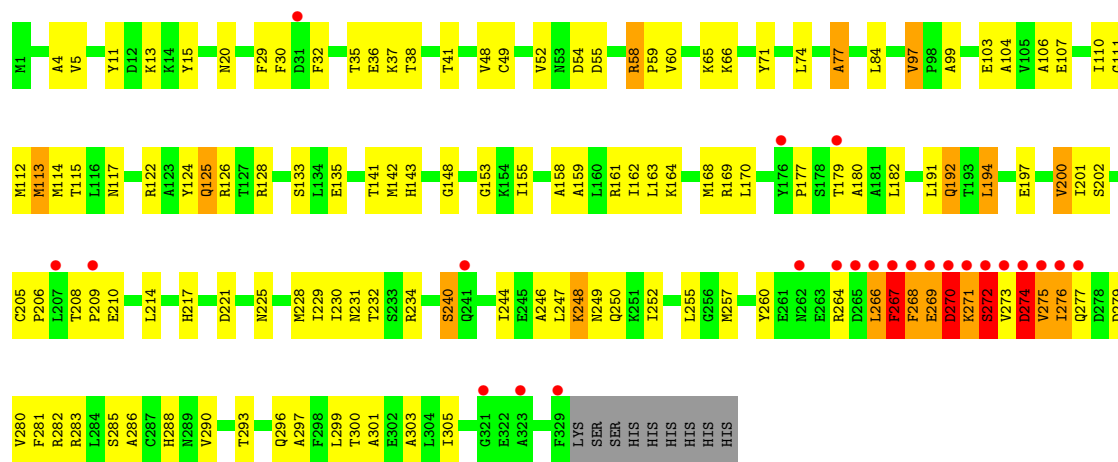


• Molecule 1: D-LACTATE DEHYDROGENASE

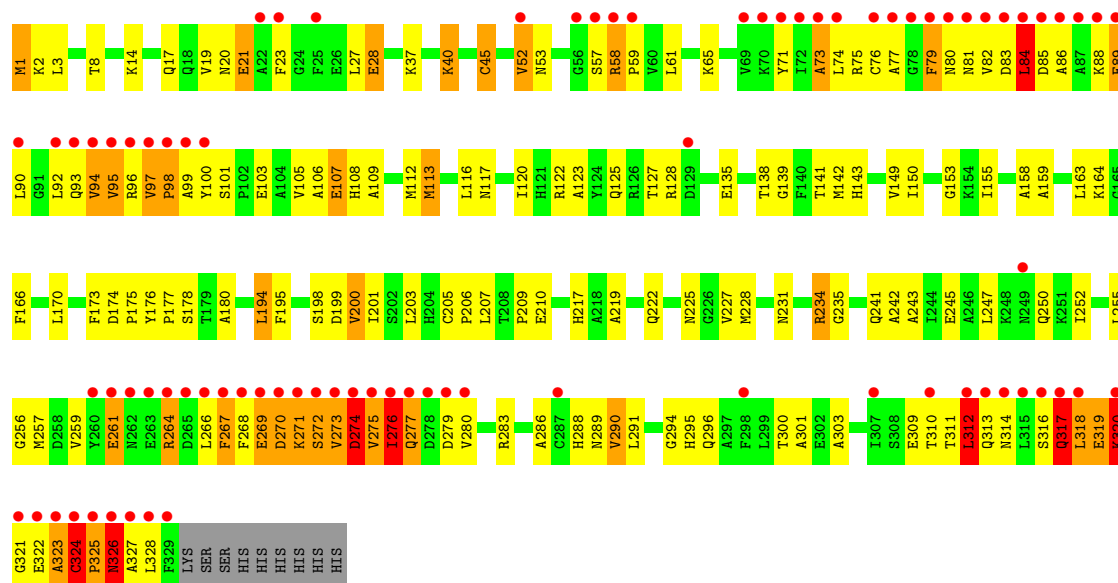


• Molecule 1: D-LACTATE DEHYDROGENASE





● Molecule 1: D-LACTATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.68Å 137.21Å 145.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.79 – 1.88 72.79 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.9 (72.79-1.88) 99.9 (72.79-1.88)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.191 , 0.233 0.208 , 0.241	Depositor DCC
R_{free} test set	6158 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10915	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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	2.04	113/2612 (4.3%)	1.10	10/3527 (0.3%)
1	B	1.94	84/2612 (3.2%)	1.13	12/3527 (0.3%)
1	C	1.98	95/2603 (3.6%)	1.13	12/3516 (0.3%)
1	D	1.93	85/2603 (3.3%)	1.32	31/3516 (0.9%)
All	All	1.97	377/10430 (3.6%)	1.17	65/14086 (0.5%)

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	3
1	B	0	2
1	C	0	1
1	D	0	6
All	All	0	12

All (377) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	162	ILE	C-O	-8.93	1.14	1.24
1	C	117	ASN	C-O	-8.63	1.14	1.24
1	C	124	TYR	C-O	-8.62	1.14	1.24
1	D	139	GLY	C-O	-8.32	1.16	1.24
1	A	252	ILE	C-O	-8.26	1.15	1.24
1	D	200	VAL	C-O	-8.17	1.15	1.24
1	A	117	ASN	C-O	-7.88	1.15	1.24
1	A	157	VAL	C-O	-7.83	1.15	1.24
1	A	246	ALA	C-O	-7.78	1.15	1.24
1	A	138	THR	C-O	-7.76	1.14	1.23
1	A	200	VAL	C-O	-7.76	1.16	1.24
1	D	180	ALA	C-O	-7.76	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	TYR	C-O	-7.74	1.15	1.24
1	B	117	ASN	C-O	-7.69	1.15	1.24
1	A	318	LEU	C-O	-7.67	1.15	1.24
1	D	117	ASN	C-O	-7.62	1.15	1.24
1	C	114	MET	C-O	-7.60	1.15	1.24
1	D	228	MET	C-O	-7.53	1.15	1.24
1	C	180	ALA	C-O	-7.50	1.15	1.24
1	C	142	MET	C-O	-7.50	1.15	1.24
1	B	229	ILE	C-O	-7.36	1.16	1.24
1	A	202	SER	C-O	-7.32	1.15	1.24
1	D	135	GLU	C-O	-7.30	1.15	1.23
1	A	12	ASP	C-O	-7.26	1.15	1.24
1	D	198	SER	C-O	-7.25	1.15	1.24
1	D	58	ARG	C-O	-7.24	1.17	1.24
1	D	310	THR	N-CA	-7.21	1.37	1.46
1	A	201	ILE	C-O	-7.18	1.16	1.24
1	A	296	GLN	C-O	-7.17	1.14	1.23
1	B	162	ILE	C-O	-7.09	1.16	1.24
1	A	173	PHE	C-O	-7.03	1.16	1.24
1	D	290	VAL	C-O	-7.01	1.16	1.24
1	D	231	ASN	C-O	-6.99	1.16	1.23
1	B	116	LEU	C-O	-6.98	1.16	1.24
1	A	139	GLY	C-O	-6.97	1.18	1.24
1	B	230	ILE	C-O	-6.96	1.16	1.24
1	A	95	VAL	C-O	-6.96	1.16	1.23
1	A	302	GLU	C-O	-6.94	1.16	1.24
1	C	221	ASP	C-O	-6.91	1.16	1.24
1	A	14	LYS	C-O	-6.91	1.16	1.24
1	A	179	THR	C-O	-6.89	1.16	1.24
1	A	255	LEU	C-O	-6.84	1.16	1.23
1	C	296	GLN	C-O	-6.83	1.14	1.23
1	A	106	ALA	C-O	-6.80	1.16	1.24
1	C	260	TYR	C-O	-6.80	1.15	1.23
1	B	154	LYS	C-O	-6.78	1.16	1.24
1	A	169	ARG	C-O	-6.78	1.15	1.24
1	C	255	LEU	C-O	-6.75	1.16	1.24
1	A	198	SER	C-O	-6.74	1.15	1.24
1	D	112	MET	C-O	-6.74	1.16	1.24
1	A	109	ALA	C-O	-6.73	1.16	1.24
1	A	11	TYR	C-O	-6.73	1.16	1.24
1	C	297	ALA	C-O	-6.71	1.15	1.24
1	B	29	PHE	C-O	-6.69	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	LYS	C-O	-6.66	1.16	1.24
1	C	143	HIS	C-O	-6.66	1.15	1.23
1	B	102	PRO	C-O	-6.63	1.15	1.24
1	C	60	VAL	C-O	-6.59	1.16	1.24
1	C	37	LYS	C-O	-6.55	1.16	1.24
1	A	135	GLU	C-O	-6.54	1.16	1.23
1	D	113	MET	C-O	-6.54	1.16	1.24
1	D	142	MET	C-O	-6.53	1.16	1.24
1	D	219	ALA	C-O	-6.52	1.16	1.24
1	C	110	ILE	C-O	-6.52	1.16	1.24
1	C	225	ASN	C-O	-6.50	1.16	1.23
1	D	317	GLN	N-CA	-6.49	1.38	1.46
1	C	106	ALA	C-O	-6.48	1.16	1.24
1	B	200	VAL	C-O	-6.48	1.17	1.24
1	C	257	MET	C-O	-6.48	1.16	1.23
1	A	122	ARG	C-O	-6.47	1.16	1.24
1	A	281	PHE	C-O	-6.46	1.16	1.24
1	A	93	GLN	C-O	-6.46	1.16	1.24
1	A	124	TYR	C-O	-6.46	1.16	1.24
1	C	301	ALA	C-O	-6.46	1.16	1.24
1	B	225	ASN	C-O	-6.46	1.16	1.23
1	C	161	ARG	C-O	-6.46	1.16	1.24
1	D	289	ASN	C-O	-6.45	1.16	1.23
1	B	101	SER	C-O	-6.44	1.16	1.24
1	C	299	LEU	C-O	-6.43	1.16	1.23
1	A	205	CYS	C-O	-6.42	1.17	1.24
1	B	213	HIS	C-O	-6.40	1.15	1.23
1	C	113	MET	C-O	-6.40	1.16	1.24
1	C	99	ALA	C-O	-6.38	1.16	1.23
1	B	253	GLY	C-O	-6.36	1.16	1.23
1	D	123	ALA	C-O	-6.36	1.16	1.24
1	C	49	CYS	C-O	-6.36	1.16	1.24
1	C	125	GLN	C-O	-6.36	1.16	1.24
1	A	293	THR	C-O	-6.31	1.15	1.23
1	D	101	SER	C-O	-6.31	1.16	1.24
1	C	5	VAL	C-O	-6.31	1.17	1.24
1	C	111	GLY	C-O	-6.31	1.16	1.23
1	C	200	VAL	C-O	-6.30	1.17	1.24
1	D	153	GLY	C-O	-6.29	1.17	1.23
1	B	301	ALA	C-O	-6.29	1.16	1.24
1	A	257	MET	C-O	-6.29	1.17	1.23
1	A	228	MET	C-O	-6.28	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	45	CYS	C-O	-6.27	1.16	1.24
1	B	84	LEU	C-O	-6.27	1.16	1.24
1	C	48	VAL	C-O	-6.26	1.17	1.24
1	D	255	LEU	C-O	-6.25	1.17	1.23
1	A	195	PHE	C-O	-6.25	1.17	1.24
1	A	182	LEU	C-O	-6.24	1.16	1.24
1	D	205	CYS	C-O	-6.24	1.17	1.24
1	C	122	ARG	C-O	-6.24	1.16	1.24
1	A	174	ASP	C-O	-6.18	1.16	1.24
1	A	43	ASN	C-O	-6.16	1.16	1.23
1	A	222	GLN	C-O	-6.16	1.16	1.24
1	C	230	ILE	C-O	-6.16	1.17	1.24
1	A	288	HIS	C-O	-6.16	1.16	1.23
1	A	217	HIS	C-O	-6.15	1.17	1.24
1	C	155	ILE	C-O	-6.15	1.17	1.24
1	A	107	GLU	C-O	-6.14	1.17	1.24
1	A	49	CYS	C-O	-6.13	1.16	1.24
1	A	189	VAL	C-O	-6.13	1.16	1.23
1	B	123	ALA	C-O	-6.13	1.17	1.24
1	A	38	THR	C-O	-6.12	1.15	1.23
1	D	108	HIS	C-O	-6.11	1.17	1.24
1	D	243	ALA	C-O	-6.11	1.17	1.24
1	D	53	ASN	C-O	-6.11	1.15	1.23
1	B	292	PHE	C-O	-6.09	1.16	1.24
1	D	141	THR	C-O	-6.08	1.16	1.23
1	C	115	THR	C-O	-6.08	1.17	1.24
1	B	136	GLY	C-O	-6.07	1.15	1.24
1	C	103	GLU	C-O	-6.07	1.17	1.24
1	D	105	VAL	C-O	-6.07	1.17	1.24
1	D	166	PHE	C-O	-6.07	1.16	1.24
1	C	36	GLU	C-O	-6.06	1.17	1.24
1	C	55	ASP	C-O	-6.06	1.16	1.24
1	B	228	MET	C-O	-6.05	1.16	1.24
1	B	166	PHE	C-O	-6.05	1.16	1.24
1	A	30	PHE	C-O	-6.05	1.16	1.24
1	A	219	ALA	C-O	-6.04	1.17	1.24
1	A	3	LEU	C-O	-6.03	1.17	1.24
1	A	113	MET	C-O	-6.03	1.17	1.24
1	B	108	HIS	C-O	-6.01	1.17	1.24
1	B	10	GLN	C-O	-6.01	1.17	1.24
1	C	38	THR	C-O	-6.00	1.16	1.24
1	A	283	ARG	C-O	-6.00	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	121	HIS	C-O	-5.99	1.17	1.24
1	D	138	THR	C-O	-5.99	1.16	1.23
1	A	22	ALA	C-O	-5.98	1.16	1.24
1	D	194	LEU	C-O	-5.98	1.17	1.24
1	C	248	LYS	C-O	-5.97	1.17	1.24
1	D	325	PRO	N-CD	5.96	1.56	1.47
1	B	155	ILE	C-O	-5.96	1.17	1.24
1	B	71	TYR	C-O	-5.95	1.16	1.23
1	B	76	CYS	C-O	-5.93	1.16	1.23
1	D	291	LEU	C-O	-5.93	1.17	1.24
1	D	107	GLU	C-O	-5.93	1.17	1.24
1	C	305	ILE	C-O	-5.92	1.17	1.24
1	A	203	LEU	C-O	-5.91	1.16	1.24
1	B	65	LYS	C-O	-5.91	1.17	1.24
1	B	159	ALA	C-O	-5.91	1.17	1.24
1	D	176	TYR	C-O	-5.90	1.17	1.24
1	D	225	ASN	C-O	-5.90	1.16	1.23
1	C	159	ALA	C-O	-5.90	1.17	1.24
1	C	113	MET	N-CA	-5.89	1.39	1.46
1	C	247	LEU	C-O	-5.89	1.17	1.24
1	A	86	ALA	C-O	-5.87	1.17	1.24
1	A	243	ALA	C-O	-5.87	1.17	1.24
1	D	164	LYS	C-O	-5.87	1.17	1.24
1	A	8	THR	C-O	-5.86	1.17	1.23
1	B	169	ARG	C-O	-5.86	1.16	1.24
1	A	149	VAL	C-O	-5.86	1.17	1.24
1	B	4	ALA	C-O	-5.86	1.16	1.24
1	B	252	ILE	C-O	-5.86	1.17	1.24
1	D	143	HIS	C-O	-5.86	1.16	1.23
1	A	29	PHE	C-O	-5.85	1.17	1.24
1	C	164	LYS	C-O	-5.84	1.17	1.24
1	C	252	ILE	C-O	-5.83	1.18	1.24
1	A	45	CYS	C-O	-5.83	1.16	1.24
1	B	218	ALA	C-O	-5.82	1.17	1.24
1	B	207	LEU	C-O	-5.79	1.17	1.24
1	B	303	ALA	C-O	-5.79	1.17	1.24
1	B	118	ARG	C-O	-5.78	1.16	1.24
1	C	290	VAL	C-O	-5.78	1.18	1.24
1	D	159	ALA	C-O	-5.78	1.17	1.24
1	D	127	THR	C-O	-5.77	1.16	1.24
1	D	40	LYS	C-O	-5.76	1.16	1.24
1	A	128	ARG	C-O	-5.75	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297	ALA	C-O	-5.75	1.17	1.24
1	C	163	LEU	C-O	-5.74	1.17	1.24
1	A	206	PRO	C-O	-5.73	1.17	1.23
1	B	142	MET	C-O	-5.73	1.17	1.24
1	A	88	LYS	C-O	-5.73	1.17	1.24
1	A	220	PHE	C-O	-5.73	1.17	1.24
1	D	158	ALA	C-O	-5.73	1.17	1.24
1	C	133	SER	C-O	-5.72	1.17	1.23
1	D	296	GLN	C-O	-5.72	1.16	1.23
1	D	245	GLU	C-O	-5.72	1.17	1.24
1	B	202	SER	C-O	-5.71	1.17	1.24
1	B	30	PHE	C-O	-5.70	1.17	1.24
1	A	166	PHE	C-O	-5.70	1.16	1.24
1	B	247	LEU	C-O	-5.69	1.17	1.24
1	C	52	VAL	C-O	-5.69	1.17	1.24
1	D	247	LEU	C-O	-5.68	1.17	1.24
1	A	108	HIS	C-O	-5.68	1.17	1.24
1	D	116	LEU	C-O	-5.67	1.17	1.24
1	A	55	ASP	C-O	-5.67	1.17	1.24
1	C	65	LYS	C-O	-5.67	1.17	1.24
1	B	161	ARG	C-O	-5.67	1.17	1.24
1	A	158	ALA	C-O	-5.65	1.17	1.24
1	A	196	ALA	C-O	-5.64	1.17	1.24
1	C	141	THR	C-O	-5.63	1.17	1.24
1	A	163	LEU	C-O	-5.60	1.17	1.24
1	C	201	ILE	C-O	-5.59	1.18	1.24
1	C	74	LEU	C-O	-5.58	1.17	1.24
1	D	301	ALA	C-O	-5.58	1.17	1.24
1	D	234	ARG	C-O	-5.56	1.17	1.23
1	B	128	ARG	C-O	-5.56	1.17	1.24
1	C	20	ASN	C-O	-5.56	1.16	1.24
1	B	206	PRO	C-O	-5.56	1.17	1.23
1	C	11	TYR	C-O	-5.55	1.17	1.24
1	D	177	PRO	C-O	-5.54	1.17	1.23
1	B	231	ASN	C-O	-5.52	1.17	1.24
1	D	199	ASP	C-O	-5.52	1.17	1.24
1	D	300	THR	C-O	-5.51	1.16	1.23
1	A	58	ARG	C-O	-5.51	1.19	1.24
1	C	54	ASP	C-O	-5.51	1.16	1.23
1	C	58	ARG	C-O	-5.51	1.19	1.24
1	C	205	CYS	C-O	-5.51	1.18	1.24
1	C	303	ALA	C-O	-5.51	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	LEU	C-O	-5.50	1.17	1.24
1	B	198	SER	C-O	-5.50	1.17	1.24
1	D	45	CYS	C-O	-5.50	1.17	1.24
1	B	47	ALA	C-O	-5.50	1.17	1.23
1	A	180	ALA	C-O	-5.49	1.17	1.24
1	D	279	ASP	C-O	-5.49	1.17	1.24
1	C	285	SER	C-O	-5.48	1.17	1.24
1	D	206	PRO	C-O	-5.48	1.17	1.23
1	A	133	SER	C-O	-5.48	1.17	1.23
1	B	37	LYS	C-O	-5.48	1.17	1.24
1	D	27	LEU	C-O	-5.48	1.17	1.24
1	A	227	VAL	C-O	-5.48	1.18	1.24
1	C	194	LEU	C-O	-5.48	1.17	1.24
1	C	84	LEU	C-O	-5.45	1.17	1.24
1	D	37	LYS	C-O	-5.45	1.17	1.24
1	A	155	ILE	C-O	-5.44	1.18	1.24
1	A	162	ILE	C-O	-5.44	1.17	1.24
1	D	242	ALA	C-O	-5.44	1.17	1.24
1	C	158	ALA	C-O	-5.42	1.17	1.24
1	B	289	ASN	C-O	-5.42	1.17	1.23
1	B	153	GLY	C-O	-5.42	1.18	1.23
1	A	99	ALA	C-O	-5.42	1.17	1.23
1	B	293	THR	C-O	-5.42	1.17	1.23
1	C	231	ASN	C-O	-5.42	1.17	1.23
1	A	74	LEU	C-O	-5.41	1.17	1.24
1	C	153	GLY	C-O	-5.41	1.18	1.23
1	D	98	PRO	C-O	-5.41	1.17	1.24
1	A	148	GLY	C-O	-5.41	1.16	1.23
1	B	222	GLN	C-O	-5.39	1.17	1.24
1	A	13	LYS	C-O	-5.39	1.17	1.24
1	A	242	ALA	C-O	-5.39	1.17	1.24
1	A	94	VAL	C-O	-5.38	1.18	1.24
1	D	3	LEU	C-O	-5.38	1.17	1.24
1	A	28	GLU	C-O	-5.38	1.17	1.24
1	D	150	ILE	C-O	-5.38	1.18	1.24
1	A	36	GLU	C-O	-5.38	1.17	1.24
1	A	186	VAL	C-O	-5.37	1.17	1.24
1	A	320	LYS	C-O	-5.37	1.17	1.24
1	D	252	ILE	C-O	-5.36	1.18	1.24
1	C	135	GLU	C-O	-5.35	1.17	1.23
1	C	282	ARG	C-O	-5.35	1.18	1.24
1	D	286	ALA	C-O	-5.35	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	HIS	C-O	-5.34	1.17	1.24
1	A	253	GLY	C-O	-5.34	1.17	1.23
1	C	112	MET	C-O	-5.33	1.17	1.24
1	B	32	PHE	C-O	-5.33	1.16	1.23
1	D	106	ALA	C-O	-5.33	1.17	1.24
1	D	14	LYS	C-O	-5.33	1.18	1.24
1	B	107	GLU	C-O	-5.33	1.17	1.24
1	B	158	ALA	C-O	-5.32	1.17	1.24
1	A	212	TYR	C-O	-5.32	1.17	1.23
1	C	246	ALA	C-O	-5.31	1.17	1.24
1	A	241	GLN	C-O	-5.31	1.18	1.24
1	C	29	PHE	C-O	-5.31	1.17	1.24
1	B	227	VAL	C-O	-5.30	1.17	1.24
1	D	303	ALA	C-O	-5.30	1.17	1.24
1	A	254	SER	C-O	-5.30	1.17	1.23
1	C	269	GLU	CA-C	5.30	1.60	1.53
1	D	207	LEU	C-O	-5.30	1.17	1.24
1	B	257	MET	C-O	-5.29	1.18	1.24
1	D	209	PRO	C-O	-5.29	1.17	1.24
1	B	55	ASP	C-O	-5.29	1.17	1.24
1	C	293	THR	C-O	-5.28	1.17	1.23
1	A	73	ALA	C-O	-5.28	1.17	1.24
1	A	234	ARG	C-O	-5.28	1.17	1.23
1	D	227	VAL	C-O	-5.28	1.18	1.24
1	D	155	ILE	C-O	-5.27	1.18	1.24
1	B	160	LEU	C-O	-5.27	1.18	1.24
1	A	114	MET	C-O	-5.27	1.17	1.24
1	C	30	PHE	C-O	-5.27	1.17	1.24
1	A	311	THR	C-O	-5.26	1.18	1.24
1	C	170	LEU	C-O	-5.26	1.17	1.24
1	B	40	LYS	C-O	-5.26	1.17	1.24
1	C	148	GLY	C-O	-5.26	1.16	1.23
1	A	123	ALA	C-O	-5.25	1.18	1.24
1	C	300	THR	C-O	-5.25	1.17	1.23
1	D	109	ALA	C-O	-5.25	1.18	1.24
1	D	222	GLN	C-O	-5.25	1.17	1.24
1	B	46	GLU	C-O	-5.25	1.17	1.24
1	C	35	THR	C-O	-5.24	1.17	1.23
1	A	153	GLY	C-O	-5.24	1.18	1.23
1	B	34	LEU	C-O	-5.24	1.17	1.24
1	B	254	SER	C-O	-5.23	1.17	1.23
1	D	195	PHE	C-O	-5.23	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	201	ILE	C-O	-5.22	1.18	1.24
1	C	4	ALA	C-O	-5.22	1.17	1.24
1	A	232	THR	C-O	-5.21	1.16	1.23
1	B	41	THR	C-O	-5.21	1.17	1.24
1	B	49	CYS	C-O	-5.21	1.17	1.24
1	C	71	TYR	C-O	-5.21	1.17	1.23
1	B	311	THR	C-O	-5.21	1.18	1.24
1	C	32	PHE	C-O	-5.21	1.17	1.23
1	C	288	HIS	C-O	-5.21	1.17	1.23
1	A	97	VAL	C-O	-5.20	1.18	1.24
1	D	8	THR	C-O	-5.20	1.17	1.23
1	D	326	ASN	N-CA	-5.20	1.40	1.46
1	B	282	ARG	C-O	-5.19	1.18	1.24
1	B	143	HIS	C-O	-5.19	1.17	1.23
1	A	199	ASP	C-O	-5.19	1.18	1.24
1	B	290	VAL	C-O	-5.18	1.19	1.24
1	C	206	PRO	C-O	-5.17	1.18	1.23
1	C	107	GLU	C-O	-5.16	1.18	1.24
1	C	169	ARG	C-O	-5.16	1.17	1.24
1	A	211	ASN	C-O	-5.15	1.17	1.24
1	B	83	ASP	C-O	-5.15	1.17	1.23
1	B	104	ALA	C-O	-5.15	1.18	1.24
1	A	290	VAL	C-O	-5.15	1.19	1.24
1	B	291	LEU	C-O	-5.14	1.18	1.24
1	D	256	GLY	C-O	-5.14	1.17	1.23
1	C	104	ALA	C-O	-5.14	1.18	1.24
1	A	154	LYS	C-O	-5.14	1.18	1.24
1	C	229	ILE	C-O	-5.14	1.18	1.24
1	D	170	LEU	C-O	-5.13	1.18	1.24
1	B	259	VAL	C-O	-5.13	1.18	1.24
1	A	146	THR	C-O	-5.13	1.17	1.24
1	C	77	ALA	C-O	-5.13	1.18	1.24
1	C	202	SER	C-O	-5.13	1.18	1.24
1	A	35	THR	C-O	-5.13	1.17	1.24
1	D	294	GLY	C-O	-5.13	1.17	1.23
1	A	305	ILE	C-O	-5.12	1.18	1.24
1	B	63	GLU	C-O	-5.12	1.18	1.24
1	B	67	HIS	C-O	-5.12	1.17	1.24
1	C	41	THR	C-O	-5.12	1.17	1.24
1	D	149	VAL	C-O	-5.11	1.18	1.24
1	C	182	LEU	C-O	-5.11	1.18	1.24
1	A	104	ALA	C-O	-5.11	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	178	SER	C-O	-5.09	1.17	1.24
1	A	213	HIS	C-O	-5.09	1.17	1.23
1	B	103	GLU	C-O	-5.08	1.18	1.24
1	A	285	SER	C-O	-5.07	1.18	1.24
1	D	17	GLN	C-O	-5.07	1.18	1.24
1	B	251	LYS	C-O	-5.07	1.18	1.24
1	A	112	MET	C-O	-5.07	1.18	1.24
1	A	34	LEU	C-O	-5.06	1.17	1.23
1	A	193	THR	C-O	-5.06	1.18	1.24
1	A	50	ILE	C-O	-5.05	1.17	1.23
1	B	296	GLN	C-O	-5.05	1.17	1.23
1	D	120	ILE	C-O	-5.05	1.18	1.24
1	C	168	MET	C-O	-5.05	1.18	1.23
1	B	221	ASP	C-O	-5.05	1.18	1.24
1	C	217	HIS	C-O	-5.05	1.18	1.24
1	D	28	GLU	C-O	-5.05	1.18	1.24
1	B	145	LYS	C-O	-5.04	1.17	1.23
1	B	150	ILE	C-O	-5.04	1.18	1.24
1	B	14	LYS	C-O	-5.04	1.18	1.24
1	D	203	LEU	C-O	-5.03	1.17	1.24
1	C	286	ALA	C-O	-5.03	1.18	1.24
1	B	43	ASN	C-O	-5.03	1.17	1.23
1	B	36	GLU	C-O	-5.02	1.18	1.24
1	D	163	LEU	C-O	-5.02	1.18	1.24
1	A	251	LYS	C-O	-5.01	1.18	1.24
1	C	232	THR	C-O	-5.01	1.17	1.24
1	D	173	PHE	C-O	-5.01	1.18	1.24
1	C	197	GLU	C-O	-5.01	1.17	1.24
1	C	279	ASP	C-O	-5.00	1.17	1.24

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	323	ALA	N-CA-C	11.96	123.87	111.07
1	D	321	GLY	N-CA-C	11.88	127.74	112.54
1	B	277	GLN	N-CA-C	10.30	125.17	108.99
1	C	270	ASP	N-CA-C	9.78	121.70	111.14
1	A	268	PHE	N-CA-C	-9.66	94.78	107.73
1	C	269	GLU	N-CA-C	9.55	125.07	109.02
1	B	77	ALA	N-CA-C	8.31	120.42	111.36
1	D	311	THR	N-CA-C	-7.44	103.17	111.28
1	D	317	GLN	CA-C-N	7.41	135.68	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	317	GLN	C-N-CA	7.41	135.68	121.54
1	A	277	GLN	N-CA-C	7.32	121.07	109.50
1	C	269	GLU	CA-C-N	7.24	130.29	120.44
1	C	269	GLU	C-N-CA	7.24	130.29	120.44
1	B	283	ARG	N-CA-C	7.05	118.61	111.07
1	D	271	LYS	N-CA-C	-6.78	96.35	110.80
1	D	81	ASN	N-CA-C	6.68	119.56	111.82
1	D	317	GLN	N-CA-C	-6.59	98.96	109.76
1	D	326	ASN	N-CA-C	-6.58	102.99	111.02
1	D	324	CYS	C-N-CD	6.57	135.05	120.60
1	D	274	ASP	N-CA-C	-6.52	100.10	109.29
1	A	277	GLN	CA-C-N	6.45	133.12	122.73
1	A	277	GLN	C-N-CA	6.45	133.12	122.73
1	D	324	CYS	N-CA-C	6.42	128.97	111.00
1	B	37	LYS	N-CA-C	6.41	118.35	111.36
1	C	126	ARG	N-CA-C	6.38	118.11	111.03
1	C	210	GLU	CB-CA-C	-6.32	100.96	110.88
1	D	312	LEU	N-CA-C	6.28	118.20	111.36
1	D	320	LYS	CA-C-N	6.25	127.60	120.53
1	D	320	LYS	C-N-CA	6.25	127.60	120.53
1	A	37	LYS	N-CA-C	6.21	119.03	111.82
1	C	97	VAL	CA-C-O	6.17	122.58	119.12
1	C	264	ARG	N-CA-C	6.17	117.67	111.07
1	A	32	PHE	N-CA-C	6.15	118.46	110.53
1	C	77	ALA	N-CA-C	6.09	118.00	111.36
1	A	15	TYR	N-CA-C	6.06	117.96	111.36
1	C	15	TYR	N-CA-C	5.95	117.85	111.36
1	A	126	ARG	N-CA-C	5.93	117.54	111.14
1	A	264	ARG	N-CA-C	5.92	117.53	111.14
1	D	94	VAL	N-CA-C	5.88	117.18	108.65
1	D	326	ASN	CB-CA-C	-5.81	101.68	110.92
1	D	314	ASN	CB-CA-C	-5.75	101.85	110.88
1	B	126	ARG	N-CA-C	5.74	117.34	111.14
1	D	320	LYS	N-CA-C	-5.71	99.46	108.14
1	D	52	VAL	N-CA-C	5.67	118.13	111.05
1	B	276	ILE	N-CA-C	5.67	117.02	109.37
1	D	274	ASP	CA-C-N	5.55	131.96	121.97
1	D	274	ASP	C-N-CA	5.55	131.96	121.97
1	A	271	LYS	N-CA-C	5.53	116.66	108.86
1	D	276	ILE	CA-C-N	5.49	131.30	122.14
1	D	276	ILE	C-N-CA	5.49	131.30	122.14
1	D	73	ALA	N-CA-C	5.37	117.15	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	84	LEU	N-CA-C	5.31	119.02	112.54
1	D	199	ASP	N-CA-C	5.23	117.06	111.36
1	D	210	GLU	N-CA-C	5.23	117.89	111.82
1	B	179	THR	N-CA-C	-5.16	105.66	111.28
1	D	92	LEU	N-CA-C	5.15	117.00	108.20
1	B	272	SER	CA-C-N	5.10	127.09	120.56
1	B	272	SER	C-N-CA	5.10	127.09	120.56
1	D	95	VAL	N-CA-C	5.07	119.89	109.34
1	D	286	ALA	N-CA-C	5.07	116.61	111.14
1	C	267	PHE	N-CA-C	-5.05	102.91	110.23
1	C	272	SER	N-CA-C	5.03	120.52	113.02
1	B	170	LEU	N-CA-C	5.02	116.91	108.73
1	B	97	VAL	CA-C-O	5.00	123.05	119.25
1	B	322	GLU	N-CA-C	5.00	116.98	110.53

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	LEU	Peptide
1	A	276	ILE	Peptide
1	A	277	GLN	Peptide
1	B	269	GLU	Peptide
1	B	276	ILE	Peptide
1	C	267	PHE	Peptide
1	D	267	PHE	Peptide
1	D	272	SER	Peptide
1	D	274	ASP	Peptide
1	D	276	ILE	Peptide
1	D	317	GLN	Peptide
1	D	75	ARG	Peptide

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	2567	0	2562	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2567	0	2562	61	0
1	C	2558	0	2546	72	1
1	D	2558	0	2547	166	0
2	A	216	0	0	1	0
2	B	164	0	0	8	0
2	C	148	0	0	2	0
2	D	137	0	0	7	0
All	All	10915	0	10217	349	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 17.

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:C:240:SER:HB3	1:C:268:PHE:CD1	1.26	1.69
1:D:324:CYS:SG	1:D:326:ASN:ND2	1.95	1.40
1:D:324:CYS:HB3	1:D:326:ASN:CG	1.48	1.38
1:C:240:SER:HB3	1:C:268:PHE:CE1	1.57	1.37
1:B:241:GLN:OE1	1:B:269:GLU:C	1.67	1.35
1:C:240:SER:CB	1:C:268:PHE:CD1	2.10	1.34
1:B:241:GLN:CD	1:B:269:GLU:O	1.69	1.31
1:C:240:SER:CB	1:C:268:PHE:CE1	2.20	1.25
1:D:83:ASP:OD1	1:D:85:ASP:OD1	1.55	1.23
1:B:275:VAL:O	1:B:277:GLN:NE2	1.72	1.22
1:B:46:GLU:HG3	2:B:2001:HOH:O	1.38	1.21
1:D:274:ASP:HB3	1:D:275:VAL:HG13	1.23	1.18
1:D:267:PHE:HA	1:D:268:PHE:HB2	1.27	1.17
1:C:266:LEU:HD23	1:C:267:PHE:N	1.60	1.17
1:D:276:ILE:HD12	1:D:277:GLN:HB2	1.19	1.14
1:A:1:MET:HE3	1:A:319:GLU:HG3	1.32	1.10
1:A:268:PHE:O	1:A:269:GLU:HB2	1.46	1.10
1:D:324:CYS:CB	1:D:326:ASN:CG	2.26	1.08
1:A:128:ARG:NH1	1:D:125:GLN:OE1	1.85	1.08
1:C:271:LYS:NZ	1:C:277:GLN:OE1	1.87	1.07
1:C:267:PHE:CD1	1:C:268:PHE:HB2	1.89	1.07
1:C:275:VAL:HG12	1:C:276:ILE:HD13	1.08	1.04
1:B:269:GLU:HB3	1:B:270:ASP:HA	1.36	1.04
1:D:277:GLN:NE2	1:D:280:VAL:HB	1.75	1.01
1:D:95:VAL:HA	1:D:328:LEU:CD2	1.90	1.01
1:A:274:ASP:CB	1:A:275:VAL:HG22	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ARG:NH1	1:C:125:GLN:HE22	1.60	0.99
1:A:274:ASP:HB2	1:A:275:VAL:HG22	1.43	0.99
1:D:276:ILE:CD1	1:D:277:GLN:HB2	1.93	0.98
1:C:275:VAL:HG12	1:C:276:ILE:CD1	1.93	0.98
1:C:240:SER:CB	1:C:268:PHE:HD1	1.61	0.96
1:A:274:ASP:HB2	1:A:275:VAL:CG2	1.94	0.96
1:D:271:LYS:NZ	1:D:276:ILE:HD13	1.81	0.96
1:D:274:ASP:HB3	1:D:275:VAL:CG1	1.95	0.96
1:A:274:ASP:CA	1:A:275:VAL:HG22	1.94	0.96
1:D:19:VAL:HG11	1:D:309:GLU:HA	1.49	0.95
1:D:271:LYS:HE3	1:D:276:ILE:HA	1.46	0.94
1:B:274:ASP:HA	1:B:275:VAL:HG12	1.47	0.94
1:D:324:CYS:CB	1:D:326:ASN:ND2	2.31	0.94
1:B:128:ARG:HH11	1:C:125:GLN:HE22	0.98	0.93
1:C:240:SER:CB	1:C:268:PHE:HE1	1.82	0.93
1:D:277:GLN:O	1:D:280:VAL:HG12	1.69	0.92
1:B:191:LEU:CD1	1:B:214:LEU:HD11	1.99	0.92
1:C:275:VAL:CG1	1:C:276:ILE:HD13	1.97	0.91
1:D:274:ASP:CB	1:D:275:VAL:HG13	2.00	0.91
1:A:264:ARG:HG2	1:A:264:ARG:HH11	1.36	0.91
1:D:276:ILE:HD12	1:D:277:GLN:CB	1.99	0.90
1:A:271:LYS:HG3	1:A:272:SER:H	1.33	0.88
1:B:128:ARG:HH11	1:C:125:GLN:NE2	1.70	0.88
1:D:1:MET:HE2	1:D:71:TYR:CD2	2.11	0.86
1:D:271:LYS:HB3	1:D:275:VAL:H	1.40	0.86
1:C:267:PHE:CE1	1:C:268:PHE:HB2	2.09	0.85
1:C:268:PHE:HB3	1:C:280:VAL:HG21	1.58	0.85
1:D:271:LYS:HB3	1:D:275:VAL:N	1.90	0.85
1:A:274:ASP:HA	1:A:275:VAL:HG22	1.59	0.82
1:B:269:GLU:HB3	1:B:270:ASP:CA	2.09	0.82
1:C:240:SER:CA	1:C:268:PHE:HE1	1.93	0.81
1:C:266:LEU:CD2	1:C:267:PHE:N	2.43	0.81
1:D:277:GLN:HE21	1:D:280:VAL:HB	1.45	0.81
1:D:271:LYS:HB3	1:D:274:ASP:C	2.06	0.80
1:D:267:PHE:CA	1:D:268:PHE:HB2	2.10	0.79
1:C:266:LEU:HD23	1:C:267:PHE:CA	2.11	0.79
1:D:1:MET:HE2	1:D:71:TYR:HD2	1.47	0.79
1:D:76:CYS:O	1:D:97:VAL:HB	1.83	0.78
1:A:276:ILE:HG13	1:A:277:GLN:H	1.46	0.78
1:D:324:CYS:HB3	1:D:326:ASN:OD1	1.83	0.78
1:D:23:PHE:HE2	1:D:313:GLN:HA	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:SER:CA	1:C:268:PHE:CE1	2.67	0.78
1:D:95:VAL:HA	1:D:328:LEU:HD23	1.64	0.78
1:A:37:LYS:NZ	1:B:28:GLU:OE2	2.17	0.77
1:D:271:LYS:HZ2	1:D:276:ILE:HD13	1.44	0.77
1:D:277:GLN:OE1	1:D:277:GLN:HA	1.85	0.77
1:A:1:MET:CE	1:A:319:GLU:HG3	2.14	0.77
1:D:271:LYS:CE	1:D:276:ILE:HA	2.15	0.77
1:A:268:PHE:O	1:A:269:GLU:CB	2.26	0.76
1:C:240:SER:HB3	1:C:268:PHE:HD1	1.05	0.76
1:B:248:LYS:NZ	1:B:269:GLU:OE2	2.18	0.76
1:A:274:ASP:O	1:C:248:LYS:NZ	2.17	0.76
1:D:319:GLU:O	1:D:320:LYS:HG3	1.86	0.76
1:C:244:ILE:HD13	1:C:269:GLU:HG3	1.67	0.76
1:B:269:GLU:H	1:B:270:ASP:HB3	1.50	0.75
1:D:65:LYS:HD2	1:D:90:LEU:HB3	1.68	0.75
1:B:191:LEU:HD11	1:B:214:LEU:HD11	1.68	0.75
1:D:82:VAL:HG12	1:D:84:LEU:HD12	1.67	0.74
1:D:318:LEU:N	1:D:320:LYS:O	2.20	0.74
1:D:267:PHE:HA	1:D:268:PHE:CB	2.15	0.73
1:C:240:SER:HA	1:C:268:PHE:HE1	1.53	0.72
1:D:1:MET:HG3	1:D:319:GLU:HG3	1.71	0.72
1:A:274:ASP:CA	1:A:275:VAL:CG2	2.68	0.71
1:D:94:VAL:C	1:D:95:VAL:HG13	2.15	0.71
1:A:271:LYS:CG	1:A:272:SER:H	2.04	0.70
1:D:58:ARG:N	1:D:59:PRO:CD	2.53	0.70
1:B:274:ASP:CA	1:B:275:VAL:HG12	2.21	0.70
1:C:267:PHE:CD1	1:C:268:PHE:CB	2.72	0.70
1:B:275:VAL:H	1:B:277:GLN:HE22	1.39	0.70
1:B:113:MET:SD	1:B:200:VAL:HG11	2.31	0.70
1:C:267:PHE:CD2	1:C:268:PHE:CD1	2.73	0.70
1:D:319:GLU:C	1:D:320:LYS:HG3	2.16	0.70
1:C:271:LYS:NZ	1:C:271:LYS:HB2	2.07	0.69
1:D:318:LEU:N	1:D:318:LEU:HD12	2.07	0.69
1:A:271:LYS:HG3	1:A:272:SER:N	2.05	0.69
1:B:191:LEU:HD13	1:B:214:LEU:HD11	1.75	0.69
1:C:267:PHE:CG	1:C:268:PHE:CG	2.72	0.69
1:A:272:SER:OG	1:A:273:VAL:N	2.26	0.69
1:A:330:LYS:HE2	1:A:330:LYS:HA	1.76	0.68
1:B:113:MET:HG3	1:B:228:MET:SD	2.33	0.68
1:C:267:PHE:CE1	1:C:281:PHE:CE1	2.82	0.68
1:D:83:ASP:OD1	1:D:85:ASP:CG	2.36	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:VAL:HG12	1:D:95:VAL:N	2.09	0.67
1:D:57:SER:HA	1:D:83:ASP:HB3	1.77	0.67
1:D:19:VAL:CG1	1:D:309:GLU:HA	2.23	0.67
1:D:324:CYS:HB3	1:D:326:ASN:CB	2.25	0.66
1:A:264:ARG:HG2	1:A:264:ARG:NH1	2.07	0.66
1:C:240:SER:OG	1:C:268:PHE:CD1	2.49	0.66
1:A:276:ILE:HG13	1:A:277:GLN:N	2.09	0.66
1:C:240:SER:HA	1:C:268:PHE:CE1	2.31	0.66
1:B:269:GLU:HG3	1:B:283:ARG:HH22	1.60	0.66
1:D:267:PHE:O	1:D:277:GLN:HB3	1.96	0.65
1:C:266:LEU:HD23	1:C:266:LEU:C	2.21	0.65
1:D:76:CYS:O	1:D:97:VAL:N	2.27	0.65
1:B:244:ILE:HG21	1:B:269:GLU:HG2	1.79	0.64
1:B:269:GLU:CB	1:B:270:ASP:HA	2.22	0.64
1:D:85:ASP:OD1	1:D:85:ASP:N	2.31	0.64
1:B:269:GLU:CB	1:B:270:ASP:CA	2.75	0.64
1:A:269:GLU:H	1:A:270:ASP:CG	2.06	0.64
1:D:23:PHE:CE2	1:D:313:GLN:HA	2.31	0.64
1:A:58:ARG:HB3	1:A:59:PRO:HD3	1.78	0.64
1:D:1:MET:CE	1:D:71:TYR:CD2	2.80	0.64
1:D:274:ASP:HB3	1:D:275:VAL:CB	2.28	0.64
1:B:274:ASP:HA	1:B:275:VAL:CG1	2.26	0.63
1:D:322:GLU:HG3	1:D:323:ALA:H	1.63	0.63
1:B:175:PRO:HA	2:B:2116:HOH:O	1.99	0.63
1:D:235:GLY:HA3	1:D:267:PHE:HZ	1.62	0.63
1:D:271:LYS:CB	1:D:275:VAL:H	2.12	0.63
1:D:269:GLU:OE1	1:D:269:GLU:HA	1.99	0.62
1:C:269:GLU:OE1	1:C:283:ARG:NH1	2.32	0.62
1:D:23:PHE:HE2	1:D:313:GLN:CA	2.11	0.62
1:D:317:GLN:OE1	1:D:324:CYS:SG	2.58	0.61
1:D:328:LEU:N	1:D:328:LEU:HD22	2.15	0.61
1:D:273:VAL:HG12	1:D:273:VAL:O	2.00	0.61
1:B:269:GLU:N	1:B:270:ASP:HB3	2.15	0.61
1:B:165:GLY:HA3	2:B:2111:HOH:O	2.00	0.60
1:C:240:SER:OG	1:C:268:PHE:CE1	2.54	0.60
1:D:257:MET:HE3	2:D:2117:HOH:O	2.01	0.60
1:D:122:ARG:HD2	2:D:2050:HOH:O	2.01	0.60
1:C:271:LYS:HB2	1:C:271:LYS:HZ3	1.65	0.60
1:D:86:ALA:O	1:D:89:GLU:HG3	2.01	0.59
1:B:228:MET:HG3	1:B:254:SER:HB2	1.84	0.59
1:D:52:VAL:HG12	1:D:76:CYS:SG	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:ILE:HD12	1:D:277:GLN:N	2.16	0.59
1:D:324:CYS:HB3	1:D:326:ASN:H	1.68	0.59
1:B:329:PHE:CB	2:B:2057:HOH:O	2.50	0.59
1:D:1:MET:HE2	1:D:71:TYR:CE2	2.37	0.59
1:C:113:MET:HG3	1:C:228:MET:SD	2.41	0.59
1:C:208:THR:HB	1:C:209:PRO:CD	2.33	0.59
1:D:241:GLN:HG2	1:D:269:GLU:HB3	1.85	0.58
1:D:57:SER:HA	1:D:83:ASP:CB	2.33	0.58
1:D:82:VAL:CG1	1:D:84:LEU:HD12	2.31	0.58
1:D:324:CYS:HB2	1:D:327:ALA:H	1.67	0.58
1:B:283:ARG:HD3	1:D:283:ARG:HD3	1.84	0.58
1:B:125:GLN:OE1	1:C:125:GLN:HG2	2.04	0.58
1:B:269:GLU:CG	1:B:283:ARG:HH22	2.17	0.58
1:D:1:MET:CE	1:D:71:TYR:HD2	2.12	0.58
1:D:323:ALA:N	1:D:324:CYS:HA	2.18	0.58
1:C:191:LEU:HD11	1:C:214:LEU:HD11	1.85	0.58
1:A:277:GLN:OE1	1:A:278:ASP:HA	2.04	0.57
1:C:267:PHE:CE1	1:C:268:PHE:CB	2.82	0.57
1:D:23:PHE:CE2	1:D:313:GLN:CA	2.87	0.57
1:D:19:VAL:HG11	1:D:309:GLU:CA	2.29	0.57
1:A:269:GLU:H	1:A:270:ASP:CB	2.18	0.56
1:A:264:ARG:HH11	1:A:264:ARG:CG	2.12	0.56
1:D:2:LYS:HG2	1:D:45:CYS:SG	2.45	0.56
1:C:249:ASN:C	1:C:250:GLN:HG2	2.28	0.56
1:C:191:LEU:CD1	1:C:214:LEU:HD11	2.36	0.56
1:C:194:LEU:C	1:C:194:LEU:HD23	2.31	0.55
1:D:23:PHE:N	1:D:23:PHE:CD1	2.73	0.55
1:D:241:GLN:HG2	1:D:269:GLU:CB	2.36	0.55
1:C:58:ARG:HB3	1:C:59:PRO:HD3	1.88	0.55
1:C:208:THR:HB	1:C:209:PRO:HD2	1.88	0.55
1:D:317:GLN:O	1:D:318:LEU:HD13	2.06	0.55
1:D:1:MET:HG3	1:D:319:GLU:CG	2.35	0.55
1:D:80:ASN:HB2	2:D:2040:HOH:O	2.06	0.55
1:D:74:LEU:HB3	1:D:76:CYS:HB3	1.88	0.55
1:D:271:LYS:HB3	1:D:274:ASP:O	2.07	0.55
1:C:267:PHE:CD1	1:C:267:PHE:C	2.85	0.55
1:A:125:GLN:HE22	1:C:128:ARG:HH22	1.53	0.55
1:B:320:LYS:HB3	1:B:322:GLU:HG3	1.89	0.55
1:A:268:PHE:HB2	1:A:270:ASP:OD1	2.06	0.55
1:D:317:GLN:OE1	1:D:326:ASN:ND2	2.39	0.55
1:A:125:GLN:OE1	1:D:125:GLN:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:PHE:N	1:A:268:PHE:CD1	2.73	0.54
1:D:57:SER:O	1:D:61:LEU:HG	2.08	0.54
1:D:318:LEU:C	1:D:320:LYS:N	2.62	0.54
1:D:324:CYS:HB3	1:D:326:ASN:N	2.23	0.54
1:C:273:VAL:O	1:C:274:ASP:HB3	2.07	0.54
1:D:21:GLU:HA	1:D:21:GLU:OE1	2.07	0.54
1:D:94:VAL:CG1	1:D:95:VAL:N	2.71	0.54
1:C:113:MET:SD	1:C:200:VAL:HG11	2.47	0.54
1:C:267:PHE:CG	1:C:268:PHE:CB	2.91	0.54
1:D:271:LYS:CE	1:D:276:ILE:HD13	2.37	0.54
1:D:23:PHE:CG	1:D:312:LEU:HB3	2.43	0.53
1:D:94:VAL:C	1:D:95:VAL:CG1	2.81	0.53
1:B:329:PHE:HB3	2:B:2057:HOH:O	2.07	0.53
1:D:79:PHE:CD1	1:D:79:PHE:N	2.76	0.53
1:D:58:ARG:N	1:D:59:PRO:HD3	2.24	0.53
1:D:85:ASP:CG	1:D:86:ALA:H	2.17	0.52
1:D:85:ASP:CG	1:D:86:ALA:N	2.67	0.52
1:D:100:TYR:CD1	1:D:100:TYR:C	2.87	0.52
1:C:267:PHE:CG	1:C:268:PHE:HB2	2.42	0.52
1:D:324:CYS:SG	1:D:326:ASN:CG	2.76	0.52
1:B:264:ARG:HH21	1:B:278:ASP:CG	2.18	0.52
1:D:261:GLU:OE1	1:D:261:GLU:N	2.32	0.52
1:D:322:GLU:HB3	1:D:324:CYS:SG	2.50	0.52
1:B:269:GLU:CB	1:B:270:ASP:CB	2.88	0.52
1:D:84:LEU:CD1	1:D:84:LEU:N	2.73	0.52
1:D:20:ASN:HB3	2:D:2019:HOH:O	2.10	0.51
1:B:241:GLN:OE1	1:B:269:GLU:O	0.54	0.51
1:A:125:GLN:OE1	1:D:125:GLN:CG	2.59	0.51
1:A:274:ASP:HB2	1:A:275:VAL:HG23	1.91	0.50
1:D:272:SER:H	1:D:274:ASP:H	1.58	0.50
1:A:277:GLN:HB2	1:A:279:ASP:H	1.76	0.50
1:D:94:VAL:O	1:D:95:VAL:HG13	2.11	0.50
1:D:259:VAL:HG12	1:D:264:ARG:HD3	1.93	0.50
1:A:277:GLN:HB2	1:A:279:ASP:N	2.27	0.50
1:D:272:SER:N	1:D:274:ASP:H	2.10	0.50
1:A:274:ASP:HA	1:A:275:VAL:CG2	2.34	0.50
1:D:271:LYS:CE	1:D:276:ILE:CA	2.87	0.50
1:D:23:PHE:CE2	1:D:313:GLN:N	2.79	0.49
1:C:269:GLU:HB3	1:C:271:LYS:HG2	1.94	0.49
1:A:274:ASP:C	1:A:275:VAL:CG2	2.85	0.49
1:D:94:VAL:O	1:D:95:VAL:CG1	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LYS:CE	1:B:28:GLU:OE2	2.60	0.49
1:A:267:PHE:HB2	1:A:277:GLN:HE21	1.78	0.49
1:B:267:PHE:HE2	1:B:284:LEU:CD1	2.26	0.49
1:A:1:MET:HE1	1:A:71:TYR:CE2	2.48	0.49
1:A:274:ASP:CB	1:A:275:VAL:CG2	2.65	0.49
1:A:192:GLN:CD	1:A:192:GLN:H	2.19	0.49
1:B:244:ILE:HG21	1:B:269:GLU:CG	2.42	0.48
1:D:241:GLN:CG	1:D:269:GLU:HB3	2.43	0.48
2:A:2042:HOH:O	1:B:40:LYS:HE3	2.14	0.48
1:C:192:GLN:H	1:C:192:GLN:NE2	2.11	0.48
1:C:274:ASP:CG	1:C:275:VAL:N	2.71	0.48
1:D:98:PRO:HD2	2:D:2042:HOH:O	2.12	0.48
1:D:1:MET:HB2	1:D:319:GLU:CD	2.39	0.48
1:D:319:GLU:C	1:D:320:LYS:CG	2.85	0.48
1:D:276:ILE:HD12	1:D:277:GLN:CA	2.44	0.47
1:D:113:MET:SD	1:D:200:VAL:HG11	2.54	0.47
1:D:95:VAL:HA	1:D:328:LEU:HD21	1.84	0.47
1:D:318:LEU:N	1:D:318:LEU:CD1	2.75	0.47
1:C:272:SER:HB2	1:C:274:ASP:O	2.15	0.47
1:D:309:GLU:OE2	2:D:2137:HOH:O	2.20	0.47
1:D:318:LEU:C	1:D:320:LYS:H	2.23	0.47
1:A:259:VAL:HG12	1:A:264:ARG:HH11	1.80	0.47
1:D:271:LYS:HZ1	1:D:276:ILE:HD13	1.73	0.47
1:C:275:VAL:HA	1:C:276:ILE:HA	1.60	0.46
1:D:84:LEU:N	1:D:84:LEU:HD13	2.29	0.46
1:B:58:ARG:N	1:B:59:PRO:CD	2.79	0.46
1:C:244:ILE:HD13	1:C:269:GLU:CG	2.42	0.46
1:D:93:GLN:C	1:D:94:VAL:HG23	2.40	0.46
1:D:325:PRO:O	1:D:326:ASN:C	2.54	0.46
1:C:269:GLU:C	1:C:271:LYS:HG3	2.41	0.46
2:C:2034:HOH:O	1:D:40:LYS:HE2	2.15	0.46
1:D:86:ALA:HA	1:D:89:GLU:HG2	1.98	0.46
1:A:267:PHE:HB2	1:A:277:GLN:NE2	2.31	0.46
1:B:257:MET:HE1	1:B:267:PHE:CD1	2.51	0.45
1:D:97:VAL:HG13	1:D:99:ALA:O	2.16	0.45
1:D:259:VAL:CG1	1:D:264:ARG:HD3	2.47	0.45
1:D:266:LEU:O	1:D:267:PHE:HD1	1.99	0.45
1:C:234:ARG:HG3	2:C:2104:HOH:O	2.17	0.45
1:C:267:PHE:CD1	1:C:268:PHE:CG	3.01	0.45
1:C:267:PHE:CD2	1:C:268:PHE:CE1	3.02	0.45
1:A:58:ARG:HH22	1:A:89:GLU:CD	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:TYR:HA	1:B:177:PRO:HD3	1.61	0.45
1:A:269:GLU:N	1:A:270:ASP:HA	2.31	0.45
1:A:277:GLN:CA	1:A:279:ASP:H	2.29	0.45
1:B:269:GLU:CB	1:B:270:ASP:HB3	2.46	0.45
1:D:84:LEU:HD13	1:D:84:LEU:H	1.82	0.45
1:C:192:GLN:H	1:C:192:GLN:HE21	1.64	0.45
1:A:40:LYS:CD	1:B:40:LYS:HG3	2.46	0.45
1:C:77:ALA:HA	1:C:97:VAL:O	2.16	0.45
1:A:192:GLN:CD	1:A:192:GLN:N	2.75	0.45
1:A:276:ILE:HG23	1:A:277:GLN:N	2.31	0.45
1:D:268:PHE:CG	1:D:269:GLU:HG2	2.51	0.45
1:A:276:ILE:CG1	1:A:277:GLN:N	2.78	0.44
1:B:191:LEU:HD23	1:B:191:LEU:HA	1.86	0.44
1:C:276:ILE:HA	1:C:276:ILE:HD12	1.83	0.44
1:B:174:ASP:OD1	1:B:175:PRO:HD2	2.18	0.44
1:B:274:ASP:CA	1:B:275:VAL:CG1	2.90	0.44
1:A:18:GLN:O	1:A:21:GLU:HG3	2.18	0.44
1:B:324:CYS:HA	1:B:325:PRO:HD2	1.90	0.44
1:D:288:HIS:HB2	1:D:290:VAL:HG23	2.00	0.43
1:B:261:GLU:HB2	2:B:2147:HOH:O	2.17	0.43
1:D:52:VAL:CG1	1:D:76:CYS:SG	3.06	0.43
1:D:73:ALA:HA	1:D:95:VAL:CG2	2.48	0.43
1:D:82:VAL:HB	1:D:84:LEU:HD11	2.01	0.43
1:D:103:GLU:O	1:D:107:GLU:HG3	2.19	0.43
1:A:1:MET:CE	1:A:71:TYR:HE2	2.31	0.43
1:B:58:ARG:HB3	1:B:59:PRO:HD3	2.01	0.43
1:D:94:VAL:O	1:D:327:ALA:HA	2.19	0.43
1:D:317:GLN:C	1:D:318:LEU:HD12	2.43	0.43
1:D:318:LEU:O	1:D:320:LYS:N	2.52	0.43
1:A:194:LEU:C	1:A:194:LEU:HD23	2.43	0.43
1:D:94:VAL:HG12	1:D:95:VAL:H	1.83	0.43
1:D:261:GLU:OE1	1:D:295:HIS:ND1	2.49	0.42
1:D:40:LYS:HB3	1:D:40:LYS:HE3	1.86	0.42
1:D:271:LYS:HE3	1:D:277:GLN:HG2	1.99	0.42
1:A:269:GLU:N	1:A:270:ASP:CB	2.82	0.42
1:B:269:GLU:CA	1:B:270:ASP:HB3	2.49	0.42
1:D:324:CYS:C	1:D:326:ASN:H	2.27	0.42
1:D:94:VAL:CG1	1:D:95:VAL:H	2.31	0.42
1:D:95:VAL:HG12	1:D:326:ASN:C	2.45	0.42
1:A:259:VAL:HG12	1:A:264:ARG:NH1	2.35	0.42
1:A:269:GLU:N	1:A:270:ASP:CA	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:ASP:HA	1:D:175:PRO:HD3	1.93	0.42
1:A:50:ILE:HG13	1:A:74:LEU:HD23	2.01	0.42
1:C:268:PHE:CB	1:C:280:VAL:HG11	2.49	0.42
1:D:317:GLN:HA	1:D:320:LYS:O	2.19	0.42
1:D:20:ASN:HA	1:D:312:LEU:HD23	2.02	0.42
1:D:77:ALA:HA	1:D:96:ARG:HD2	2.02	0.42
1:C:58:ARG:N	1:C:59:PRO:CD	2.83	0.41
1:D:268:PHE:CD1	1:D:269:GLU:N	2.88	0.41
1:A:267:PHE:C	1:A:268:PHE:HD1	2.28	0.41
1:A:277:GLN:OE1	1:A:278:ASP:CA	2.69	0.41
1:B:271:LYS:O	1:B:273:VAL:HG22	2.21	0.41
1:C:268:PHE:HB2	1:C:280:VAL:HG11	2.03	0.41
1:A:328:LEU:O	1:A:329:PHE:HB3	2.19	0.41
1:B:288:HIS:HB2	1:B:290:VAL:HG23	2.02	0.41
1:D:235:GLY:HA3	1:D:267:PHE:CZ	2.49	0.41
1:A:329:PHE:CD1	1:A:329:PHE:C	2.98	0.41
1:B:269:GLU:HB2	1:B:270:ASP:HB3	2.03	0.41
1:C:268:PHE:H	1:C:271:LYS:CE	2.33	0.41
1:D:23:PHE:CD2	1:D:312:LEU:HB3	2.55	0.41
1:D:194:LEU:HD23	1:D:194:LEU:C	2.45	0.41
1:C:268:PHE:H	1:C:271:LYS:HD3	1.83	0.41
1:D:82:VAL:O	1:D:84:LEU:HD13	2.21	0.41
1:D:274:ASP:CG	1:D:275:VAL:HG13	2.46	0.41
1:C:266:LEU:CD2	1:C:266:LEU:C	2.89	0.41
1:D:217:HIS:CD2	2:D:2041:HOH:O	2.73	0.41
1:C:274:ASP:OD1	1:C:275:VAL:N	2.54	0.40
1:D:274:ASP:HB3	1:D:275:VAL:CG2	2.51	0.40
1:A:40:LYS:HE2	2:B:2038:HOH:O	2.21	0.40
1:A:264:ARG:NH1	1:A:264:ARG:CG	2.73	0.40
1:D:273:VAL:O	1:D:273:VAL:CG1	2.69	0.40
1:B:125:GLN:HE22	1:D:128:ARG:HH22	1.67	0.40
1:D:271:LYS:HE3	1:D:276:ILE:CD1	2.51	0.40
1:B:269:GLU:HB2	1:B:270:ASP:CB	2.51	0.40
1:B:329:PHE:HB2	2:B:2057:HOH:O	2.20	0.40
1:B:1:MET:HE2	1:B:319:GLU:HG3	2.03	0.40
1:D:270:ASP:O	1:D:271:LYS:CD	2.70	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:C:66:LYS:NZ	1:C:270:ASP:O[4_445]	1.89	0.31

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	328/338 (97%)	320 (98%)	6 (2%)	2 (1%)	21	10
1	B	328/338 (97%)	324 (99%)	4 (1%)	0	100	100
1	C	327/338 (97%)	320 (98%)	6 (2%)	1 (0%)	36	26
1	D	327/338 (97%)	315 (96%)	9 (3%)	3 (1%)	14	4
All	All	1310/1352 (97%)	1279 (98%)	25 (2%)	6 (0%)	24	13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	GLU
1	C	274	ASP
1	D	318	LEU
1	D	273	VAL
1	D	269	GLU
1	A	276	ILE

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	273/281 (97%)	264 (97%)	9 (3%)	33	16
1	B	273/281 (97%)	261 (96%)	12 (4%)	25	9
1	C	272/281 (97%)	258 (95%)	14 (5%)	21	7
1	D	272/281 (97%)	250 (92%)	22 (8%)	11	2
All	All	1090/1124 (97%)	1033 (95%)	57 (5%)	21	6

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	88	LYS
1	A	110	ILE
1	A	264	ARG
1	A	266	LEU
1	A	268	PHE
1	A	273	VAL
1	A	275	VAL
1	A	330	LYS
1	B	110	ILE
1	B	215	LEU
1	B	241	GLN
1	B	266	LEU
1	B	269	GLU
1	B	271	LYS
1	B	273	VAL
1	B	275	VAL
1	B	276	ILE
1	B	277	GLN
1	B	320	LYS
1	B	330	LYS
1	C	13	LYS
1	C	177	PRO
1	C	179	THR
1	C	192	GLN
1	C	240	SER
1	C	266	LEU
1	C	267	PHE
1	C	268	PHE
1	C	270	ASP
1	C	271	LYS
1	C	272	SER
1	C	274	ASP

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Mol	Chain	Res	Type
1	C	275	VAL
1	C	276	ILE
1	D	1	MET
1	D	21	GLU
1	D	28	GLU
1	D	79	PHE
1	D	84	LEU
1	D	88	LYS
1	D	89	GLU
1	D	97	VAL
1	D	234	ARG
1	D	250	GLN
1	D	261	GLU
1	D	264	ARG
1	D	270	ASP
1	D	275	VAL
1	D	277	GLN
1	D	312	LEU
1	D	316	SER
1	D	317	GLN
1	D	319	GLU
1	D	320	LYS
1	D	324	CYS
1	D	326	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	213	HIS
1	A	222	GLN
1	A	296	GLN
1	B	17	GLN
1	B	80	ASN
1	B	241	GLN
1	B	277	GLN
1	B	296	GLN
1	C	53	ASN
1	C	125	GLN
1	C	192	GLN
1	C	296	GLN
1	D	10	GLN

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Mol	Chain	Res	Type
1	D	80	ASN
1	D	296	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 [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	330/338 (97%)	0.31	20 (6%)	27 29	8, 19, 44, 120	1 (0%)
1	B	330/338 (97%)	0.75	32 (9%)	13 15	10, 25, 57, 130	0
1	C	329/338 (97%)	0.61	24 (7%)	21 24	10, 22, 51, 132	0
1	D	329/338 (97%)	1.13	82 (24%)	2 1	8, 23, 65, 146	1 (0%)
All	All	1318/1352 (97%)	0.70	158 (11%)	9 10	8, 22, 58, 146	2 (0%)

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	273	VAL	14.9
1	C	268	PHE	10.9
1	D	323	ALA	10.4
1	D	267	PHE	10.0
1	C	267	PHE	9.9
1	B	276	ILE	9.7
1	D	268	PHE	8.7
1	A	267	PHE	8.5
1	A	276	ILE	8.5
1	B	275	VAL	8.5
1	D	266	LEU	8.0
1	B	268	PHE	7.9
1	A	275	VAL	7.8
1	B	273	VAL	7.8
1	A	273	VAL	7.8
1	D	273	VAL	7.7
1	D	329	PHE	7.3
1	C	266	LEU	7.1
1	D	275	VAL	6.6
1	B	271	LYS	6.5
1	C	276	ILE	6.5

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Mol	Chain	Res	Type	RSRZ
1	D	327	ALA	6.5
1	D	97	VAL	6.5
1	A	268	PHE	6.4
1	C	274	ASP	6.4
1	D	324	CYS	6.3
1	D	276	ILE	6.3
1	C	275	VAL	6.2
1	C	329	PHE	6.2
1	C	272	SER	6.1
1	D	326	ASN	6.1
1	D	84	LEU	6.1
1	D	78	GLY	5.9
1	B	266	LEU	5.8
1	D	321	GLY	5.7
1	D	79	PHE	5.7
1	C	271	LYS	5.5
1	B	323	ALA	5.4
1	B	267	PHE	5.3
1	D	325	PRO	5.2
1	B	272	SER	5.2
1	D	98	PRO	5.2
1	D	328	LEU	5.0
1	A	266	LEU	5.0
1	D	95	VAL	5.0
1	D	100	TYR	4.8
1	C	269	GLU	4.8
1	A	274	ASP	4.7
1	D	77	ALA	4.6
1	D	92	LEU	4.6
1	D	269	GLU	4.5
1	D	82	VAL	4.5
1	B	270	ASP	4.4
1	B	274	ASP	4.4
1	C	323	ALA	4.4
1	D	272	SER	4.3
1	D	94	VAL	4.3
1	A	265	ASP	4.3
1	D	81	ASN	4.3
1	A	264	ARG	4.2
1	C	277	GLN	4.1
1	D	99	ALA	4.1
1	D	76	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	329	PHE	4.0
1	A	271	LYS	4.0
1	C	262	ASN	4.0
1	D	274	ASP	3.9
1	D	315	LEU	3.9
1	D	316	SER	3.9
1	D	318	LEU	3.8
1	C	270	ASP	3.8
1	A	329	PHE	3.8
1	D	74	LEU	3.7
1	D	87	ALA	3.7
1	D	265	ASP	3.6
1	A	330	LYS	3.6
1	B	321	GLY	3.5
1	B	264	ARG	3.4
1	D	264	ARG	3.4
1	D	22	ALA	3.4
1	D	270	ASP	3.4
1	C	264	ARG	3.3
1	D	310	THR	3.3
1	C	265	ASP	3.3
1	D	80	ASN	3.3
1	D	57	SER	3.3
1	D	71	TYR	3.2
1	D	72	ILE	3.2
1	B	175	PRO	3.2
1	D	262	ASN	3.2
1	D	86	ALA	3.2
1	B	179	THR	3.2
1	D	52	VAL	3.2
1	D	271	LYS	3.2
1	D	85	ASP	3.2
1	B	176	TYR	3.1
1	B	182	LEU	3.1
1	D	25	PHE	3.1
1	D	260	TYR	3.1
1	B	330	LYS	3.1
1	A	272	SER	3.0
1	A	277	GLN	3.0
1	D	313	GLN	3.0
1	B	277	GLN	3.0
1	D	73	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	277	GLN	2.9
1	D	314	ASN	2.8
1	D	96	ARG	2.8
1	D	317	GLN	2.8
1	A	269	GLU	2.8
1	D	322	GLU	2.7
1	B	177	PRO	2.7
1	B	269	GLU	2.7
1	D	320	LYS	2.7
1	D	83	ASP	2.7
1	A	43	ASN	2.7
1	B	241	GLN	2.6
1	B	324	CYS	2.6
1	D	312	LEU	2.6
1	D	89	GLU	2.6
1	B	262	ASN	2.6
1	B	193	THR	2.6
1	D	280	VAL	2.6
1	D	93	GLN	2.5
1	D	90	LEU	2.5
1	D	70	LYS	2.5
1	A	262	ASN	2.5
1	B	90	LEU	2.5
1	D	307	ILE	2.5
1	D	58	ARG	2.5
1	B	180	ALA	2.5
1	D	59	PRO	2.5
1	C	176	TYR	2.4
1	D	249	ASN	2.4
1	D	23	PHE	2.4
1	A	270	ASP	2.4
1	B	265	ASP	2.3
1	D	261	GLU	2.3
1	D	263	GLU	2.3
1	A	279	ASP	2.3
1	C	321	GLY	2.2
1	B	191	LEU	2.2
1	D	69	VAL	2.2
1	C	31	ASP	2.2
1	D	88	LYS	2.2
1	C	179	THR	2.2
1	A	278	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	279	ASP	2.2
1	C	207	LEU	2.2
1	C	209	PRO	2.2
1	B	320	LYS	2.2
1	D	298	PHE	2.1
1	D	278	ASP	2.1
1	C	241	GLN	2.1
1	D	129	ASP	2.1
1	B	214	LEU	2.0
1	D	287	CYS	2.0
1	D	56	GLY	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.