Full wwPDB X-ray Structure Validation Report ⓘ

Dec 7, 2023 – 03:00 pm GMT

PDB ID	:	1OFP
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:

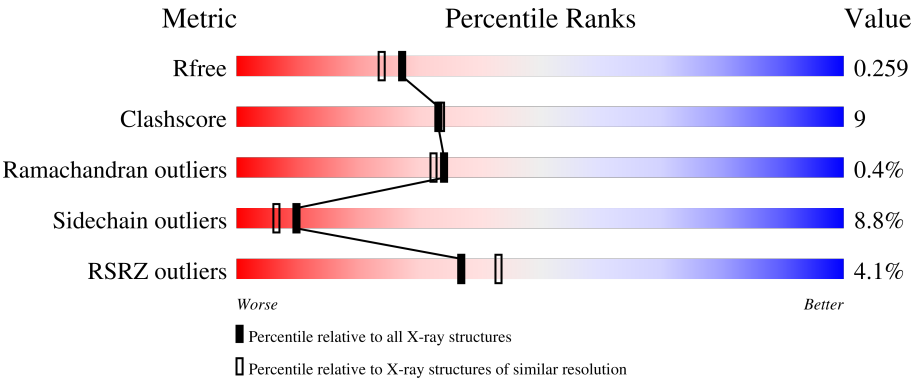
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 <=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	4% 55% 21% 6% • 17%
1	B	370	4% 58% 23% 5% • 13%
1	C	370	3% 60% 19% 7% 14%
1	D	370	4% 58% 21% 5% • 15%

2 Entry composition (i)

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.

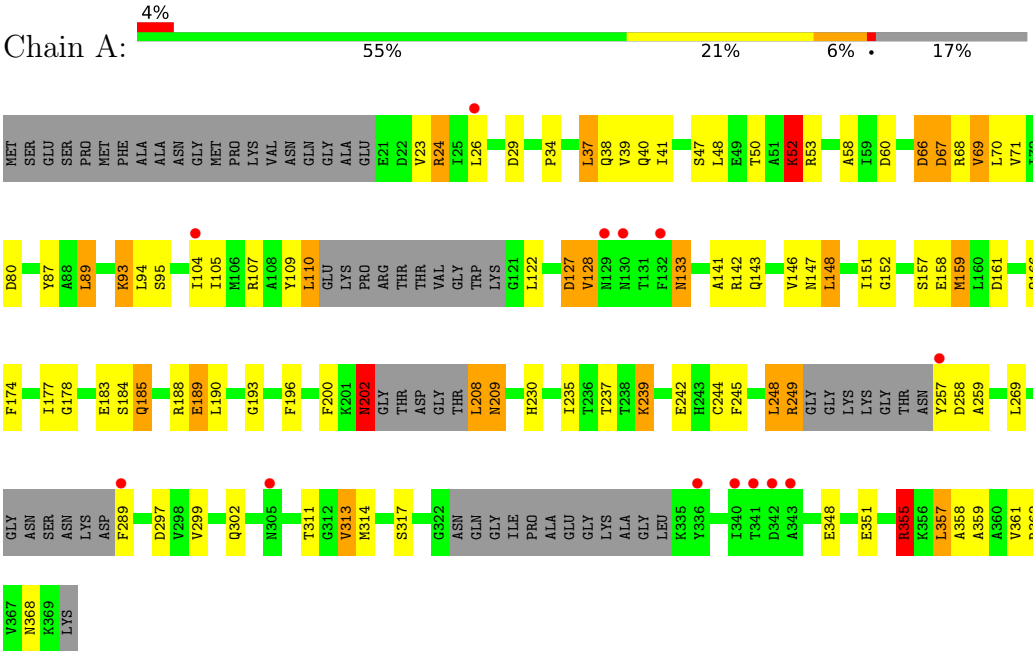
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	B	33	Total	O	0	0
			33	33		
2	C	23	Total	O	0	0
			23	23		
2	D	26	Total	O	0	0
			26	26		

3 Residue-property plots (i)

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

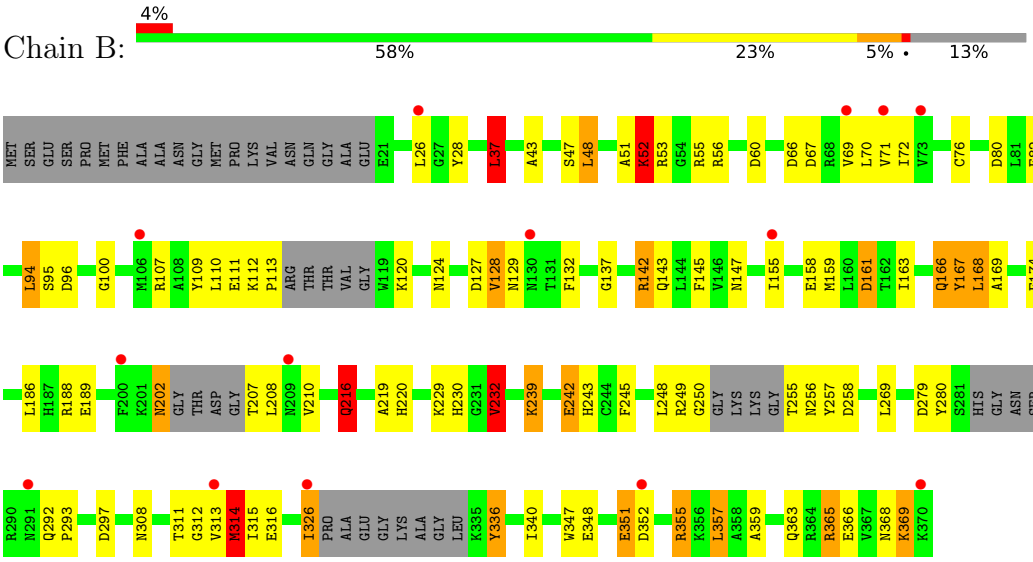
• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain A:



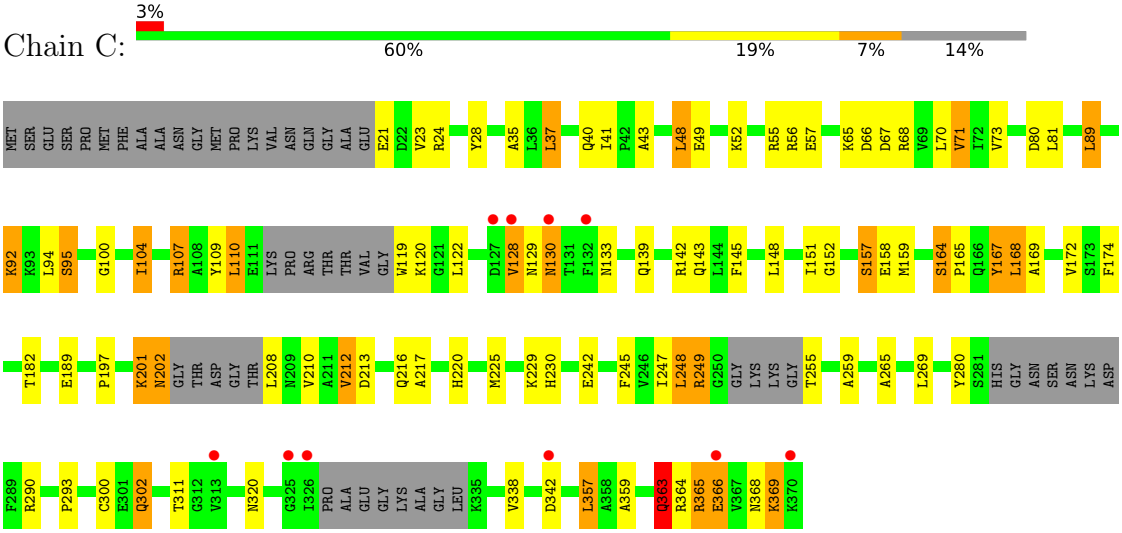
• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain B:



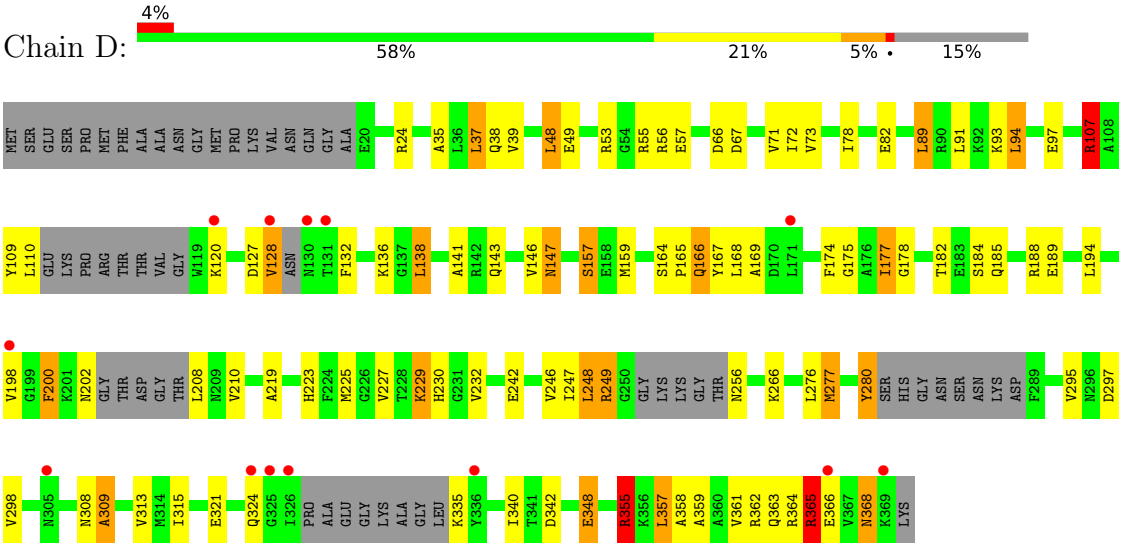
• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

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 19.87 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.88-2.10) 98.6 (19.87-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.205 , 0.260 0.210 , 0.259	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)	0.36 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.97	48/2250 (2.1%)	1.62	38/3058 (1.2%)
1	B	1.92	49/2408 (2.0%)	1.51	32/3270 (1.0%)
1	C	1.92	48/2353 (2.0%)	1.53	22/3200 (0.7%)
1	D	1.95	54/2335 (2.3%)	1.58	33/3169 (1.0%)
All	All	1.94	199/9346 (2.1%)	1.56	125/12697 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (199) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	35	ALA	CA-CB	9.73	1.72	1.52
1	B	359	ALA	CA-CB	9.66	1.72	1.52
1	B	52	LYS	CD-CE	9.20	1.74	1.51
1	C	172	VAL	CB-CG1	-9.03	1.33	1.52
1	C	71	VAL	CB-CG1	-8.86	1.34	1.52
1	D	157	SER	CB-OG	8.76	1.53	1.42
1	A	242	GLU	CD-OE2	8.70	1.35	1.25
1	B	189	GLU	CG-CD	8.69	1.65	1.51
1	B	232	VAL	CB-CG2	-8.64	1.34	1.52
1	C	157	SER	CB-OG	8.58	1.53	1.42
1	A	348	GLU	CA-CB	8.50	1.72	1.53
1	C	57	GLU	CD-OE2	8.43	1.34	1.25
1	D	227	VAL	CB-CG2	-8.21	1.35	1.52
1	B	355	ARG	CG-CD	8.15	1.72	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	189	GLU	CG-CD	8.09	1.64	1.51
1	B	142	ARG	CB-CG	-7.90	1.31	1.52
1	A	351	GLU	CD-OE2	7.88	1.34	1.25
1	B	47	SER	CB-OG	-7.87	1.32	1.42
1	B	51	ALA	CA-CB	-7.85	1.35	1.52
1	A	178	GLY	C-O	7.79	1.36	1.23
1	C	212	VAL	CB-CG2	-7.78	1.36	1.52
1	D	107	ARG	CG-CD	7.76	1.71	1.51
1	A	183	GLU	CD-OE2	7.75	1.34	1.25
1	A	93	LYS	CD-CE	7.53	1.70	1.51
1	D	184	SER	CB-OG	7.47	1.51	1.42
1	C	70	LEU	C-O	-7.46	1.09	1.23
1	C	365	ARG	CG-CD	7.46	1.70	1.51
1	D	242	GLU	CD-OE2	7.44	1.33	1.25
1	B	351	GLU	CD-OE2	7.34	1.33	1.25
1	B	159	MET	CG-SD	-7.29	1.62	1.81
1	B	316	GLU	CD-OE2	7.29	1.33	1.25
1	C	202	ASN	CB-CG	-7.27	1.34	1.51
1	B	69	VAL	CB-CG2	7.24	1.68	1.52
1	C	159	MET	CG-SD	-7.23	1.62	1.81
1	D	348	GLU	CG-CD	7.14	1.62	1.51
1	A	107	ARG	CG-CD	7.12	1.69	1.51
1	A	184	SER	CB-OG	7.09	1.51	1.42
1	C	169	ALA	CA-CB	7.07	1.67	1.52
1	A	189	GLU	CG-CD	7.06	1.62	1.51
1	A	52	LYS	CG-CD	7.05	1.76	1.52
1	D	169	ALA	CA-CB	7.02	1.67	1.52
1	D	248	LEU	CG-CD2	-7.01	1.25	1.51
1	A	183	GLU	CG-CD	6.96	1.62	1.51
1	A	146	VAL	CB-CG1	6.93	1.67	1.52
1	B	111	GLU	CA-CB	6.91	1.69	1.53
1	B	52	LYS	CE-NZ	6.90	1.66	1.49
1	A	172	VAL	CB-CG1	-6.88	1.38	1.52
1	C	242	GLU	CD-OE2	6.88	1.33	1.25
1	C	359	ALA	CA-CB	6.86	1.66	1.52
1	A	71	VAL	C-O	-6.85	1.10	1.23
1	B	336	TYR	CG-CD1	-6.83	1.30	1.39
1	B	167	TYR	CZ-OH	-6.82	1.26	1.37
1	C	56	ARG	CG-CD	6.79	1.69	1.51
1	C	247	ILE	CA-CB	-6.79	1.39	1.54
1	A	355	ARG	CG-CD	6.77	1.68	1.51
1	B	155	ILE	CA-CB	-6.75	1.39	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	73	VAL	CB-CG1	-6.75	1.38	1.52
1	B	169	ALA	CA-CB	6.73	1.66	1.52
1	D	309	ALA	CA-CB	-6.72	1.38	1.52
1	B	158	GLU	CA-CB	6.68	1.68	1.53
1	B	336	TYR	CE2-CZ	-6.67	1.29	1.38
1	D	82	GLU	CA-CB	6.66	1.68	1.53
1	B	178	GLY	C-O	6.65	1.34	1.23
1	D	93	LYS	CD-CE	6.64	1.67	1.51
1	A	128	VAL	CA-CB	6.60	1.68	1.54
1	A	148	LEU	C-O	6.60	1.35	1.23
1	C	210	VAL	CA-CB	6.56	1.68	1.54
1	C	217	ALA	CA-CB	6.53	1.66	1.52
1	D	210	VAL	CB-CG1	6.52	1.66	1.52
1	D	219	ALA	CA-CB	6.51	1.66	1.52
1	D	49	GLU	CD-OE1	6.47	1.32	1.25
1	A	69	VAL	CB-CG2	-6.46	1.39	1.52
1	C	364	ARG	CG-CD	6.37	1.67	1.51
1	B	311	THR	CB-CG2	6.34	1.73	1.52
1	D	132	PHE	CG-CD2	6.34	1.48	1.38
1	D	189	GLU	CD-OE1	6.33	1.32	1.25
1	B	316	GLU	CG-CD	6.32	1.61	1.51
1	D	359	ALA	CA-CB	6.30	1.65	1.52
1	A	299	VAL	CB-CG1	6.29	1.66	1.52
1	A	60	ASP	CB-CG	6.24	1.64	1.51
1	B	210	VAL	CB-CG1	6.15	1.65	1.52
1	A	52	LYS	CB-CG	6.15	1.69	1.52
1	A	248	LEU	CG-CD2	-6.15	1.29	1.51
1	B	76	CYS	CB-SG	6.11	1.92	1.82
1	D	128	VAL	CB-CG2	6.10	1.65	1.52
1	C	28	TYR	CD1-CE1	6.07	1.48	1.39
1	C	302	GLN	CB-CG	-6.06	1.36	1.52
1	C	95	SER	CB-OG	-6.02	1.34	1.42
1	C	167	TYR	CD2-CE2	-6.02	1.30	1.39
1	D	167	TYR	CD2-CE2	-6.00	1.30	1.39
1	A	364	ARG	CG-CD	6.00	1.67	1.51
1	D	355	ARG	CG-CD	5.99	1.67	1.51
1	D	97	GLU	CD-OE1	5.98	1.32	1.25
1	D	178	GLY	C-O	5.98	1.33	1.23
1	D	35	ALA	CA-CB	5.97	1.65	1.52
1	A	158	GLU	CB-CG	-5.95	1.40	1.52
1	B	128	VAL	CB-CG2	5.95	1.65	1.52
1	B	188	ARG	CZ-NH1	-5.94	1.25	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	280	TYR	CE2-CZ	-5.94	1.30	1.38
1	A	167	TYR	CD1-CE1	-5.93	1.30	1.39
1	B	239	LYS	CB-CG	-5.93	1.36	1.52
1	B	340	ILE	C-O	-5.92	1.12	1.23
1	C	220	HIS	C-O	5.92	1.34	1.23
1	D	277	MET	SD-CE	5.92	2.10	1.77
1	A	188	ARG	CZ-NH1	-5.91	1.25	1.33
1	B	80	ASP	CB-CG	5.90	1.64	1.51
1	A	289	PHE	CA-CB	5.90	1.67	1.53
1	C	107	ARG	CG-CD	5.90	1.66	1.51
1	B	280	TYR	CG-CD1	-5.89	1.31	1.39
1	B	137	GLY	CA-C	-5.85	1.42	1.51
1	A	358	ALA	C-O	5.84	1.34	1.23
1	D	57	GLU	CG-CD	5.84	1.60	1.51
1	D	78	ILE	C-O	5.82	1.34	1.23
1	D	71	VAL	C-O	-5.80	1.12	1.23
1	D	109	TYR	CG-CD2	-5.75	1.31	1.39
1	C	57	GLU	CG-CD	5.72	1.60	1.51
1	C	213	ASP	CB-CG	5.71	1.63	1.51
1	D	295	VAL	CB-CG2	-5.70	1.40	1.52
1	C	158	GLU	CA-CB	5.70	1.66	1.53
1	C	128	VAL	CA-CB	5.70	1.66	1.54
1	A	159	MET	CG-SD	-5.69	1.66	1.81
1	A	313	VAL	CA-CB	5.68	1.66	1.54
1	B	351	GLU	CD-OE1	5.68	1.31	1.25
1	B	145	PHE	CE1-CZ	-5.65	1.26	1.37
1	D	185	GLN	CB-CG	5.65	1.67	1.52
1	B	279	ASP	C-O	-5.64	1.12	1.23
1	D	247	ILE	CA-CB	-5.63	1.42	1.54
1	C	280	TYR	CD1-CE1	-5.63	1.30	1.39
1	D	168	LEU	CG-CD2	-5.63	1.31	1.51
1	A	363	GLN	C-O	5.62	1.34	1.23
1	B	248	LEU	CG-CD2	-5.60	1.31	1.51
1	A	23	VAL	CB-CG1	5.58	1.64	1.52
1	A	185	GLN	C-O	5.58	1.33	1.23
1	C	119	TRP	CE3-CZ3	5.57	1.48	1.38
1	B	112	LYS	C-O	5.55	1.33	1.23
1	A	311	THR	CB-OG1	5.55	1.54	1.43
1	D	358	ALA	N-CA	-5.54	1.35	1.46
1	C	201	LYS	CB-CG	-5.53	1.37	1.52
1	B	168	LEU	CG-CD2	-5.52	1.31	1.51
1	A	313	VAL	C-O	-5.51	1.12	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	189	GLU	CG-CD	5.50	1.60	1.51
1	A	68	ARG	C-O	5.50	1.33	1.23
1	B	109	TYR	CG-CD1	5.49	1.46	1.39
1	B	219	ALA	CA-CB	5.49	1.64	1.52
1	D	39	VAL	CB-CG2	-5.48	1.41	1.52
1	D	120	LYS	CA-C	5.46	1.67	1.52
1	A	93	LYS	CE-NZ	5.45	1.62	1.49
1	D	298	VAL	CA-CB	-5.45	1.43	1.54
1	B	82	GLU	CA-CB	5.44	1.66	1.53
1	A	87	TYR	CG-CD2	5.43	1.46	1.39
1	A	47	SER	CB-OG	-5.42	1.35	1.42
1	D	109	TYR	CG-CD1	5.41	1.46	1.39
1	D	147	ASN	N-CA	5.41	1.57	1.46
1	D	167	TYR	CD1-CE1	-5.41	1.31	1.39
1	D	141	ALA	CA-CB	-5.40	1.41	1.52
1	A	365	ARG	CG-CD	5.40	1.65	1.51
1	D	365	ARG	CG-CD	5.40	1.65	1.51
1	A	80	ASP	CB-CG	5.39	1.63	1.51
1	A	104	ILE	C-O	-5.39	1.13	1.23
1	B	242	GLU	CD-OE2	5.38	1.31	1.25
1	C	28	TYR	CD2-CE2	5.37	1.47	1.39
1	C	197	PRO	N-CD	-5.35	1.40	1.47
1	D	321	GLU	CB-CG	-5.33	1.42	1.52
1	C	120	LYS	CA-CB	5.32	1.65	1.53
1	D	136	LYS	CD-CE	5.29	1.64	1.51
1	C	143	GLN	CD-NE2	-5.29	1.19	1.32
1	D	37	LEU	C-O	-5.29	1.13	1.23
1	A	39	VAL	CB-CG2	-5.29	1.41	1.52
1	C	164	SER	CB-OG	-5.28	1.35	1.42
1	C	225	MET	CG-SD	5.25	1.94	1.81
1	D	146	VAL	CB-CG1	5.25	1.63	1.52
1	A	58	ALA	CA-CB	5.23	1.63	1.52
1	D	361	VAL	CB-CG1	-5.23	1.41	1.52
1	B	229	LYS	CA-CB	5.22	1.65	1.53
1	D	56	ARG	CG-CD	5.22	1.65	1.51
1	B	347	TRP	CB-CG	-5.19	1.41	1.50
1	D	174	PHE	CE1-CZ	-5.19	1.27	1.37
1	C	245	PHE	CD2-CE2	-5.18	1.28	1.39
1	A	41	ILE	CB-CG2	5.16	1.68	1.52
1	A	193	GLY	N-CA	-5.15	1.38	1.46
1	B	257	TYR	CD1-CE1	5.13	1.47	1.39
1	A	242	GLU	CG-CD	5.12	1.59	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	348	GLU	CA-CB	5.11	1.65	1.53
1	C	145	PHE	CE1-CZ	-5.11	1.27	1.37
1	B	56	ARG	CG-CD	5.11	1.64	1.51
1	D	368	ASN	C-N	-5.09	1.22	1.34
1	C	142	ARG	CZ-NH2	-5.09	1.26	1.33
1	C	56	ARG	CB-CG	5.08	1.66	1.52
1	B	181	THR	C-O	-5.08	1.13	1.23
1	C	104	ILE	C-O	-5.08	1.13	1.23
1	D	200	PHE	C-O	5.08	1.32	1.23
1	C	363	GLN	CB-CG	5.08	1.66	1.52
1	D	298	VAL	CB-CG1	-5.07	1.42	1.52
1	B	71	VAL	CB-CG2	5.04	1.63	1.52
1	C	65	LYS	CG-CD	5.04	1.69	1.52
1	C	49	GLU	CA-CB	5.03	1.65	1.53
1	A	314	MET	CG-SD	5.01	1.94	1.81
1	C	311	THR	CB-CG2	5.01	1.68	1.52
1	D	159	MET	CG-SD	-5.00	1.68	1.81

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	365	ARG	NE-CZ-NH1	-15.75	112.42	120.30
1	A	365	ARG	NE-CZ-NH1	-14.78	112.91	120.30
1	D	368	ASN	O-C-N	-14.57	99.39	122.70
1	D	355	ARG	NE-CZ-NH1	-14.16	113.22	120.30
1	A	67	ASP	CB-CG-OD2	12.77	129.79	118.30
1	C	66	ASP	CB-CG-OD2	12.73	129.76	118.30
1	A	364	ARG	NE-CZ-NH2	-12.41	114.09	120.30
1	A	368	ASN	O-C-N	-11.52	104.26	122.70
1	A	365	ARG	NE-CZ-NH2	11.47	126.03	120.30
1	C	202	ASN	CB-CA-C	-11.18	88.03	110.40
1	C	369	LYS	O-C-N	11.11	140.48	122.70
1	B	127	ASP	CB-CG-OD2	10.59	127.83	118.30
1	B	53	ARG	NE-CZ-NH1	10.22	125.41	120.30
1	A	355	ARG	NE-CZ-NH1	-10.09	115.26	120.30
1	B	67	ASP	CB-CG-OD2	9.81	127.13	118.30
1	A	29	ASP	CB-CG-OD2	9.74	127.07	118.30
1	D	67	ASP	CB-CG-OD2	9.71	127.03	118.30
1	B	355	ARG	NE-CZ-NH1	-9.49	115.56	120.30
1	C	67	ASP	CB-CG-OD2	9.46	126.82	118.30
1	D	368	ASN	CA-C-O	9.46	139.97	120.10
1	D	342	ASP	CB-CG-OD1	9.22	126.60	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	96	ASP	CB-CG-OD2	8.97	126.37	118.30
1	B	202	ASN	CB-CA-C	-8.95	92.50	110.40
1	A	188	ARG	NE-CZ-NH1	-8.84	115.88	120.30
1	A	364	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	D	24	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	C	364	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	B	56	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	C	248	LEU	CB-CG-CD2	-8.23	97.02	111.00
1	A	297	ASP	CB-CG-OD2	8.21	125.68	118.30
1	D	365	ARG	NE-CZ-NH2	8.03	124.31	120.30
1	A	188	ARG	NE-CZ-NH2	7.90	124.25	120.30
1	A	24	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	C	365	ARG	NE-CZ-NH2	7.79	124.20	120.30
1	A	142	ARG	NE-CZ-NH2	7.77	124.18	120.30
1	C	68	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	B	53	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	B	94	LEU	CB-CG-CD1	7.58	123.88	111.00
1	C	365	ARG	NE-CZ-NH1	-7.57	116.51	120.30
1	B	232	VAL	CG1-CB-CG2	-7.49	98.92	110.90
1	A	202	ASN	CB-CA-C	-7.47	95.45	110.40
1	B	80	ASP	CB-CG-OD1	7.43	124.99	118.30
1	C	66	ASP	CB-CG-OD1	-7.34	111.69	118.30
1	D	53	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	B	369	LYS	O-C-N	-7.31	111.00	122.70
1	D	56	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	C	55	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	B	352	ASP	CB-CG-OD2	6.93	124.54	118.30
1	D	348	GLU	OE1-CD-OE2	-6.92	115.00	123.30
1	A	66	ASP	CB-CG-OD1	6.89	124.50	118.30
1	D	297	ASP	CB-CG-OD1	6.79	124.41	118.30
1	B	60	ASP	CB-CG-OD2	6.77	124.39	118.30
1	A	368	ASN	CA-C-O	6.73	134.23	120.10
1	A	249	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	258	ASP	CB-CG-OD2	6.64	124.28	118.30
1	C	73	VAL	CG1-CB-CG2	-6.54	100.43	110.90
1	D	66	ASP	CB-CG-OD1	6.52	124.16	118.30
1	C	37	LEU	CB-CG-CD2	6.51	122.06	111.00
1	A	237	THR	OG1-CB-CG2	-6.51	95.03	110.00
1	D	280	TYR	CA-C-O	-6.48	106.48	120.10
1	B	365	ARG	NE-CZ-NH1	-6.45	117.07	120.30
1	D	357	LEU	CB-CG-CD1	-6.42	100.09	111.00
1	A	142	ARG	NE-CZ-NH1	-6.40	117.10	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	212	VAL	CG1-CB-CG2	-6.39	100.68	110.90
1	A	40	GLN	CB-CA-C	-6.34	97.72	110.40
1	D	362	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	C	81	LEU	CB-CG-CD1	6.30	121.71	111.00
1	B	113	PRO	CA-C-O	-6.29	105.11	120.20
1	B	129	ASN	C-N-CA	-6.24	106.09	121.70
1	B	314	MET	CG-SD-CE	-6.23	90.23	100.20
1	A	280	TYR	CA-C-O	-6.22	107.03	120.10
1	C	213	ASP	CB-CG-OD2	6.19	123.87	118.30
1	D	168	LEU	CA-CB-CG	6.19	129.54	115.30
1	B	66	ASP	CB-CG-OD1	6.17	123.85	118.30
1	D	48	LEU	CB-CG-CD1	6.13	121.42	111.00
1	C	80	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	67	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	B	161	ASP	CB-CG-OD2	6.07	123.77	118.30
1	B	55	ARG	NE-CZ-NH2	6.05	123.32	120.30
1	C	41	ILE	CG1-CB-CG2	-5.87	98.49	111.40
1	A	269	LEU	CB-CG-CD1	-5.85	101.06	111.00
1	D	223	HIS	CB-CA-C	-5.84	98.72	110.40
1	C	342	ASP	CB-CG-OD1	5.84	123.55	118.30
1	A	248	LEU	CB-CG-CD2	-5.81	101.12	111.00
1	B	96	ASP	CB-CG-OD1	-5.76	113.12	118.30
1	D	94	LEU	CB-CG-CD1	5.75	120.78	111.00
1	B	60	ASP	CB-CG-OD1	-5.74	113.14	118.30
1	A	196	PHE	CB-CA-C	5.71	121.82	110.40
1	A	279	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	37	LEU	CB-CG-CD2	5.69	120.67	111.00
1	C	24	ARG	NE-CZ-NH2	5.67	123.13	120.30
1	B	202	ASN	CA-C-O	-5.64	108.25	120.10
1	B	129	ASN	O-C-N	-5.64	113.68	122.70
1	D	138	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	A	80	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	216	GLN	CA-CB-CG	5.58	125.68	113.40
1	D	249	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	D	249	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	D	364	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	177	ILE	CG1-CB-CG2	-5.51	99.28	111.40
1	C	142	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	326	ILE	CG1-CB-CG2	-5.41	99.49	111.40
1	B	297	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	249	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	D	55	ARG	NE-CZ-NH2	5.31	122.96	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	26	LEU	CB-CG-CD1	5.30	120.01	111.00
1	B	56	ARG	CA-CB-CG	5.30	125.06	113.40
1	A	257	TYR	N-CA-C	5.29	125.29	111.00
1	D	256	ASN	N-CA-C	5.28	125.26	111.00
1	D	194	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	A	364	ARG	CG-CD-NE	-5.24	100.79	111.80
1	A	190	LEU	CB-CG-CD2	5.23	119.89	111.00
1	D	246	VAL	CG1-CB-CG2	-5.22	102.55	110.90
1	A	53	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	66	ASP	OD1-CG-OD2	-5.21	113.39	123.30
1	B	269	LEU	CB-CG-CD2	5.20	119.84	111.00
1	D	188	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	D	89	LEU	CB-CG-CD1	5.17	119.78	111.00
1	A	37	LEU	CA-CB-CG	5.16	127.16	115.30
1	D	340	ILE	CG1-CB-CG2	-5.13	100.11	111.40
1	C	71	VAL	CG1-CB-CG2	-5.10	102.74	110.90
1	A	244	CYS	CA-CB-SG	-5.10	104.83	114.00
1	D	138	LEU	CB-CG-CD1	5.09	119.65	111.00
1	A	122	LEU	CA-CB-CG	5.07	126.96	115.30
1	A	208	LEU	N-CA-C	5.05	124.62	111.00

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	42	0
1	B	2376	0	2344	53	0
1	C	2322	0	2241	38	0
1	D	2305	0	2253	34	0
2	A	21	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	156	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 (156) 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
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: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:C:167:TYR:C	1:C:168:LEU:HD22	2.15	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:89:LEU:CD1	1:A:151:ILE:HD13	2.35	0.57
1:A:133:ASN:C	1:A:133:ASN:HD22	2.07	0.57
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:C:164:SER:HB3	1:D:225:MET:HE3	1.88	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:D:348:GLU:H	1:D:348:GLU:CD	2.12	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:239:LYS:CG	1:B:26:LEU:HD21	2.42	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
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:A:109:TYR:C	1:A:110:LEU:HD23	2.38	0.44
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:167:TYR:C	1:B:168:LEU:HD22	2.38	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:C:109:TYR:C	1:C:110:LEU:HD23	2.39	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
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:355:ARG:NH1	1:A:355:ARG:CG	2.77	0.41
1:C:21:GLU:OE2	1:D:229:LYS:HE2	2.20	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:280:TYR:CD1	1:D:315:ILE:HG12	2.56	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	295/370 (80%)	282 (96%)	11 (4%)	2 (1%)	22 18
1	B	310/370 (84%)	299 (96%)	10 (3%)	1 (0%)	41 41
1	C	307/370 (83%)	293 (95%)	12 (4%)	2 (1%)	22 18
1	D	301/370 (81%)	293 (97%)	8 (3%)	0	100 100
All	All	1213/1480 (82%)	1167 (96%)	41 (3%)	5 (0%)	34 32

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 (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	221/298 (74%)	198 (90%)	23 (10%)	7 4
1	B	245/298 (82%)	229 (94%)	16 (6%)	17 14
1	C	233/298 (78%)	207 (89%)	26 (11%)	6 3
1	D	231/298 (78%)	214 (93%)	17 (7%)	13 10
All	All	930/1192 (78%)	848 (91%)	82 (9%)	10 6

All (82) 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
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	209	ASN
1	A	230	HIS
1	A	239	LYS
1	A	317	SER
1	A	355	ARG
1	A	357	LEU
1	A	363	GLN
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	166	GLN
1	B	216	GLN
1	B	230	HIS
1	B	232	VAL
1	B	314	MET
1	B	326	ILE
1	B	357	LEU
1	B	363	GLN
1	B	366	GLU
1	C	23	VAL
1	C	37	LEU
1	C	48	LEU
1	C	52	LYS
1	C	89	LEU
1	C	92	LYS
1	C	94	LEU
1	C	95	SER
1	C	107	ARG
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	249	ARG
1	C	255	THR
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	94	LEU
1	D	107	ARG
1	D	110	LEU
1	D	157	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	85	GLN
1	A	133	ASN
1	A	147	ASN
1	A	166	GLN
1	A	202	ASN
1	A	274	ASN
1	A	302	GLN
1	B	85	GLN
1	B	124	ASN
1	B	147	ASN
1	B	166	GLN
1	B	220	HIS
1	B	256	ASN
1	B	274	ASN
1	B	291	ASN
1	B	296	ASN
1	B	302	GLN
1	B	308	ASN
1	C	85	GLN
1	C	133	ASN
1	C	139	GLN
1	C	143	GLN
1	C	147	ASN
1	C	202	ASN
1	C	216	GLN
1	C	274	ASN
1	D	40	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	85	GLN
1	D	124	ASN
1	D	130	ASN
1	D	147	ASN
1	D	166	GLN
1	D	220	HIS
1	D	274	ASN
1	D	296	ASN
1	D	302	GLN
1	D	308	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 monosaccharides 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, 95^{th} 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%)	0.29	15 (4%)	29	35	32, 50, 66, 79	0
1	B	322/370 (87%)	0.18	14 (4%)	35	41	31, 46, 63, 75	0
1	C	319/370 (86%)	0.18	10 (3%)	49	55	32, 48, 66, 73	0
1	D	315/370 (85%)	0.29	13 (4%)	37	43	32, 48, 66, 78	0
All	All	1263/1480 (85%)	0.23	52 (4%)	37	43	31, 48, 66, 79	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	369	LYS	5.8
1	A	129	ASN	5.3
1	A	336	TYR	4.8
1	B	370	LYS	4.7
1	D	326	ILE	4.6
1	A	76	CYS	4.1
1	D	325	GLY	4.0
1	A	341	THR	3.8
1	C	128	VAL	3.6
1	D	336	TYR	3.5
1	B	326	ILE	3.3
1	C	130	ASN	3.2
1	A	342	ASP	3.1
1	C	132	PHE	3.0
1	A	132	PHE	3.0
1	D	131	THR	2.9
1	D	324	GLN	2.7
1	D	130	ASN	2.7
1	B	71	VAL	2.7
1	D	198	VAL	2.7
1	D	128	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	342	ASP	2.7
1	B	313	VAL	2.6
1	D	120	LYS	2.6
1	C	326	ILE	2.6
1	A	130	ASN	2.5
1	D	366	GLU	2.5
1	D	171	LEU	2.5
1	A	257	TYR	2.5
1	B	130	ASN	2.5
1	A	340	ILE	2.4
1	A	305	ASN	2.4
1	C	313	VAL	2.4
1	B	291	ASN	2.3
1	B	69	VAL	2.3
1	B	26	LEU	2.3
1	B	155	ILE	2.3
1	C	370	LYS	2.2
1	B	352	ASP	2.2
1	A	26	LEU	2.2
1	A	289	PHE	2.2
1	B	200	PHE	2.2
1	B	209	ASN	2.1
1	A	343	ALA	2.1
1	A	73	VAL	2.1
1	C	325	GLY	2.1
1	C	366	GLU	2.1
1	C	127	ASP	2.1
1	B	106	MET	2.0
1	D	305	ASN	2.0
1	A	104	ILE	2.0
1	B	73	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.