



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:03 AM UTC

PDB ID : 1OF6 / pdb_00001of6
Title : crystal structure of the tyrosine-regulated 3-deoxy-d-arabino-heptulosonate-7-phosphate synthase from saccharomyces cerevisiae complexed with tyrosine and manganese
Authors : Koenig, V.; Pfeil, A.; Heinrich, G.; Braus, G.; Schneider, T.R.
Deposited on : 2003-04-08
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
Mogul : 2022.3.0, CSD as543be (2022)
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

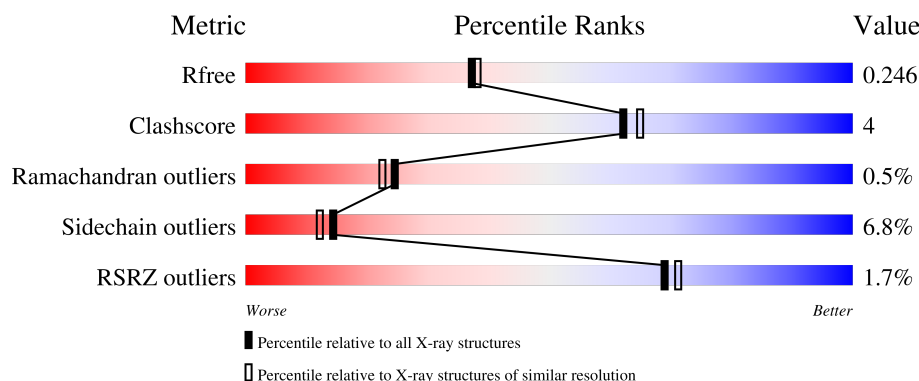
1 Overall quality at a glance

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% 82% 11% • 5%
1	B	370	% 79% 13% • 6%
1	C	370	% 79% 14% •• 5%
1	D	370	% 78% 15% • 6%
1	E	370	3% 74% 15% • 8%

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Mol	Chain	Length	Quality of chain
1	F	370	 % 79% 14% • 6%
1	G	370	 3% 69% 19% • 8%
1	H	370	 % 78% 14% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DTY	A	1370	X	-	-	-
3	DTY	B	1370	X	-	-	-
3	DTY	C	1371	X	-	-	-
3	DTY	D	1370	X	-	-	-
3	DTY	E	1370	X	-	-	-
3	DTY	F	1370	X	-	-	-
3	DTY	G	1369	X	-	-	-
3	DTY	H	1369	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21605 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, TYROSINE-INHIBITED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2630	1635	473	512	10			
1	B	346	Total	C	N	O	S	0	0	0
			2608	1623	466	509	10			
1	C	350	Total	C	N	O	S	0	0	0
			2634	1639	472	513	10			
1	D	349	Total	C	N	O	S	0	0	0
			2617	1627	468	512	10			
1	E	339	Total	C	N	O	S	0	0	0
			2559	1590	459	500	10			
1	F	347	Total	C	N	O	S	0	0	0
			2607	1622	467	508	10			
1	G	342	Total	C	N	O	S	0	0	0
			2572	1601	459	502	10			
1	H	347	Total	C	N	O	S	0	0	0
			2599	1615	465	509	10			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

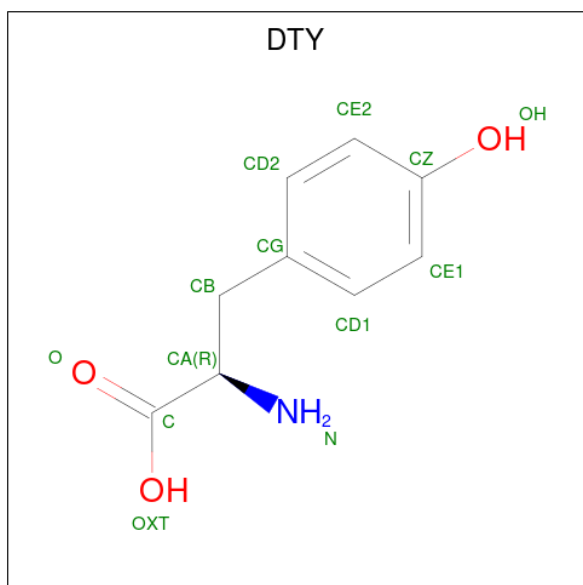
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mn	0	0
			1	1		
2	H	1	Total	Mn	0	0
			1	1		

- Molecule 3 is D-TYROSINE (CCD ID: DTY) (formula: $C_9H_{11}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	9	1	3		
3	B	1	Total	C	N	O	0	0
			13	9	1	3		
3	C	1	Total	C	N	O	0	0
			13	9	1	3		
3	D	1	Total	C	N	O	0	0
			13	9	1	3		
3	E	1	Total	C	N	O	0	0
			13	9	1	3		
3	F	1	Total	C	N	O	0	0
			13	9	1	3		
3	G	1	Total	C	N	O	0	0
			13	9	1	3		
3	H	1	Total	C	N	O	0	0
			13	9	1	3		

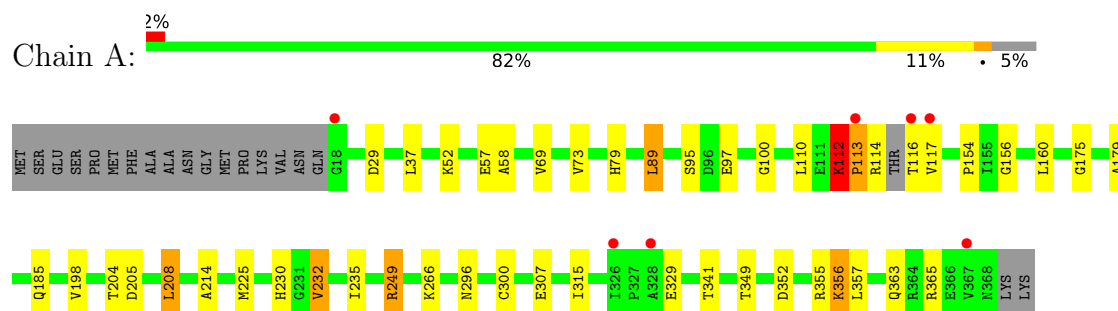
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	106	Total 106	O 106	0	0
4	B	91	Total 91	O 91	0	0
4	C	83	Total 83	O 83	0	0
4	D	113	Total 113	O 113	0	0
4	E	63	Total 63	O 63	0	0
4	F	88	Total 88	O 88	0	0
4	G	58	Total 58	O 58	0	0
4	H	65	Total 65	O 65	0	0

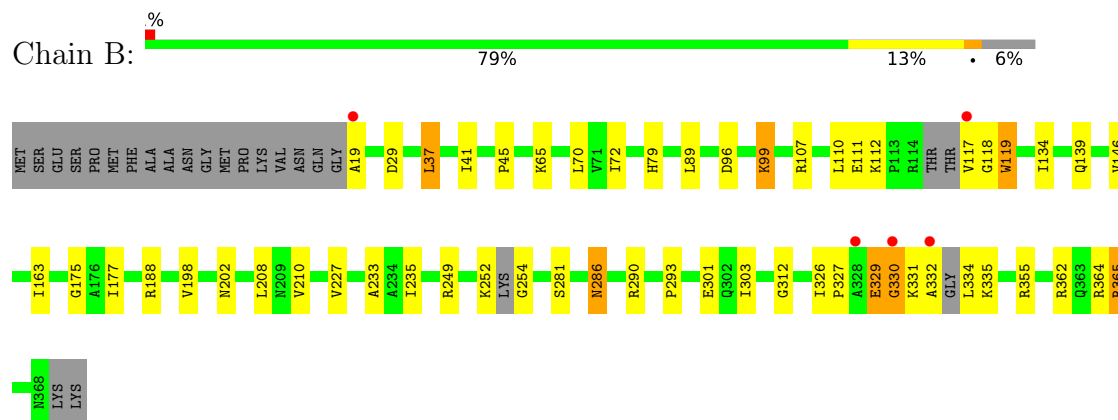
3 Residue-property plots [i](#)

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

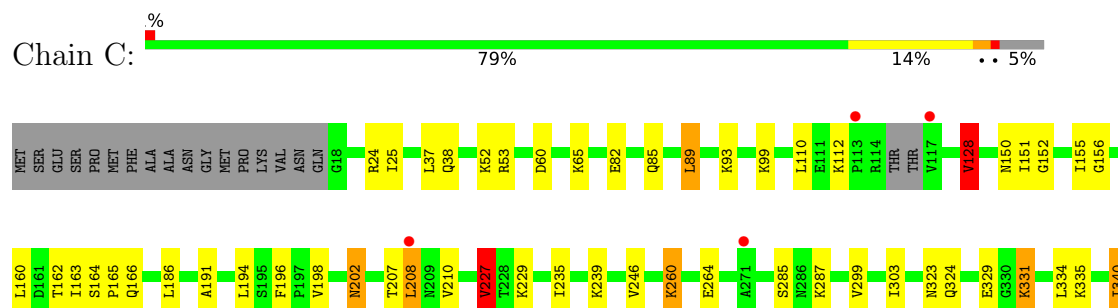
- Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE, TYROSINE-INHIBITED



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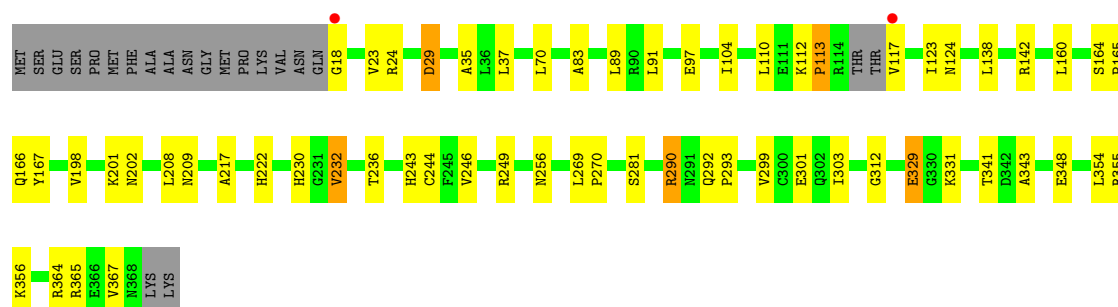
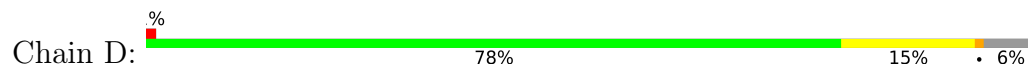


- Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE, TYROSINE-INHIBITED

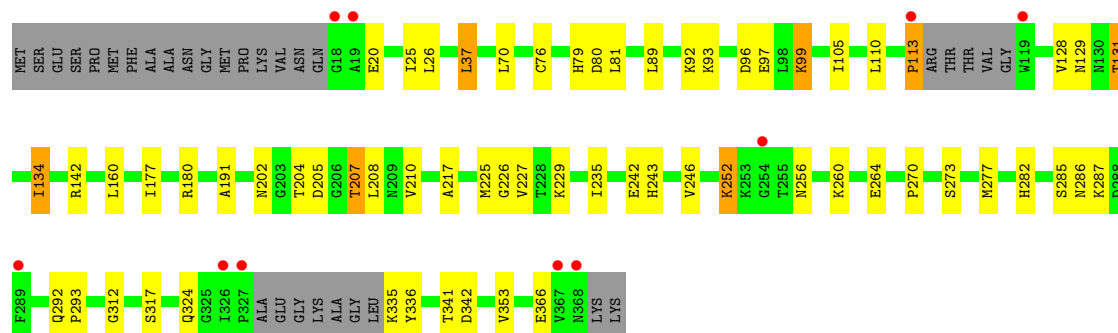
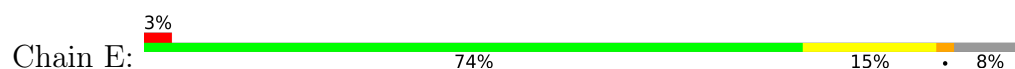




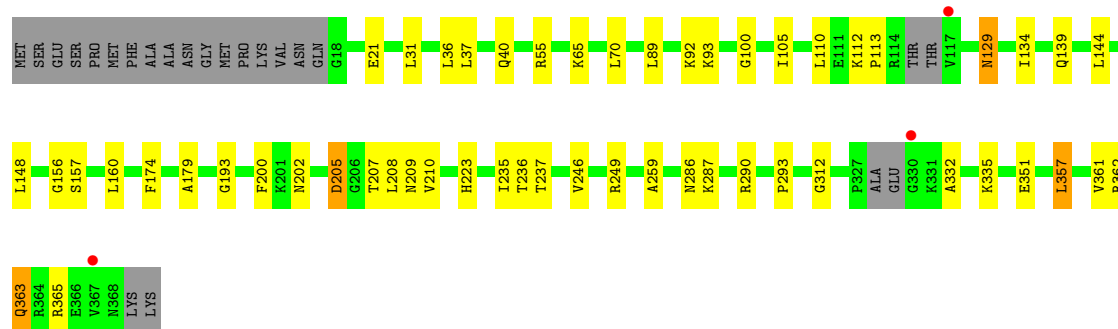
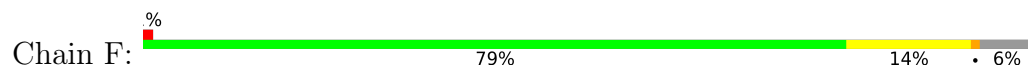
- Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE, TYROSINE-INHIBITED



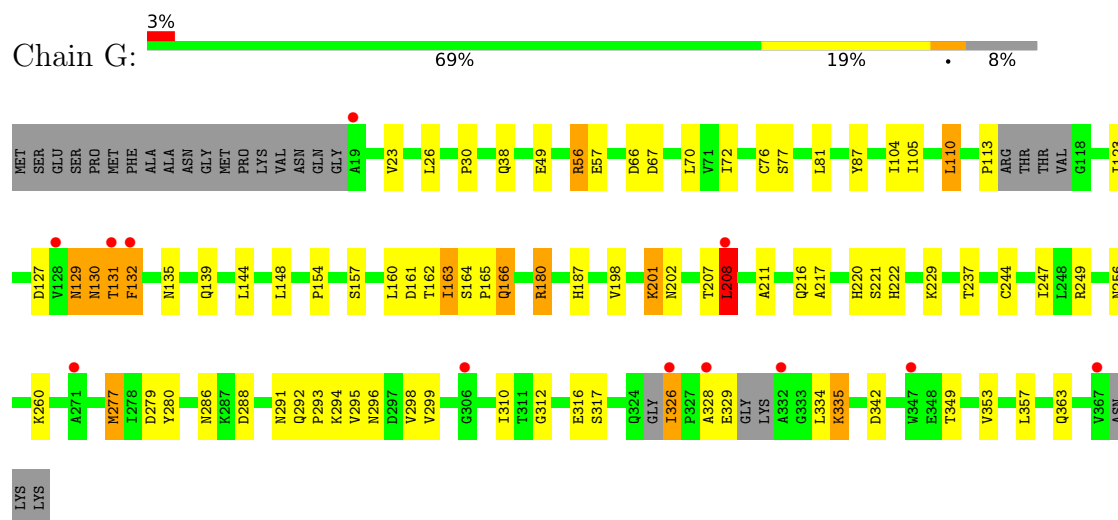
- Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE, TYROSINE-INHIBITED



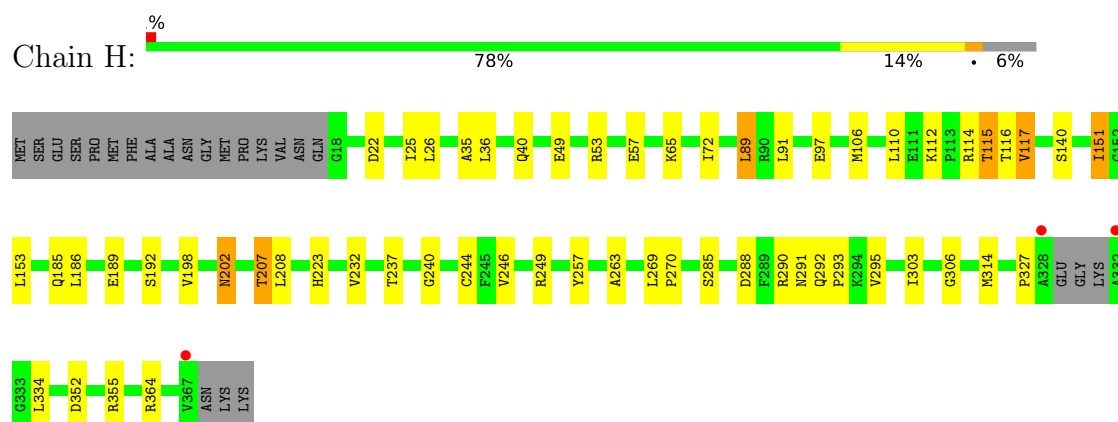
- Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE, TYROSINE-INHIBITED



• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE, TYROSINE-INHIBITED



• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE, TYROSINE-INHIBITED



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.13Å 94.70Å 104.84Å 64.71° 85.51° 75.61°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-2.10) 97.1 (20.00-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.195 , 0.237 (Not available) , 0.246	Depositor DCC
R_{free} test set	4949 reflections (3.16%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.001 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21605	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.6318e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.43	9/2668 (0.3%)	1.25	4/3612 (0.1%)
1	B	1.47	7/2644 (0.3%)	1.26	1/3577 (0.0%)
1	C	1.39	11/2672 (0.4%)	1.24	7/3615 (0.2%)
1	D	1.45	10/2655 (0.4%)	1.26	9/3596 (0.3%)
1	E	1.39	8/2595 (0.3%)	1.29	7/3512 (0.2%)
1	F	1.34	4/2644 (0.2%)	1.26	4/3578 (0.1%)
1	G	1.39	15/2608 (0.6%)	1.28	9/3531 (0.3%)
1	H	1.36	3/2637 (0.1%)	1.29	3/3576 (0.1%)
All	All	1.40	67/21123 (0.3%)	1.27	44/28597 (0.2%)

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	H	0	1

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	256	ASN	C-O	-10.46	1.14	1.24
1	F	193	GLY	C-O	-9.05	1.17	1.24
1	C	163	ILE	CA-CB	8.76	1.62	1.55
1	F	200	PHE	CA-C	-7.11	1.44	1.52
1	B	146	VAL	C-O	-7.03	1.16	1.24
1	A	341	THR	C-O	-6.98	1.17	1.23
1	G	201	LYS	CE-NZ	6.92	1.70	1.49
1	G	310	ILE	CA-C	-6.62	1.44	1.52
1	B	227	VAL	C-O	-6.43	1.17	1.24
1	D	113	PRO	CA-C	6.42	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	142	ARG	C-O	-6.41	1.16	1.24
1	A	69	VAL	CA-CB	-6.25	1.47	1.54
1	G	72	ILE	CA-CB	6.11	1.61	1.54
1	A	58	ALA	C-O	-6.05	1.17	1.24
1	D	35	ALA	CA-CB	6.03	1.62	1.53
1	C	128	VAL	CA-CB	6.00	1.62	1.54
1	B	188	ARG	CA-C	5.96	1.60	1.52
1	B	119	TRP	N-CA	5.91	1.53	1.46
1	E	277	MET	C-O	5.83	1.31	1.24
1	C	299	VAL	CA-CB	5.83	1.61	1.54
1	A	112	LYS	CA-C	5.81	1.59	1.52
1	E	226	GLY	N-CA	5.76	1.49	1.44
1	G	104	ILE	C-O	-5.72	1.17	1.24
1	G	277	MET	CG-SD	-5.70	1.66	1.80
1	G	237	THR	CA-CB	5.70	1.61	1.53
1	H	115	THR	CA-CB	5.65	1.61	1.53
1	F	179	ALA	CA-CB	-5.63	1.44	1.53
1	B	233	ALA	CA-CB	-5.58	1.44	1.53
1	A	208	LEU	CA-C	-5.51	1.45	1.52
1	G	132	PHE	CA-C	5.51	1.60	1.52
1	B	118	GLY	CA-C	5.51	1.59	1.51
1	A	214	ALA	C-O	-5.44	1.17	1.24
1	E	217	ALA	CA-CB	5.44	1.62	1.53
1	B	177	ILE	CA-C	5.43	1.59	1.52
1	E	282	HIS	C-O	5.41	1.29	1.24
1	C	303	ILE	CA-CB	5.39	1.60	1.54
1	C	191	ALA	CA-CB	-5.38	1.44	1.53
1	C	160	LEU	C-O	-5.37	1.17	1.24
1	D	138	LEU	C-O	-5.37	1.17	1.24
1	E	210	VAL	CA-CB	5.37	1.61	1.54
1	C	38	GLN	C-O	-5.36	1.17	1.24
1	A	185	GLN	C-O	-5.36	1.18	1.24
1	D	138	LEU	CA-C	-5.35	1.45	1.52
1	G	187	HIS	C-O	-5.34	1.17	1.24
1	C	229	LYS	C-O	-5.32	1.17	1.24
1	C	210	VAL	CA-CB	5.30	1.61	1.54
1	H	106	MET	SD-CE	-5.28	1.66	1.79
1	D	301	GLU	CD-OE2	5.28	1.35	1.25
1	G	57	GLU	C-O	-5.27	1.17	1.24
1	A	179	ALA	C-O	5.26	1.30	1.24
1	G	310	ILE	CA-CB	5.26	1.60	1.53
1	G	211	ALA	CA-C	5.23	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	365	ARG	CA-C	5.21	1.59	1.52
1	A	156	GLY	CA-C	-5.19	1.47	1.52
1	G	166	GLN	C-O	-5.18	1.17	1.24
1	H	263	ALA	N-CA	5.17	1.52	1.46
1	D	301	GLU	CG-CD	5.16	1.65	1.52
1	D	343	ALA	CA-CB	5.15	1.61	1.53
1	G	221	SER	C-O	-5.12	1.17	1.24
1	E	341	THR	CA-CB	5.10	1.61	1.52
1	C	151	ILE	CA-CB	-5.08	1.47	1.54
1	G	208	LEU	CG-CD1	5.08	1.69	1.52
1	G	56	ARG	CG-CD	5.08	1.67	1.52
1	C	198	VAL	C-O	-5.08	1.18	1.24
1	F	210	VAL	C-O	-5.02	1.18	1.24
1	E	191	ALA	CA-CB	-5.02	1.45	1.53
1	E	177	ILE	CA-CB	-5.02	1.48	1.54

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	29	ASP	N-CA-C	-7.58	99.56	110.40
1	D	299	VAL	N-CA-C	-7.07	104.08	111.58
1	C	227	VAL	CB-CA-C	-7.05	99.96	110.82
1	C	128	VAL	CB-CA-C	6.34	121.69	111.29
1	E	97	GLU	N-CA-C	6.31	118.71	111.02
1	H	112	LYS	N-CA-C	-6.11	101.88	110.31
1	F	259	ALA	N-CA-C	6.05	118.65	111.33
1	G	256	ASN	N-CA-C	6.05	117.55	110.41
1	D	348	GLU	N-CA-C	-5.85	104.99	111.36
1	C	156	GLY	CA-C-O	-5.83	116.50	121.57
1	H	306	GLY	N-CA-C	5.72	123.34	115.27
1	A	205	ASP	N-CA-C	5.71	119.98	113.19
1	E	256	ASN	N-CA-C	5.65	117.07	110.41
1	D	124	ASN	N-CA-C	5.64	117.23	111.14
1	F	100	GLY	N-CA-C	-5.63	107.35	114.16
1	E	81	LEU	N-CA-C	5.57	118.12	111.71
1	E	252	LYS	N-CA-C	5.57	117.35	111.28
1	H	35	ALA	N-CA-C	5.57	117.80	111.11
1	D	301	GLU	N-CA-C	-5.52	105.27	111.28
1	C	340	ILE	N-CA-C	5.50	116.81	111.91
1	E	336	TYR	N-CA-C	5.49	118.77	110.64
1	G	291	ASN	N-CA-C	5.46	119.57	113.01
1	G	201	LYS	CD-CE-NZ	5.40	129.19	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	264	GLU	N-CA-C	-5.40	104.79	111.33
1	C	155	ILE	N-CA-C	5.37	117.81	108.95
1	C	163	ILE	CB-CA-C	-5.37	107.15	111.71
1	G	298	VAL	N-CA-C	5.36	116.09	110.62
1	B	210	VAL	N-CA-C	5.36	116.09	110.62
1	F	210	VAL	N-CA-C	5.29	116.02	110.62
1	G	201	LYS	CB-CA-C	5.29	119.27	109.54
1	C	196	PHE	N-CA-C	5.22	112.72	108.07
1	D	354	LEU	N-CA-C	5.19	117.02	111.36
1	G	279	ASP	CA-C-N	5.17	129.47	120.68
1	G	279	ASP	C-N-CA	5.17	129.47	120.68
1	A	154	PRO	N-CD-CG	-5.17	95.45	103.20
1	G	237	THR	OG1-CB-CG2	-5.14	99.03	109.30
1	D	83	ALA	N-CA-C	5.12	117.52	111.33
1	E	99	LYS	N-CA-C	5.11	117.59	111.71
1	G	201	LYS	CB-CG-CD	5.11	123.05	111.30
1	A	204	THR	OG1-CB-CG2	-5.09	99.11	109.30
1	A	57	GLU	N-CA-C	5.09	116.51	111.07
1	D	367	VAL	N-CA-C	5.02	117.36	111.09
1	F	332	ALA	N-CA-C	5.01	117.63	111.82
1	D	356	LYS	N-CA-C	5.00	116.42	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	207	THR	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	2630	0	2628	19	0
1	B	2608	0	2604	20	0
1	C	2634	0	2638	22	0
1	D	2617	0	2603	24	0
1	E	2559	0	2557	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2607	0	2602	23	0
1	G	2572	0	2558	37	0
1	H	2599	0	2578	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	13	0	9	0	0
3	B	13	0	9	0	0
3	C	13	0	9	1	0
3	D	13	0	9	0	0
3	E	13	0	9	0	0
3	F	13	0	9	0	0
3	G	13	0	9	0	0
3	H	13	0	9	0	0
4	A	106	0	0	1	0
4	B	91	0	0	1	0
4	C	83	0	0	0	0
4	D	113	0	0	1	0
4	E	63	0	0	0	0
4	F	88	0	0	2	0
4	G	58	0	0	2	0
4	H	65	0	0	1	0
All	All	21605	0	20840	171	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 4.

All (171) 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:G:201:LYS:CE	1:G:201:LYS:NZ	1.70	1.53
1:D:208:LEU:HD11	1:D:246:VAL:HG11	1.56	0.88
1:A:97:GLU:OE2	1:A:355:ARG:NH1	2.08	0.86
1:D:303:ILE:O	1:D:364:ARG:HB2	1.80	0.81
1:C:208:LEU:HD21	1:C:246:VAL:HG11	1.64	0.80
1:G:129:ASN:ND2	1:G:129:ASN:C	2.43	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:ASN:C	1:G:129:ASN:HD22	1.91	0.77
1:A:52:LYS:HZ1	1:B:19:ALA:N	1.82	0.77
1:G:76:CYS:SG	1:G:342:ASP:HB2	2.28	0.73
1:H:223:HIS:CE1	1:H:237:THR:HG23	2.29	0.68
1:F:70:LEU:HD11	1:F:105:ILE:HD12	1.78	0.66
1:B:355:ARG:HH11	1:B:355:ARG:HG2	1.61	0.66
1:B:96:ASP:O	1:B:99:LYS:HD3	1.97	0.65
1:G:334:LEU:O	1:G:335:LYS:O	2.16	0.64
1:C:52:LYS:HE2	1:D:18:GLY:O	1.99	0.63
1:C:208:LEU:HD22	1:C:208:LEU:O	1.99	0.63
1:E:205:ASP:OD1	1:E:207:THR:OG1	2.16	0.62
1:F:357:LEU:O	1:F:361:VAL:HG23	2.00	0.62
1:G:202:ASN:HB2	1:G:207:THR:O	2.01	0.60
1:F:290:ARG:O	1:F:293:PRO:HD2	2.01	0.60
1:F:362:ARG:O	1:F:365:ARG:HB2	2.02	0.59
1:D:112:LYS:HD2	1:D:341:THR:HB	1.85	0.59
1:H:303:ILE:O	1:H:364:ARG:HB2	2.01	0.59
1:F:36:LEU:O	1:F:40:GLN:HG3	2.03	0.59
1:E:76:CYS:SG	1:E:342:ASP:HB2	2.44	0.58
1:G:207:THR:HA	1:G:208:LEU:HD12	1.85	0.58
1:D:217:ALA:O	1:D:222:HIS:HE1	1.87	0.57
1:E:208:LEU:HD11	1:E:246:VAL:HG11	1.86	0.56
1:D:208:LEU:HD11	1:D:246:VAL:CG1	2.30	0.56
1:G:217:ALA:O	1:G:222:HIS:HE1	1.89	0.55
1:A:232:VAL:HG11	1:D:230:HIS:HB3	1.89	0.55
1:D:37:LEU:HD12	1:D:167:TYR:CD2	2.41	0.55
1:C:128:VAL:HG13	1:C:331:LYS:HG2	1.87	0.54
1:H:207:THR:OG1	4:H:2044:HOH:O	2.18	0.54
1:E:92:LYS:NZ	1:E:96:ASP:OD1	2.40	0.54
1:B:37:LEU:HD13	1:B:41:ILE:HD12	1.90	0.54
1:B:252:LYS:O	1:B:254:GLY:N	2.41	0.54
1:B:175:GLY:O	1:B:198:VAL:HA	2.07	0.54
1:C:53:ARG:NH2	1:C:152:GLY:O	2.41	0.54
1:E:113:PRO:HB3	1:E:180:ARG:NH1	2.23	0.53
1:C:323:ASN:C	1:C:323:ASN:OD1	2.50	0.53
1:E:324:GLN:OE1	1:E:335:LYS:HB3	2.09	0.53
1:F:205:ASP:OD2	1:F:207:THR:HG23	2.08	0.53
1:H:36:LEU:O	1:H:40:GLN:HG3	2.09	0.53
1:B:290:ARG:O	1:B:293:PRO:HD2	2.09	0.53
1:A:266:LYS:NZ	1:A:307:GLU:OE2	2.40	0.53
1:D:97:GLU:OE2	1:D:355:ARG:NH1	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:288:ASP:HA	4:G:2052:HOH:O	2.08	0.52
1:G:326:ILE:HA	1:G:334:LEU:HD21	1.90	0.52
1:H:53:ARG:O	1:H:57:GLU:HG3	2.09	0.52
1:G:328:ALA:O	1:G:329:GLU:HB2	2.10	0.52
1:H:290:ARG:O	1:H:293:PRO:HD2	2.10	0.52
1:C:24:ARG:HH22	1:D:243:HIS:CD2	2.28	0.52
1:C:260:LYS:O	1:C:264:GLU:HG2	2.10	0.52
1:G:76:CYS:HA	1:G:316:GLU:OE2	2.10	0.52
1:G:113:PRO:HB3	1:G:180:ARG:NH1	2.25	0.51
1:G:110:LEU:HD23	1:G:123:ILE:HD11	1.92	0.51
1:B:330:GLY:C	1:B:332:ALA:H	2.18	0.51
1:A:230:HIS:HB3	1:D:232:VAL:HG11	1.92	0.51
1:D:290:ARG:O	1:D:293:PRO:HD2	2.11	0.51
1:G:66:ASP:OD1	1:G:67:ASP:N	2.44	0.51
1:A:29:ASP:HB2	1:B:235:ILE:HB	1.94	0.50
1:E:129:ASN:OD1	1:E:131:THR:HB	2.11	0.50
1:G:164:SER:N	1:G:165:PRO:CD	2.75	0.49
1:G:280:TYR:HA	1:G:295:VAL:HG11	1.94	0.49
1:A:112:LYS:HG2	1:A:113:PRO:HD2	1.95	0.49
1:C:166:GLN:HG3	1:C:227:VAL:HG23	1.94	0.49
1:E:270:PRO:HD2	1:E:273:SER:OG	2.11	0.49
1:G:180:ARG:HG3	4:G:2029:HOH:O	2.13	0.49
1:C:85:GLN:O	1:C:89:LEU:HD22	2.13	0.48
1:C:150:ASN:CG	1:C:150:ASN:O	2.56	0.48
1:H:91:LEU:HD23	1:H:153:LEU:HD21	1.94	0.48
1:A:352:ASP:O	1:A:356:LYS:HG2	2.14	0.48
1:B:72:ILE:HG22	1:B:107:ARG:HG3	1.94	0.48
1:B:119:TRP:HB2	1:B:326:ILE:HD11	1.94	0.48
1:G:296:ASN:CG	1:G:353:VAL:HG13	2.39	0.48
1:C:235:ILE:HB	1:D:29:ASP:HB2	1.96	0.48
1:E:205:ASP:CG	1:E:207:THR:OG1	2.57	0.47
1:E:225:MET:HE2	1:F:134:ILE:HG21	1.94	0.47
1:F:156:GLY:HA2	1:F:174:PHE:O	2.13	0.47
1:E:25:ILE:HD12	1:F:236:THR:CG2	2.45	0.47
1:G:105:ILE:HG12	1:G:154:PRO:HB2	1.97	0.47
1:A:73:VAL:HG23	1:A:315:ILE:HB	1.96	0.47
1:G:70:LEU:O	1:G:312:GLY:HA2	2.14	0.47
1:G:349:THR:O	1:G:353:VAL:HG23	2.14	0.47
1:F:363:GLN:HA	1:F:363:GLN:OE1	2.15	0.47
1:H:22:ASP:HB3	1:H:25:ILE:HB	1.97	0.47
1:F:335:LYS:NZ	4:F:2079:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:VAL:O	1:D:244:CYS:HA	2.15	0.47
1:H:257:TYR:CG	1:H:295:VAL:HG13	2.50	0.47
1:C:25:ILE:HD12	1:D:236:THR:HG22	1.97	0.46
1:E:205:ASP:OD2	1:E:207:THR:OG1	2.33	0.46
1:C:60:ASP:OD1	1:C:65:LYS:HE2	2.16	0.46
1:E:37:LEU:HD12	1:E:142:ARG:HD3	1.97	0.46
1:G:162:THR:OG1	1:G:163:ILE:HD13	2.15	0.46
1:E:292:GLN:HB2	1:E:293:PRO:HD3	1.97	0.46
1:E:242:GLU:HG2	1:E:243:HIS:CD2	2.51	0.45
1:H:208:LEU:HD11	1:H:246:VAL:HG11	1.98	0.45
1:C:348:GLU:H	1:C:348:GLU:CD	2.24	0.45
1:C:164:SER:N	1:C:165:PRO:CD	2.80	0.45
1:H:291:ASN:O	1:H:295:VAL:HG23	2.17	0.45
1:C:194:LEU:O	1:D:24:ARG:HD2	2.17	0.45
1:H:198:VAL:O	1:H:244:CYS:HA	2.17	0.45
1:B:70:LEU:O	1:B:312:GLY:HA2	2.17	0.44
1:C:208:LEU:HD21	1:C:246:VAL:CG1	2.43	0.44
1:E:235:ILE:HG13	1:F:31:LEU:HD13	1.99	0.44
1:A:89:LEU:HD13	1:A:89:LEU:HA	1.87	0.44
1:B:37:LEU:HD11	1:B:139:GLN:HA	1.99	0.44
1:E:225:MET:HE2	1:F:134:ILE:CG2	2.48	0.44
1:E:229:LYS:HZ1	1:F:21:GLU:CD	2.26	0.44
1:A:249:ARG:C	1:A:249:ARG:HD3	2.42	0.44
1:G:292:GLN:HB2	1:G:293:PRO:HD3	2.00	0.43
1:H:89:LEU:HD13	1:H:151:ILE:HD12	2.00	0.43
1:D:292:GLN:N	1:D:293:PRO:CD	2.81	0.43
1:H:202:ASN:HB2	1:H:207:THR:O	2.18	0.43
1:A:175:GLY:O	1:A:198:VAL:HA	2.18	0.43
1:H:288:ASP:OD1	1:H:290:ARG:HB2	2.18	0.43
1:E:70:LEU:O	1:E:312:GLY:HA2	2.18	0.43
1:G:295:VAL:O	1:G:299:VAL:HG23	2.19	0.43
1:G:135:ASN:O	1:G:139:GLN:HG3	2.19	0.43
1:D:70:LEU:O	1:D:312:GLY:HA2	2.18	0.43
1:H:97:GLU:CD	1:H:355:ARG:HH21	2.26	0.43
1:A:100:GLY:O	1:A:365:ARG:NH2	2.49	0.43
1:G:127:ASP:HB2	1:G:129:ASN:OD1	2.19	0.43
1:H:192:SER:HB2	1:H:240:GLY:HA2	2.01	0.43
1:E:20:GLU:HG3	1:F:55:ARG:NH1	2.33	0.43
1:F:112:LYS:O	1:F:113:PRO:C	2.62	0.43
1:D:201:LYS:HE3	4:D:2030:HOH:O	2.18	0.43
1:G:130:ASN:O	1:G:130:ASN:OD1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:292:GLN:N	1:H:293:PRO:CD	2.82	0.43
1:A:235:ILE:HB	1:B:29:ASP:HB2	1.99	0.43
1:E:79:HIS:CD2	1:E:80:ASP:HB2	2.54	0.43
1:A:296:ASN:O	1:A:300:CYS:HB2	2.20	0.42
1:A:225:MET:HE3	1:B:163:ILE:HB	2.01	0.42
1:C:357:LEU:O	1:C:361:VAL:HG23	2.19	0.42
1:H:185:GLN:O	1:H:189:GLU:HG3	2.19	0.42
1:D:112:LYS:O	1:D:113:PRO:C	2.60	0.42
1:D:164:SER:N	1:D:165:PRO:CD	2.83	0.42
1:B:327:PRO:O	1:B:329:GLU:O	2.37	0.42
1:C:324:GLN:OE1	1:C:335:LYS:HG3	2.19	0.42
1:D:91:LEU:HD11	1:D:104:ILE:HG21	2.02	0.42
1:F:70:LEU:O	1:F:312:GLY:HA2	2.19	0.42
1:G:38:GLN:OE1	1:G:229:LYS:HE2	2.19	0.42
1:G:87:TYR:CD1	1:G:87:TYR:C	2.97	0.42
1:A:112:LYS:HE3	1:A:112:LYS:HB3	1.90	0.42
1:B:303:ILE:O	1:B:364:ARG:HB2	2.19	0.42
1:F:129:ASN:C	1:F:129:ASN:HD22	2.28	0.42
1:H:72:ILE:O	1:H:314:MET:HA	2.20	0.42
1:A:112:LYS:HA	1:A:113:PRO:HD2	1.84	0.41
1:F:223:HIS:CE1	1:F:237:THR:HG23	2.55	0.41
1:H:269:LEU:HA	1:H:270:PRO:HD2	1.90	0.41
1:C:202:ASN:HB2	1:C:207:THR:O	2.21	0.41
1:G:247:ILE:HG12	1:G:277:MET:HB3	2.03	0.41
1:F:208:LEU:HD11	1:F:246:VAL:HG11	2.03	0.41
1:G:144:LEU:O	1:G:148:LEU:HG	2.20	0.41
1:C:162:THR:O	3:C:1371:DTY:OH	2.39	0.41
1:G:161:ASP:HB3	1:H:186:LEU:HD12	2.02	0.41
1:B:330:GLY:C	1:B:332:ALA:N	2.79	0.41
1:F:144:LEU:HD11	1:F:148:LEU:HD11	2.03	0.41
1:A:79:HIS:HD2	4:A:2019:HOH:O	2.04	0.41
1:D:123:ILE:HD13	1:D:123:ILE:HG21	1.89	0.40
1:E:70:LEU:HD11	1:E:105:ILE:HD12	2.02	0.40
1:E:134:ILE:HB	1:F:235:ILE:HG12	2.02	0.40
1:G:30:PRO:O	1:G:135:ASN:ND2	2.54	0.40
1:G:198:VAL:O	1:G:244:CYS:HA	2.21	0.40
1:B:79:HIS:HD2	4:B:2010:HOH:O	2.04	0.40
1:G:129:ASN:OD1	1:G:131:THR:OG1	2.39	0.40
1:B:362:ARG:O	1:B:365:ARG:HB2	2.21	0.40
1:G:216:GLN:O	1:G:220:HIS:HD2	2.04	0.40
1:D:269:LEU:HA	1:D:270:PRO:HD3	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:LYS:NZ	4:F:2022:HOH:O	2.55	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	346/370 (94%)	331 (96%)	13 (4%)	2 (1%)	21	18
1	B	338/370 (91%)	324 (96%)	11 (3%)	3 (1%)	14	10
1	C	346/370 (94%)	334 (96%)	11 (3%)	1 (0%)	36	36
1	D	345/370 (93%)	332 (96%)	12 (4%)	1 (0%)	36	36
1	E	333/370 (90%)	314 (94%)	18 (5%)	1 (0%)	36	36
1	F	341/370 (92%)	324 (95%)	16 (5%)	1 (0%)	36	36
1	G	334/370 (90%)	311 (93%)	20 (6%)	3 (1%)	14	10
1	H	343/370 (93%)	328 (96%)	13 (4%)	2 (1%)	21	18
All	All	2726/2960 (92%)	2598 (95%)	114 (4%)	14 (0%)	24	22

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	329	GLU
1	F	286	ASN
1	G	335	LYS
1	A	329	GLU
1	B	286	ASN
1	B	331	LYS
1	C	329	GLU
1	G	132	PHE
1	H	327	PRO

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Mol	Chain	Res	Type
1	A	113	PRO
1	G	130	ASN
1	H	117	VAL
1	B	330	GLY
1	E	128	VAL

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	279/298 (94%)	263 (94%)	16 (6%)	18	17
1	B	278/298 (93%)	258 (93%)	20 (7%)	13	11
1	C	280/298 (94%)	258 (92%)	22 (8%)	11	9
1	D	277/298 (93%)	263 (95%)	14 (5%)	21	21
1	E	274/298 (92%)	252 (92%)	22 (8%)	11	8
1	F	277/298 (93%)	260 (94%)	17 (6%)	17	15
1	G	273/298 (92%)	250 (92%)	23 (8%)	10	7
1	H	275/298 (92%)	258 (94%)	17 (6%)	16	14
All	All	2213/2384 (93%)	2062 (93%)	151 (7%)	14	12

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	89	LEU
1	A	95	SER
1	A	110	LEU
1	A	112	LYS
1	A	114	ARG
1	A	116	THR
1	A	117	VAL
1	A	160	LEU
1	A	208	LEU

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Mol	Chain	Res	Type
1	A	232	VAL
1	A	249	ARG
1	A	349	THR
1	A	356	LYS
1	A	357	LEU
1	A	363	GLN
1	B	37	LEU
1	B	45	PRO
1	B	65	LYS
1	B	89	LEU
1	B	99	LYS
1	B	110	LEU
1	B	111	GLU
1	B	112	LYS
1	B	117	VAL
1	B	134	ILE
1	B	202	ASN
1	B	208	LEU
1	B	249	ARG
1	B	281	SER
1	B	286	ASN
1	B	301	GLU
1	B	329	GLU
1	B	334	LEU
1	B	335	LYS
1	B	365	ARG
1	C	37	LEU
1	C	82	GLU
1	C	89	LEU
1	C	93	LYS
1	C	99	LYS
1	C	110	LEU
1	C	112	LYS
1	C	128	VAL
1	C	186	LEU
1	C	202	ASN
1	C	208	LEU
1	C	227	VAL
1	C	239	LYS
1	C	260	LYS
1	C	285	SER
1	C	287	LYS

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Mol	Chain	Res	Type
1	C	331	LYS
1	C	334	LEU
1	C	340	ILE
1	C	348	GLU
1	C	353	VAL
1	C	369	LYS
1	D	23	VAL
1	D	89	LEU
1	D	110	LEU
1	D	117	VAL
1	D	160	LEU
1	D	166	GLN
1	D	202	ASN
1	D	209	ASN
1	D	232	VAL
1	D	249	ARG
1	D	281	SER
1	D	290	ARG
1	D	329	GLU
1	D	331	LYS
1	E	26	LEU
1	E	37	LEU
1	E	89	LEU
1	E	93	LYS
1	E	99	LYS
1	E	110	LEU
1	E	113	PRO
1	E	131	THR
1	E	134	ILE
1	E	160	LEU
1	E	202	ASN
1	E	204	THR
1	E	207	THR
1	E	227	VAL
1	E	252	LYS
1	E	260	LYS
1	E	285	SER
1	E	286	ASN
1	E	287	LYS
1	E	317	SER
1	E	353	VAL
1	E	366	GLU

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Mol	Chain	Res	Type
1	F	37	LEU
1	F	65	LYS
1	F	89	LEU
1	F	93	LYS
1	F	110	LEU
1	F	129	ASN
1	F	139	GLN
1	F	157	SER
1	F	160	LEU
1	F	202	ASN
1	F	205	ASP
1	F	209	ASN
1	F	249	ARG
1	F	287	LYS
1	F	351	GLU
1	F	357	LEU
1	F	363	GLN
1	G	23	VAL
1	G	26	LEU
1	G	49	GLU
1	G	56	ARG
1	G	77	SER
1	G	81	LEU
1	G	110	LEU
1	G	129	ASN
1	G	131	THR
1	G	157	SER
1	G	160	LEU
1	G	163	ILE
1	G	166	GLN
1	G	180	ARG
1	G	208	LEU
1	G	249	ARG
1	G	260	LYS
1	G	286	ASN
1	G	294	LYS
1	G	317	SER
1	G	326	ILE
1	G	357	LEU
1	G	363	GLN
1	H	26	LEU
1	H	49	GLU

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Mol	Chain	Res	Type
1	H	65	LYS
1	H	89	LEU
1	H	110	LEU
1	H	114	ARG
1	H	115	THR
1	H	116	THR
1	H	117	VAL
1	H	140	SER
1	H	151	ILE
1	H	202	ASN
1	H	232	VAL
1	H	249	ARG
1	H	285	SER
1	H	334	LEU
1	H	352	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	150	ASN
1	A	223	HIS
1	A	286	ASN
1	A	308	ASN
1	A	368	ASN
1	B	40	GLN
1	B	143	GLN
1	B	220	HIS
1	B	223	HIS
1	B	286	ASN
1	C	40	GLN
1	D	139	GLN
1	D	143	GLN
1	D	150	ASN
1	D	222	HIS
1	D	243	HIS
1	E	124	ASN
1	E	143	GLN
1	E	286	ASN
1	E	320	ASN
1	F	129	ASN
1	F	143	GLN

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Mol	Chain	Res	Type
1	F	230	HIS
1	F	268	GLN
1	F	308	ASN
1	F	368	ASN
1	G	143	GLN
1	G	220	HIS
1	G	222	HIS
1	G	223	HIS
1	G	363	GLN
1	H	79	HIS
1	H	143	GLN
1	H	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	DTY	C	1371	-	12,13,13	1.35	2 (16%)	13,17,17	0.87	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DTY	D	1370	-	12,13,13	1.75	4 (33%)	13,17,17	1.59	4 (30%)
3	DTY	G	1369	-	12,13,13	1.31	2 (16%)	13,17,17	0.94	0
3	DTY	E	1370	-	12,13,13	1.42	2 (16%)	13,17,17	1.28	1 (7%)
3	DTY	B	1370	-	12,13,13	2.09	3 (25%)	13,17,17	1.12	2 (15%)
3	DTY	A	1370	-	12,13,13	1.53	2 (16%)	13,17,17	1.16	1 (7%)
3	DTY	F	1370	-	12,13,13	1.47	2 (16%)	13,17,17	1.14	2 (15%)
3	DTY	H	1369	-	12,13,13	1.88	2 (16%)	13,17,17	1.09	2 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DTY	C	1371	-	1/1/2/2	0/8/8/8	0/1/1/1
3	DTY	D	1370	-	1/1/2/2	0/8/8/8	0/1/1/1
3	DTY	G	1369	-	1/1/2/2	0/8/8/8	0/1/1/1
3	DTY	E	1370	-	1/1/2/2	0/8/8/8	0/1/1/1
3	DTY	B	1370	-	1/1/2/2	0/8/8/8	0/1/1/1
3	DTY	A	1370	-	1/1/2/2	0/8/8/8	0/1/1/1
3	DTY	F	1370	-	1/1/2/2	1/8/8/8	0/1/1/1
3	DTY	H	1369	-	1/1/2/2	0/8/8/8	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1370	DTY	OH-CZ	-5.80	1.24	1.37
3	H	1369	DTY	OH-CZ	-4.90	1.26	1.37
3	F	1370	DTY	OH-CZ	-4.34	1.27	1.37
3	A	1370	DTY	OH-CZ	-4.10	1.27	1.37
3	E	1370	DTY	OXT-C	-3.50	1.19	1.30
3	D	1370	DTY	CE1-CD1	3.35	1.44	1.38
3	E	1370	DTY	OH-CZ	-3.18	1.29	1.37
3	C	1371	DTY	OH-CZ	-3.18	1.29	1.37
3	G	1369	DTY	OH-CZ	-3.02	1.30	1.37
3	C	1371	DTY	OXT-C	-2.78	1.21	1.30
3	D	1370	DTY	OH-CZ	-2.64	1.31	1.37
3	D	1370	DTY	CE2-CD2	2.62	1.43	1.38
3	H	1369	DTY	OXT-C	-2.61	1.22	1.30
3	G	1369	DTY	OXT-C	-2.52	1.22	1.30
3	B	1370	DTY	O-C	2.51	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1370	DTY	CD1-CG	2.45	1.43	1.38
3	A	1370	DTY	OXT-C	-2.29	1.23	1.30
3	F	1370	DTY	OXT-C	-2.29	1.23	1.30
3	D	1370	DTY	CE2-CZ	2.23	1.43	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1370	DTY	OXT-C-O	-3.48	116.17	124.08
3	D	1370	DTY	CD2-CE2-CZ	2.85	122.89	119.88
3	D	1370	DTY	CE2-CZ-CE1	-2.84	115.24	119.77
3	C	1371	DTY	OXT-C-O	-2.61	118.17	124.08
3	D	1370	DTY	OXT-C-O	-2.44	118.54	124.08
3	A	1370	DTY	CD2-CE2-CZ	-2.42	117.32	119.88
3	F	1370	DTY	CG-CB-CA	-2.35	109.32	114.13
3	F	1370	DTY	OXT-C-O	-2.31	118.84	124.08
3	B	1370	DTY	OXT-C-O	-2.23	119.02	124.08
3	B	1370	DTY	CB-CA-N	-2.21	102.92	111.40
3	H	1369	DTY	CE1-CD1-CG	-2.13	118.20	121.00
3	H	1369	DTY	CD2-CG-CD1	2.08	121.32	118.23
3	D	1370	DTY	CB-CA-N	-2.01	103.70	111.40

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1370	DTY	CA
3	B	1370	DTY	CA
3	C	1371	DTY	CA
3	D	1370	DTY	CA
3	E	1370	DTY	CA
3	F	1370	DTY	CA
3	G	1369	DTY	CA
3	H	1369	DTY	CA

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1370	DTY	O-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1371	DTY	1	0

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	350/370 (94%)	-0.02	7 (2%) 65 67	31, 43, 60, 77	0
1	B	346/370 (93%)	-0.04	5 (1%) 73 75	29, 42, 56, 81	0
1	C	350/370 (94%)	0.08	5 (1%) 73 75	33, 45, 63, 83	0
1	D	349/370 (94%)	-0.10	2 (0%) 85 87	31, 40, 55, 70	0
1	E	339/370 (91%)	0.36	10 (2%) 53 56	34, 51, 66, 79	0
1	F	347/370 (93%)	0.09	3 (0%) 81 83	35, 46, 60, 71	0
1	G	342/370 (92%)	0.43	12 (3%) 47 49	35, 50, 66, 80	0
1	H	347/370 (93%)	0.15	3 (0%) 81 83	35, 46, 62, 78	0
All	All	2770/2960 (93%)	0.12	47 (1%) 69 71	29, 45, 63, 83	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	117	VAL	4.4
1	B	332	ALA	4.3
1	D	117	VAL	4.3
1	H	328	ALA	3.8
1	H	332	ALA	3.8
1	H	367	VAL	3.7
1	G	131	THR	3.7
1	G	367	VAL	3.6
1	A	18	GLY	3.4
1	A	113	PRO	3.4
1	B	117	VAL	3.3
1	G	208	LEU	3.3
1	A	116	THR	3.3
1	G	128	VAL	3.3
1	F	117	VAL	3.1
1	E	113	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	327	PRO	3.0
1	E	289	PHE	3.0
1	D	18	GLY	2.9
1	E	119	TRP	2.9
1	E	367	VAL	2.8
1	C	271	ALA	2.8
1	A	117	VAL	2.7
1	C	113	PRO	2.7
1	B	19	ALA	2.7
1	G	271	ALA	2.6
1	B	328	ALA	2.6
1	G	332	ALA	2.6
1	E	18	GLY	2.5
1	F	330	GLY	2.4
1	E	368	ASN	2.4
1	G	326	ILE	2.4
1	G	132	PHE	2.3
1	F	367	VAL	2.3
1	C	208	LEU	2.3
1	A	367	VAL	2.2
1	E	254	GLY	2.2
1	A	326	ILE	2.2
1	E	326	ILE	2.2
1	E	19	ALA	2.2
1	G	347	TRP	2.2
1	C	367	VAL	2.1
1	A	328	ALA	2.1
1	B	330	GLY	2.1
1	G	306	GLY	2.1
1	G	19	ALA	2.1
1	G	328	ALA	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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DTY	C	1371	13/13	0.95	0.06	33,34,38,39	0
3	DTY	B	1370	13/13	0.96	0.06	33,35,37,38	0
3	DTY	A	1370	13/13	0.96	0.05	28,33,34,34	0
3	DTY	D	1370	13/13	0.96	0.05	30,33,35,35	0
3	DTY	F	1370	13/13	0.96	0.05	33,38,41,43	0
3	DTY	G	1369	13/13	0.96	0.06	35,40,41,41	0
3	DTY	H	1369	13/13	0.96	0.06	35,38,40,41	0
3	DTY	E	1370	13/13	0.97	0.05	31,34,37,38	0
2	MN	G	1368	1/1	0.97	0.07	45,45,45,45	0
2	MN	H	1368	1/1	0.98	0.04	37,37,37,37	0
2	MN	E	1369	1/1	0.98	0.06	45,45,45,45	0
2	MN	C	1370	1/1	0.98	0.06	38,38,38,38	0
2	MN	D	1369	1/1	0.99	0.05	30,30,30,30	0
2	MN	A	1369	1/1	0.99	0.04	33,33,33,33	0
2	MN	B	1369	1/1	1.00	0.09	31,31,31,31	0
2	MN	F	1369	1/1	1.00	0.05	33,33,33,33	0

6.5 Other polymers

There are no such residues in this entry.