



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:22 PM GMT

PDB ID : 1OF6
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

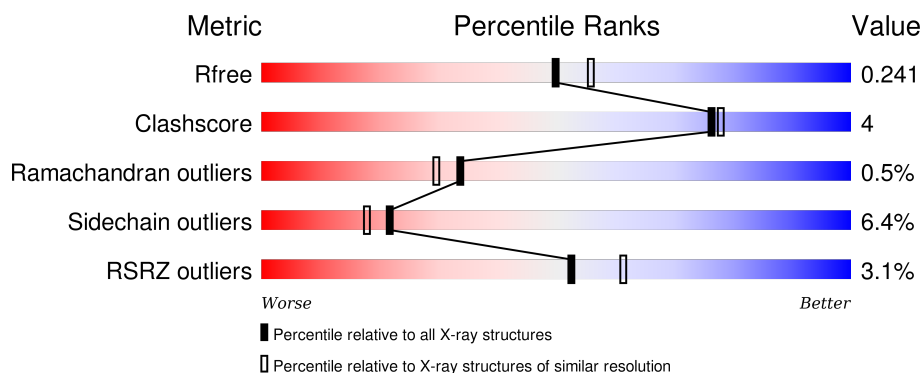
1 Overall quality at a glance ⓘ

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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div>81% 12% • 5%</div> </div>
1	B	370	<div> <div>2%</div> <div>78% 12% • 6%</div> </div>
1	C	370	<div> <div>2%</div> <div>79% 14% •• 5%</div> </div>
1	D	370	<div> <div>2%</div> <div>81% 11% • 6%</div> </div>
1	E	370	<div> <div>4%</div> <div>77% 14% • 8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	370	
1	G	370	
1	H	370	

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 (three-letter code: MN) (formula: Mn).

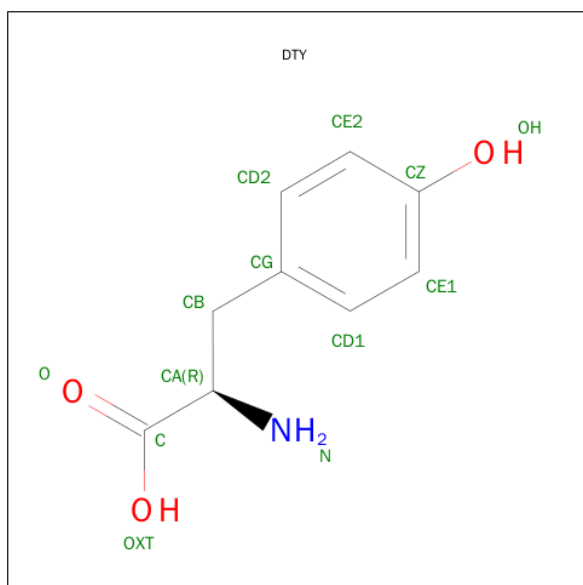
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	H	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

- Molecule 3 is D-TYROSINE (three-letter code: 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		

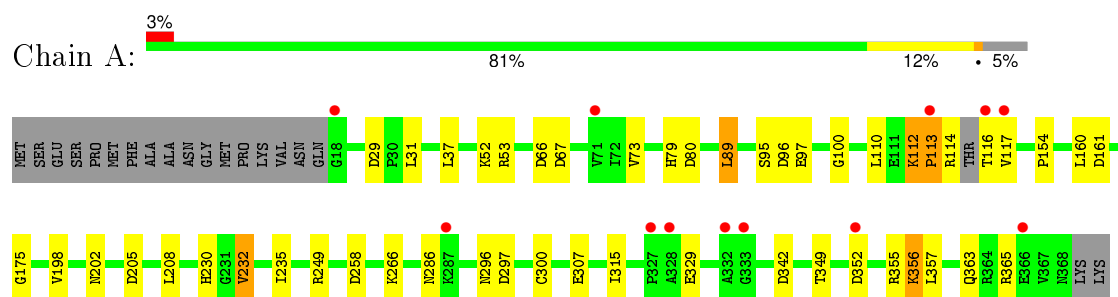
- Molecule 4 is water.

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

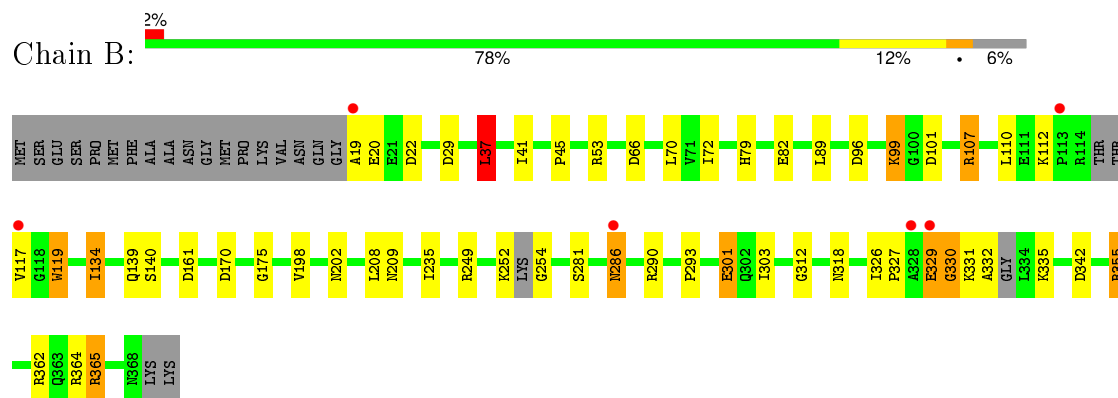
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

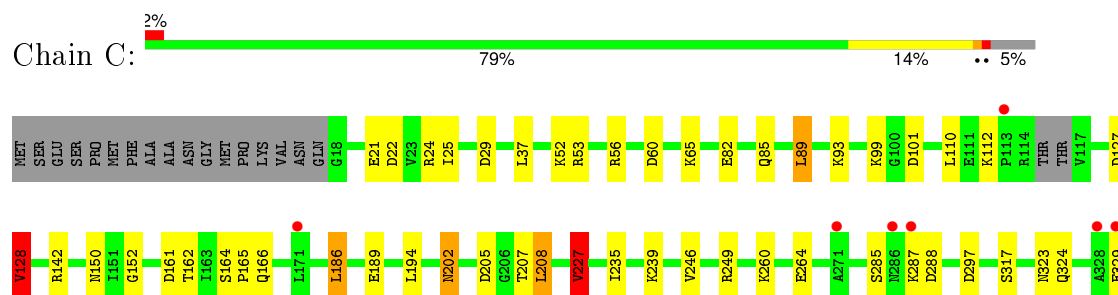
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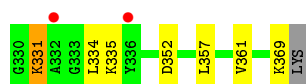


- Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE, TYROSINE-INHIBITED

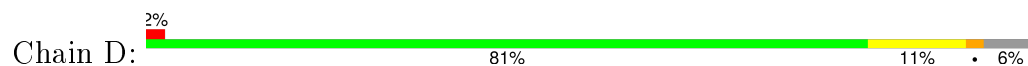


- Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE, TYROSINE-INHIBITED

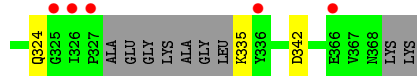




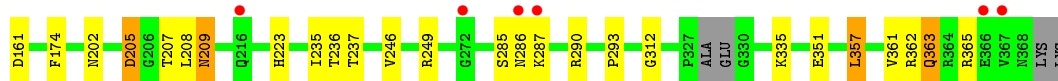
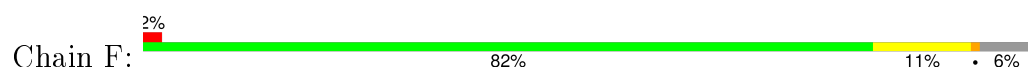
- Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE, TYROSINE-INHIBITED



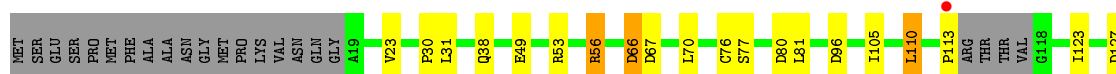
- Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE, TYROSINE-INHIBITED

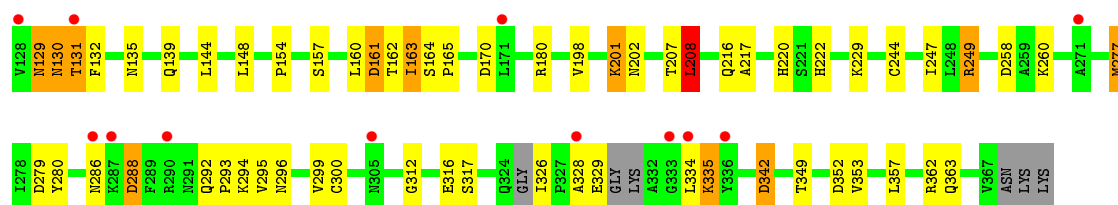


- Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE, TYROSINE-INHIBITED

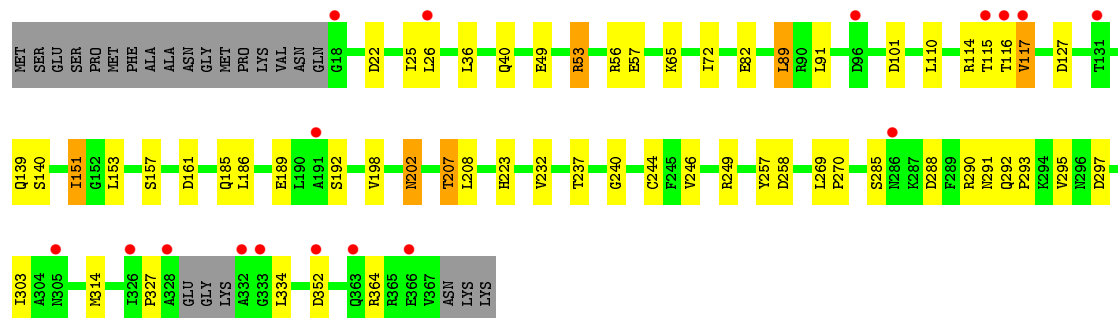
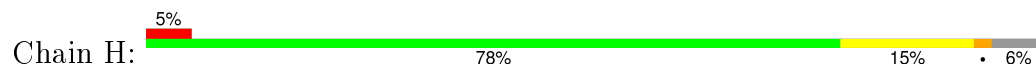


- Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE, TYROSINE-INHIBITED





• 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 19.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-2.10) 83.4 (19.99-2.10)	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 0.201 , 0.241	Depositor DCC
R_{free} test set	4949 reflections (3.26%)	DCC
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.9	EDS
Estimated twinning fraction	0.001 for -h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 156678 reflections	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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.12	0/2668	1.08	12/3612 (0.3%)
1	B	1.18	7/2644 (0.3%)	1.07	12/3577 (0.3%)
1	C	1.08	4/2672 (0.1%)	1.11	15/3615 (0.4%)
1	D	1.15	4/2655 (0.2%)	1.06	7/3596 (0.2%)
1	E	1.06	0/2595	1.10	11/3512 (0.3%)
1	F	1.04	1/2644 (0.0%)	1.06	6/3578 (0.2%)
1	G	1.11	4/2608 (0.2%)	1.12	17/3531 (0.5%)
1	H	1.05	1/2637 (0.0%)	1.08	8/3576 (0.2%)
All	All	1.10	21/21123 (0.1%)	1.08	88/28597 (0.3%)

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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	301	GLU	CD-OE2	8.84	1.35	1.25
1	D	301	GLU	CG-CD	8.67	1.65	1.51
1	G	201	LYS	CE-NZ	8.42	1.70	1.49
1	B	301	GLU	CD-OE1	7.46	1.33	1.25
1	B	301	GLU	CG-CD	7.08	1.62	1.51
1	G	56	ARG	CG-CD	6.30	1.67	1.51
1	B	119	TRP	CB-CG	6.03	1.61	1.50
1	C	56	ARG	CG-CD	5.92	1.66	1.51
1	F	209	ASN	CB-CG	5.73	1.64	1.51
1	D	246	VAL	CB-CG1	-5.68	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	300	CYS	CB-SG	-5.67	1.72	1.81
1	G	277	MET	CG-SD	-5.64	1.66	1.81
1	C	189	GLU	CD-OE1	5.46	1.31	1.25
1	D	301	GLU	CD-OE1	5.37	1.31	1.25
1	C	227	VAL	CB-CG1	-5.33	1.41	1.52
1	H	82	GLU	CG-CD	5.33	1.59	1.51
1	B	82	GLU	CD-OE1	5.31	1.31	1.25
1	B	140	SER	CB-OG	-5.23	1.35	1.42
1	B	209	ASN	CB-CG	5.21	1.63	1.51
1	C	21	GLU	CD-OE1	5.03	1.31	1.25
1	B	20	GLU	CD-OE1	5.01	1.31	1.25

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	161	ASP	CB-CG-OD2	10.21	127.49	118.30
1	F	161	ASP	CB-CG-OD2	8.86	126.28	118.30
1	E	161	ASP	CB-CG-OD2	8.86	126.27	118.30
1	H	161	ASP	CB-CG-OD2	8.67	126.11	118.30
1	G	279	ASP	CB-CG-OD1	8.34	125.80	118.30
1	B	161	ASP	CB-CG-OD2	8.27	125.74	118.30
1	C	101	ASP	CB-CG-OD2	8.24	125.72	118.30
1	C	297	ASP	CB-CG-OD2	7.93	125.44	118.30
1	A	161	ASP	CB-CG-OD2	7.89	125.40	118.30
1	H	53	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	G	208	LEU	CB-CG-CD1	7.78	124.22	111.00
1	G	53	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	E	258	ASP	CB-CG-OD2	7.67	125.20	118.30
1	G	201	LYS	CD-CE-NZ	7.60	129.19	111.70
1	C	288	ASP	CB-CG-OD2	7.56	125.11	118.30
1	B	101	ASP	CB-CG-OD2	7.41	124.97	118.30
1	G	362	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	G	161	ASP	CB-CG-OD2	7.34	124.91	118.30
1	E	96	ASP	CB-CG-OD2	7.29	124.86	118.30
1	D	66	ASP	CB-CG-OD2	7.25	124.83	118.30
1	C	56	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	E	53	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	F	125	ASP	CB-CG-OD1	7.04	124.63	118.30
1	H	53	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	B	170	ASP	CB-CG-OD1	6.80	124.42	118.30
1	C	205	ASP	CB-CG-OD2	6.67	124.30	118.30
1	G	96	ASP	CB-CG-OD2	6.65	124.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	66	ASP	CB-CG-OD2	6.62	124.26	118.30
1	C	352	ASP	CB-CG-OD2	6.52	124.17	118.30
1	B	342	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	96	ASP	CB-CG-OD2	6.40	124.06	118.30
1	C	142	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	C	186	LEU	CA-CB-CG	6.29	129.77	115.30
1	G	342	ASP	CB-CG-OD2	6.26	123.93	118.30
1	E	22	ASP	CB-CG-OD2	6.25	123.93	118.30
1	G	170	ASP	CB-CG-OD2	6.13	123.81	118.30
1	B	355	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	E	90	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	G	258	ASP	CB-CG-OD2	6.07	123.76	118.30
1	D	29	ASP	CB-CG-OD2	6.03	123.72	118.30
1	C	227	VAL	CB-CA-C	-6.02	99.96	111.40
1	B	355	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	E	53	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	22	ASP	CB-CG-OD1	5.96	123.66	118.30
1	G	288	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	67	ASP	CB-CG-OD1	5.82	123.53	118.30
1	A	205	ASP	CB-CG-OD1	5.81	123.53	118.30
1	E	127	ASP	CB-CG-OD2	5.79	123.51	118.30
1	C	142	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	E	56	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	E	101	ASP	CB-CG-OD2	5.67	123.41	118.30
1	D	101	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	107	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	D	160	LEU	CA-CB-CG	5.51	127.97	115.30
1	B	66	ASP	CB-CG-OD2	5.47	123.22	118.30
1	G	80	ASP	CB-CG-OD1	5.46	123.22	118.30
1	H	127	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	53	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	128	VAL	CB-CA-C	5.41	121.69	111.40
1	E	205	ASP	CB-CG-OD2	5.41	123.17	118.30
1	G	31	LEU	CA-CB-CG	5.38	127.68	115.30
1	H	56	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	G	352	ASP	CB-CG-OD1	5.36	123.13	118.30
1	A	342	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	53	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	G	249	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	C	29	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	127	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	89	LEU	CB-CG-CD1	5.28	119.97	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	37	LEU	CB-CG-CD2	5.27	119.96	111.00
1	F	160	LEU	CB-CG-CD1	5.26	119.95	111.00
1	G	249	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	161	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	31	LEU	CA-CB-CG	5.24	127.34	115.30
1	B	134	ILE	CG1-CB-CG2	-5.23	99.89	111.40
1	A	80	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	297	ASP	CB-CG-OD1	5.21	122.99	118.30
1	H	297	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	154	PRO	N-CD-CG	-5.17	95.45	103.20
1	D	89	LEU	CA-CB-CG	5.14	127.12	115.30
1	F	53	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	F	22	ASP	CB-CG-OD2	5.13	122.92	118.30
1	F	53	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	H	101	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	66	ASP	CB-CG-OD2	5.09	122.88	118.30
1	H	258	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	258	ASP	CB-CG-OD1	5.00	122.80	118.30

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	17	0
1	B	2608	0	2604	18	0
1	C	2634	0	2638	21	0
1	D	2617	0	2603	23	0
1	E	2559	0	2557	20	0
1	F	2607	0	2602	17	0
1	G	2572	0	2558	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2599	0	2578	21	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	1	0
4	G	58	0	0	2	0
4	H	65	0	0	1	0
All	All	21605	0	20840	158	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 (158) 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: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:G:129:ASN:HD22	1:G:129:ASN:C	1.91	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:ASN:C	1:G:129:ASN:ND2	2.43	0.72
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:252:LYS:O	1:B:254:GLY:N	2.41	0.54
1:B:37:LEU:HD13	1:B:41:ILE:HD12	1.90	0.54
1:C:53:ARG:NH2	1:C:152:GLY:O	2.41	0.54
1:B:175:GLY:O	1:B:198:VAL:HA	2.07	0.54
1:E:113:PRO:HB3	1:E:180:ARG:NH1	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:290:ARG:O	1:H:293:PRO:HD2	2.10	0.52
1:G:328:ALA:O	1:G:329:GLU:HB2	2.10	0.52
1:C:260:LYS:O	1:C:264:GLU:HG2	2.10	0.52
1:C:24:ARG:HH22	1:D:243:HIS:CD2	2.28	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: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:323:ASN:C	1:C:323:ASN:OD1	2.50	0.49
1:C:85:GLN:O	1:C:89:LEU:HD22	2.13	0.48
1:H:91:LEU:HD23	1:H:153:LEU:HD21	1.94	0.48
1:B:72:ILE:HG22	1:B:107:ARG:HG3	1.94	0.48
1:A:352:ASP:O	1:A:356:LYS:HG2	2.14	0.48
1:B:119:TRP:HB2	1:B:326:ILE:HD11	1.94	0.48
1:C:235:ILE:HB	1:D:29:ASP:HB2	1.96	0.48
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:B:330:GLY:C	1:B:332:ALA:H	2.18	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:OE1	1:F:363:GLN:HA	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
1:H:257:TYR:CG	1:H:295:VAL:HG13	2.50	0.47
1:D:198:VAL:O	1:D:244:CYS:HA	2.15	0.47
1:E:205:ASP:OD2	1:E:207:THR:OG1	2.33	0.46
1:C:25:ILE:HD12	1:D:236:THR:HG22	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:37:LEU:HD11	1:B:139:GLN:HA	1.99	0.44
1:A:89:LEU:HD13	1:A:89:LEU:HA	1.87	0.44
1:C:150:ASN:O	1:C:150:ASN:CG	2.56	0.43
1:H:89:LEU:HD13	1:H:151:ILE:HD12	2.00	0.43
1:G:292:GLN:HB2	1:G:293:PRO:HD3	2.00	0.43
1:H:202:ASN:HB2	1:H:207:THR:O	2.18	0.43
1:D:292:GLN:N	1:D:293:PRO:CD	2.81	0.43
1:H:288:ASP:OD1	1:H:290:ARG:HB2	2.18	0.43
1:G:296:ASN:CG	1:G:353:VAL:HG13	2.39	0.43
1:A:175:GLY:O	1:A:198:VAL:HA	2.18	0.43
1:G:295:VAL:O	1:G:299:VAL:HG23	2.19	0.43
1:E:70:LEU:O	1:E:312:GLY:HA2	2.18	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: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:A:100:GLY:O	1:A:365:ARG:NH2	2.49	0.43
1:E:20:GLU:HG3	1:F:55:ARG:NH1	2.33	0.43
1:H:292:GLN:N	1:H:293:PRO:CD	2.82	0.43
1:G:130:ASN:O	1:G:130:ASN:OD1	2.37	0.43
1:D:201:LYS:HE3	4:D:2030:HOH:O	2.18	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: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: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:F:70:LEU:O	1:F:312:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:GLN:OE1	1:G:229:LYS:HE2	2.19	0.42
1:D:91:LEU:HD11	1:D:104:ILE:HG21	2.02	0.42
1:E:205:ASP:CG	1:E:207:THR:OG1	2.57	0.42
1:A:112:LYS:HB3	1:A:112:LYS:HE3	1.90	0.42
1:B:303:ILE:O	1:B:364:ARG:HB2	2.19	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: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:E:70:LEU:HD11	1:E:105:ILE:HD12	2.02	0.40
1:G:30:PRO:O	1:G:135:ASN:ND2	2.54	0.40
1:E:134:ILE:HB	1:F:235:ILE:HG12	2.02	0.40
1:D:123:ILE:HG21	1:D:123:ILE:HD13	1.89	0.40
1:G:198:VAL:O	1:G:244:CYS:HA	2.21	0.40
1:G:129:ASN:OD1	1:G:131:THR:OG1	2.39	0.40
1:B:79:HIS:HD2	4:B:2010:HOH:O	2.04	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

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	30	24
1	B	338/370 (91%)	324 (96%)	11 (3%)	3 (1%)	21	15
1	C	346/370 (94%)	334 (96%)	11 (3%)	1 (0%)	46	45
1	D	345/370 (93%)	332 (96%)	12 (4%)	1 (0%)	46	45
1	E	333/370 (90%)	314 (94%)	18 (5%)	1 (0%)	46	45
1	F	341/370 (92%)	324 (95%)	16 (5%)	1 (0%)	46	45
1	G	334/370 (90%)	311 (93%)	20 (6%)	3 (1%)	21	15
1	H	343/370 (93%)	328 (96%)	13 (4%)	2 (1%)	30	24
All	All	2726/2960 (92%)	2598 (95%)	114 (4%)	14 (0%)	34	30

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
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%)	261 (94%)	18 (6%)	21	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	278/298 (93%)	260 (94%)	18 (6%)	21	17
1	C	280/298 (94%)	260 (93%)	20 (7%)	18	14
1	D	277/298 (93%)	264 (95%)	13 (5%)	32	30
1	E	274/298 (92%)	256 (93%)	18 (7%)	21	17
1	F	277/298 (93%)	261 (94%)	16 (6%)	25	21
1	G	273/298 (92%)	254 (93%)	19 (7%)	19	15
1	H	275/298 (92%)	256 (93%)	19 (7%)	19	15
All	All	2213/2384 (93%)	2072 (94%)	141 (6%)	22	18

All (141) 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	202	ASN
1	A	208	LEU
1	A	232	VAL
1	A	249	ARG
1	A	286	ASN
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	89	LEU
1	B	99	LYS
1	B	110	LEU
1	B	112	LYS
1	B	117	VAL
1	B	134	ILE
1	B	202	ASN
1	B	208	LEU

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Mol	Chain	Res	Type
1	B	249	ARG
1	B	281	SER
1	B	286	ASN
1	B	301	GLU
1	B	318	ASN
1	B	329	GLU
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	249	ARG
1	C	285	SER
1	C	287	LYS
1	C	317	SER
1	C	331	LYS
1	C	334	LEU
1	C	369	LYS
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

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Mol	Chain	Res	Type
1	E	37	LEU
1	E	89	LEU
1	E	93	LYS
1	E	110	LEU
1	E	113	PRO
1	E	130	ASN
1	E	160	LEU
1	E	202	ASN
1	E	204	THR
1	E	207	THR
1	E	227	VAL
1	E	249	ARG
1	E	252	LYS
1	E	260	LYS
1	E	285	SER
1	E	286	ASN
1	E	317	SER
1	F	37	LEU
1	F	89	LEU
1	F	93	LYS
1	F	110	LEU
1	F	129	ASN
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	285	SER
1	F	287	LYS
1	F	351	GLU
1	F	357	LEU
1	F	363	GLN
1	G	23	VAL
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

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Mol	Chain	Res	Type
1	G	160	LEU
1	G	163	ILE
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	357	LEU
1	G	363	GLN
1	H	26	LEU
1	H	49	GLU
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	139	GLN
1	H	140	SER
1	H	151	ILE
1	H	157	SER
1	H	202	ASN
1	H	232	VAL
1	H	249	ARG
1	H	285	SER
1	H	334	LEU
1	H	352	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	223	HIS
1	A	286	ASN
1	B	223	HIS
1	B	286	ASN
1	D	222	HIS
1	D	243	HIS
1	E	286	ASN
1	F	129	ASN

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Mol	Chain	Res	Type
1	G	220	HIS
1	G	222	HIS
1	G	223	HIS
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 carbohydrates 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	A	1370	-	10,13,13	1.35	1 (10%)	11,17,17	1.11	1 (9%)
3	DTY	B	1370	-	10,13,13	1.99	2 (20%)	11,17,17	0.70	0
3	DTY	C	1371	-	10,13,13	1.14	1 (10%)	11,17,17	0.48	0
3	DTY	D	1370	-	10,13,13	1.73	4 (40%)	11,17,17	1.44	2 (18%)
3	DTY	E	1370	-	10,13,13	1.05	1 (10%)	11,17,17	0.84	0
3	DTY	F	1370	-	10,13,13	1.35	1 (10%)	11,17,17	0.95	1 (9%)
3	DTY	G	1369	-	10,13,13	1.09	1 (10%)	11,17,17	0.85	0
3	DTY	H	1369	-	10,13,13	1.78	1 (10%)	11,17,17	1.09	1 (9%)

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	A	1370	-	1/1/2/2	0/4/8/8	0/1/1/1
3	DTY	B	1370	-	1/1/2/2	0/4/8/8	0/1/1/1
3	DTY	C	1371	-	1/1/2/2	0/4/8/8	0/1/1/1
3	DTY	D	1370	-	1/1/2/2	0/4/8/8	0/1/1/1
3	DTY	E	1370	-	1/1/2/2	0/4/8/8	0/1/1/1
3	DTY	F	1370	-	1/1/2/2	0/4/8/8	0/1/1/1
3	DTY	G	1369	-	1/1/2/2	0/4/8/8	0/1/1/1
3	DTY	H	1369	-	1/1/2/2	0/4/8/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1370	DTY	OH-CZ	-5.49	1.24	1.37
3	H	1369	DTY	OH-CZ	-4.64	1.26	1.37
3	F	1370	DTY	OH-CZ	-4.12	1.27	1.37
3	A	1370	DTY	OH-CZ	-3.89	1.27	1.37
3	E	1370	DTY	OH-CZ	-3.02	1.29	1.37
3	C	1371	DTY	OH-CZ	-3.02	1.29	1.37
3	G	1369	DTY	OH-CZ	-2.88	1.30	1.37
3	D	1370	DTY	OH-CZ	-2.52	1.31	1.37
3	D	1370	DTY	CE2-CZ	2.12	1.43	1.38
3	B	1370	DTY	CD1-CG	2.33	1.43	1.38
3	D	1370	DTY	CE2-CD2	2.38	1.43	1.38
3	D	1370	DTY	CE1-CD1	3.04	1.44	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1370	DTY	CE2-CZ-CE1	-3.19	115.24	119.79
3	A	1370	DTY	CD2-CE2-CZ	-2.20	117.32	119.87
3	F	1370	DTY	CG-CB-CA	-2.17	109.32	114.34
3	H	1369	DTY	CE1-CD1-CG	-2.07	118.20	121.04
3	D	1370	DTY	CD2-CE2-CZ	2.62	122.89	119.87

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	1371	DTY	CA

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

There are no torsion outliers.

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%)	0.00	12 (3%) 49 58	31, 43, 60, 77	0
1	B	346/370 (93%)	-0.03	6 (1%) 73 78	29, 42, 56, 81	0
1	C	350/370 (94%)	0.02	9 (2%) 59 66	33, 45, 63, 83	0
1	D	349/370 (94%)	-0.03	6 (1%) 73 78	31, 40, 55, 70	0
1	E	339/370 (91%)	0.19	15 (4%) 38 47	34, 51, 66, 79	0
1	F	347/370 (93%)	0.05	9 (2%) 59 66	35, 46, 61, 71	0
1	G	342/370 (92%)	0.22	13 (3%) 44 53	35, 50, 66, 80	0
1	H	347/370 (93%)	0.10	17 (4%) 33 42	35, 46, 62, 78	0
All	All	2770/2960 (93%)	0.07	87 (3%) 52 61	29, 45, 63, 83	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	117	VAL	5.0
1	A	328	ALA	4.7
1	C	328	ALA	4.6
1	C	113	PRO	4.6
1	H	115	THR	4.6
1	E	287	LYS	4.3
1	D	18	GLY	4.1
1	C	332	ALA	3.9
1	D	328	ALA	3.7
1	A	117	VAL	3.6
1	G	286	ASN	3.5
1	H	333	GLY	3.5
1	E	325	GLY	3.5
1	F	18	GLY	3.5
1	G	128	VAL	3.3
1	C	329	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	113	PRO	3.3
1	E	336	TYR	3.2
1	D	286	ASN	3.2
1	A	116	THR	3.2
1	E	130	ASN	3.1
1	B	328	ALA	3.1
1	G	131	THR	3.1
1	G	328	ALA	3.0
1	G	113	PRO	3.0
1	E	327	PRO	3.0
1	H	286	ASN	3.0
1	B	329	GLU	2.9
1	H	116	THR	2.9
1	C	287	LYS	2.9
1	H	18	GLY	2.9
1	G	171	LEU	2.9
1	A	366	GLU	2.9
1	E	286	ASN	2.8
1	D	117	VAL	2.8
1	A	327	PRO	2.8
1	H	332	ALA	2.8
1	H	363	GLN	2.7
1	E	366	GLU	2.7
1	A	333	GLY	2.7
1	E	326	ILE	2.6
1	E	18	GLY	2.6
1	E	290	ARG	2.6
1	D	78	ILE	2.5
1	E	289	PHE	2.5
1	B	117	VAL	2.5
1	B	286	ASN	2.5
1	H	117	VAL	2.5
1	C	336	TYR	2.4
1	F	272	GLY	2.4
1	F	130	ASN	2.4
1	E	113	PRO	2.4
1	C	286	ASN	2.4
1	A	18	GLY	2.3
1	A	352	ASP	2.3
1	G	290	ARG	2.3
1	H	352	ASP	2.3
1	F	367	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	287	LYS	2.3
1	G	336	TYR	2.3
1	H	366	GLU	2.3
1	F	286	ASN	2.3
1	B	19	ALA	2.2
1	F	216	GLN	2.2
1	H	305	ASN	2.2
1	F	287	LYS	2.2
1	H	328	ALA	2.2
1	G	333	GLY	2.1
1	D	329	GLU	2.1
1	H	26	LEU	2.1
1	H	131	THR	2.1
1	E	119	TRP	2.1
1	A	332	ALA	2.1
1	H	191	ALA	2.1
1	B	113	PRO	2.1
1	E	26	LEU	2.1
1	H	96	ASP	2.1
1	F	366	GLU	2.1
1	G	287	LYS	2.1
1	C	171	LEU	2.1
1	C	271	ALA	2.1
1	G	305	ASN	2.1
1	G	334	LEU	2.1
1	E	82	GLU	2.0
1	H	326	ILE	2.0
1	G	271	ALA	2.0
1	A	71	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	DTY	A	1370	13/13	0.96	0.13	0.50	28,33,34,34	0
3	DTY	H	1369	13/13	0.96	0.12	0.15	35,38,40,41	0
3	DTY	C	1371	13/13	0.97	0.11	-0.18	33,34,38,39	0
3	DTY	G	1369	13/13	0.97	0.11	-0.27	35,40,41,41	0
3	DTY	B	1370	13/13	0.97	0.10	-0.42	33,35,37,38	0
3	DTY	D	1370	13/13	0.96	0.09	-0.55	30,33,35,35	0
3	DTY	F	1370	13/13	0.96	0.10	-0.65	33,38,41,43	0
2	MN	H	1368	1/1	0.96	0.05	-1.51	37,37,37,37	0
2	MN	E	1369	1/1	0.99	0.05	-1.58	45,45,45,45	0
3	DTY	E	1370	13/13	0.97	0.07	-1.71	31,34,37,38	0
2	MN	A	1369	1/1	0.98	0.04	-1.83	33,33,33,33	0
2	MN	C	1370	1/1	0.96	0.03	-1.91	38,38,38,38	0
2	MN	D	1369	1/1	0.99	0.03	-1.93	30,30,30,30	0
2	MN	G	1368	1/1	0.98	0.04	-2.01	45,45,45,45	0
2	MN	B	1369	1/1	1.00	0.02	-	31,31,31,31	0
2	MN	F	1369	1/1	1.00	0.02	-	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.