



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:02 PM UTC

PDB ID : 1OFP / pdb_00001ofp
Title : CRYSTAL STRUCTURE OF THE TYROSINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE FROM SACCHAROMYCES CEREVISIAE
Authors : Koenig, V.; Pfeil, A.; Heinrich, G.; Braus, G.H.; Schneider, T.R.
Deposited on : 2003-04-17
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

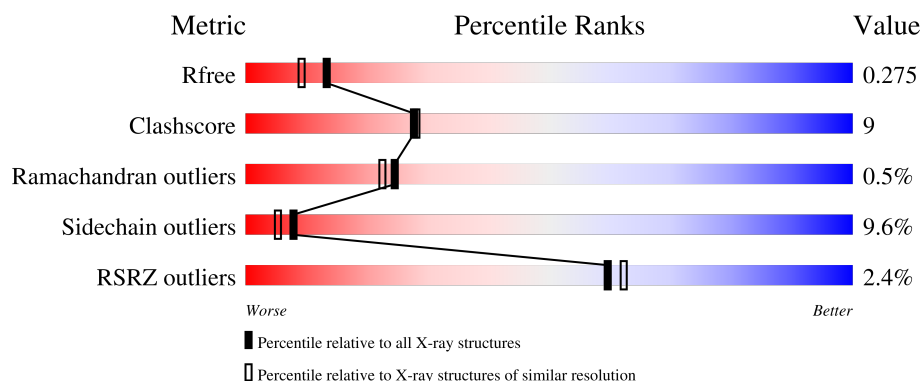
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	370	2% 37% 35% 9% • 17%
1	B	370	% 44% 35% 7% • 13%
1	C	370	2% 44% 35% 6% • 14%
1	D	370	2% 45% 34% 5% • 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9328 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 PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	1
			2222	1400	395	418	9			
1	B	322	Total	C	N	O	S	0	0	1
			2376	1489	429	448	10			
1	C	319	Total	C	N	O	S	0	0	1
			2322	1454	415	444	9			
1	D	315	Total	C	N	O	S	0	0	1
			2305	1448	416	432	9			

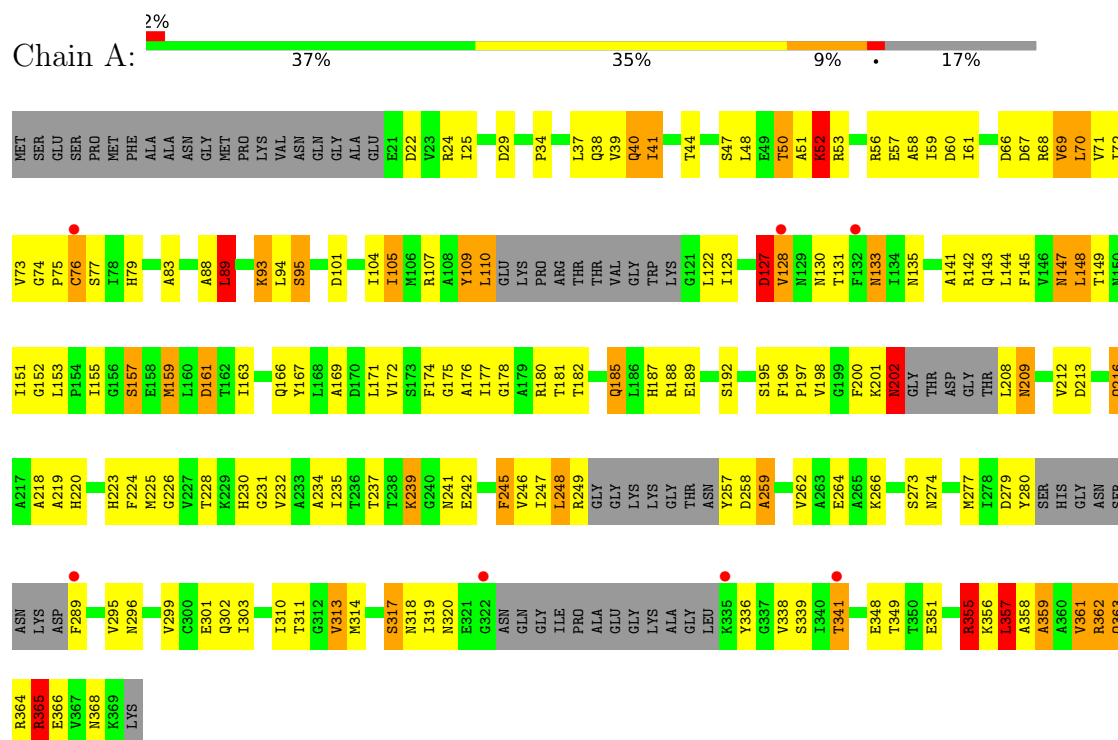
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	B	33	Total	O	0	0
			33	33		
2	C	23	Total	O	0	0
			23	23		
2	D	26	Total	O	0	0
			26	26		

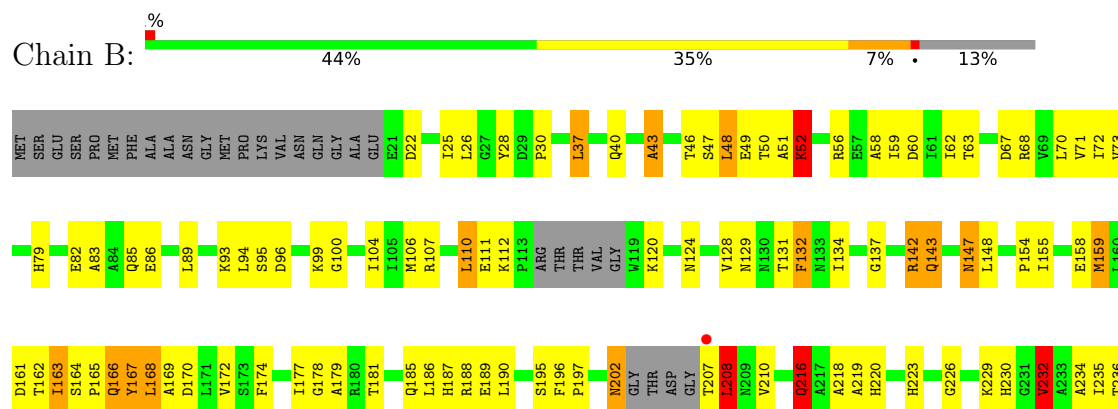
3 Residue-property plots

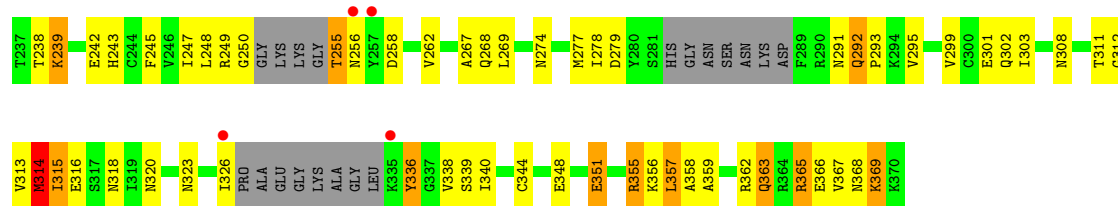
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

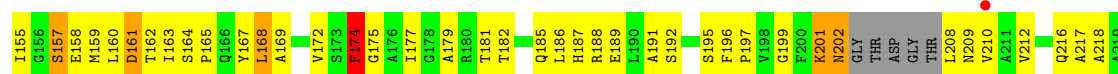
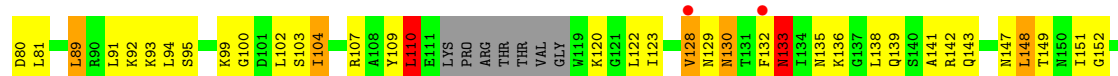
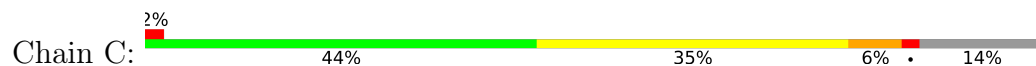


• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

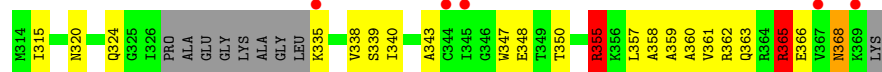
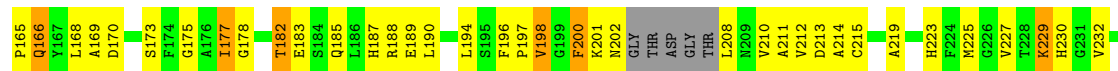
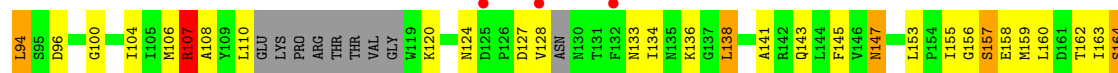
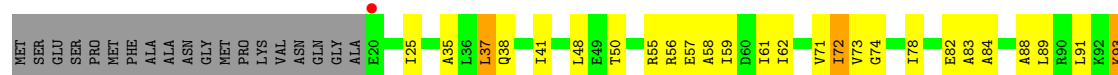




• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE



• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.59Å 69.00Å 102.45Å 106.38° 101.48° 94.81°	Depositor
Resolution (Å)	19.88 – 2.10 19.88 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.88-2.10) 98.5 (19.88-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.205 , 0.260 (Not available) , 0.275	Depositor DCC
R_{free} test set	3800 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9328	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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	2.61	147/2250 (6.5%)	1.86	50/3058 (1.6%)
1	B	2.46	129/2408 (5.4%)	1.74	30/3270 (0.9%)
1	C	2.50	119/2353 (5.1%)	1.80	32/3200 (1.0%)
1	D	2.54	129/2335 (5.5%)	1.86	41/3169 (1.3%)
All	All	2.53	524/9346 (5.6%)	1.82	153/12697 (1.2%)

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	1
1	C	0	1
All	All	0	2

All (524) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	VAL	C-O	-12.88	1.10	1.24
1	C	35	ALA	CA-CB	12.61	1.72	1.53
1	D	277	MET	SD-CE	12.58	2.10	1.79
1	B	359	ALA	CA-CB	12.24	1.72	1.53
1	C	70	LEU	C-O	-12.22	1.09	1.24
1	C	210	VAL	CA-CB	12.08	1.68	1.54
1	C	247	ILE	CA-CB	-11.86	1.39	1.54
1	A	348	GLU	CA-CB	11.66	1.72	1.53
1	B	51	ALA	CA-CB	-10.89	1.35	1.53
1	D	71	VAL	C-O	-10.84	1.12	1.24
1	B	158	GLU	CA-CB	10.68	1.68	1.53
1	D	120	LYS	CA-C	10.55	1.67	1.52
1	D	247	ILE	CA-CB	-10.48	1.42	1.54
1	A	128	VAL	CA-CB	10.41	1.68	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	ILE	C-O	-10.28	1.13	1.24
1	A	148	LEU	C-O	10.15	1.35	1.24
1	A	313	VAL	C-O	-10.05	1.12	1.23
1	B	111	GLU	CA-CB	9.82	1.69	1.53
1	D	82	GLU	CA-CB	9.48	1.68	1.53
1	C	104	ILE	C-O	-9.43	1.13	1.24
1	B	279	ASP	C-O	-9.42	1.12	1.24
1	A	311	THR	CA-C	-9.28	1.40	1.52
1	B	155	ILE	CA-CB	-9.25	1.39	1.54
1	D	358	ALA	N-CA	-9.25	1.35	1.46
1	A	59	ILE	CA-CB	9.20	1.65	1.54
1	C	158	GLU	CA-CB	9.17	1.66	1.53
1	D	104	ILE	C-O	-9.15	1.14	1.24
1	D	147	ASN	N-CA	9.01	1.57	1.46
1	D	62	ILE	CA-CB	9.01	1.65	1.54
1	C	128	VAL	CA-CB	9.01	1.66	1.54
1	A	358	ALA	C-O	8.99	1.34	1.24
1	D	59	ILE	C-O	-8.97	1.14	1.24
1	D	310	ILE	CA-C	-8.91	1.43	1.52
1	A	318	ASN	CA-C	8.86	1.64	1.52
1	C	169	ALA	CA-CB	8.80	1.67	1.53
1	B	137	GLY	CA-C	-8.79	1.42	1.52
1	D	78	ILE	C-O	8.71	1.34	1.24
1	C	359	ALA	CA-CB	8.69	1.66	1.53
1	D	41	ILE	CA-C	-8.67	1.43	1.52
1	D	309	ALA	CA-CB	-8.67	1.38	1.53
1	D	196	PHE	C-O	-8.66	1.15	1.24
1	B	177	ILE	CA-CB	-8.63	1.43	1.54
1	A	178	GLY	C-O	8.63	1.36	1.23
1	A	176	ALA	C-O	-8.57	1.14	1.24
1	D	37	LEU	C-O	-8.55	1.13	1.24
1	A	73	VAL	CA-C	-8.51	1.41	1.52
1	A	58	ALA	CA-C	-8.47	1.41	1.52
1	B	112	LYS	CA-C	8.46	1.61	1.52
1	D	61	ILE	CA-C	-8.40	1.41	1.52
1	D	169	ALA	CA-CB	8.37	1.67	1.53
1	A	185	GLN	C-O	8.34	1.33	1.24
1	C	220	HIS	C-O	8.34	1.34	1.23
1	A	247	ILE	CA-CB	-8.33	1.44	1.54
1	C	314	MET	C-O	-8.27	1.14	1.24
1	B	112	LYS	C-O	8.26	1.33	1.24
1	B	340	ILE	C-O	-8.15	1.12	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	106	MET	C-O	-8.14	1.14	1.24
1	A	155	ILE	C-O	8.13	1.32	1.24
1	D	159	MET	SD-CE	8.11	1.99	1.79
1	B	169	ALA	CA-CB	8.09	1.66	1.53
1	D	134	ILE	C-O	-8.09	1.14	1.24
1	D	248	LEU	CG-CD2	-8.07	1.25	1.52
1	D	298	VAL	CA-CB	-8.01	1.43	1.54
1	A	52	LYS	CG-CD	7.99	1.76	1.52
1	B	104	ILE	C-O	-7.98	1.15	1.24
1	A	363	GLN	C-O	7.96	1.34	1.24
1	B	82	GLU	CA-CB	7.92	1.66	1.53
1	A	277	MET	SD-CE	7.90	1.99	1.79
1	D	141	ALA	CA-CB	-7.90	1.41	1.53
1	B	314	MET	SD-CE	-7.88	1.59	1.79
1	D	368	ASN	C-N	-7.87	1.22	1.33
1	A	72	ILE	C-O	-7.86	1.15	1.24
1	C	217	ALA	CA-CB	7.85	1.66	1.53
1	B	223	HIS	C-O	-7.84	1.15	1.24
1	C	187	HIS	C-O	-7.82	1.14	1.24
1	A	69	VAL	C-O	-7.80	1.14	1.24
1	D	359	ALA	CA-CB	7.78	1.65	1.53
1	C	189	GLU	CA-C	-7.76	1.42	1.52
1	C	223	HIS	CA-C	-7.75	1.43	1.52
1	D	219	ALA	CA-CB	7.74	1.66	1.53
1	D	25	ILE	CA-CB	-7.72	1.44	1.53
1	B	106	MET	CA-C	-7.70	1.43	1.52
1	C	369	LYS	C-N	-7.69	1.22	1.33
1	B	51	ALA	N-CA	7.66	1.55	1.46
1	A	159	MET	SD-CE	7.64	1.98	1.79
1	A	224	PHE	CA-C	7.60	1.62	1.52
1	B	235	ILE	CA-CB	-7.58	1.45	1.53
1	C	25	ILE	CA-CB	-7.55	1.45	1.53
1	B	134	ILE	CA-CB	-7.55	1.44	1.54
1	A	104	ILE	N-CA	-7.53	1.37	1.46
1	C	149	THR	CA-CB	-7.51	1.40	1.53
1	D	340	ILE	C-O	-7.51	1.13	1.24
1	B	181	THR	C-O	-7.51	1.13	1.24
1	C	209	ASN	C-O	-7.51	1.15	1.24
1	B	348	GLU	CA-CB	7.50	1.65	1.53
1	D	200	PHE	C-O	7.49	1.32	1.24
1	D	57	GLU	CA-C	-7.46	1.42	1.52
1	C	41	ILE	CA-CB	-7.44	1.44	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	MET	CG-SD	-7.43	1.62	1.80
1	A	61	ILE	CA-C	-7.41	1.43	1.52
1	C	49	GLU	CA-CB	7.38	1.65	1.53
1	D	59	ILE	CA-CB	7.37	1.63	1.54
1	D	35	ALA	CA-CB	7.36	1.65	1.53
1	C	159	MET	CG-SD	-7.36	1.62	1.80
1	B	358	ALA	C-O	7.36	1.32	1.24
1	C	138	LEU	CA-C	-7.35	1.43	1.52
1	A	357	LEU	CA-CB	7.35	1.64	1.53
1	A	107	ARG	CA-C	-7.35	1.43	1.52
1	D	338	VAL	CA-CB	7.35	1.63	1.54
1	B	303	ILE	N-CA	-7.34	1.37	1.46
1	A	41	ILE	CA-CB	-7.34	1.44	1.54
1	C	277	MET	SD-CE	7.33	1.97	1.79
1	B	295	VAL	N-CA	-7.30	1.37	1.46
1	A	368	ASN	C-N	-7.28	1.23	1.33
1	B	210	VAL	C-O	-7.28	1.14	1.24
1	B	158	GLU	CA-C	-7.28	1.43	1.52
1	A	70	LEU	C-N	-7.27	1.24	1.33
1	B	52	LYS	CD-CE	7.27	1.74	1.52
1	B	302	GLN	N-CA	7.27	1.55	1.46
1	A	232	VAL	C-O	-7.24	1.16	1.24
1	B	49	GLU	CA-CB	7.20	1.64	1.53
1	D	347	TRP	C-O	7.19	1.32	1.24
1	D	73	VAL	CA-CB	7.18	1.63	1.54
1	A	358	ALA	N-CA	-7.17	1.37	1.46
1	A	159	MET	C-O	7.16	1.32	1.24
1	A	187	HIS	C-O	-7.14	1.15	1.24
1	A	338	VAL	C-O	7.13	1.31	1.24
1	A	248	LEU	CG-CD2	-7.10	1.29	1.52
1	C	202	ASN	CB-CG	-7.09	1.34	1.52
1	B	178	GLY	C-O	7.08	1.34	1.23
1	B	142	ARG	CB-CG	-7.08	1.31	1.52
1	A	68	ARG	C-O	7.07	1.33	1.23
1	C	358	ALA	C-O	7.07	1.32	1.24
1	A	218	ALA	N-CA	-7.07	1.36	1.46
1	D	177	ILE	CA-CB	-7.06	1.45	1.54
1	A	163	ILE	C-O	-7.06	1.17	1.24
1	A	358	ALA	CA-CB	-7.05	1.42	1.53
1	A	181	THR	C-O	-7.04	1.15	1.24
1	C	61	ILE	CA-C	-7.04	1.44	1.52
1	D	246	VAL	CA-CB	-7.04	1.45	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	153	LEU	CA-C	7.02	1.60	1.52
1	A	295	VAL	CA-CB	7.01	1.62	1.54
1	A	73	VAL	C-O	-7.00	1.16	1.23
1	C	155	ILE	CA-C	-6.99	1.44	1.52
1	C	350	THR	C-O	-6.98	1.16	1.24
1	D	160	LEU	N-CA	6.93	1.55	1.46
1	D	59	ILE	C-N	-6.93	1.25	1.33
1	A	247	ILE	C-O	6.91	1.31	1.24
1	B	339	SER	C-O	6.91	1.31	1.23
1	D	163	ILE	CA-C	-6.89	1.45	1.53
1	A	313	VAL	CA-CB	6.87	1.66	1.55
1	A	279	ASP	CA-C	6.86	1.61	1.52
1	A	220	HIS	C-O	6.86	1.32	1.23
1	C	277	MET	N-CA	-6.85	1.37	1.46
1	C	39	VAL	CA-CB	6.81	1.63	1.54
1	C	290	ARG	CA-CB	6.77	1.64	1.53
1	C	135	ASN	N-CA	6.76	1.54	1.46
1	D	73	VAL	C-O	-6.75	1.17	1.24
1	C	120	LYS	CA-CB	6.75	1.65	1.53
1	A	289	PHE	CA-CB	6.74	1.67	1.53
1	D	350	THR	N-CA	6.74	1.54	1.46
1	A	163	ILE	CA-C	-6.71	1.45	1.53
1	B	59	ILE	CA-CB	6.70	1.62	1.54
1	C	148	LEU	C-O	6.70	1.32	1.24
1	A	262	VAL	CA-CB	-6.67	1.46	1.54
1	D	189	GLU	CA-C	-6.65	1.44	1.52
1	D	359	ALA	CA-C	-6.64	1.43	1.52
1	D	56	ARG	N-CA	6.64	1.54	1.46
1	A	105	ILE	C-O	-6.63	1.17	1.24
1	B	355	ARG	CG-CD	6.63	1.72	1.52
1	A	311	THR	CB-OG1	6.62	1.54	1.43
1	D	120	LYS	N-CA	6.62	1.54	1.46
1	A	182	THR	CA-CB	6.62	1.63	1.53
1	D	262	VAL	CA-CB	-6.61	1.45	1.54
1	D	164	SER	CA-C	6.61	1.61	1.52
1	D	182	THR	C-O	-6.60	1.16	1.24
1	C	160	LEU	C-O	-6.60	1.15	1.23
1	D	50	THR	CA-CB	-6.58	1.43	1.53
1	A	147	ASN	N-CA	6.58	1.54	1.46
1	B	358	ALA	CA-CB	-6.57	1.43	1.53
1	A	198	VAL	C-O	-6.56	1.17	1.24
1	B	164	SER	C-O	-6.54	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	123	ILE	CA-C	-6.53	1.43	1.52
1	D	299	VAL	CA-C	-6.53	1.44	1.52
1	D	213	ASP	CA-C	6.53	1.61	1.52
1	D	168	LEU	CG-CD2	-6.52	1.31	1.52
1	B	63	THR	CA-C	6.52	1.62	1.52
1	A	219	ALA	CA-C	6.51	1.61	1.52
1	D	93	LYS	N-CA	6.51	1.53	1.46
1	A	231	GLY	C-O	-6.50	1.15	1.24
1	B	248	LEU	CG-CD2	-6.49	1.31	1.52
1	C	143	GLN	CD-NE2	-6.49	1.19	1.33
1	B	132	PHE	C-O	6.49	1.32	1.23
1	B	229	LYS	CA-CB	6.46	1.65	1.53
1	B	362	ARG	N-CA	6.46	1.54	1.46
1	A	171	LEU	CA-CB	-6.45	1.42	1.53
1	D	104	ILE	N-CA	-6.44	1.38	1.46
1	B	369	LYS	C-N	-6.43	1.24	1.33
1	A	127	ASP	CA-C	6.42	1.61	1.52
1	B	168	LEU	CG-CD2	-6.40	1.31	1.52
1	A	153	LEU	CA-C	6.39	1.60	1.52
1	A	58	ALA	CA-CB	6.39	1.63	1.53
1	A	224	PHE	C-O	-6.37	1.15	1.23
1	D	178	GLY	C-O	6.37	1.33	1.23
1	A	89	LEU	CA-CB	-6.37	1.43	1.53
1	C	232	VAL	C-O	-6.37	1.16	1.24
1	A	228	THR	C-O	-6.36	1.15	1.23
1	B	99	LYS	N-CA	6.33	1.54	1.46
1	B	82	GLU	CA-C	-6.33	1.43	1.52
1	C	69	VAL	C-O	-6.33	1.15	1.24
1	D	247	ILE	CA-C	6.32	1.60	1.52
1	C	163	ILE	C-O	-6.32	1.18	1.24
1	D	155	ILE	CA-C	-6.32	1.45	1.52
1	D	107	ARG	CG-CD	6.30	1.71	1.52
1	D	187	HIS	C-O	-6.30	1.16	1.24
1	D	197	PRO	N-CA	-6.29	1.39	1.47
1	B	311	THR	CB-CG2	6.28	1.73	1.52
1	B	235	ILE	C-O	-6.27	1.16	1.23
1	B	219	ALA	CA-CB	6.27	1.64	1.53
1	B	269	LEU	CA-C	6.26	1.59	1.52
1	C	365	ARG	CA-C	6.26	1.61	1.52
1	C	132	PHE	C-O	6.24	1.31	1.23
1	D	362	ARG	N-CA	6.24	1.53	1.46
1	C	162	THR	CA-CB	-6.22	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	MET	CA-C	6.20	1.60	1.52
1	B	355	ARG	N-CA	6.20	1.54	1.46
1	D	106	MET	CA-CB	-6.20	1.44	1.53
1	D	41	ILE	CA-CB	-6.19	1.46	1.54
1	B	85	GLN	CA-CB	6.19	1.62	1.53
1	A	51	ALA	N-CA	6.19	1.53	1.46
1	B	358	ALA	CA-C	6.18	1.61	1.52
1	C	310	ILE	CA-CB	6.18	1.60	1.53
1	C	102	LEU	CA-C	-6.17	1.44	1.52
1	C	52	LYS	N-CA	6.16	1.53	1.46
1	A	226	GLY	N-CA	6.16	1.50	1.45
1	D	147	ASN	CA-C	6.15	1.60	1.52
1	A	75	PRO	C-O	6.14	1.30	1.23
1	B	52	LYS	CA-CB	6.14	1.62	1.53
1	A	180	ARG	CA-C	6.14	1.61	1.52
1	D	360	ALA	CA-CB	-6.12	1.42	1.53
1	A	365	ARG	CA-C	6.12	1.61	1.52
1	B	50	THR	CA-CB	-6.11	1.43	1.53
1	A	83	ALA	C-O	6.11	1.31	1.24
1	C	225	MET	C-O	-6.11	1.16	1.24
1	C	362	ARG	N-CA	6.09	1.53	1.46
1	A	209	ASN	C-O	-6.08	1.16	1.24
1	B	236	THR	C-O	-6.08	1.16	1.24
1	B	367	VAL	CA-CB	-6.06	1.47	1.54
1	A	52	LYS	CA-CB	6.06	1.62	1.53
1	C	365	ARG	CG-CD	6.05	1.70	1.52
1	B	262	VAL	C-O	-6.04	1.17	1.24
1	A	213	ASP	CG-OD1	6.04	1.36	1.25
1	B	131	THR	CA-CB	6.04	1.63	1.53
1	B	163	ILE	CA-C	-6.03	1.46	1.52
1	C	99	LYS	CA-C	-6.03	1.44	1.52
1	B	58	ALA	N-CA	6.01	1.53	1.46
1	A	144	LEU	C-O	-6.01	1.17	1.24
1	A	310	ILE	CA-C	-6.00	1.46	1.52
1	D	155	ILE	CA-CB	-6.00	1.44	1.54
1	A	339	SER	CA-C	6.00	1.60	1.52
1	C	188	ARG	C-O	-6.00	1.17	1.24
1	B	277	MET	N-CA	-5.99	1.38	1.46
1	A	192	SER	CA-C	-5.96	1.44	1.52
1	C	296	ASN	C-O	5.96	1.31	1.24
1	B	170	ASP	CG-OD1	5.95	1.36	1.25
1	D	72	ILE	C-O	-5.95	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	215	CYS	N-CA	-5.95	1.39	1.46
1	A	39	VAL	CA-CB	5.95	1.62	1.54
1	A	301	GLU	C-O	5.94	1.31	1.24
1	C	355	ARG	CA-C	-5.94	1.45	1.52
1	D	358	ALA	C-O	5.92	1.30	1.24
1	A	245	PHE	C-O	5.92	1.31	1.23
1	A	22	ASP	CA-CB	5.91	1.62	1.53
1	D	237	THR	CA-CB	5.90	1.62	1.53
1	A	131	THR	C-O	5.90	1.31	1.23
1	B	147	ASN	N-CA	5.89	1.53	1.46
1	C	302	GLN	C-O	-5.89	1.17	1.24
1	C	120	LYS	CA-C	5.88	1.61	1.52
1	A	77	SER	CA-C	-5.87	1.45	1.52
1	A	93	LYS	CD-CE	5.87	1.70	1.52
1	C	366	GLU	N-CA	5.86	1.53	1.46
1	B	142	ARG	NE-CZ	-5.86	1.26	1.33
1	A	155	ILE	CA-CB	-5.85	1.46	1.55
1	C	348	GLU	CA-CB	5.85	1.62	1.53
1	B	278	ILE	CA-CB	5.85	1.61	1.54
1	A	122	LEU	N-CA	5.84	1.53	1.46
1	B	234	ALA	CA-CB	-5.82	1.44	1.53
1	A	44	THR	CA-C	-5.82	1.45	1.52
1	D	313	VAL	CA-CB	5.82	1.65	1.55
1	C	99	LYS	CA-CB	5.79	1.63	1.53
1	B	268	GLN	CA-C	-5.79	1.44	1.52
1	B	106	MET	N-CA	-5.79	1.38	1.46
1	C	53	ARG	N-CA	-5.79	1.39	1.46
1	B	110	LEU	C-O	5.78	1.31	1.24
1	D	133	ASN	C-O	-5.77	1.17	1.23
1	A	107	ARG	CG-CD	5.77	1.69	1.52
1	C	236	THR	C-O	-5.76	1.17	1.24
1	D	108	ALA	CA-C	-5.76	1.44	1.53
1	A	159	MET	CG-SD	-5.76	1.66	1.80
1	C	224	PHE	C-O	-5.75	1.17	1.23
1	D	211	ALA	CA-CB	-5.75	1.44	1.53
1	D	157	SER	CB-OG	5.75	1.53	1.42
1	B	185	GLN	N-CA	-5.74	1.39	1.46
1	D	214	ALA	C-O	-5.74	1.17	1.24
1	C	357	LEU	C-O	-5.73	1.17	1.24
1	B	165	PRO	CA-CB	5.73	1.62	1.53
1	C	195	SER	N-CA	-5.73	1.38	1.46
1	A	212	VAL	CA-CB	5.73	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	ASN	CA-C	5.72	1.60	1.52
1	D	83	ALA	C-O	5.71	1.30	1.24
1	C	65	LYS	CG-CD	5.71	1.69	1.52
1	D	157	SER	CA-C	-5.71	1.45	1.52
1	A	359	ALA	CA-CB	5.71	1.62	1.53
1	A	311	THR	C-O	-5.69	1.16	1.24
1	A	22	ASP	N-CA	-5.69	1.38	1.46
1	D	358	ALA	CA-CB	-5.68	1.44	1.53
1	C	33	SER	CA-C	-5.66	1.45	1.53
1	C	172	VAL	CB-CG1	-5.66	1.33	1.52
1	C	148	LEU	CG-CD1	-5.65	1.33	1.52
1	C	43	ALA	N-CA	-5.65	1.38	1.45
1	B	52	LYS	CE-NZ	5.65	1.66	1.49
1	C	296	ASN	N-CA	-5.65	1.39	1.46
1	D	279	ASP	C-O	-5.65	1.17	1.24
1	D	343	ALA	CA-CB	5.64	1.61	1.53
1	B	104	ILE	CA-CB	5.64	1.61	1.54
1	D	261	SER	N-CA	5.63	1.53	1.46
1	A	79	HIS	CA-C	5.62	1.59	1.52
1	C	54	GLY	CA-C	5.62	1.58	1.52
1	C	157	SER	CB-OG	5.62	1.53	1.42
1	B	167	TYR	CZ-OH	-5.62	1.26	1.38
1	C	225	MET	CG-SD	5.62	1.94	1.80
1	A	336	TYR	C-O	5.61	1.30	1.24
1	D	194	LEU	CA-C	-5.60	1.45	1.52
1	A	180	ARG	CA-CB	5.60	1.62	1.53
1	A	274	ASN	N-CA	-5.59	1.38	1.45
1	D	74	GLY	N-CA	5.58	1.52	1.44
1	A	101	ASP	CA-C	5.57	1.59	1.52
1	B	226	GLY	C-O	-5.57	1.16	1.23
1	A	52	LYS	CB-CG	5.57	1.69	1.52
1	A	188	ARG	NE-CZ	-5.56	1.26	1.33
1	D	58	ALA	CA-CB	5.56	1.62	1.53
1	A	145	PHE	N-CA	-5.55	1.39	1.46
1	C	177	ILE	CG1-CD1	-5.55	1.30	1.51
1	B	148	LEU	C-O	5.54	1.30	1.24
1	C	71	VAL	CB-CG1	-5.54	1.34	1.52
1	D	290	ARG	CA-CB	5.54	1.63	1.53
1	D	183	GLU	C-O	-5.54	1.16	1.24
1	A	41	ILE	CG1-CD1	-5.54	1.30	1.51
1	D	159	MET	C-O	5.53	1.30	1.23
1	B	172	VAL	N-CA	-5.53	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	SER	CA-C	-5.53	1.45	1.52
1	A	365	ARG	C-O	5.52	1.30	1.24
1	B	239	LYS	CA-C	-5.52	1.45	1.52
1	C	158	GLU	CA-C	-5.52	1.46	1.52
1	B	292	GLN	CA-CB	5.51	1.60	1.53
1	C	78	ILE	CG1-CD1	-5.51	1.30	1.51
1	D	365	ARG	NE-CZ	-5.50	1.26	1.33
1	C	56	ARG	CG-CD	5.49	1.69	1.52
1	C	358	ALA	N-CA	-5.49	1.39	1.46
1	A	169	ALA	CA-CB	5.49	1.62	1.53
1	A	355	ARG	CG-CD	5.48	1.68	1.52
1	B	154	PRO	CA-CB	5.47	1.61	1.53
1	B	59	ILE	C-O	-5.47	1.18	1.24
1	A	364	ARG	CD-NE	-5.47	1.38	1.46
1	A	259	ALA	CA-CB	5.46	1.62	1.53
1	C	295	VAL	N-CA	-5.46	1.39	1.46
1	A	88	ALA	CA-C	5.46	1.59	1.52
1	C	229	LYS	CA-C	-5.46	1.45	1.52
1	A	41	ILE	CA-C	-5.46	1.47	1.52
1	D	136	LYS	C-O	-5.46	1.17	1.24
1	B	338	VAL	CA-CB	5.46	1.61	1.54
1	A	172	VAL	CA-C	-5.45	1.46	1.52
1	A	25	ILE	C-O	-5.45	1.18	1.24
1	B	190	LEU	N-CA	5.45	1.52	1.46
1	D	170	ASP	CA-C	5.45	1.60	1.52
1	B	262	VAL	N-CA	-5.44	1.40	1.46
1	B	277	MET	SD-CE	5.43	1.93	1.79
1	C	185	GLN	N-CA	-5.43	1.39	1.46
1	C	93	LYS	N-CA	5.42	1.52	1.46
1	C	302	GLN	CB-CG	-5.42	1.36	1.52
1	B	197	PRO	N-CA	-5.42	1.40	1.47
1	C	192	SER	CA-C	-5.42	1.45	1.52
1	B	43	ALA	N-CA	-5.41	1.39	1.46
1	B	60	ASP	CG-OD2	5.41	1.35	1.25
1	C	297	ASP	CA-C	-5.41	1.45	1.52
1	A	356	LYS	C-O	5.41	1.30	1.24
1	B	232	VAL	CB-CG2	-5.41	1.34	1.52
1	B	238	THR	CA-CB	-5.41	1.45	1.53
1	D	201	LYS	CA-C	-5.41	1.45	1.52
1	D	302	GLN	CA-C	-5.41	1.45	1.52
1	C	72	ILE	C-O	-5.40	1.18	1.24
1	C	43	ALA	CA-CB	-5.40	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	143	GLN	N-CA	5.40	1.52	1.46
1	B	226	GLY	CA-C	5.40	1.59	1.51
1	A	225	MET	CA-C	-5.39	1.45	1.52
1	C	142	ARG	CZ-NH2	-5.39	1.26	1.33
1	B	315	ILE	CA-CB	5.39	1.61	1.54
1	C	312	GLY	C-O	-5.39	1.18	1.24
1	D	156	GLY	N-CA	-5.38	1.39	1.45
1	B	73	VAL	C-O	-5.38	1.18	1.24
1	A	314	MET	CG-SD	5.37	1.94	1.80
1	C	181	THR	C-O	-5.37	1.17	1.24
1	C	340	ILE	CA-CB	5.36	1.61	1.54
1	C	324	GLN	C-O	5.36	1.30	1.23
1	B	355	ARG	C-O	-5.36	1.17	1.24
1	C	210	VAL	CA-C	5.35	1.59	1.52
1	D	273	SER	CA-C	-5.35	1.46	1.52
1	B	168	LEU	CA-CB	5.35	1.61	1.54
1	B	247	ILE	C-O	5.35	1.30	1.24
1	B	83	ALA	N-CA	-5.35	1.39	1.46
1	C	136	LYS	C-O	-5.35	1.17	1.24
1	C	242	GLU	C-O	-5.34	1.17	1.24
1	A	76	CYS	N-CA	5.34	1.52	1.46
1	B	25	ILE	CA-CB	-5.34	1.47	1.53
1	D	141	ALA	C-O	-5.34	1.18	1.24
1	A	355	ARG	N-CA	5.33	1.53	1.46
1	B	179	ALA	C-O	-5.33	1.17	1.24
1	B	68	ARG	C-O	5.33	1.31	1.23
1	D	309	ALA	N-CA	-5.32	1.39	1.46
1	B	67	ASP	CA-C	5.32	1.60	1.52
1	D	84	ALA	CA-CB	5.32	1.62	1.53
1	B	218	ALA	C-O	5.31	1.30	1.24
1	A	264	GLU	CA-C	5.31	1.59	1.52
1	A	22	ASP	C-O	-5.31	1.15	1.24
1	C	357	LEU	CG-CD2	-5.31	1.35	1.52
1	C	262	VAL	N-CA	-5.30	1.40	1.46
1	B	239	LYS	CB-CG	-5.30	1.36	1.52
1	B	188	ARG	CZ-NH1	-5.30	1.25	1.32
1	C	202	ASN	N-CA	5.30	1.56	1.46
1	D	240	GLY	C-O	-5.30	1.16	1.23
1	A	135	ASN	N-CA	5.29	1.52	1.46
1	C	110	LEU	C-O	5.29	1.30	1.24
1	A	339	SER	N-CA	5.29	1.52	1.46
1	C	197	PRO	N-CD	-5.28	1.40	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	312	GLY	C-O	-5.28	1.17	1.24
1	D	96	ASP	C-O	-5.27	1.18	1.24
1	A	188	ARG	CZ-NH1	-5.27	1.25	1.32
1	C	160	LEU	N-CA	5.27	1.52	1.46
1	A	57	GLU	N-CA	5.26	1.52	1.46
1	A	296	ASN	C-O	5.26	1.30	1.24
1	A	175	GLY	C-O	-5.26	1.17	1.23
1	A	320	ASN	C-O	5.26	1.30	1.23
1	B	159	MET	N-CA	-5.25	1.39	1.46
1	D	58	ALA	CA-C	-5.25	1.46	1.52
1	A	167	TYR	C-O	-5.24	1.17	1.24
1	C	302	GLN	N-CA	5.24	1.52	1.46
1	B	216	GLN	C-O	5.23	1.30	1.24
1	C	355	ARG	N-CA	5.23	1.52	1.46
1	A	349	THR	CA-C	5.23	1.59	1.52
1	B	96	ASP	C-O	-5.22	1.18	1.24
1	C	355	ARG	C-O	-5.22	1.17	1.24
1	A	216	GLN	N-CA	5.22	1.52	1.46
1	B	79	HIS	C-O	-5.21	1.17	1.24
1	A	53	ARG	CA-C	-5.21	1.46	1.52
1	D	88	ALA	CA-C	5.21	1.59	1.52
1	B	356	LYS	N-CA	-5.21	1.39	1.46
1	D	158	GLU	C-O	-5.21	1.17	1.24
1	C	161	ASP	C-O	-5.20	1.17	1.23
1	A	220	HIS	CA-C	-5.20	1.45	1.53
1	D	339	SER	N-CA	5.20	1.52	1.46
1	C	53	ARG	C-O	-5.20	1.18	1.24
1	A	242	GLU	CD-OE2	5.19	1.35	1.25
1	C	141	ALA	C-O	-5.19	1.18	1.24
1	B	93	LYS	N-CA	5.18	1.52	1.46
1	D	173	SER	CA-C	-5.18	1.45	1.52
1	B	189	GLU	CG-CD	5.17	1.65	1.52
1	B	320	ASN	C-O	5.17	1.30	1.23
1	A	109	TYR	N-CA	5.17	1.52	1.46
1	D	365	ARG	C-O	5.17	1.30	1.24
1	D	291	ASN	CA-C	5.16	1.59	1.52
1	C	48	LEU	N-CA	-5.16	1.39	1.46
1	D	107	ARG	CA-C	-5.15	1.46	1.52
1	C	364	ARG	CG-CD	5.14	1.67	1.52
1	D	56	ARG	NE-CZ	5.14	1.38	1.33
1	D	227	VAL	CB-CG2	-5.14	1.35	1.52
1	C	228	THR	C-O	-5.13	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	93	LYS	CD-CE	5.13	1.67	1.52
1	D	292	GLN	CA-CB	5.13	1.60	1.53
1	B	320	ASN	N-CA	5.13	1.52	1.45
1	C	346	GLY	CA-C	-5.13	1.45	1.52
1	C	93	LYS	C-O	-5.12	1.18	1.24
1	A	60	ASP	CB-CG	5.12	1.64	1.52
1	D	185	GLN	CB-CG	5.11	1.67	1.52
1	D	304	ALA	C-O	-5.11	1.17	1.24
1	B	62	ILE	CB-CG1	-5.11	1.43	1.53
1	D	299	VAL	C-O	-5.11	1.18	1.24
1	A	197	PRO	N-CA	-5.11	1.40	1.47
1	D	362	ARG	C-N	-5.11	1.26	1.34
1	D	320	ASN	C-O	5.10	1.30	1.23
1	B	238	THR	CA-C	5.09	1.59	1.52
1	D	56	ARG	CA-C	-5.09	1.46	1.52
1	A	341	THR	CA-CB	5.09	1.62	1.53
1	A	157	SER	N-CA	-5.09	1.39	1.45
1	A	234	ALA	C-O	-5.08	1.17	1.23
1	B	302	GLN	C-N	-5.08	1.27	1.33
1	D	302	GLN	C-O	-5.08	1.18	1.24
1	A	241	ASN	C-O	5.08	1.29	1.24
1	C	103	SER	C-O	5.07	1.30	1.24
1	A	149	THR	C-O	-5.06	1.17	1.24
1	B	47	SER	CB-OG	-5.06	1.32	1.42
1	D	190	LEU	CA-C	5.06	1.59	1.52
1	C	273	SER	N-CA	5.06	1.52	1.45
1	A	157	SER	CA-C	-5.05	1.46	1.52
1	B	46	THR	CA-C	5.05	1.59	1.52
1	B	187	HIS	N-CA	5.05	1.52	1.46
1	C	132	PHE	CA-C	5.05	1.59	1.53
1	B	316	GLU	CA-CB	5.05	1.59	1.53
1	B	318	ASN	CA-C	5.05	1.59	1.52
1	B	363	GLN	C-O	5.05	1.30	1.24
1	B	30	PRO	CA-CB	-5.04	1.47	1.53
1	C	57	GLU	CD-OE2	5.04	1.34	1.25
1	D	159	MET	CG-SD	-5.04	1.68	1.80
1	D	212	VAL	C-O	-5.04	1.17	1.24
1	C	191	ALA	CA-C	5.04	1.59	1.52
1	D	210	VAL	C-O	-5.03	1.17	1.24
1	B	344	CYS	CA-C	5.03	1.58	1.52
1	D	55	ARG	CA-CB	5.02	1.61	1.53
1	D	311	THR	CA-C	-5.02	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	120	LYS	CA-CB	5.01	1.62	1.53
1	C	218	ALA	N-CA	-5.01	1.39	1.46
1	A	279	ASP	C-O	-5.00	1.17	1.24
1	B	71	VAL	C-O	-5.00	1.18	1.24
1	A	40	GLN	CA-CB	-5.00	1.45	1.53
1	A	56	ARG	N-CA	5.00	1.52	1.46

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	368	ASN	O-C-N	-14.76	99.39	123.00
1	A	368	ASN	O-C-N	-11.71	104.26	123.00
1	C	202	ASN	CB-CA-C	-11.61	88.03	110.10
1	D	299	VAL	N-CA-C	-11.43	99.73	110.82
1	D	368	ASN	CA-C-O	11.28	139.97	120.80
1	C	369	LYS	O-C-N	10.93	140.48	123.00
1	A	361	VAL	N-CA-C	-10.61	100.53	110.82
1	A	153	LEU	CB-CA-C	-9.41	100.86	110.17
1	B	202	ASN	CB-CA-C	-9.26	92.50	110.10
1	D	365	ARG	NE-CZ-NH1	-9.07	112.42	121.50
1	C	336	TYR	N-CA-C	8.82	123.19	109.96
1	A	365	ARG	NE-CZ-NH1	-8.59	112.91	121.50
1	C	348	GLU	N-CA-C	-8.53	101.49	112.23
1	D	280	TYR	CA-C-O	-8.42	106.48	120.80
1	A	196	PHE	CB-CA-C	8.36	121.82	110.37
1	D	355	ARG	NE-CZ-NH1	-8.28	113.22	121.50
1	D	301	GLU	N-CA-C	-8.21	102.27	111.14
1	A	280	TYR	CA-C-O	-8.10	107.03	120.80
1	B	129	ASN	CA-C-N	-8.09	106.09	121.54
1	B	129	ASN	C-N-CA	-8.09	106.09	121.54
1	C	295	VAL	N-CA-C	-8.03	102.61	110.72
1	A	368	ASN	CA-C-O	7.90	134.23	120.80
1	D	223	HIS	CB-CA-C	-7.88	98.72	110.62
1	D	246	VAL	N-CA-C	7.88	119.14	109.30
1	B	295	VAL	N-CA-C	-7.75	102.89	110.72
1	A	202	ASN	CB-CA-C	-7.71	95.45	110.10
1	A	365	ARG	NE-CZ-NH2	7.59	126.03	119.20
1	B	369	LYS	O-C-N	-7.50	111.00	123.00
1	B	202	ASN	CA-C-O	-7.38	108.25	120.80
1	D	156	GLY	CA-C-O	-7.30	114.90	121.47
1	B	162	THR	N-CA-C	7.28	121.76	113.02
1	A	163	ILE	N-CA-C	-7.25	105.72	112.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	THR	OG1-CB-CG2	-7.13	95.03	109.30
1	D	73	VAL	N-CA-C	7.06	118.31	107.78
1	A	273	SER	N-CA-C	7.05	119.94	110.35
1	D	347	TRP	N-CA-C	7.05	118.96	111.28
1	B	208	LEU	N-CA-C	6.99	122.06	112.90
1	A	57	GLU	N-CA-C	6.96	118.86	111.28
1	B	299	VAL	N-CA-C	-6.76	103.63	111.00
1	A	40	GLN	CB-CA-C	-6.75	97.72	110.67
1	D	294	LYS	N-CA-C	-6.70	104.04	111.82
1	B	129	ASN	O-C-N	-6.70	113.68	122.59
1	A	299	VAL	N-CA-C	-6.62	105.30	111.45
1	A	123	ILE	N-CA-C	-6.54	104.12	110.72
1	C	202	ASN	CA-C-O	-6.52	109.72	120.80
1	A	198	VAL	CA-C-N	-6.50	115.36	122.38
1	A	198	VAL	C-N-CA	-6.50	115.36	122.38
1	A	195	SER	N-CA-C	6.48	120.66	113.21
1	B	195	SER	CB-CA-C	-6.43	103.25	111.22
1	C	81	LEU	N-CA-C	6.28	118.92	111.33
1	D	188	ARG	N-CA-C	-6.27	103.98	111.69
1	A	355	ARG	NE-CZ-NH1	-6.24	115.26	121.50
1	B	365	ARG	N-CA-C	-6.13	104.60	111.28
1	D	201	LYS	CA-C-O	-6.09	114.11	121.05
1	B	22	ASP	N-CA-C	6.08	120.02	112.47
1	B	269	LEU	N-CA-C	6.08	117.69	109.24
1	D	124	ASN	N-CA-C	-6.05	104.61	112.23
1	D	71	VAL	CB-CA-C	-6.02	103.17	110.99
1	B	355	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	C	223	HIS	CB-CA-C	-5.89	100.71	110.14
1	C	291	ASN	N-CA-C	5.89	119.56	112.38
1	B	336	TYR	N-CA-C	5.87	118.85	110.10
1	B	196	PHE	CB-CA-C	5.87	117.97	110.22
1	D	320	ASN	CA-C-N	5.86	131.63	120.97
1	D	320	ASN	C-N-CA	5.86	131.63	120.97
1	C	155	ILE	N-CA-C	5.81	118.06	108.99
1	B	216	GLN	CA-CB-CG	5.79	125.68	114.10
1	A	29	ASP	N-CA-C	-5.79	101.25	110.10
1	B	274	ASN	N-CA-C	-5.75	101.48	110.17
1	D	145	PHE	N-CA-C	-5.74	105.10	111.36
1	D	212	VAL	N-CA-C	-5.73	104.75	111.00
1	D	361	VAL	N-CA-C	-5.70	104.79	111.00
1	D	365	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	D	100	GLY	N-CA-C	-5.68	107.62	114.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	ARG	NE-CZ-NH2	-5.67	114.09	119.20
1	A	303	ILE	N-CA-C	-5.65	105.22	110.53
1	D	273	SER	N-CA-C	5.65	118.03	110.35
1	C	179	ALA	N-CA-C	5.64	119.67	112.34
1	A	188	ARG	NE-CZ-NH1	-5.62	115.88	121.50
1	A	188	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	A	201	LYS	CA-C-O	-5.61	114.66	121.05
1	C	357	LEU	N-CA-C	-5.61	105.17	111.28
1	A	202	ASN	CA-C-O	-5.61	111.27	120.80
1	A	122	LEU	N-CA-C	5.60	118.32	111.82
1	C	196	PHE	CB-CA-C	5.58	117.57	110.76
1	C	365	ARG	NE-CZ-NH2	5.55	124.20	119.20
1	D	163	ILE	N-CA-C	-5.54	107.42	112.96
1	A	142	ARG	NE-CZ-NH2	5.54	124.18	119.20
1	D	94	LEU	N-CA-C	5.53	117.31	111.28
1	C	271	ALA	N-CA-C	-5.52	103.25	110.53
1	B	178	GLY	N-CA-C	-5.51	106.26	112.33
1	D	355	ARG	CD-NE-CZ	-5.51	116.68	124.40
1	B	104	ILE	N-CA-C	5.51	115.88	108.17
1	D	189	GLU	N-CA-C	5.49	117.35	111.36
1	B	302	GLN	CA-C-O	5.49	126.37	120.55
1	A	95	SER	N-CA-C	-5.49	105.38	111.36
1	B	56	ARG	CA-CB-CG	5.48	125.06	114.10
1	B	339	SER	N-CA-C	5.47	117.96	110.24
1	A	246	VAL	N-CA-C	5.47	116.11	108.89
1	A	362	ARG	N-CA-C	5.46	117.67	111.11
1	B	291	ASN	N-CA-C	5.46	119.81	113.20
1	D	138	LEU	N-CA-C	-5.45	105.26	111.14
1	A	157	SER	N-CA-C	5.40	117.60	109.23
1	B	232	VAL	CG1-CB-CG2	-5.40	98.92	110.80
1	D	365	ARG	CD-NE-CZ	-5.38	116.87	124.40
1	D	162	THR	CA-C-N	-5.35	115.79	121.84
1	D	162	THR	C-N-CA	-5.35	115.79	121.84
1	C	91	LEU	CB-CA-C	5.34	119.66	110.79
1	A	223	HIS	CB-CA-C	-5.34	101.59	110.14
1	D	197	PRO	CA-C-O	-5.32	115.27	121.34
1	C	163	ILE	N-CA-C	-5.31	107.65	112.96
1	A	319	ILE	N-CA-CB	5.30	116.19	110.62
1	C	147	ASN	CB-CA-C	-5.30	101.98	110.79
1	A	212	VAL	N-CA-C	-5.27	105.39	110.72
1	D	198	VAL	CA-C-N	-5.26	116.69	122.38
1	D	198	VAL	C-N-CA	-5.26	116.69	122.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	ASN	CA-C-N	5.26	130.06	122.16
1	A	130	ASN	C-N-CA	5.26	130.06	122.16
1	D	347	TRP	CA-C-O	5.24	126.10	120.55
1	C	201	LYS	CA-C-O	-5.23	115.09	121.05
1	B	323	ASN	N-CA-C	5.21	115.16	108.34
1	C	133	ASN	N-CA-C	-5.20	99.51	108.56
1	C	266	LYS	N-CA-C	5.20	117.69	111.71
1	C	232	VAL	N-CA-C	5.19	116.78	108.89
1	B	267	ALA	N-CA-C	-5.19	106.95	113.28
1	A	266	LYS	N-CA-C	5.18	119.07	112.34
1	C	43	ALA	CA-C-O	-5.17	115.53	121.47
1	D	196	PHE	CB-CA-C	5.17	117.45	110.37
1	A	172	VAL	N-CA-C	5.16	116.40	108.71
1	C	64	GLY	N-CA-C	5.16	121.89	114.10
1	C	25	ILE	N-CA-CB	-5.16	104.96	111.41
1	D	104	ILE	N-CA-C	5.15	115.38	108.17
1	A	319	ILE	N-CA-C	-5.15	104.88	110.23
1	C	55	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	257	TYR	N-CA-C	5.10	125.29	111.00
1	C	186	LEU	CB-CA-C	-5.10	102.32	110.79
1	A	364	ARG	CG-CD-NE	-5.09	100.79	112.00
1	D	256	ASN	N-CA-C	5.09	125.26	111.00
1	B	301	GLU	CA-C-O	-5.08	115.16	120.55
1	A	50	THR	CA-C-N	-5.08	113.47	120.28
1	A	50	THR	C-N-CA	-5.08	113.47	120.28
1	C	199	GLY	N-CA-C	5.08	120.60	111.62
1	D	278	ILE	CA-CB-CG1	-5.07	101.78	110.40
1	C	107	ARG	CB-CA-C	-5.06	102.66	110.26
1	A	161	ASP	N-CA-CB	-5.06	102.60	110.29
1	A	202	ASN	N-CA-CB	5.06	119.09	110.50
1	A	107	ARG	CB-CA-C	-5.05	102.69	110.26
1	B	40	GLN	CB-CA-C	-5.04	100.99	110.67
1	A	355	ARG	N-CA-C	-5.04	105.88	112.23
1	C	175	GLY	CA-C-O	5.03	125.95	121.57
1	A	40	GLN	N-CA-C	5.01	117.63	111.82
1	C	174	PHE	CA-C-N	5.01	125.46	121.61
1	C	174	PHE	C-N-CA	5.01	125.46	121.61

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	ASP	Peptide
1	C	368	ASN	Peptide

5.2 Too-close contacts [i](#)

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	2222	0	2172	46	0
1	B	2376	0	2344	53	0
1	C	2322	0	2241	41	0
1	D	2305	0	2253	35	0
2	A	21	0	0	1	0
2	B	33	0	0	0	0
2	C	23	0	0	1	0
2	D	26	0	0	1	0
All	All	9328	0	9010	164	0

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

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LYS:CD	1:A:52:LYS:CG	1.76	1.61
1:D:277:MET:CE	1:D:277:MET:SD	2.11	1.39
1:B:202:ASN:HD21	1:B:256:ASN:HD21	1.10	0.97
1:B:202:ASN:HD21	1:B:256:ASN:ND2	1.65	0.94
1:B:202:ASN:ND2	1:B:256:ASN:HD21	1.66	0.92
1:D:355:ARG:HH11	1:D:355:ARG:HG3	1.39	0.88
1:A:365:ARG:HG2	1:A:365:ARG:HH11	1.39	0.87
1:B:355:ARG:HH11	1:B:355:ARG:HG3	1.42	0.83
1:B:308:ASN:HD21	1:B:368:ASN:HD21	1.22	0.83
1:B:143:GLN:HE21	1:B:147:ASN:HD21	1.24	0.81
1:D:182:THR:OG1	2:D:2012:HOH:O	1.98	0.81
1:D:365:ARG:NH1	1:D:365:ARG:HG2	1.98	0.79
1:A:365:ARG:HH11	1:A:365:ARG:CG	1.92	0.78
1:B:43:ALA:HB1	1:B:48:LEU:HD13	1.64	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ILE:HG22	1:D:107:ARG:HG2	1.66	0.78
1:D:355:ARG:HG3	1:D:355:ARG:NH1	2.00	0.76
1:C:182:THR:OG1	2:C:2009:HOH:O	2.04	0.74
1:B:202:ASN:ND2	1:B:256:ASN:ND2	2.26	0.74
1:D:365:ARG:HH11	1:D:365:ARG:CG	2.02	0.72
1:A:202:ASN:HD21	1:A:249:ARG:H	1.36	0.72
1:D:355:ARG:HH11	1:D:355:ARG:CG	1.96	0.71
1:C:167:TYR:C	1:C:168:LEU:HD22	2.15	0.71
1:B:100:GLY:O	1:B:365:ARG:NH2	2.24	0.69
1:B:250:GLY:H	1:B:256:ASN:ND2	1.90	0.69
1:A:365:ARG:CG	1:A:365:ARG:NH1	2.55	0.68
1:B:128:VAL:O	1:B:128:VAL:HG12	1.94	0.67
1:B:143:GLN:HE21	1:B:147:ASN:ND2	1.92	0.67
1:C:248:LEU:HD22	1:C:248:LEU:N	2.10	0.66
1:B:72:ILE:HG22	1:B:107:ARG:HG2	1.78	0.65
1:D:355:ARG:NH1	1:D:355:ARG:CG	2.57	0.65
1:D:248:LEU:HD21	1:D:276:LEU:HD22	1.79	0.65
1:D:127:ASP:O	1:D:128:VAL:HG23	1.96	0.65
1:A:313:VAL:HG21	1:A:357:LEU:HD11	1.79	0.64
1:B:48:LEU:O	1:B:52:LYS:HE2	1.97	0.64
1:C:365:ARG:HH11	1:C:365:ARG:CG	2.11	0.64
1:C:365:ARG:HH11	1:C:365:ARG:HG2	1.61	0.64
1:B:355:ARG:HH11	1:B:355:ARG:CG	2.06	0.64
1:A:143:GLN:HE21	1:A:147:ASN:ND2	1.96	0.63
1:B:308:ASN:HD21	1:B:368:ASN:ND2	1.94	0.63
1:B:249:ARG:N	1:B:256:ASN:HD22	1.96	0.63
1:A:202:ASN:ND2	1:A:249:ARG:H	1.96	0.63
1:A:143:GLN:HE21	1:A:147:ASN:HD21	1.47	0.62
1:C:168:LEU:HD22	1:C:168:LEU:N	2.14	0.62
1:A:133:ASN:C	1:A:133:ASN:HD22	2.07	0.61
1:B:37:LEU:HD13	1:B:142:ARG:HD3	1.80	0.61
1:A:355:ARG:HH11	1:A:355:ARG:HG3	1.65	0.61
1:C:71:VAL:CG1	1:C:104:ILE:HG12	2.31	0.61
1:C:202:ASN:ND2	1:C:249:ARG:H	1.98	0.61
1:C:366:GLU:HA	1:C:366:GLU:OE2	2.00	0.61
1:D:313:VAL:HG21	1:D:357:LEU:HD11	1.82	0.59
1:B:43:ALA:CB	1:B:48:LEU:HD13	2.33	0.58
1:D:365:ARG:HG2	1:D:365:ARG:HH11	1.61	0.58
1:A:355:ARG:HG3	1:A:355:ARG:NH1	2.18	0.58
1:D:348:GLU:H	1:D:348:GLU:CD	2.12	0.57
1:A:89:LEU:CD1	1:A:151:ILE:HD13	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:VAL:HG13	1:C:71:VAL:O	2.04	0.56
1:C:129:ASN:O	1:C:130:ASN:CB	2.52	0.56
1:A:365:ARG:HG2	1:A:365:ARG:NH1	2.14	0.56
1:C:365:ARG:CG	1:C:365:ARG:NH1	2.67	0.56
1:A:174:PHE:HE2	1:A:245:PHE:HZ	1.53	0.56
1:C:40:GLN:HE22	1:C:139:GLN:HE21	1.54	0.56
1:A:24:ARG:HA	1:B:239:LYS:CG	2.35	0.56
1:B:355:ARG:HG3	1:B:355:ARG:NH1	2.18	0.55
1:A:239:LYS:HG3	1:B:26:LEU:HD21	1.88	0.55
1:A:66:ASP:OD2	1:A:67:ASP:N	2.40	0.55
1:A:248:LEU:HD22	1:A:248:LEU:N	2.22	0.55
1:A:143:GLN:NE2	1:A:147:ASN:HD21	2.04	0.54
1:A:110:LEU:HA	2:A:2006:HOH:O	2.08	0.54
1:B:249:ARG:H	1:B:256:ASN:HD22	1.55	0.54
1:D:365:ARG:NH1	1:D:365:ARG:CG	2.57	0.53
1:A:355:ARG:HH11	1:A:355:ARG:CG	2.21	0.53
1:A:34:PRO:O	1:A:38:GLN:HG3	2.08	0.52
1:A:189:GLU:OE2	1:B:120:LYS:HE2	2.09	0.52
1:C:92:LYS:HE3	1:C:152:GLY:O	2.09	0.52
1:D:308:ASN:HD21	1:D:368:ASN:HD21	1.58	0.52
1:C:168:LEU:N	1:C:168:LEU:CD2	2.72	0.52
1:C:248:LEU:HD22	1:C:248:LEU:H	1.73	0.52
1:C:40:GLN:HE22	1:C:139:GLN:NE2	2.08	0.51
1:C:290:ARG:O	1:C:293:PRO:HD2	2.10	0.51
1:B:355:ARG:CG	1:B:355:ARG:NH1	2.74	0.51
1:A:70:LEU:HD11	1:A:105:ILE:HD12	1.92	0.50
1:A:89:LEU:HD13	1:A:151:ILE:HD13	1.94	0.49
1:A:109:TYR:C	1:A:110:LEU:HD23	2.38	0.49
1:C:202:ASN:HD22	1:C:249:ARG:HG3	1.76	0.49
1:C:167:TYR:HB2	1:C:168:LEU:CD2	2.43	0.48
1:C:161:ASP:OD2	1:D:225:MET:HE3	2.13	0.48
1:A:239:LYS:CG	1:B:26:LEU:HD21	2.42	0.48
1:B:167:TYR:C	1:B:168:LEU:HD22	2.38	0.48
1:C:109:TYR:C	1:C:110:LEU:HD23	2.39	0.48
1:A:76:CYS:SG	1:A:341:THR:OG1	2.67	0.48
1:A:259:ALA:HA	1:A:302:GLN:NE2	2.29	0.48
1:B:250:GLY:H	1:B:256:ASN:HD22	1.57	0.48
1:C:43:ALA:HB1	1:C:48:LEU:HD13	1.96	0.47
1:B:351:GLU:OE2	1:B:355:ARG:NH1	2.38	0.47
1:D:38:GLN:OE1	1:D:229:LYS:NZ	2.37	0.47
1:A:67:ASP:OD1	1:A:365:ARG:NH1	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:GLN:HE21	1:D:166:GLN:HA	1.80	0.47
1:A:239:LYS:HG3	1:B:26:LEU:CD2	2.45	0.47
1:D:164:SER:N	1:D:165:PRO:CD	2.78	0.47
1:B:207:THR:HG22	1:B:208:LEU:N	2.30	0.46
1:B:167:TYR:CB	1:B:168:LEU:HD22	2.45	0.46
1:B:313:VAL:HG21	1:B:357:LEU:HD11	1.97	0.46
1:C:167:TYR:CB	1:C:168:LEU:HD22	2.45	0.46
1:D:127:ASP:O	1:D:128:VAL:CG2	2.63	0.46
1:B:216:GLN:O	1:B:220:HIS:HD2	1.98	0.46
1:D:72:ILE:HG22	1:D:107:ARG:CG	2.40	0.46
1:A:161:ASP:HA	1:B:186:LEU:HD21	1.98	0.45
1:B:70:LEU:O	1:B:312:GLY:HA2	2.15	0.45
1:B:166:GLN:HA	1:B:166:GLN:HE21	1.81	0.45
1:A:185:GLN:HG2	1:B:120:LYS:NZ	2.30	0.45
1:C:259:ALA:HA	1:C:302:GLN:OE1	2.17	0.45
1:D:248:LEU:HD22	1:D:248:LEU:N	2.31	0.45
1:B:43:ALA:CB	1:B:48:LEU:CD1	2.95	0.45
1:B:242:GLU:HG2	1:B:243:HIS:CD2	2.52	0.44
1:C:89:LEU:HD13	1:C:151:ILE:HD13	1.99	0.44
1:D:266:LYS:HD3	1:D:309:ALA:CB	2.46	0.44
1:B:207:THR:HG22	1:B:208:LEU:H	1.82	0.44
1:A:177:ILE:HG13	1:A:200:PHE:CE2	2.53	0.44
1:B:174:PHE:HE2	1:B:245:PHE:HZ	1.65	0.44
1:B:124:ASN:O	1:B:132:PHE:HA	2.18	0.44
1:A:110:LEU:HD12	1:A:141:ALA:HB1	2.00	0.44
1:B:255:THR:HG22	1:B:258:ASP:OD2	2.18	0.43
1:A:110:LEU:CD1	1:A:141:ALA:HB1	2.49	0.43
1:A:209:ASN:OD1	1:A:209:ASN:N	2.51	0.43
1:B:365:ARG:HH11	1:B:365:ARG:HG2	1.83	0.43
1:C:80:ASP:OD1	1:C:80:ASP:C	2.61	0.43
1:B:202:ASN:ND2	1:B:249:ARG:H	2.16	0.43
1:C:265:ALA:O	1:C:269:LEU:HG	2.18	0.43
1:D:324:GLN:OE1	1:D:335:LYS:CB	2.66	0.43
1:C:201:LYS:HB3	1:C:249:ARG:HD2	2.01	0.43
1:C:110:LEU:HD13	1:C:122:LEU:HD23	1.99	0.43
1:B:232:VAL:HG11	1:D:232:VAL:HG11	2.01	0.43
1:C:71:VAL:HG13	1:C:104:ILE:HG12	2.00	0.43
1:C:363:GLN:OE1	1:C:363:GLN:HA	2.19	0.43
1:D:138:LEU:HD23	1:D:138:LEU:HA	1.88	0.42
1:D:177:ILE:HG13	1:D:200:PHE:CE2	2.54	0.42
1:A:50:THR:OG1	1:A:152:GLY:HA2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:VAL:HG23	1:A:361:VAL:HG22	2.00	0.42
1:C:320:ASN:HB2	1:C:338:VAL:HG22	2.02	0.42
1:D:127:ASP:O	1:D:128:VAL:CB	2.67	0.42
1:A:359:ALA:HA	1:A:362:ARG:CZ	2.50	0.42
1:B:314:MET:HG3	1:B:315:ILE:N	2.33	0.42
1:C:300:CYS:SG	1:C:357:LEU:HA	2.60	0.42
1:A:74:GLY:C	1:A:317:SER:O	2.63	0.41
1:A:355:ARG:NH1	1:A:355:ARG:CG	2.77	0.41
1:A:40:GLN:C	1:A:41:ILE:HG13	2.43	0.41
1:C:21:GLU:OE2	1:D:229:LYS:HE2	2.20	0.41
1:D:258:ASP:O	1:D:259:ALA:C	2.63	0.41
1:B:143:GLN:NE2	1:B:147:ASN:HD21	2.05	0.41
1:C:71:VAL:HG11	1:C:104:ILE:HG12	2.03	0.41
1:C:202:ASN:HD21	1:C:249:ARG:H	1.67	0.41
1:D:91:LEU:HD12	1:D:91:LEU:HA	1.84	0.41
1:A:235:ILE:O	1:B:28:TYR:HA	2.21	0.41
1:D:143:GLN:HE21	1:D:147:ASN:ND2	2.17	0.41
1:B:86:GLU:OE1	1:B:336:TYR:OH	2.33	0.41
1:A:258:ASP:O	1:A:259:ALA:C	2.63	0.41
1:C:100:GLY:O	1:C:365:ARG:NH2	2.53	0.41
1:B:292:GLN:HB2	1:B:293:PRO:HD3	2.03	0.41
1:B:161:ASP:OD1	1:B:163:ILE:N	2.36	0.40
1:C:164:SER:N	1:C:165:PRO:CD	2.84	0.40
1:D:175:GLY:O	1:D:198:VAL:HA	2.21	0.40
1:C:133:ASN:C	1:C:133:ASN:HD22	2.30	0.40
1:D:280:TYR:CD1	1:D:315:ILE:HG12	2.56	0.40
1:C:174:PHE:CD1	1:C:174:PHE:C	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	259/370 (70%)	250 (96%)	7 (3%)	2 (1%)	16	12
1	B	221/370 (60%)	213 (96%)	7 (3%)	1 (0%)	24	22
1	C	307/370 (83%)	293 (95%)	12 (4%)	2 (1%)	18	15
1	D	301/370 (81%)	293 (97%)	8 (3%)	0	100	100
All	All	1088/1480 (74%)	1049 (96%)	34 (3%)	5 (0%)	24	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	VAL
1	B	369	LYS
1	C	369	LYS
1	C	130	ASN
1	A	127	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	221/298 (74%)	196 (89%)	25 (11%)	5	3
1	B	245/298 (82%)	225 (92%)	20 (8%)	10	8
1	C	233/298 (78%)	207 (89%)	26 (11%)	6	3
1	D	231/298 (78%)	213 (92%)	18 (8%)	11	9
All	All	930/1192 (78%)	841 (90%)	89 (10%)	8	5

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	48	LEU
1	A	52	LYS
1	A	89	LEU
1	A	93	LYS
1	A	94	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	95	SER
1	A	110	LEU
1	A	133	ASN
1	A	148	LEU
1	A	157	SER
1	A	159	MET
1	A	166	GLN
1	A	202	ASN
1	A	208	LEU
1	A	216	GLN
1	A	230	HIS
1	A	239	LYS
1	A	317	SER
1	A	351	GLU
1	A	355	ARG
1	A	357	LEU
1	A	363	GLN
1	A	365	ARG
1	A	366	GLU
1	B	37	LEU
1	B	48	LEU
1	B	52	LYS
1	B	89	LEU
1	B	94	LEU
1	B	95	SER
1	B	110	LEU
1	B	159	MET
1	B	166	GLN
1	B	208	LEU
1	B	216	GLN
1	B	230	HIS
1	B	232	VAL
1	B	255	THR
1	B	314	MET
1	B	326	ILE
1	B	351	GLU
1	B	357	LEU
1	B	363	GLN
1	B	366	GLU
1	C	23	VAL
1	C	37	LEU
1	C	48	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	52	LYS
1	C	89	LEU
1	C	94	LEU
1	C	95	SER
1	C	110	LEU
1	C	128	VAL
1	C	133	ASN
1	C	148	LEU
1	C	157	SER
1	C	168	LEU
1	C	174	PHE
1	C	208	LEU
1	C	212	VAL
1	C	216	GLN
1	C	229	LYS
1	C	230	HIS
1	C	232	VAL
1	C	249	ARG
1	C	255	THR
1	C	353	VAL
1	C	357	LEU
1	C	363	GLN
1	C	366	GLU
1	D	37	LEU
1	D	48	LEU
1	D	89	LEU
1	D	93	LYS
1	D	94	LEU
1	D	107	ARG
1	D	110	LEU
1	D	157	SER
1	D	166	GLN
1	D	202	ASN
1	D	208	LEU
1	D	229	LYS
1	D	230	HIS
1	D	249	ARG
1	D	355	ARG
1	D	363	GLN
1	D	365	ARG
1	D	366	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	124	ASN
1	A	133	ASN
1	A	143	GLN
1	A	147	ASN
1	A	166	GLN
1	A	223	HIS
1	A	274	ASN
1	A	302	GLN
1	B	85	GLN
1	B	143	GLN
1	B	147	ASN
1	B	150	ASN
1	B	166	GLN
1	B	220	HIS
1	B	256	ASN
1	B	268	GLN
1	B	274	ASN
1	B	291	ASN
1	B	302	GLN
1	B	308	ASN
1	B	323	ASN
1	C	40	GLN
1	C	85	GLN
1	C	133	ASN
1	C	143	GLN
1	C	147	ASN
1	C	202	ASN
1	C	223	HIS
1	C	274	ASN
1	D	40	GLN
1	D	85	GLN
1	D	130	ASN
1	D	147	ASN
1	D	166	GLN
1	D	220	HIS
1	D	268	GLN
1	D	274	ASN
1	D	296	ASN
1	D	302	GLN
1	D	320	ASN
1	D	368	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	307/370 (82%)	0.26	7 (2%) 61 64	32, 50, 66, 79	0
1	B	322/370 (87%)	0.04	5 (1%) 70 73	31, 46, 63, 75	0
1	C	319/370 (86%)	0.20	9 (2%) 55 57	32, 48, 66, 73	0
1	D	315/370 (85%)	0.16	9 (2%) 53 56	32, 48, 66, 78	0
All	All	1263/1480 (85%)	0.16	30 (2%) 59 62	31, 48, 66, 79	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	128	VAL	3.5
1	A	128	VAL	3.5
1	A	289	PHE	3.4
1	B	207	THR	3.2
1	B	326	ILE	3.1
1	C	326	ILE	3.1
1	A	76	CYS	3.0
1	C	344	CYS	2.9
1	C	210	VAL	2.8
1	C	132	PHE	2.8
1	B	335	LYS	2.7
1	B	256	ASN	2.6
1	D	128	VAL	2.5
1	D	344	CYS	2.5
1	D	345	ILE	2.4
1	A	341	THR	2.3
1	A	322	GLY	2.3
1	A	335	LYS	2.2
1	D	125	ASP	2.2
1	D	132	PHE	2.2
1	D	335	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	20	GLU	2.2
1	C	289	PHE	2.1
1	C	367	VAL	2.1
1	A	132	PHE	2.1
1	C	223	HIS	2.1
1	D	369	LYS	2.1
1	B	257	TYR	2.0
1	C	49	GLU	2.0
1	D	367	VAL	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.