



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:39 PM UTC

PDB ID : 5OLC / pdb_00005olc
Title : Crystal structure of the 3,6-anhydro-D-galactonate cycloisomerase from *Zobellia galactanivorans*
Authors : Michel, G.; Czjzek, M.; Jam, M.
Deposited on : 2017-07-27
Resolution : 2.79 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

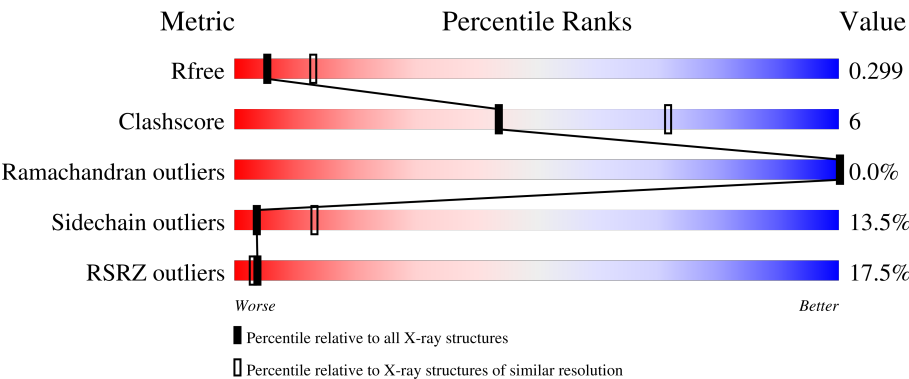
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	396	14% 67%19%•11%
1	B	396	15% 65%21%••11%
1	C	396	16% 65%20%•11%
1	D	396	15% 69%17%•11%
1	E	396	15% 67%18%•11%

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Mol	Chain	Length	Quality of chain
1	F	396	15% 65% 20% • 11%
1	G	396	16% 65% 19% • 11%
1	H	396	17% 66% 19% • 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21906 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 Galactonate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	0	0
			2721	1749	446	513	13			
1	B	351	Total	C	N	O	S	0	0	0
			2709	1742	444	510	13			
1	C	351	Total	C	N	O	S	0	0	0
			2717	1748	446	510	13			
1	D	351	Total	C	N	O	S	0	0	0
			2711	1745	443	510	13			
1	E	351	Total	C	N	O	S	0	0	0
			2735	1758	451	513	13			
1	F	351	Total	C	N	O	S	0	0	0
			2741	1764	451	513	13			
1	G	351	Total	C	N	O	S	0	0	0
			2730	1755	449	513	13			
1	H	351	Total	C	N	O	S	0	0	0
			2745	1767	452	513	13			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP G0L7B8
A	-6	HIS	-	expression tag	UNP G0L7B8
A	-5	HIS	-	expression tag	UNP G0L7B8
A	-4	HIS	-	expression tag	UNP G0L7B8
A	-3	HIS	-	expression tag	UNP G0L7B8
A	-2	HIS	-	expression tag	UNP G0L7B8
A	-1	HIS	-	expression tag	UNP G0L7B8
A	0	GLY	-	expression tag	UNP G0L7B8
A	1	SER	-	expression tag	UNP G0L7B8
B	-7	MET	-	initiating methionine	UNP G0L7B8
B	-6	HIS	-	expression tag	UNP G0L7B8
B	-5	HIS	-	expression tag	UNP G0L7B8
B	-4	HIS	-	expression tag	UNP G0L7B8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP G0L7B8
B	-2	HIS	-	expression tag	UNP G0L7B8
B	-1	HIS	-	expression tag	UNP G0L7B8
B	0	GLY	-	expression tag	UNP G0L7B8
B	1	SER	-	expression tag	UNP G0L7B8
C	-7	MET	-	initiating methionine	UNP G0L7B8
C	-6	HIS	-	expression tag	UNP G0L7B8
C	-5	HIS	-	expression tag	UNP G0L7B8
C	-4	HIS	-	expression tag	UNP G0L7B8
C	-3	HIS	-	expression tag	UNP G0L7B8
C	-2	HIS	-	expression tag	UNP G0L7B8
C	-1	HIS	-	expression tag	UNP G0L7B8
C	0	GLY	-	expression tag	UNP G0L7B8
C	1	SER	-	expression tag	UNP G0L7B8
D	-7	MET	-	initiating methionine	UNP G0L7B8
D	-6	HIS	-	expression tag	UNP G0L7B8
D	-5	HIS	-	expression tag	UNP G0L7B8
D	-4	HIS	-	expression tag	UNP G0L7B8
D	-3	HIS	-	expression tag	UNP G0L7B8
D	-2	HIS	-	expression tag	UNP G0L7B8
D	-1	HIS	-	expression tag	UNP G0L7B8
D	0	GLY	-	expression tag	UNP G0L7B8
D	1	SER	-	expression tag	UNP G0L7B8
E	-7	MET	-	initiating methionine	UNP G0L7B8
E	-6	HIS	-	expression tag	UNP G0L7B8
E	-5	HIS	-	expression tag	UNP G0L7B8
E	-4	HIS	-	expression tag	UNP G0L7B8
E	-3	HIS	-	expression tag	UNP G0L7B8
E	-2	HIS	-	expression tag	UNP G0L7B8
E	-1	HIS	-	expression tag	UNP G0L7B8
E	0	GLY	-	expression tag	UNP G0L7B8
E	1	SER	-	expression tag	UNP G0L7B8
F	-7	MET	-	initiating methionine	UNP G0L7B8
F	-6	HIS	-	expression tag	UNP G0L7B8
F	-5	HIS	-	expression tag	UNP G0L7B8
F	-4	HIS	-	expression tag	UNP G0L7B8
F	-3	HIS	-	expression tag	UNP G0L7B8
F	-2	HIS	-	expression tag	UNP G0L7B8
F	-1	HIS	-	expression tag	UNP G0L7B8
F	0	GLY	-	expression tag	UNP G0L7B8
F	1	SER	-	expression tag	UNP G0L7B8
G	-7	MET	-	initiating methionine	UNP G0L7B8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	HIS	-	expression tag	UNP G0L7B8
G	-5	HIS	-	expression tag	UNP G0L7B8
G	-4	HIS	-	expression tag	UNP G0L7B8
G	-3	HIS	-	expression tag	UNP G0L7B8
G	-2	HIS	-	expression tag	UNP G0L7B8
G	-1	HIS	-	expression tag	UNP G0L7B8
G	0	GLY	-	expression tag	UNP G0L7B8
G	1	SER	-	expression tag	UNP G0L7B8
H	-7	MET	-	initiating methionine	UNP G0L7B8
H	-6	HIS	-	expression tag	UNP G0L7B8
H	-5	HIS	-	expression tag	UNP G0L7B8
H	-4	HIS	-	expression tag	UNP G0L7B8
H	-3	HIS	-	expression tag	UNP G0L7B8
H	-2	HIS	-	expression tag	UNP G0L7B8
H	-1	HIS	-	expression tag	UNP G0L7B8
H	0	GLY	-	expression tag	UNP G0L7B8
H	1	SER	-	expression tag	UNP G0L7B8

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	13	Total O 13 13	0	0
3	B	9	Total O 9 9	0	0
3	C	12	Total O 12 12	0	0
3	D	8	Total O 8 8	0	0

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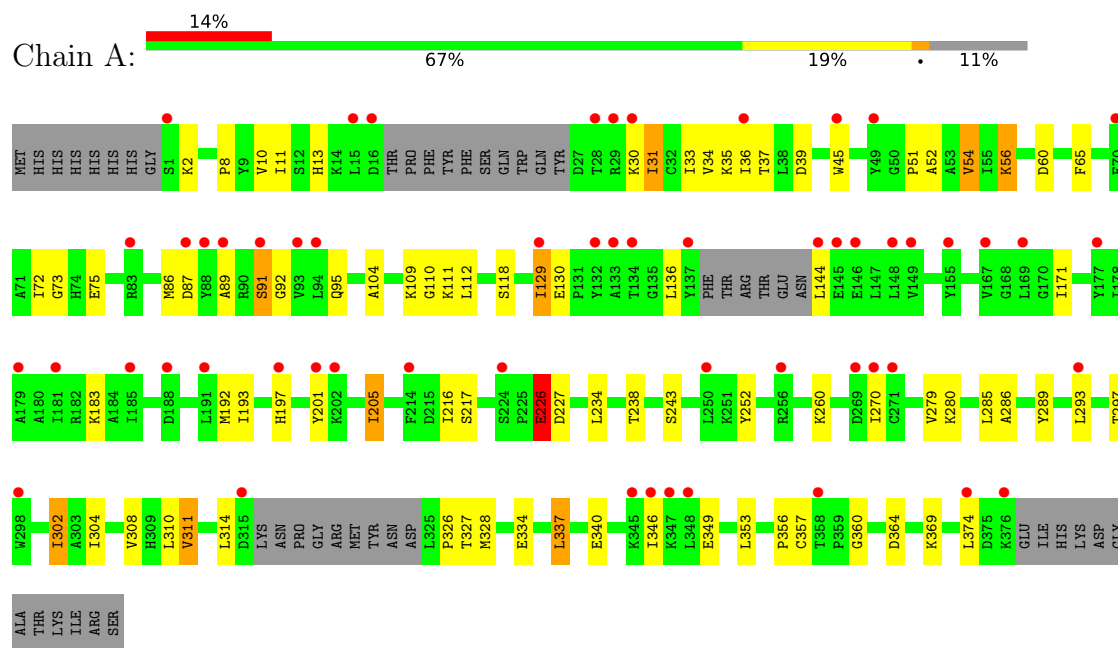
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	9	Total 9	O 9	0	0
3	F	11	Total 11	O 11	0	0
3	G	19	Total 19	O 19	0	0
3	H	11	Total 11	O 11	0	0

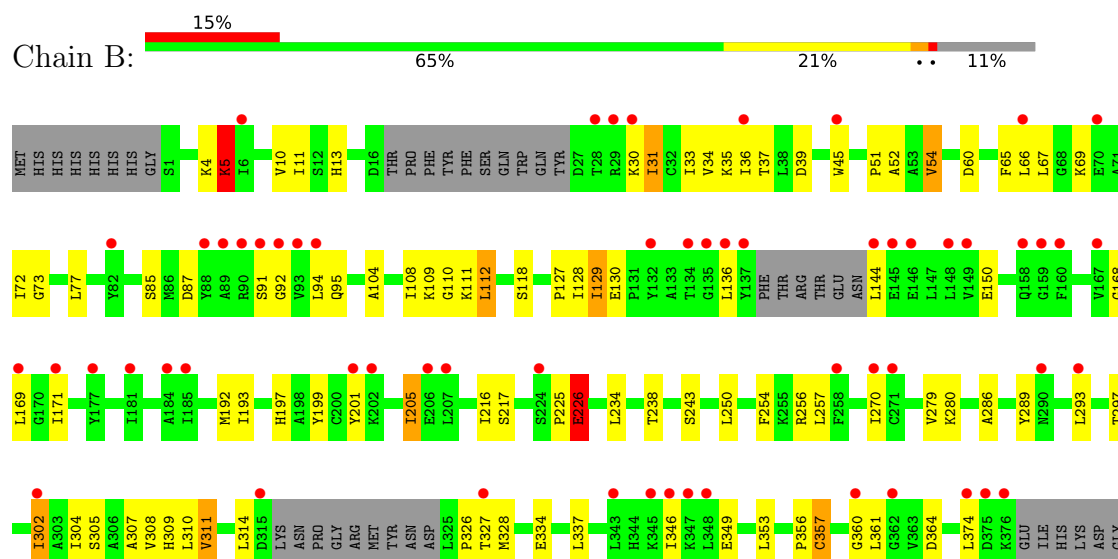
3 Residue-property plots [i](#)

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: Galactonate dehydratase



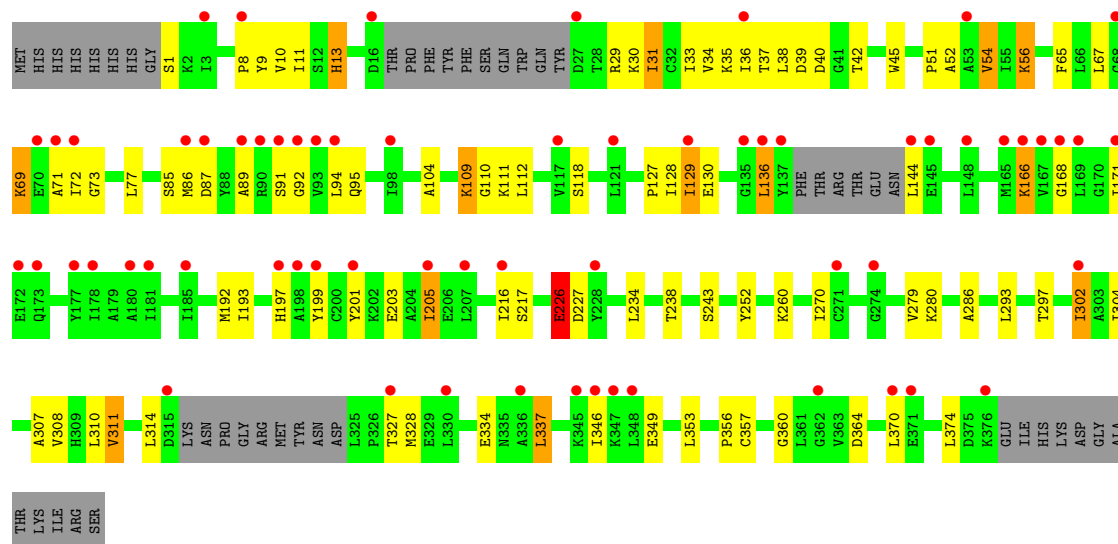
• Molecule 1: Galactonate dehydratase



ALA
THR
LYS
ILE
ARG
SER

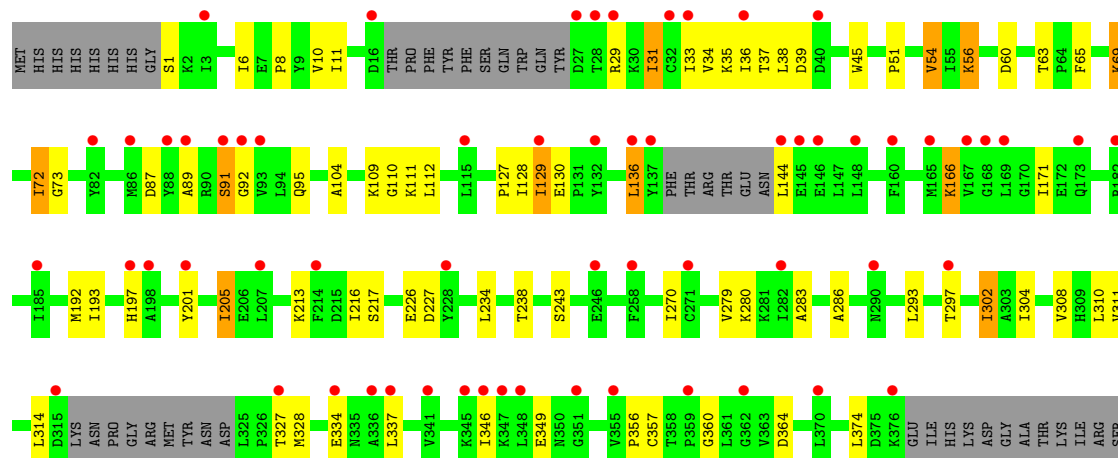
• Molecule 1: Galactonate dehydratase

Chain C: 16% 65% 20% 11%



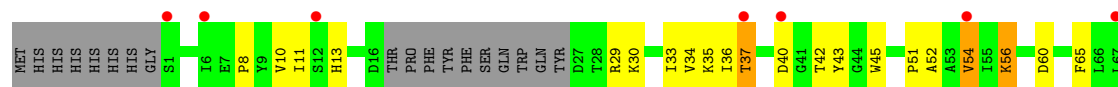
• Molecule 1: Galactonate dehydratase

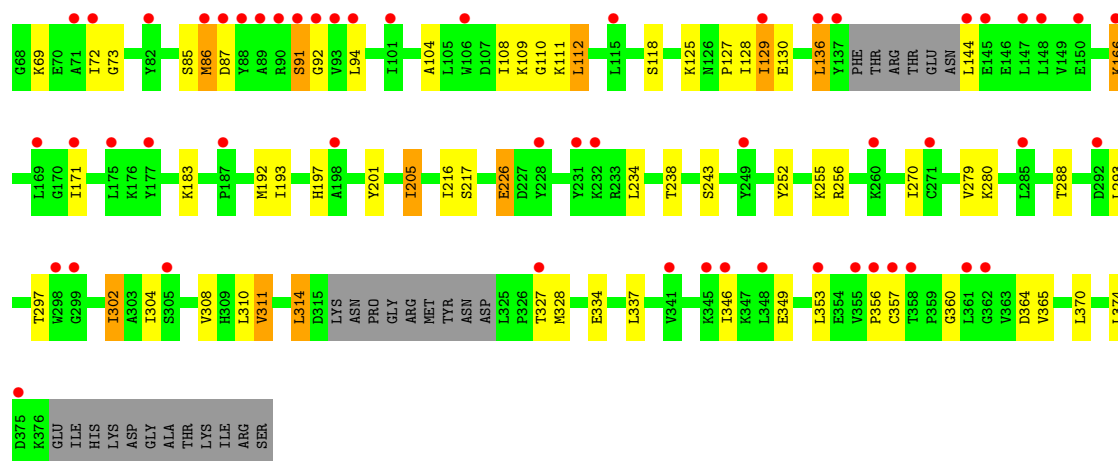
Chain D: 15% 69% 17% 11%



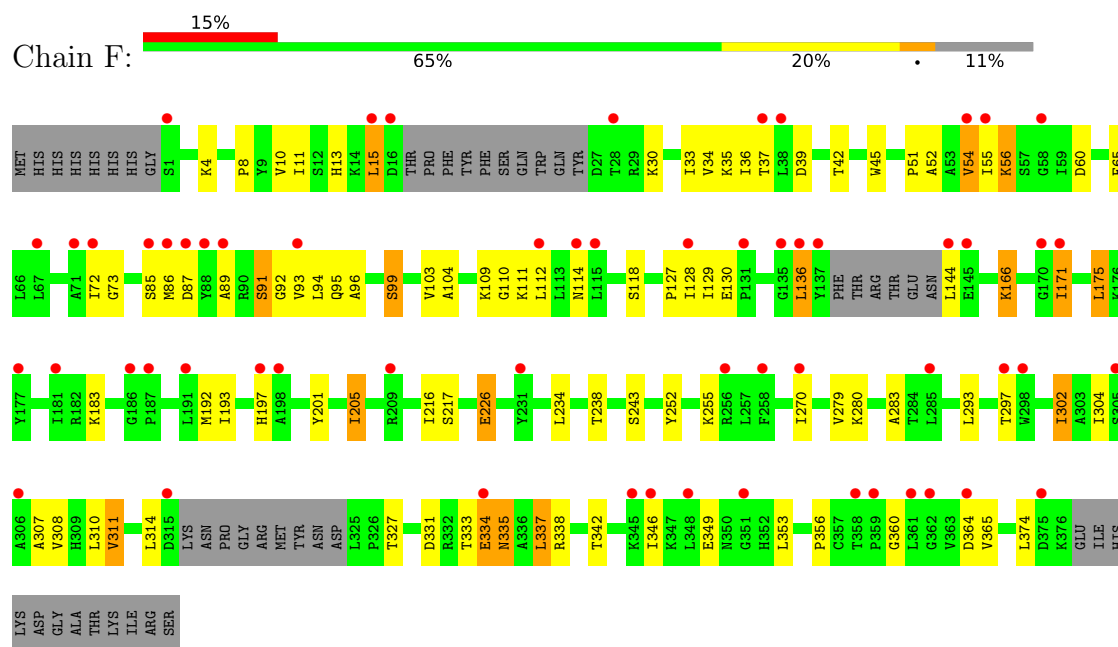
• Molecule 1: Galactonate dehydratase

Chain E: 15% 67% 18% 11%

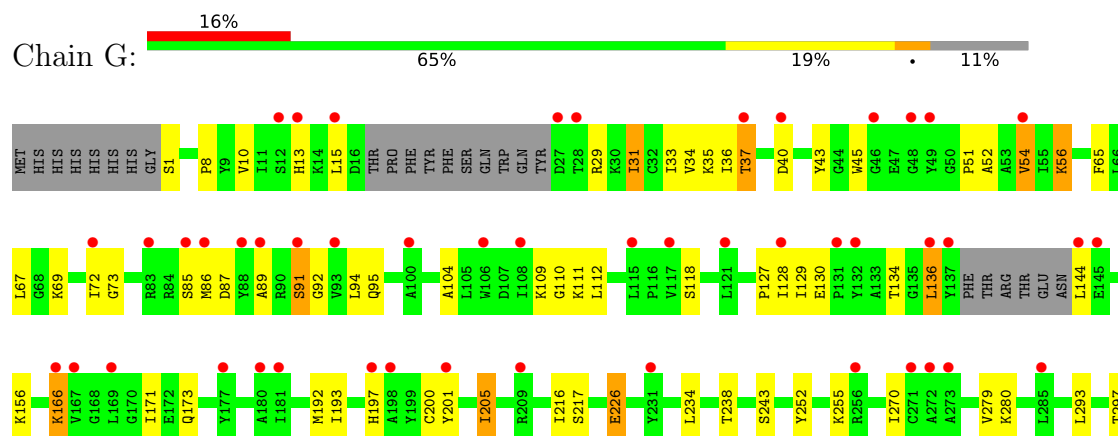


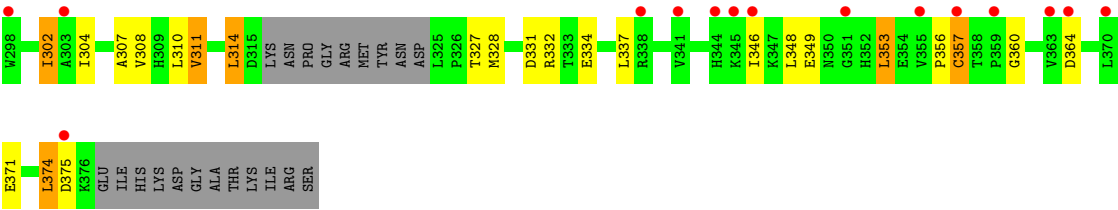


• Molecule 1: Galactonate dehydratase

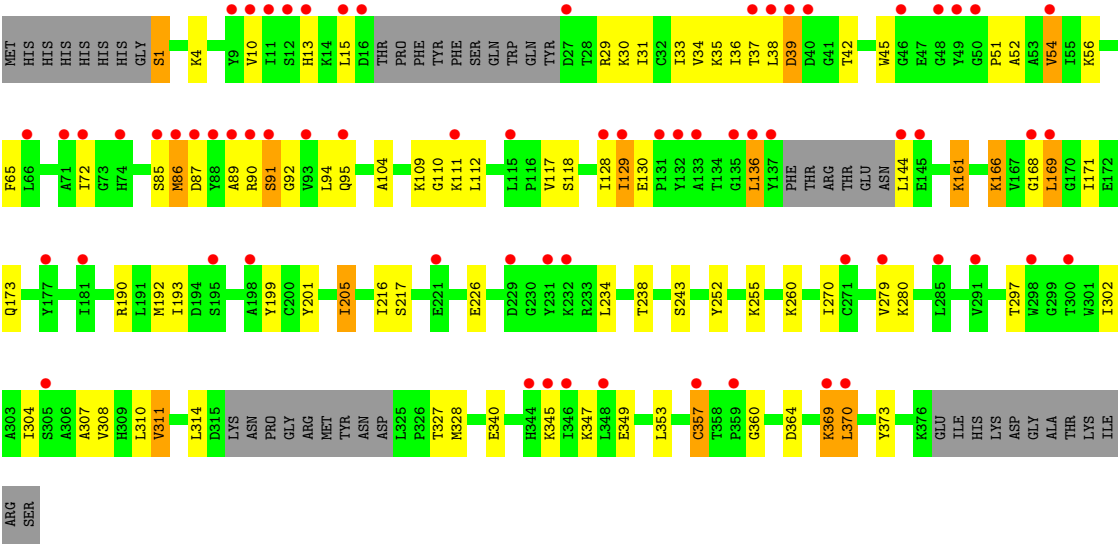


• Molecule 1: Galactonate dehydratase





● Molecule 1: Galactonate dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.84Å 154.07Å 150.87Å 90.00° 104.38° 90.00°	Depositor
Resolution (Å)	49.17 – 2.79 49.17 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.17-2.79) 99.0 (49.17-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.231 , 0.266 0.263 , 0.299	Depositor DCC
R_{free} test set	4656 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	21906	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.90	0/2777	1.40	14/3766 (0.4%)
1	B	0.91	0/2765	1.41	19/3752 (0.5%)
1	C	0.88	0/2773	1.41	15/3760 (0.4%)
1	D	0.90	0/2767	1.41	17/3753 (0.5%)
1	E	0.89	0/2791	1.40	12/3781 (0.3%)
1	F	0.90	0/2797	1.42	21/3789 (0.6%)
1	G	0.90	0/2786	1.40	15/3777 (0.4%)
1	H	0.91	0/2801	1.42	17/3793 (0.4%)
All	All	0.90	0/22257	1.41	130/30171 (0.4%)

There are no bond length outliers.

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	GLY	CA-C-N	8.36	131.72	120.77
1	C	92	GLY	C-N-CA	8.36	131.72	120.77
1	F	92	GLY	CA-C-N	8.33	131.68	120.77
1	F	92	GLY	C-N-CA	8.33	131.68	120.77
1	F	114	ASN	CA-CB-CG	8.11	120.71	112.60
1	A	92	GLY	CA-C-N	7.85	131.05	120.77
1	A	92	GLY	C-N-CA	7.85	131.05	120.77
1	D	92	GLY	CA-C-N	7.81	131.00	120.77
1	D	92	GLY	C-N-CA	7.81	131.00	120.77
1	B	92	GLY	CA-C-N	7.71	130.87	120.77
1	B	92	GLY	C-N-CA	7.71	130.87	120.77
1	G	92	GLY	CA-C-N	7.44	130.52	120.77
1	G	92	GLY	C-N-CA	7.44	130.52	120.77
1	H	92	GLY	CA-C-N	7.43	130.50	120.77
1	H	92	GLY	C-N-CA	7.43	130.50	120.77
1	E	92	GLY	CA-C-N	7.15	130.13	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	92	GLY	C-N-CA	7.15	130.13	120.77
1	H	345	LYS	CA-C-N	7.10	130.29	120.49
1	H	345	LYS	C-N-CA	7.10	130.29	120.49
1	H	226	GLU	CB-CG-CD	6.99	124.48	112.60
1	D	111	LYS	CA-C-N	6.34	130.33	120.82
1	D	111	LYS	C-N-CA	6.34	130.33	120.82
1	C	39	ASP	CA-CB-CG	6.32	118.92	112.60
1	H	111	LYS	CA-C-N	6.29	130.26	120.82
1	H	111	LYS	C-N-CA	6.29	130.26	120.82
1	A	39	ASP	CA-CB-CG	6.28	118.88	112.60
1	E	111	LYS	CA-C-N	6.25	130.20	120.82
1	E	111	LYS	C-N-CA	6.25	130.20	120.82
1	B	111	LYS	CA-C-N	6.22	130.16	120.82
1	B	111	LYS	C-N-CA	6.22	130.16	120.82
1	C	111	LYS	CA-C-N	6.20	130.11	120.82
1	C	111	LYS	C-N-CA	6.20	130.11	120.82
1	A	111	LYS	CA-C-N	6.18	130.10	120.82
1	A	111	LYS	C-N-CA	6.18	130.10	120.82
1	E	86	MET	CA-C-N	6.17	129.17	120.28
1	E	86	MET	C-N-CA	6.17	129.17	120.28
1	F	111	LYS	CA-C-N	6.08	129.94	120.82
1	F	111	LYS	C-N-CA	6.08	129.94	120.82
1	G	111	LYS	CA-C-N	6.01	129.84	120.82
1	G	111	LYS	C-N-CA	6.01	129.84	120.82
1	C	73	GLY	CA-C-N	5.89	128.44	120.38
1	C	73	GLY	C-N-CA	5.89	128.44	120.38
1	B	302	ILE	CA-C-N	5.80	127.98	120.44
1	B	302	ILE	C-N-CA	5.80	127.98	120.44
1	B	60	ASP	CA-CB-CG	5.72	118.32	112.60
1	D	39	ASP	CA-CB-CG	5.70	118.30	112.60
1	G	302	ILE	CA-C-N	5.70	127.84	120.44
1	G	302	ILE	C-N-CA	5.70	127.84	120.44
1	A	302	ILE	CA-C-N	5.67	128.15	120.44
1	A	302	ILE	C-N-CA	5.67	128.15	120.44
1	B	69	LYS	CA-C-N	5.66	128.87	120.95
1	B	69	LYS	C-N-CA	5.66	128.87	120.95
1	F	99	SER	CA-C-N	5.64	127.77	120.44
1	F	99	SER	C-N-CA	5.64	127.77	120.44
1	F	86	MET	CA-C-N	5.61	128.36	120.28
1	F	86	MET	C-N-CA	5.61	128.36	120.28
1	D	302	ILE	CA-C-N	5.60	128.06	120.44
1	D	302	ILE	C-N-CA	5.60	128.06	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	86	MET	CA-C-N	5.57	128.30	120.28
1	H	86	MET	C-N-CA	5.57	128.30	120.28
1	H	302	ILE	CA-C-N	5.57	128.01	120.44
1	H	302	ILE	C-N-CA	5.57	128.01	120.44
1	A	286	ALA	CA-C-N	5.55	127.65	120.44
1	A	286	ALA	C-N-CA	5.55	127.65	120.44
1	G	226	GLU	CB-CG-CD	5.48	121.92	112.60
1	E	302	ILE	CA-C-N	5.48	127.89	120.44
1	E	302	ILE	C-N-CA	5.48	127.89	120.44
1	D	73	GLY	CA-C-N	5.42	127.80	120.38
1	D	73	GLY	C-N-CA	5.42	127.80	120.38
1	C	302	ILE	CA-C-N	5.41	127.80	120.44
1	C	302	ILE	C-N-CA	5.41	127.80	120.44
1	F	302	ILE	N-CA-C	-5.41	105.44	110.53
1	D	286	ALA	CA-C-N	5.39	127.45	120.44
1	D	286	ALA	C-N-CA	5.39	127.45	120.44
1	D	60	ASP	CA-CB-CG	5.37	117.97	112.60
1	D	69	LYS	CA-C-N	5.37	128.47	120.95
1	D	69	LYS	C-N-CA	5.37	128.47	120.95
1	H	357	CYS	CA-C-N	5.37	127.85	120.39
1	H	357	CYS	C-N-CA	5.37	127.85	120.39
1	B	286	ALA	CA-C-N	5.35	127.39	120.44
1	B	286	ALA	C-N-CA	5.35	127.39	120.44
1	C	286	ALA	CA-C-N	5.33	127.37	120.44
1	C	286	ALA	C-N-CA	5.33	127.37	120.44
1	F	60	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	254	PHE	CA-CB-CG	-5.29	108.52	113.80
1	H	370	LEU	N-CA-C	-5.27	105.44	111.14
1	G	40	ASP	CA-CB-CG	5.26	117.86	112.60
1	F	39	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	5	LYS	N-CA-C	5.22	116.70	107.61
1	F	226	GLU	CB-CG-CD	5.22	121.48	112.60
1	F	73	GLY	CA-C-N	5.22	128.00	120.38
1	F	73	GLY	C-N-CA	5.22	128.00	120.38
1	G	357	CYS	CA-C-N	5.22	127.64	120.39
1	G	357	CYS	C-N-CA	5.22	127.64	120.39
1	B	226	GLU	CB-CG-CD	5.21	121.47	112.60
1	E	60	ASP	CA-CB-CG	5.20	117.80	112.60
1	F	302	ILE	CA-C-N	5.20	127.19	120.44
1	F	302	ILE	C-N-CA	5.20	127.19	120.44
1	A	60	ASP	CA-CB-CG	5.18	117.78	112.60
1	C	40	ASP	CA-CB-CG	5.18	117.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	283	ALA	CA-C-N	5.17	127.17	120.44
1	D	283	ALA	C-N-CA	5.17	127.17	120.44
1	A	226	GLU	CB-CG-CD	5.17	121.38	112.60
1	B	39	ASP	CA-CB-CG	5.17	117.77	112.60
1	H	369	LYS	CA-C-N	5.17	127.47	120.44
1	H	369	LYS	C-N-CA	5.17	127.47	120.44
1	B	357	CYS	CA-C-N	5.15	127.55	120.39
1	B	357	CYS	C-N-CA	5.15	127.55	120.39
1	D	227	ASP	CA-CB-CG	5.13	117.73	112.60
1	E	226	GLU	CB-CG-CD	5.13	121.32	112.60
1	C	227	ASP	CA-CB-CG	5.13	117.73	112.60
1	C	226	GLU	CB-CG-CD	5.12	121.31	112.60
1	H	92	GLY	N-CA-C	5.12	120.42	111.50
1	A	227	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	92	GLY	N-CA-C	5.11	120.53	111.02
1	A	73	GLY	CA-C-N	5.11	127.84	120.38
1	A	73	GLY	C-N-CA	5.11	127.84	120.38
1	G	69	LYS	CA-C-N	5.10	128.09	120.95
1	G	69	LYS	C-N-CA	5.10	128.09	120.95
1	F	283	ALA	CA-C-N	5.10	127.07	120.44
1	F	283	ALA	C-N-CA	5.10	127.07	120.44
1	G	73	GLY	CA-C-N	5.08	127.80	120.38
1	G	73	GLY	C-N-CA	5.08	127.80	120.38
1	F	93	VAL	N-CA-C	5.08	115.52	110.23
1	G	92	GLY	N-CA-C	5.07	120.33	111.50
1	E	73	GLY	CA-C-N	5.06	127.77	120.38
1	E	73	GLY	C-N-CA	5.06	127.77	120.38
1	B	73	GLY	CA-C-N	5.04	127.74	120.38
1	B	73	GLY	C-N-CA	5.04	127.74	120.38
1	F	337	LEU	N-CA-C	-5.02	107.01	113.23

There are no chirality outliers.

There are no planarity outliers.

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	2721	0	2689	32	0
1	B	2709	0	2668	35	0
1	C	2717	0	2690	39	0
1	D	2711	0	2679	27	0
1	E	2735	0	2722	37	0
1	F	2741	0	2740	38	0
1	G	2730	0	2709	36	0
1	H	2745	0	2751	36	0
2	C	1	0	0	0	0
2	D	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	0	0	0
3	B	9	0	0	0	0
3	C	12	0	0	1	0
3	D	8	0	0	0	0
3	E	9	0	0	2	0
3	F	11	0	0	0	0
3	G	19	0	0	0	0
3	H	11	0	0	0	0
All	All	21906	0	21648	265	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 6.

All (265) 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:F:333:THR:O	1:F:338:ARG:NH2	2.01	0.93
1:F:33:ILE:HD12	1:F:302:ILE:HD12	1.61	0.82
1:H:1:SER:HB3	1:H:38:LEU:HD13	1.62	0.81
1:H:169:LEU:HD22	1:H:173:GLN:HG2	1.64	0.78
1:H:136:LEU:HB3	1:H:166:LYS:HD3	1.68	0.76
1:D:136:LEU:HB3	1:D:166:LYS:HD2	1.69	0.74
1:C:129:ILE:HD11	1:C:328:MET:HG2	1.71	0.73
1:D:129:ILE:HD11	1:D:328:MET:HG2	1.71	0.72
1:E:129:ILE:HD11	1:E:328:MET:HG2	1.71	0.71
1:F:331:ASP:OD1	1:F:333:THR:OG1	2.09	0.71
1:H:130:GLU:HB2	1:H:161:LYS:HD2	1.73	0.70
1:F:136:LEU:HB3	1:F:166:LYS:HD3	1.74	0.69
1:C:136:LEU:HB3	1:C:166:LYS:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:LEU:HB3	1:G:166:LYS:HD3	1.77	0.66
1:D:1:SER:HB3	1:D:38:LEU:HD13	1.76	0.66
1:G:33:ILE:HD12	1:G:302:ILE:HD12	1.77	0.66
1:E:136:LEU:HB3	1:E:166:LYS:HD3	1.77	0.65
1:B:129:ILE:HD11	1:B:328:MET:HG2	1.78	0.65
1:B:91:SER:HB2	1:H:91:SER:HB2	1.79	0.65
1:A:33:ILE:HD12	1:A:302:ILE:HD12	1.78	0.65
1:A:129:ILE:HD11	1:A:328:MET:HG2	1.79	0.64
1:A:340:GLU:HB3	1:A:369:LYS:HD2	1.79	0.64
1:C:33:ILE:HD12	1:C:302:ILE:HD12	1.81	0.63
1:B:33:ILE:HD12	1:B:302:ILE:HD12	1.79	0.63
1:G:85:SER:HB2	1:G:94:LEU:HD13	1.82	0.62
1:E:33:ILE:HD12	1:E:302:ILE:HD12	1.80	0.62
1:A:91:SER:HB2	1:G:91:SER:HB2	1.82	0.61
1:C:308:VAL:HG22	1:C:328:MET:HE1	1.83	0.61
1:D:91:SER:HB2	1:F:91:SER:HB2	1.83	0.61
1:C:11:ILE:HD12	1:C:337:LEU:HD13	1.82	0.61
1:H:4:LYS:HD3	1:H:39:ASP:HA	1.83	0.61
1:F:85:SER:HB2	1:F:94:LEU:HD13	1.82	0.60
1:A:31:ILE:HD11	1:A:33:ILE:HD11	1.82	0.60
1:A:308:VAL:HG22	1:A:328:MET:HE1	1.84	0.60
1:B:308:VAL:HG22	1:B:328:MET:HE1	1.83	0.60
1:D:31:ILE:HD11	1:D:33:ILE:HD11	1.84	0.59
1:B:95:GLN:NE2	1:B:250:LEU:HD21	2.17	0.59
1:D:308:VAL:HG22	1:D:328:MET:HE1	1.85	0.59
1:C:1:SER:HB3	1:C:38:LEU:HD13	1.84	0.59
1:B:31:ILE:HD11	1:B:33:ILE:HD11	1.84	0.59
1:H:308:VAL:HG22	1:H:328:MET:HE1	1.84	0.58
1:G:308:VAL:HG22	1:G:328:MET:HE1	1.86	0.58
1:E:85:SER:HB2	1:E:94:LEU:HD13	1.85	0.58
1:E:308:VAL:HG22	1:E:328:MET:HE1	1.86	0.58
1:B:226:GLU:HG2	1:H:252:TYR:CG	2.38	0.57
1:E:51:PRO:HB2	1:E:54:VAL:HG23	1.86	0.57
1:C:91:SER:HB2	1:E:91:SER:HB2	1.86	0.57
1:C:13:HIS:HB3	1:C:337:LEU:HD23	1.86	0.56
1:F:51:PRO:HB2	1:F:54:VAL:HG23	1.87	0.56
1:A:226:GLU:HG2	1:G:252:TYR:CG	2.39	0.56
1:C:85:SER:HB2	1:C:94:LEU:HD13	1.87	0.56
1:D:33:ILE:HD12	1:D:302:ILE:HD12	1.86	0.56
1:G:51:PRO:HB2	1:G:54:VAL:HG23	1.87	0.56
1:D:11:ILE:HD12	1:D:337:LEU:HG	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:51:PRO:HB2	1:H:54:VAL:HG23	1.88	0.55
1:E:37:THR:HG23	3:E:401:HOH:O	2.06	0.55
1:G:348:LEU:HD13	1:G:353:LEU:HD12	1.89	0.54
1:D:51:PRO:HB2	1:D:54:VAL:HG23	1.90	0.54
1:C:51:PRO:HB2	1:C:54:VAL:HG23	1.90	0.54
1:B:110:GLY:HA3	1:B:360:GLY:HA2	1.90	0.53
1:A:11:ILE:HD12	1:A:337:LEU:HB3	1.90	0.53
1:A:51:PRO:HB2	1:A:54:VAL:HG23	1.91	0.53
1:F:36:ILE:HD12	1:F:104:ALA:HB3	1.90	0.53
1:H:89:ALA:HB1	1:H:95:GLN:HE21	1.73	0.53
1:F:35:LYS:HB2	1:F:45:TRP:CZ3	2.43	0.53
1:G:37:THR:HG23	1:G:43:TYR:HB3	1.91	0.53
1:B:11:ILE:HD12	1:B:337:LEU:HB3	1.89	0.53
1:D:36:ILE:HD12	1:D:104:ALA:HB3	1.90	0.53
1:C:89:ALA:HB1	1:C:95:GLN:HE21	1.74	0.52
1:G:89:ALA:HB1	1:G:95:GLN:HE21	1.74	0.52
1:D:110:GLY:HA3	1:D:360:GLY:HA2	1.91	0.52
1:A:89:ALA:HB1	1:A:95:GLN:HE21	1.75	0.52
1:B:51:PRO:HB2	1:B:54:VAL:HG23	1.91	0.52
1:C:199:TYR:HD1	1:C:203:GLU:HB3	1.75	0.52
1:G:36:ILE:HD12	1:G:104:ALA:HB3	1.91	0.52
1:B:304:ILE:O	1:B:308:VAL:HG23	2.10	0.52
1:G:31:ILE:HD11	1:G:33:ILE:HD11	1.92	0.52
1:B:4:LYS:HG3	1:B:5:LYS:HG2	1.92	0.51
1:B:66:LEU:HD22	1:B:77:LEU:HD22	1.93	0.51
1:C:199:TYR:CD1	1:C:203:GLU:HB3	2.46	0.51
1:H:36:ILE:HD12	1:H:104:ALA:HB3	1.92	0.51
1:H:110:GLY:HA3	1:H:360:GLY:HA2	1.92	0.51
1:C:36:ILE:HD12	1:C:104:ALA:HB3	1.93	0.50
1:B:305:SER:HB3	1:B:361:LEU:HB3	1.93	0.50
1:E:346:ILE:HG22	1:E:356:PRO:HG3	1.94	0.50
1:F:89:ALA:HB1	1:F:95:GLN:OE1	2.11	0.50
1:E:110:GLY:HA3	1:E:360:GLY:HA2	1.93	0.50
1:H:193:ILE:HG12	1:H:216:ILE:HG21	1.94	0.50
1:A:110:GLY:HA3	1:A:360:GLY:HA2	1.94	0.50
1:B:193:ILE:HG12	1:B:216:ILE:HG21	1.94	0.50
1:G:130:GLU:O	1:G:327:THR:HG22	2.11	0.50
1:H:1:SER:CB	1:H:38:LEU:HD13	2.38	0.50
1:D:193:ILE:HG12	1:D:216:ILE:HG21	1.94	0.49
1:C:110:GLY:HA3	1:C:360:GLY:HA2	1.93	0.49
1:A:193:ILE:HG12	1:A:216:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:193:ILE:HG12	1:F:216:ILE:HG21	1.94	0.49
1:B:36:ILE:HD12	1:B:104:ALA:HB3	1.94	0.49
1:D:89:ALA:HB1	1:D:95:GLN:HE21	1.77	0.49
1:F:45:TRP:CZ2	1:F:365:VAL:HB	2.47	0.49
1:F:130:GLU:O	1:F:327:THR:HG22	2.12	0.49
1:D:226:GLU:HG2	1:F:252:TYR:CG	2.47	0.49
1:E:36:ILE:HD12	1:E:104:ALA:HB3	1.94	0.49
1:A:129:ILE:HD13	1:A:311:VAL:HG21	1.95	0.49
1:C:234:LEU:O	1:C:238:THR:HG22	2.13	0.49
1:F:110:GLY:HA3	1:F:360:GLY:HA2	1.95	0.49
1:D:8:PRO:HB2	1:D:56:LYS:HG2	1.94	0.48
1:B:346:ILE:HG22	1:B:356:PRO:HG3	1.95	0.48
1:B:10:VAL:HG13	1:B:52:ALA:HB1	1.96	0.48
1:C:193:ILE:HG12	1:C:216:ILE:HG21	1.94	0.48
1:C:346:ILE:HG22	1:C:356:PRO:HG3	1.96	0.48
1:G:110:GLY:HA3	1:G:360:GLY:HA2	1.95	0.48
1:A:130:GLU:O	1:A:327:THR:HG22	2.14	0.48
1:A:234:LEU:O	1:A:238:THR:HG22	2.14	0.48
1:B:234:LEU:O	1:B:238:THR:HG22	2.14	0.48
1:F:129:ILE:HG12	1:F:311:VAL:CG2	2.43	0.48
1:A:346:ILE:HG22	1:A:356:PRO:HG3	1.95	0.48
1:C:130:GLU:O	1:C:327:THR:HG22	2.14	0.48
1:E:130:GLU:O	1:E:327:THR:HG22	2.14	0.48
1:A:35:LYS:HB2	1:A:45:TRP:CZ3	2.48	0.47
1:B:35:LYS:HB2	1:B:45:TRP:CZ3	2.49	0.47
1:E:193:ILE:HG12	1:E:216:ILE:HG21	1.95	0.47
1:F:171:ILE:O	1:F:175:LEU:HD22	2.13	0.47
1:H:234:LEU:O	1:H:238:THR:HG22	2.14	0.47
1:D:130:GLU:O	1:D:327:THR:HG22	2.14	0.47
1:D:234:LEU:O	1:D:238:THR:HG22	2.14	0.47
1:G:193:ILE:HG12	1:G:216:ILE:HG21	1.95	0.47
1:G:234:LEU:O	1:G:238:THR:HG22	2.14	0.47
1:A:289:TYR:CE1	1:E:255:LYS:HE2	2.50	0.47
1:F:346:ILE:HG22	1:F:356:PRO:HG3	1.95	0.47
1:H:35:LYS:HB2	1:H:45:TRP:CZ3	2.50	0.47
1:H:190:ARG:HH22	1:H:327:THR:HG21	1.79	0.47
1:D:346:ILE:HG22	1:D:356:PRO:HG3	1.95	0.47
1:G:134:THR:OG1	1:G:331:ASP:HA	2.13	0.47
1:H:340:GLU:HB3	1:H:369:LYS:HD3	1.97	0.47
1:A:8:PRO:HB2	1:A:56:LYS:HG2	1.96	0.47
1:B:130:GLU:O	1:B:327:THR:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:PRO:HB2	1:C:56:LYS:HG2	1.96	0.47
1:C:35:LYS:HB2	1:C:45:TRP:CZ3	2.50	0.47
1:D:201:TYR:O	1:D:205:ILE:HG13	2.15	0.47
1:G:35:LYS:HB2	1:G:45:TRP:CZ3	2.49	0.47
1:H:130:GLU:O	1:H:327:THR:HG22	2.14	0.47
1:E:365:VAL:HG11	1:E:370:LEU:HD12	1.96	0.47
1:H:10:VAL:HG13	1:H:52:ALA:HB1	1.97	0.47
1:A:201:TYR:O	1:A:205:ILE:HG13	2.15	0.47
1:G:8:PRO:HB2	1:G:56:LYS:HG2	1.97	0.47
1:A:36:ILE:HD12	1:A:104:ALA:HB3	1.95	0.46
1:C:201:TYR:O	1:C:205:ILE:HG13	2.15	0.46
1:E:10:VAL:HG13	1:E:52:ALA:HB1	1.97	0.46
1:H:201:TYR:O	1:H:205:ILE:HG13	2.15	0.46
1:C:226:GLU:HG2	1:E:252:TYR:CG	2.50	0.46
3:E:406:HOH:O	1:G:200:CYS:HB2	2.14	0.46
1:E:201:TYR:O	1:E:205:ILE:HG13	2.16	0.46
1:G:129:ILE:HG12	1:G:311:VAL:CG2	2.44	0.46
1:E:8:PRO:HB2	1:E:56:LYS:HG2	1.97	0.46
1:E:234:LEU:O	1:E:238:THR:HG22	2.15	0.46
1:F:201:TYR:O	1:F:205:ILE:HG13	2.14	0.46
1:H:304:ILE:O	1:H:308:VAL:HG23	2.16	0.46
1:A:10:VAL:HG13	1:A:52:ALA:HB1	1.97	0.46
1:C:168:GLY:HA2	1:C:199:TYR:CE2	2.51	0.46
1:E:35:LYS:HB2	1:E:45:TRP:CZ3	2.51	0.46
1:F:234:LEU:O	1:F:238:THR:HG22	2.15	0.46
1:G:346:ILE:HG22	1:G:356:PRO:HG3	1.97	0.46
1:E:30:LYS:O	1:E:52:ALA:HB2	2.16	0.46
1:F:331:ASP:CG	1:F:333:THR:HG1	2.17	0.46
1:G:10:VAL:HG23	1:G:56:LYS:HG3	1.98	0.46
1:G:201:TYR:O	1:G:205:ILE:HG13	2.16	0.46
1:B:201:TYR:O	1:B:205:ILE:HG13	2.16	0.46
1:C:10:VAL:HG13	1:C:52:ALA:HB1	1.98	0.45
1:F:331:ASP:CG	1:F:333:THR:OG1	2.59	0.45
1:F:342:THR:HG22	1:F:365:VAL:HG22	1.97	0.45
1:H:270:ILE:HA	1:H:279:VAL:HG21	1.98	0.45
1:A:10:VAL:HG23	1:A:56:LYS:HG3	1.98	0.45
1:E:37:THR:HG22	1:E:43:TYR:HB3	1.98	0.45
1:G:304:ILE:O	1:G:308:VAL:HG23	2.15	0.45
1:A:252:TYR:CG	1:G:226:GLU:HG2	2.52	0.45
1:D:10:VAL:HG23	1:D:56:LYS:HG3	1.98	0.45
1:B:85:SER:HB2	1:B:94:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:LEU:HD12	1:C:42:THR:HB	1.96	0.45
1:E:304:ILE:O	1:E:308:VAL:HG23	2.17	0.45
1:F:127:PRO:HG2	1:F:128:ILE:HD12	1.97	0.45
1:G:127:PRO:HG2	1:G:128:ILE:HD12	1.98	0.45
1:H:168:GLY:HA2	1:H:199:TYR:CE2	2.51	0.45
1:A:304:ILE:O	1:A:308:VAL:HG23	2.17	0.45
1:F:192:MET:HG3	1:F:217:SER:HB2	1.99	0.45
1:H:4:LYS:HB3	1:H:39:ASP:OD1	2.16	0.45
1:C:109:LYS:HD2	3:C:503:HOH:O	2.16	0.45
1:D:304:ILE:O	1:D:308:VAL:HG23	2.17	0.45
1:G:270:ILE:HA	1:G:279:VAL:HG21	1.99	0.45
1:A:31:ILE:HD11	1:A:33:ILE:CD1	2.47	0.44
1:G:10:VAL:HG13	1:G:52:ALA:HB1	1.99	0.44
1:D:270:ILE:HA	1:D:279:VAL:HG21	1.98	0.44
1:A:129:ILE:HB	1:A:326:PRO:HG2	2.00	0.44
1:C:270:ILE:HA	1:C:279:VAL:HG21	1.98	0.44
1:D:192:MET:HG3	1:D:217:SER:HB2	1.99	0.44
1:E:127:PRO:HG2	1:E:128:ILE:HD12	2.00	0.44
1:A:270:ILE:HA	1:A:279:VAL:HG21	1.99	0.44
1:F:8:PRO:HB2	1:F:56:LYS:HG2	1.99	0.44
1:H:129:ILE:HG13	1:H:353:LEU:HB3	2.00	0.44
1:A:192:MET:HG3	1:A:217:SER:HB2	2.00	0.43
1:F:10:VAL:HG23	1:F:56:LYS:HG3	2.00	0.43
1:E:270:ILE:HA	1:E:279:VAL:HG21	1.99	0.43
1:A:285:LEU:HD11	1:E:288:THR:HG21	2.00	0.43
1:G:51:PRO:HB2	1:G:54:VAL:CG2	2.48	0.43
1:E:51:PRO:HB2	1:E:54:VAL:CG2	2.48	0.43
1:H:51:PRO:HB2	1:H:54:VAL:CG2	2.49	0.43
1:H:190:ARG:HH22	1:H:327:THR:CG2	2.31	0.43
1:H:205:ILE:HG13	1:H:205:ILE:H	1.70	0.43
1:C:127:PRO:HG2	1:C:128:ILE:HD12	1.99	0.43
1:E:192:MET:HG3	1:E:217:SER:HB2	2.01	0.43
1:B:129:ILE:HB	1:B:326:PRO:HG2	2.01	0.43
1:C:252:TYR:CG	1:E:226:GLU:HG2	2.54	0.43
1:G:192:MET:HG3	1:G:217:SER:HB2	2.01	0.43
1:B:31:ILE:HD11	1:B:33:ILE:CD1	2.49	0.43
1:B:309:HIS:HE2	1:B:356:PRO:HG2	1.84	0.43
1:B:192:MET:HG3	1:B:217:SER:HB2	2.01	0.43
1:D:127:PRO:HG2	1:D:128:ILE:HD12	2.00	0.42
1:B:270:ILE:HA	1:B:279:VAL:HG21	2.01	0.42
1:B:289:TYR:CZ	1:F:255:LYS:HE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:346:ILE:HD12	1:G:353:LEU:HD21	2.01	0.42
1:F:304:ILE:O	1:F:308:VAL:HG23	2.18	0.42
1:G:307:ALA:O	1:G:311:VAL:HG13	2.19	0.42
1:H:85:SER:HB2	1:H:94:LEU:HD13	2.01	0.42
1:H:307:ALA:O	1:H:311:VAL:HG13	2.19	0.42
1:E:37:THR:HG22	1:E:43:TYR:CB	2.49	0.42
1:C:205:ILE:HG13	1:C:205:ILE:H	1.70	0.42
1:F:51:PRO:HB2	1:F:54:VAL:CG2	2.50	0.42
1:H:192:MET:HG3	1:H:217:SER:HB2	2.00	0.42
1:H:13:HIS:ND1	1:H:373:TYR:HE1	2.18	0.42
1:E:108:ILE:O	1:E:112:LEU:HB2	2.20	0.42
1:E:40:ASP:OD1	1:E:42:THR:HB	2.20	0.42
1:F:55:ILE:HG12	1:F:96:ALA:HB3	2.02	0.42
1:B:127:PRO:HG2	1:B:128:ILE:HD12	2.02	0.41
1:C:304:ILE:O	1:C:308:VAL:HG23	2.19	0.41
1:C:192:MET:HG3	1:C:217:SER:HB2	2.00	0.41
1:C:69:LYS:HB3	1:C:77:LEU:HD21	2.02	0.41
1:A:75:GLU:HB3	1:E:125:LYS:NZ	2.35	0.41
1:F:307:ALA:O	1:F:311:VAL:HG13	2.21	0.41
1:G:205:ILE:HG13	1:G:205:ILE:H	1.71	0.41
1:G:371:GLU:HA	1:G:374:LEU:HD12	2.02	0.41
1:A:51:PRO:HB2	1:A:54:VAL:CG2	2.51	0.41
1:C:31:ILE:HD11	1:C:33:ILE:HD11	2.03	0.41
1:F:13:HIS:NE2	1:F:15:LEU:HD12	2.35	0.41
1:F:99:SER:O	1:F:103:VAL:HG23	2.21	0.41
1:F:270:ILE:HA	1:F:279:VAL:HG21	2.01	0.41
1:F:10:VAL:HG13	1:F:52:ALA:HB1	2.03	0.41
1:F:334:GLU:O	1:F:335:ASN:HB2	2.21	0.41
1:B:225:PRO:HB2	1:H:90:ARG:NH2	2.35	0.41
1:D:35:LYS:HB2	1:D:45:TRP:CZ3	2.56	0.41
1:E:205:ILE:HG13	1:E:205:ILE:H	1.71	0.41
1:F:11:ILE:HD12	1:F:337:LEU:HB3	2.03	0.41
1:H:130:GLU:HB2	1:H:161:LYS:CD	2.48	0.41
1:B:108:ILE:O	1:B:112:LEU:HB2	2.21	0.41
1:C:10:VAL:HG23	1:C:56:LYS:HG3	2.04	0.40
1:C:38:LEU:HD21	1:C:71:ALA:HB2	2.02	0.40
1:D:6:ILE:HD12	1:D:63:THR:HG23	2.04	0.40
1:D:72:ILE:H	1:D:72:ILE:HG13	1.76	0.40
1:E:11:ILE:HD12	1:E:337:LEU:HB3	2.03	0.40
1:B:51:PRO:HB2	1:B:54:VAL:CG2	2.51	0.40
1:B:307:ALA:O	1:B:311:VAL:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:ALA:O	1:C:311:VAL:HG13	2.21	0.40
1:C:9:TYR:CD1	1:C:370:LEU:HD11	2.57	0.40
1:G:311:VAL:HA	1:G:314:LEU:HB2	2.04	0.40
1:H:117:VAL:HG23	1:H:360:GLY:C	2.46	0.40
1:B:168:GLY:HA2	1:B:199:TYR:CE2	2.57	0.40
1:E:311:VAL:HA	1:E:314:LEU:HB2	2.03	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	343/396 (87%)	322 (94%)	21 (6%)	0	100	100
1	B	343/396 (87%)	322 (94%)	21 (6%)	0	100	100
1	C	343/396 (87%)	321 (94%)	22 (6%)	0	100	100
1	D	343/396 (87%)	323 (94%)	20 (6%)	0	100	100
1	E	343/396 (87%)	321 (94%)	22 (6%)	0	100	100
1	F	343/396 (87%)	318 (93%)	24 (7%)	1 (0%)	36	66
1	G	343/396 (87%)	321 (94%)	22 (6%)	0	100	100
1	H	343/396 (87%)	321 (94%)	22 (6%)	0	100	100
All	All	2744/3168 (87%)	2569 (94%)	174 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	335	ASN

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	284/337 (84%)	245 (86%)	39 (14%)	3	13
1	B	281/337 (83%)	243 (86%)	38 (14%)	4	13
1	C	283/337 (84%)	243 (86%)	40 (14%)	3	12
1	D	282/337 (84%)	249 (88%)	33 (12%)	5	18
1	E	287/337 (85%)	250 (87%)	37 (13%)	4	14
1	F	289/337 (86%)	253 (88%)	36 (12%)	4	15
1	G	286/337 (85%)	243 (85%)	43 (15%)	3	10
1	H	290/337 (86%)	248 (86%)	42 (14%)	3	11
All	All	2282/2696 (85%)	1974 (86%)	308 (14%)	4	13

All (308) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	13	HIS
1	A	30	LYS
1	A	31	ILE
1	A	34	VAL
1	A	37	THR
1	A	54	VAL
1	A	56	LYS
1	A	65	PHE
1	A	72	ILE
1	A	86	MET
1	A	87	ASP
1	A	91	SER
1	A	109	LYS
1	A	112	LEU
1	A	118	SER
1	A	129	ILE
1	A	136	LEU
1	A	144	LEU

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Mol	Chain	Res	Type
1	A	171	ILE
1	A	183	LYS
1	A	197	HIS
1	A	205	ILE
1	A	226	GLU
1	A	243	SER
1	A	260	LYS
1	A	280	LYS
1	A	293	LEU
1	A	297	THR
1	A	310	LEU
1	A	311	VAL
1	A	314	LEU
1	A	334	GLU
1	A	337	LEU
1	A	349	GLU
1	A	353	LEU
1	A	357	CYS
1	A	364	ASP
1	A	374	LEU
1	B	5	LYS
1	B	13	HIS
1	B	30	LYS
1	B	31	ILE
1	B	34	VAL
1	B	37	THR
1	B	54	VAL
1	B	65	PHE
1	B	67	LEU
1	B	72	ILE
1	B	87	ASP
1	B	109	LYS
1	B	112	LEU
1	B	118	SER
1	B	129	ILE
1	B	136	LEU
1	B	144	LEU
1	B	150	GLU
1	B	169	LEU
1	B	171	ILE
1	B	197	HIS
1	B	205	ILE

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Mol	Chain	Res	Type
1	B	226	GLU
1	B	243	SER
1	B	256	ARG
1	B	257	LEU
1	B	280	LYS
1	B	293	LEU
1	B	297	THR
1	B	310	LEU
1	B	311	VAL
1	B	314	LEU
1	B	334	GLU
1	B	349	GLU
1	B	353	LEU
1	B	357	CYS
1	B	364	ASP
1	B	374	LEU
1	C	13	HIS
1	C	29	ARG
1	C	30	LYS
1	C	31	ILE
1	C	34	VAL
1	C	37	THR
1	C	54	VAL
1	C	56	LYS
1	C	65	PHE
1	C	67	LEU
1	C	69	LYS
1	C	72	ILE
1	C	86	MET
1	C	87	ASP
1	C	109	LYS
1	C	112	LEU
1	C	118	SER
1	C	129	ILE
1	C	136	LEU
1	C	144	LEU
1	C	166	LYS
1	C	171	ILE
1	C	197	HIS
1	C	205	ILE
1	C	226	GLU
1	C	243	SER

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Mol	Chain	Res	Type
1	C	260	LYS
1	C	280	LYS
1	C	293	LEU
1	C	297	THR
1	C	310	LEU
1	C	311	VAL
1	C	314	LEU
1	C	334	GLU
1	C	337	LEU
1	C	349	GLU
1	C	353	LEU
1	C	357	CYS
1	C	364	ASP
1	C	374	LEU
1	D	29	ARG
1	D	31	ILE
1	D	34	VAL
1	D	37	THR
1	D	54	VAL
1	D	56	LYS
1	D	65	PHE
1	D	69	LYS
1	D	72	ILE
1	D	87	ASP
1	D	91	SER
1	D	109	LYS
1	D	112	LEU
1	D	129	ILE
1	D	136	LEU
1	D	144	LEU
1	D	166	LYS
1	D	171	ILE
1	D	197	HIS
1	D	205	ILE
1	D	213	LYS
1	D	243	SER
1	D	280	LYS
1	D	293	LEU
1	D	297	THR
1	D	310	LEU
1	D	311	VAL
1	D	314	LEU

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Mol	Chain	Res	Type
1	D	334	GLU
1	D	349	GLU
1	D	357	CYS
1	D	364	ASP
1	D	374	LEU
1	E	13	HIS
1	E	29	ARG
1	E	34	VAL
1	E	37	THR
1	E	54	VAL
1	E	56	LYS
1	E	65	PHE
1	E	69	LYS
1	E	72	ILE
1	E	86	MET
1	E	87	ASP
1	E	91	SER
1	E	109	LYS
1	E	112	LEU
1	E	118	SER
1	E	129	ILE
1	E	136	LEU
1	E	144	LEU
1	E	166	LYS
1	E	171	ILE
1	E	183	LYS
1	E	197	HIS
1	E	205	ILE
1	E	243	SER
1	E	256	ARG
1	E	280	LYS
1	E	293	LEU
1	E	297	THR
1	E	310	LEU
1	E	311	VAL
1	E	314	LEU
1	E	334	GLU
1	E	349	GLU
1	E	353	LEU
1	E	357	CYS
1	E	364	ASP
1	E	374	LEU

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Mol	Chain	Res	Type
1	F	4	LYS
1	F	15	LEU
1	F	30	LYS
1	F	34	VAL
1	F	37	THR
1	F	42	THR
1	F	54	VAL
1	F	56	LYS
1	F	65	PHE
1	F	72	ILE
1	F	87	ASP
1	F	91	SER
1	F	109	LYS
1	F	112	LEU
1	F	118	SER
1	F	136	LEU
1	F	144	LEU
1	F	166	LYS
1	F	171	ILE
1	F	175	LEU
1	F	183	LYS
1	F	197	HIS
1	F	205	ILE
1	F	226	GLU
1	F	243	SER
1	F	280	LYS
1	F	293	LEU
1	F	297	THR
1	F	310	LEU
1	F	311	VAL
1	F	314	LEU
1	F	334	GLU
1	F	349	GLU
1	F	353	LEU
1	F	364	ASP
1	F	374	LEU
1	G	1	SER
1	G	13	HIS
1	G	15	LEU
1	G	29	ARG
1	G	31	ILE
1	G	34	VAL

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Mol	Chain	Res	Type
1	G	37	THR
1	G	54	VAL
1	G	56	LYS
1	G	65	PHE
1	G	67	LEU
1	G	72	ILE
1	G	86	MET
1	G	87	ASP
1	G	91	SER
1	G	109	LYS
1	G	112	LEU
1	G	118	SER
1	G	136	LEU
1	G	144	LEU
1	G	156	LYS
1	G	166	LYS
1	G	171	ILE
1	G	173	GLN
1	G	197	HIS
1	G	205	ILE
1	G	243	SER
1	G	255	LYS
1	G	280	LYS
1	G	293	LEU
1	G	297	THR
1	G	310	LEU
1	G	311	VAL
1	G	314	LEU
1	G	332	ARG
1	G	334	GLU
1	G	337	LEU
1	G	349	GLU
1	G	353	LEU
1	G	357	CYS
1	G	364	ASP
1	G	374	LEU
1	G	375	ASP
1	H	1	SER
1	H	15	LEU
1	H	29	ARG
1	H	30	LYS
1	H	31	ILE

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Mol	Chain	Res	Type
1	H	33	ILE
1	H	34	VAL
1	H	37	THR
1	H	39	ASP
1	H	42	THR
1	H	54	VAL
1	H	56	LYS
1	H	65	PHE
1	H	72	ILE
1	H	86	MET
1	H	87	ASP
1	H	91	SER
1	H	109	LYS
1	H	112	LEU
1	H	118	SER
1	H	128	ILE
1	H	129	ILE
1	H	136	LEU
1	H	144	LEU
1	H	161	LYS
1	H	166	LYS
1	H	169	LEU
1	H	171	ILE
1	H	205	ILE
1	H	243	SER
1	H	255	LYS
1	H	260	LYS
1	H	280	LYS
1	H	297	THR
1	H	310	LEU
1	H	311	VAL
1	H	314	LEU
1	H	347	LYS
1	H	349	GLU
1	H	357	CYS
1	H	364	ASP
1	H	370	LEU

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	74	HIS

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Mol	Chain	Res	Type
1	A	95	GLN
1	A	114	ASN
1	A	173	GLN
1	A	267	GLN
1	A	313	ASN
1	B	74	HIS
1	B	114	ASN
1	B	313	ASN
1	C	13	HIS
1	C	74	HIS
1	C	95	GLN
1	C	114	ASN
1	C	313	ASN
1	C	335	ASN
1	D	74	HIS
1	D	95	GLN
1	D	114	ASN
1	D	267	GLN
1	D	313	ASN
1	D	335	ASN
1	E	74	HIS
1	E	114	ASN
1	E	173	GLN
1	E	313	ASN
1	E	344	HIS
1	F	74	HIS
1	F	158	GLN
1	F	313	ASN
1	F	344	HIS
1	G	74	HIS
1	G	95	GLN
1	G	114	ASN
1	G	313	ASN
1	H	74	HIS
1	H	95	GLN
1	H	114	ASN
1	H	313	ASN

5.3.3 RNA ⓘ

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 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	351/396 (88%)	1.21	56 (15%) 5 4	38, 69, 101, 116	0
1	B	351/396 (88%)	1.30	59 (16%) 4 3	39, 68, 99, 117	0
1	C	351/396 (88%)	1.32	64 (18%) 3 2	38, 68, 103, 132	0
1	D	351/396 (88%)	1.31	61 (17%) 4 3	39, 69, 102, 118	0
1	E	351/396 (88%)	1.27	61 (17%) 4 3	35, 64, 94, 118	0
1	F	351/396 (88%)	1.24	59 (16%) 4 3	35, 63, 93, 123	0
1	G	351/396 (88%)	1.28	63 (17%) 3 3	38, 64, 94, 106	0
1	H	351/396 (88%)	1.30	67 (19%) 3 2	38, 64, 94, 108	0
All	All	2808/3168 (88%)	1.28	490 (17%) 4 3	35, 66, 99, 132	0

All (490) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	144	LEU	5.8
1	F	86	MET	5.5
1	A	346	ILE	5.5
1	C	137	TYR	5.4
1	G	89	ALA	5.3
1	G	144	LEU	5.1
1	A	93	VAL	5.1
1	F	144	LEU	4.9
1	D	346	ILE	4.9
1	E	345	LYS	4.7
1	H	39	ASP	4.7
1	C	169	LEU	4.7
1	D	271	CYS	4.7
1	B	137	TYR	4.6
1	F	137	TYR	4.6
1	E	144	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	H	12	SER	4.4
1	D	144	LEU	4.4
1	A	91	SER	4.3
1	C	168	GLY	4.2
1	H	40	ASP	4.1
1	A	376	LYS	4.1
1	E	137	TYR	4.1
1	A	144	LEU	4.1
1	F	136	LEU	4.1
1	H	38	LEU	4.1
1	D	165	MET	4.1
1	B	136	LEU	4.1
1	H	72	ILE	4.0
1	A	201	TYR	4.0
1	G	198	ALA	4.0
1	C	345	LYS	4.0
1	B	146	GLU	4.0
1	C	86	MET	3.9
1	G	346	ILE	3.9
1	G	137	TYR	3.9
1	H	48	GLY	3.9
1	E	93	VAL	3.9
1	D	345	LYS	3.8
1	A	89	ALA	3.8
1	C	346	ILE	3.8
1	F	198	ALA	3.8
1	B	93	VAL	3.8
1	B	90	ARG	3.8
1	D	376	LYS	3.7
1	E	89	ALA	3.7
1	A	16	ASP	3.7
1	B	185	ILE	3.7
1	D	36	ILE	3.7
1	A	345	LYS	3.7
1	D	167	VAL	3.7
1	A	70	GLU	3.7
1	C	207	LEU	3.6
1	D	137	TYR	3.6
1	C	93	VAL	3.6
1	E	54	VAL	3.6
1	C	144	LEU	3.6
1	G	27	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	106	TRP	3.6
1	F	145	GLU	3.6
1	A	145	GLU	3.5
1	F	88	TYR	3.5
1	G	345	LYS	3.5
1	B	258	PHE	3.5
1	E	357	CYS	3.5
1	H	37	THR	3.5
1	B	89	ALA	3.4
1	C	167	VAL	3.4
1	C	271	CYS	3.4
1	A	29	ARG	3.4
1	E	86	MET	3.4
1	D	136	LEU	3.4
1	D	93	VAL	3.4
1	G	298	TRP	3.3
1	H	137	TYR	3.3
1	H	86	MET	3.3
1	B	346	ILE	3.3
1	F	115	LEU	3.3
1	D	89	ALA	3.3
1	B	91	SER	3.3
1	E	37	THR	3.3
1	C	135	GLY	3.3
1	B	144	LEU	3.2
1	B	375	ASP	3.2
1	B	376	LYS	3.2
1	C	148	LEU	3.2
1	H	169	LEU	3.2
1	E	92	GLY	3.2
1	C	177	TYR	3.2
1	B	345	LYS	3.2
1	A	148	LEU	3.2
1	H	136	LEU	3.2
1	G	46	GLY	3.2
1	H	89	ALA	3.2
1	D	290	ASN	3.2
1	F	345	LYS	3.2
1	A	169	LEU	3.2
1	G	15	LEU	3.2
1	G	48	GLY	3.2
1	C	336	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	129	ILE	3.2
1	A	88	TYR	3.2
1	A	87	ASP	3.1
1	A	256	ARG	3.1
1	C	87	ASP	3.1
1	D	348	LEU	3.1
1	C	71	ALA	3.1
1	C	181	ILE	3.1
1	B	343	LEU	3.1
1	C	91	SER	3.1
1	E	177	TYR	3.1
1	C	136	LEU	3.1
1	E	145	GLU	3.1
1	F	135	GLY	3.1
1	B	177	TYR	3.1
1	D	145	GLU	3.1
1	C	89	ALA	3.1
1	F	89	ALA	3.1
1	E	91	SER	3.1
1	F	305	SER	3.1
1	G	12	SER	3.1
1	E	87	ASP	3.0
1	H	345	LYS	3.0
1	B	29	ARG	3.0
1	H	93	VAL	3.0
1	F	348	LEU	3.0
1	D	132	TYR	3.0
1	C	315	ASP	3.0
1	C	36	ILE	3.0
1	G	100	ALA	3.0
1	A	137	TYR	3.0
1	E	88	TYR	3.0
1	B	315	ASP	3.0
1	F	315	ASP	3.0
1	C	178	ILE	3.0
1	F	37	THR	3.0
1	F	93	VAL	3.0
1	B	201	TYR	3.0
1	E	346	ILE	3.0
1	C	94	LEU	2.9
1	A	298	TRP	2.9
1	F	298	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	91	SER	2.9
1	G	49	TYR	2.9
1	C	72	ILE	2.9
1	G	341	VAL	2.9
1	B	169	LEU	2.9
1	G	166	LYS	2.9
1	F	231	TYR	2.9
1	B	135	GLY	2.9
1	D	337	LEU	2.9
1	E	136	LEU	2.9
1	H	370	LEU	2.9
1	B	271	CYS	2.9
1	E	260	LYS	2.9
1	G	359	PRO	2.9
1	H	11	ILE	2.9
1	A	315	ASP	2.9
1	D	347	LYS	2.9
1	E	169	LEU	2.9
1	H	15	LEU	2.9
1	C	197	HIS	2.9
1	G	145	GLU	2.8
1	H	85	SER	2.8
1	B	92	GLY	2.8
1	F	362	GLY	2.8
1	H	88	TYR	2.8
1	A	94	LEU	2.8
1	A	15	LEU	2.8
1	E	285	LEU	2.8
1	F	177	TYR	2.8
1	G	115	LEU	2.8
1	H	115	LEU	2.8
1	H	71	ALA	2.8
1	E	341	VAL	2.8
1	G	86	MET	2.8
1	E	67	LEU	2.8
1	F	38	LEU	2.8
1	H	27	ASP	2.8
1	A	146	GLU	2.8
1	E	348	LEU	2.8
1	G	285	LEU	2.8
1	H	145	GLU	2.8
1	D	173	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	171	ILE	2.7
1	D	88	TYR	2.7
1	E	249	TYR	2.7
1	C	376	LYS	2.7
1	H	111	LYS	2.7
1	A	36	ILE	2.7
1	F	361	LEU	2.7
1	B	159	GLY	2.7
1	C	68	GLY	2.7
1	G	85	SER	2.7
1	H	298	TRP	2.7
1	F	87	ASP	2.7
1	A	177	TYR	2.7
1	C	228	TYR	2.7
1	C	171	ILE	2.7
1	D	185	ILE	2.7
1	H	181	ILE	2.7
1	E	94	LEU	2.7
1	F	15	LEU	2.7
1	B	224	SER	2.7
1	B	70	GLU	2.7
1	B	206	GLU	2.7
1	F	359	PRO	2.7
1	G	231	TYR	2.7
1	F	285	LEU	2.7
1	B	347	LYS	2.7
1	D	148	LEU	2.6
1	G	271	CYS	2.6
1	D	168	GLY	2.6
1	B	167	VAL	2.6
1	D	214	PHE	2.6
1	D	336	ALA	2.6
1	E	231	TYR	2.6
1	H	177	TYR	2.6
1	A	197	HIS	2.6
1	E	166	LYS	2.6
1	G	351	GLY	2.6
1	D	258	PHE	2.6
1	G	93	VAL	2.6
1	G	167	VAL	2.6
1	B	88	TYR	2.6
1	A	83	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	13	HIS	2.6
1	A	30	LYS	2.6
1	C	145	GLU	2.6
1	H	50	GLY	2.6
1	E	71	ALA	2.6
1	H	291	VAL	2.6
1	D	91	SER	2.6
1	G	28	THR	2.6
1	C	70	GLU	2.6
1	H	271	CYS	2.6
1	A	133	ALA	2.6
1	F	114	ASN	2.6
1	F	85	SER	2.5
1	C	129	ILE	2.5
1	B	148	LEU	2.5
1	G	344	HIS	2.5
1	H	279	VAL	2.5
1	A	270	ILE	2.5
1	G	136	LEU	2.5
1	A	132	TYR	2.5
1	E	12	SER	2.5
1	A	185	ILE	2.5
1	C	302	ILE	2.5
1	B	374	LEU	2.5
1	C	172	GLU	2.5
1	D	82	TYR	2.5
1	B	360	GLY	2.5
1	A	214	PHE	2.5
1	H	133	ALA	2.5
1	B	134	THR	2.5
1	E	358	THR	2.5
1	H	357	CYS	2.5
1	C	216	ILE	2.5
1	G	209	ARG	2.5
1	C	16	ASP	2.5
1	B	362	GLY	2.5
1	H	135	GLY	2.5
1	H	131	PRO	2.5
1	H	231	TYR	2.5
1	G	303	ALA	2.5
1	B	290	ASN	2.4
1	A	374	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	94	LEU	2.4
1	A	188	ASP	2.4
1	C	8	PRO	2.4
1	E	187	PRO	2.4
1	H	46	GLY	2.4
1	C	201	TYR	2.4
1	C	117	VAL	2.4
1	D	160	PHE	2.4
1	H	198	ALA	2.4
1	A	28	THR	2.4
1	G	37	THR	2.4
1	G	72	ILE	2.4
1	H	346	ILE	2.4
1	A	1	SER	2.4
1	D	197	HIS	2.4
1	A	45	TRP	2.4
1	D	16	ASP	2.4
1	F	16	ASP	2.4
1	D	86	MET	2.4
1	D	92	GLY	2.4
1	H	359	PRO	2.4
1	F	54	VAL	2.4
1	H	132	TYR	2.4
1	C	198	ALA	2.4
1	D	182	ARG	2.4
1	D	297	THR	2.4
1	G	121	LEU	2.4
1	H	91	SER	2.4
1	A	271	CYS	2.4
1	D	146	GLU	2.4
1	D	246	GLU	2.4
1	F	334	GLU	2.4
1	B	158	GLN	2.4
1	B	28	THR	2.4
1	B	171	ILE	2.4
1	D	327	THR	2.4
1	F	128	ILE	2.4
1	F	358	THR	2.4
1	D	32	CYS	2.4
1	C	173	GLN	2.4
1	G	363	VAL	2.4
1	H	54	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	207	LEU	2.3
1	F	181	ILE	2.3
1	D	27	ASP	2.3
1	D	315	ASP	2.3
1	G	40	ASP	2.3
1	F	351	GLY	2.3
1	B	149	VAL	2.3
1	E	355	VAL	2.3
1	G	128	ILE	2.3
1	H	128	ILE	2.3
1	D	228	TYR	2.3
1	G	132	TYR	2.3
1	H	9	TYR	2.3
1	H	16	ASP	2.3
1	B	45	TRP	2.3
1	H	90	ARG	2.3
1	H	10	VAL	2.3
1	D	169	LEU	2.3
1	E	147	LEU	2.3
1	F	71	ALA	2.3
1	D	282	ILE	2.3
1	E	101	ILE	2.3
1	H	129	ILE	2.3
1	G	88	TYR	2.3
1	B	30	LYS	2.3
1	C	166	LYS	2.3
1	E	1	SER	2.3
1	F	1	SER	2.3
1	F	364	ASP	2.3
1	H	305	SER	2.3
1	F	256	ARG	2.3
1	E	148	LEU	2.3
1	E	175	LEU	2.3
1	G	357	CYS	2.3
1	F	72	ILE	2.3
1	E	82	TYR	2.3
1	G	177	TYR	2.3
1	C	371	GLU	2.3
1	E	40	ASP	2.3
1	E	298	TRP	2.3
1	F	170	GLY	2.3
1	A	191	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	36	ILE	2.2
1	C	185	ILE	2.2
1	H	74	HIS	2.2
1	A	202	LYS	2.2
1	A	347	LYS	2.2
1	C	199	TYR	2.2
1	F	187	PRO	2.2
1	G	131	PRO	2.2
1	E	305	SER	2.2
1	B	293	LEU	2.2
1	C	370	LEU	2.2
1	E	115	LEU	2.2
1	H	348	LEU	2.2
1	E	171	ILE	2.2
1	F	258	PHE	2.2
1	B	184	ALA	2.2
1	F	197	HIS	2.2
1	F	346	ILE	2.2
1	G	273	ALA	2.2
1	H	232	LYS	2.2
1	C	121	LEU	2.2
1	E	353	LEU	2.2
1	E	361	LEU	2.2
1	F	67	LEU	2.2
1	A	149	VAL	2.2
1	D	3	ILE	2.2
1	A	179	ALA	2.2
1	E	150	GLU	2.2
1	G	338	ARG	2.2
1	A	49	TYR	2.2
1	B	132	TYR	2.2
1	F	131	PRO	2.2
1	B	66	LEU	2.2
1	C	274	GLY	2.2
1	G	375	ASP	2.2
1	A	129	ILE	2.2
1	B	270	ILE	2.2
1	B	302	ILE	2.2
1	E	198	ALA	2.2
1	G	272	ALA	2.2
1	B	145	GLU	2.2
1	F	28	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	202	LYS	2.2
1	C	347	LYS	2.2
1	A	250	LEU	2.2
1	G	370	LEU	2.2
1	H	285	LEU	2.2
1	D	341	VAL	2.2
1	G	13	HIS	2.2
1	F	306	ALA	2.1
1	A	358	THR	2.1
1	E	271	CYS	2.1
1	C	165	MET	2.1
1	H	66	LEU	2.1
1	C	362	GLY	2.1
1	D	351	GLY	2.1
1	D	362	GLY	2.1
1	A	181	ILE	2.1
1	C	205	ILE	2.1
1	E	129	ILE	2.1
1	F	270	ILE	2.1
1	G	54	VAL	2.1
1	G	181	ILE	2.1
1	G	197	HIS	2.1
1	H	229	ASP	2.1
1	C	53	ALA	2.1
1	C	180	ALA	2.1
1	A	134	THR	2.1
1	B	327	THR	2.1
1	E	232	LYS	2.1
1	H	95	GLN	2.1
1	A	155	TYR	2.1
1	A	348	LEU	2.1
1	B	348	LEU	2.1
1	E	362	GLY	2.1
1	F	58	GLY	2.1
1	C	3	ILE	2.1
1	D	40	ASP	2.1
1	D	198	ALA	2.1
1	D	334	GLU	2.1
1	F	209	ARG	2.1
1	G	256	ARG	2.1
1	D	28	THR	2.1
1	A	293	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	370	LEU	2.1
1	F	191	LEU	2.1
1	C	92	GLY	2.1
1	E	299	GLY	2.1
1	G	201	TYR	2.1
1	B	6	ILE	2.1
1	E	6	ILE	2.1
1	G	108	ILE	2.1
1	G	355	VAL	2.1
1	A	269	ASP	2.1
1	B	160	PHE	2.1
1	D	29	ARG	2.1
1	G	180	ALA	2.1
1	H	221	GLU	2.1
1	E	327	THR	2.1
1	D	359	PRO	2.1
1	C	330	LEU	2.1
1	C	348	LEU	2.1
1	D	115	LEU	2.1
1	F	112	LEU	2.1
1	G	169	LEU	2.1
1	F	186	GLY	2.1
1	H	344	HIS	2.1
1	B	181	ILE	2.1
1	D	201	TYR	2.1
1	E	72	ILE	2.1
1	H	49	TYR	2.1
1	C	27	ASP	2.0
1	C	90	ARG	2.0
1	E	292	ASP	2.0
1	F	375	ASP	2.0
1	G	83	ARG	2.0
1	G	364	ASP	2.0
1	A	224	SER	2.0
1	E	106	TRP	2.0
1	C	327	THR	2.0
1	F	297	THR	2.0
1	E	356	PRO	2.0
1	D	207	LEU	2.0
1	C	98	ILE	2.0
1	D	33	ILE	2.0
1	A	167	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	82	TYR	2.0
1	D	355	VAL	2.0
1	E	228	TYR	2.0
1	G	117	VAL	2.0
1	E	375	ASP	2.0
1	H	87	ASP	2.0
1	H	369	LYS	2.0
1	H	195	SER	2.0
1	H	300	THR	2.0
1	F	55	ILE	2.0
1	H	168	GLY	2.0
1	E	90	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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(Å ²)	Q<0.9
2	MG	D	401	1/1	0.81	0.13	100,100,100,100	0
2	MG	F	401	1/1	0.86	0.11	64,64,64,64	0
2	MG	G	401	1/1	0.87	0.10	61,61,61,61	0
2	MG	H	401	1/1	0.88	0.09	73,73,73,73	0
2	MG	C	401	1/1	0.92	0.09	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.