



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:58 pm BST

PDB ID : 6VXC
Title : Crystal structure of hydroxyproline dehydratase (HypD) from *Clostridioides difficile*
Authors : Backman, L.R.F.; Drennan, C.L.
Deposited on : 2020-02-21
Resolution : 2.05 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

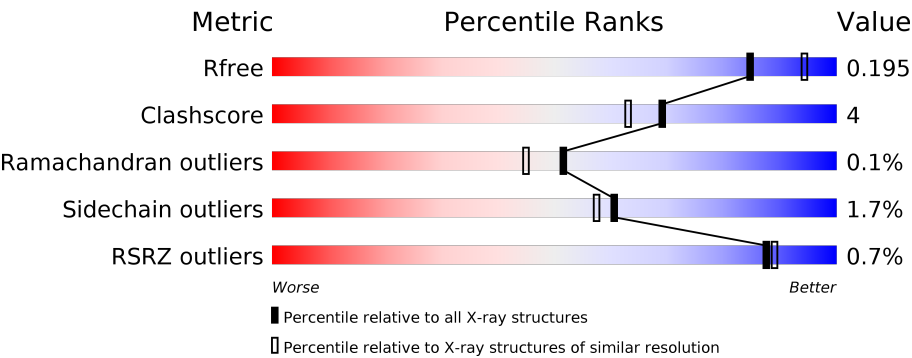
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 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	809	<div><div>%</div><div>89%7%..</div></div>
1	B	809	<div><div>2%</div><div>89%8%.</div></div>
1	C	809	<div><div></div><div>90%7%..</div></div>
1	D	809	<div><div>%</div><div>89%8%.</div></div>
1	E	809	<div><div></div><div>88%9%..</div></div>
1	F	809	<div><div></div><div>87%10%..</div></div>

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Mol	Chain	Length	Quality of chain
1	G	809	<div><div></div><div>89%</div><div>8% ..</div></div>
1	H	809	<div><div></div><div>88%</div><div>8% ..</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 54911 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 Trans-4-hydroxy-L-proline dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	789	Total	C	N	O	S	0	0	0
			6256	3946	1060	1210	40			
1	B	789	Total	C	N	O	S	0	0	0
			6256	3946	1060	1210	40			
1	C	789	Total	C	N	O	S	0	0	0
			6256	3946	1060	1210	40			
1	D	789	Total	C	N	O	S	0	0	0
			6256	3946	1060	1210	40			
1	E	789	Total	C	N	O	S	0	0	0
			6256	3946	1060	1210	40			
1	F	789	Total	C	N	O	S	0	0	0
			6256	3946	1060	1210	40			
1	G	789	Total	C	N	O	S	0	0	0
			6256	3946	1060	1210	40			
1	H	789	Total	C	N	O	S	0	0	0
			6256	3946	1060	1210	40			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A031WDE4
A	-18	GLY	-	expression tag	UNP A0A031WDE4
A	-17	SER	-	expression tag	UNP A0A031WDE4
A	-16	SER	-	expression tag	UNP A0A031WDE4
A	-15	HIS	-	expression tag	UNP A0A031WDE4
A	-14	HIS	-	expression tag	UNP A0A031WDE4
A	-13	HIS	-	expression tag	UNP A0A031WDE4
A	-12	HIS	-	expression tag	UNP A0A031WDE4
A	-11	HIS	-	expression tag	UNP A0A031WDE4
A	-10	HIS	-	expression tag	UNP A0A031WDE4
A	-9	SER	-	expression tag	UNP A0A031WDE4
A	-8	SER	-	expression tag	UNP A0A031WDE4
A	-7	GLY	-	expression tag	UNP A0A031WDE4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP A0A031WDE4
A	-5	VAL	-	expression tag	UNP A0A031WDE4
A	-4	PRO	-	expression tag	UNP A0A031WDE4
A	-3	ARG	-	expression tag	UNP A0A031WDE4
A	-2	GLY	-	expression tag	UNP A0A031WDE4
A	-1	SER	-	expression tag	UNP A0A031WDE4
A	0	HIS	-	expression tag	UNP A0A031WDE4
B	-19	MET	-	initiating methionine	UNP A0A031WDE4
B	-18	GLY	-	expression tag	UNP A0A031WDE4
B	-17	SER	-	expression tag	UNP A0A031WDE4
B	-16	SER	-	expression tag	UNP A0A031WDE4
B	-15	HIS	-	expression tag	UNP A0A031WDE4
B	-14	HIS	-	expression tag	UNP A0A031WDE4
B	-13	HIS	-	expression tag	UNP A0A031WDE4
B	-12	HIS	-	expression tag	UNP A0A031WDE4
B	-11	HIS	-	expression tag	UNP A0A031WDE4
B	-10	HIS	-	expression tag	UNP A0A031WDE4
B	-9	SER	-	expression tag	UNP A0A031WDE4
B	-8	SER	-	expression tag	UNP A0A031WDE4
B	-7	GLY	-	expression tag	UNP A0A031WDE4
B	-6	LEU	-	expression tag	UNP A0A031WDE4
B	-5	VAL	-	expression tag	UNP A0A031WDE4
B	-4	PRO	-	expression tag	UNP A0A031WDE4
B	-3	ARG	-	expression tag	UNP A0A031WDE4
B	-2	GLY	-	expression tag	UNP A0A031WDE4
B	-1	SER	-	expression tag	UNP A0A031WDE4
B	0	HIS	-	expression tag	UNP A0A031WDE4
C	-19	MET	-	initiating methionine	UNP A0A031WDE4
C	-18	GLY	-	expression tag	UNP A0A031WDE4
C	-17	SER	-	expression tag	UNP A0A031WDE4
C	-16	SER	-	expression tag	UNP A0A031WDE4
C	-15	HIS	-	expression tag	UNP A0A031WDE4
C	-14	HIS	-	expression tag	UNP A0A031WDE4
C	-13	HIS	-	expression tag	UNP A0A031WDE4
C	-12	HIS	-	expression tag	UNP A0A031WDE4
C	-11	HIS	-	expression tag	UNP A0A031WDE4
C	-10	HIS	-	expression tag	UNP A0A031WDE4
C	-9	SER	-	expression tag	UNP A0A031WDE4
C	-8	SER	-	expression tag	UNP A0A031WDE4
C	-7	GLY	-	expression tag	UNP A0A031WDE4
C	-6	LEU	-	expression tag	UNP A0A031WDE4
C	-5	VAL	-	expression tag	UNP A0A031WDE4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP A0A031WDE4
C	-3	ARG	-	expression tag	UNP A0A031WDE4
C	-2	GLY	-	expression tag	UNP A0A031WDE4
C	-1	SER	-	expression tag	UNP A0A031WDE4
C	0	HIS	-	expression tag	UNP A0A031WDE4
D	-19	MET	-	initiating methionine	UNP A0A031WDE4
D	-18	GLY	-	expression tag	UNP A0A031WDE4
D	-17	SER	-	expression tag	UNP A0A031WDE4
D	-16	SER	-	expression tag	UNP A0A031WDE4
D	-15	HIS	-	expression tag	UNP A0A031WDE4
D	-14	HIS	-	expression tag	UNP A0A031WDE4
D	-13	HIS	-	expression tag	UNP A0A031WDE4
D	-12	HIS	-	expression tag	UNP A0A031WDE4
D	-11	HIS	-	expression tag	UNP A0A031WDE4
D	-10	HIS	-	expression tag	UNP A0A031WDE4
D	-9	SER	-	expression tag	UNP A0A031WDE4
D	-8	SER	-	expression tag	UNP A0A031WDE4
D	-7	GLY	-	expression tag	UNP A0A031WDE4
D	-6	LEU	-	expression tag	UNP A0A031WDE4
D	-5	VAL	-	expression tag	UNP A0A031WDE4
D	-4	PRO	-	expression tag	UNP A0A031WDE4
D	-3	ARG	-	expression tag	UNP A0A031WDE4
D	-2	GLY	-	expression tag	UNP A0A031WDE4
D	-1	SER	-	expression tag	UNP A0A031WDE4
D	0	HIS	-	expression tag	UNP A0A031WDE4
E	-19	MET	-	initiating methionine	UNP A0A031WDE4
E	-18	GLY	-	expression tag	UNP A0A031WDE4
E	-17	SER	-	expression tag	UNP A0A031WDE4
E	-16	SER	-	expression tag	UNP A0A031WDE4
E	-15	HIS	-	expression tag	UNP A0A031WDE4
E	-14	HIS	-	expression tag	UNP A0A031WDE4
E	-13	HIS	-	expression tag	UNP A0A031WDE4
E	-12	HIS	-	expression tag	UNP A0A031WDE4
E	-11	HIS	-	expression tag	UNP A0A031WDE4
E	-10	HIS	-	expression tag	UNP A0A031WDE4
E	-9	SER	-	expression tag	UNP A0A031WDE4
E	-8	SER	-	expression tag	UNP A0A031WDE4
E	-7	GLY	-	expression tag	UNP A0A031WDE4
E	-6	LEU	-	expression tag	UNP A0A031WDE4
E	-5	VAL	-	expression tag	UNP A0A031WDE4
E	-4	PRO	-	expression tag	UNP A0A031WDE4
E	-3	ARG	-	expression tag	UNP A0A031WDE4

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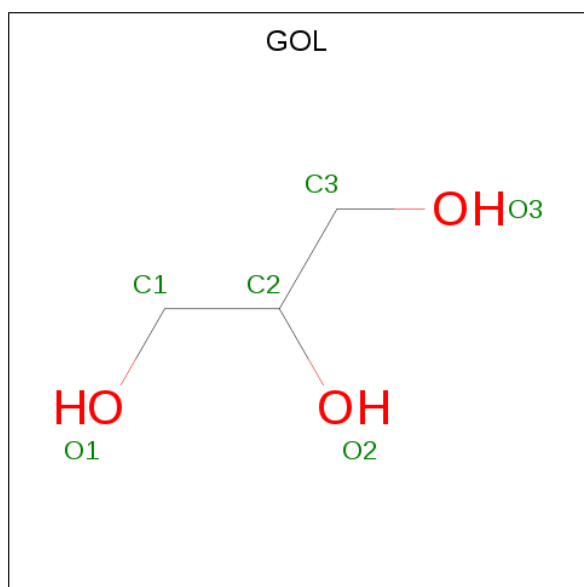
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP A0A031WDE4
E	-1	SER	-	expression tag	UNP A0A031WDE4
E	0	HIS	-	expression tag	UNP A0A031WDE4
F	-19	MET	-	initiating methionine	UNP A0A031WDE4
F	-18	GLY	-	expression tag	UNP A0A031WDE4
F	-17	SER	-	expression tag	UNP A0A031WDE4
F	-16	SER	-	expression tag	UNP A0A031WDE4
F	-15	HIS	-	expression tag	UNP A0A031WDE4
F	-14	HIS	-	expression tag	UNP A0A031WDE4
F	-13	HIS	-	expression tag	UNP A0A031WDE4
F	-12	HIS	-	expression tag	UNP A0A031WDE4
F	-11	HIS	-	expression tag	UNP A0A031WDE4
F	-10	HIS	-	expression tag	UNP A0A031WDE4
F	-9	SER	-	expression tag	UNP A0A031WDE4
F	-8	SER	-	expression tag	UNP A0A031WDE4
F	-7	GLY	-	expression tag	UNP A0A031WDE4
F	-6	LEU	-	expression tag	UNP A0A031WDE4
F	-5	VAL	-	expression tag	UNP A0A031WDE4
F	-4	PRO	-	expression tag	UNP A0A031WDE4
F	-3	ARG	-	expression tag	UNP A0A031WDE4
F	-2	GLY	-	expression tag	UNP A0A031WDE4
F	-1	SER	-	expression tag	UNP A0A031WDE4
F	0	HIS	-	expression tag	UNP A0A031WDE4
G	-19	MET	-	initiating methionine	UNP A0A031WDE4
G	-18	GLY	-	expression tag	UNP A0A031WDE4
G	-17	SER	-	expression tag	UNP A0A031WDE4
G	-16	SER	-	expression tag	UNP A0A031WDE4
G	-15	HIS	-	expression tag	UNP A0A031WDE4
G	-14	HIS	-	expression tag	UNP A0A031WDE4
G	-13	HIS	-	expression tag	UNP A0A031WDE4
G	-12	HIS	-	expression tag	UNP A0A031WDE4
G	-11	HIS	-	expression tag	UNP A0A031WDE4
G	-10	HIS	-	expression tag	UNP A0A031WDE4
G	-9	SER	-	expression tag	UNP A0A031WDE4
G	-8	SER	-	expression tag	UNP A0A031WDE4
G	-7	GLY	-	expression tag	UNP A0A031WDE4
G	-6	LEU	-	expression tag	UNP A0A031WDE4
G	-5	VAL	-	expression tag	UNP A0A031WDE4
G	-4	PRO	-	expression tag	UNP A0A031WDE4
G	-3	ARG	-	expression tag	UNP A0A031WDE4
G	-2	GLY	-	expression tag	UNP A0A031WDE4
G	-1	SER	-	expression tag	UNP A0A031WDE4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP A0A031WDE4
H	-19	MET	-	initiating methionine	UNP A0A031WDE4
H	-18	GLY	-	expression tag	UNP A0A031WDE4
H	-17	SER	-	expression tag	UNP A0A031WDE4
H	-16	SER	-	expression tag	UNP A0A031WDE4
H	-15	HIS	-	expression tag	UNP A0A031WDE4
H	-14	HIS	-	expression tag	UNP A0A031WDE4
H	-13	HIS	-	expression tag	UNP A0A031WDE4
H	-12	HIS	-	expression tag	UNP A0A031WDE4
H	-11	HIS	-	expression tag	UNP A0A031WDE4
H	-10	HIS	-	expression tag	UNP A0A031WDE4
H	-9	SER	-	expression tag	UNP A0A031WDE4
H	-8	SER	-	expression tag	UNP A0A031WDE4
H	-7	GLY	-	expression tag	UNP A0A031WDE4
H	-6	LEU	-	expression tag	UNP A0A031WDE4
H	-5	VAL	-	expression tag	UNP A0A031WDE4
H	-4	PRO	-	expression tag	UNP A0A031WDE4
H	-3	ARG	-	expression tag	UNP A0A031WDE4
H	-2	GLY	-	expression tag	UNP A0A031WDE4
H	-1	SER	-	expression tag	UNP A0A031WDE4
H	0	HIS	-	expression tag	UNP A0A031WDE4

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

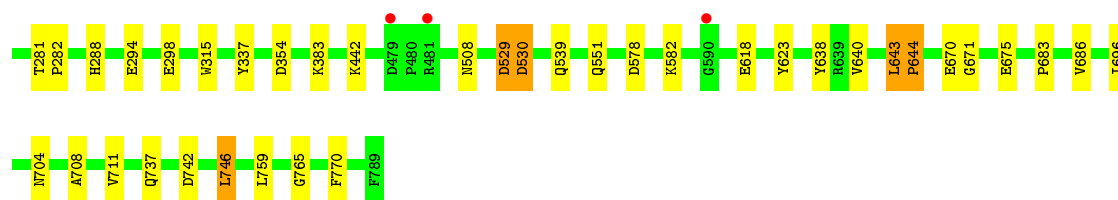
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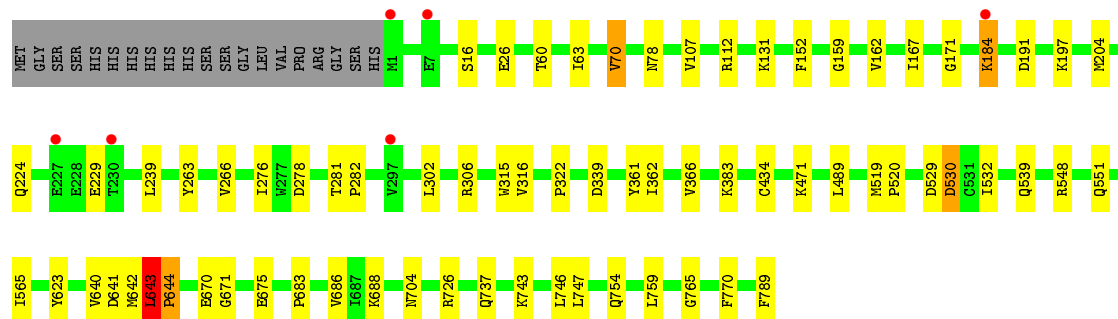
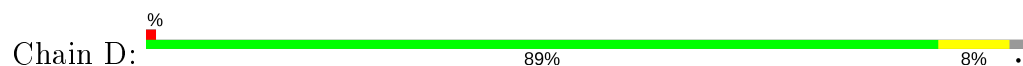
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

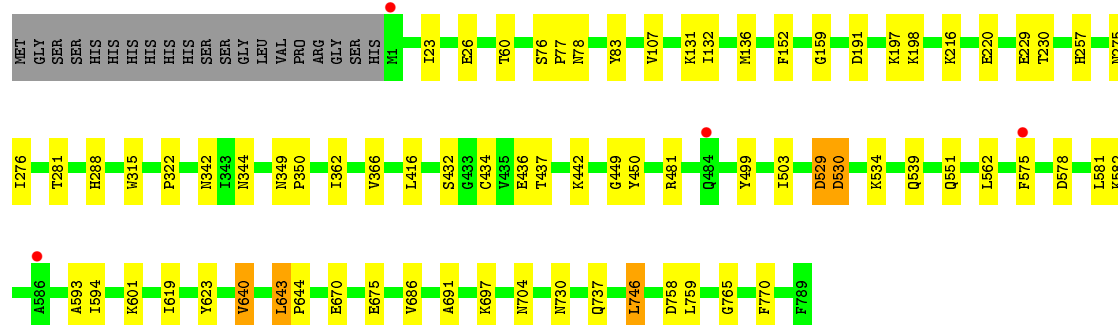
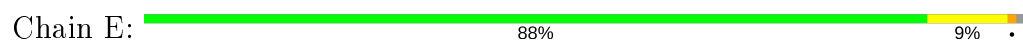
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	657	Total	O	0	0
			657	657		
3	B	427	Total	O	0	0
			427	427		
3	C	612	Total	O	0	0
			612	612		
3	D	516	Total	O	0	0
			516	516		
3	E	646	Total	O	0	0
			646	646		
3	F	664	Total	O	0	0
			664	664		
3	G	676	Total	O	0	0
			676	676		
3	H	617	Total	O	0	0
			617	617		



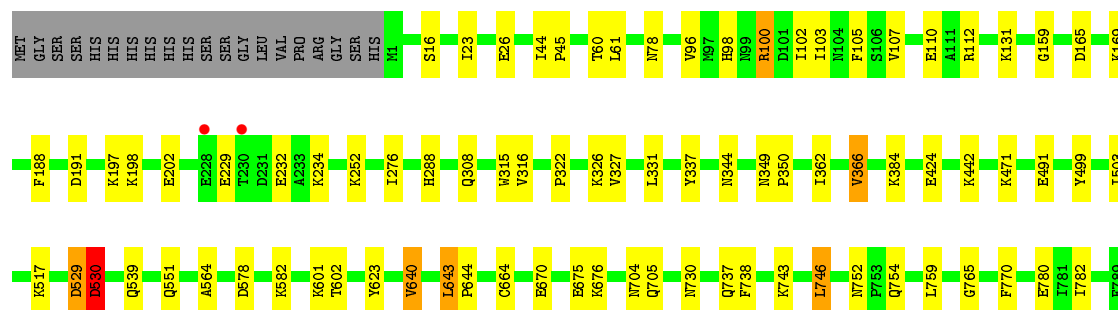
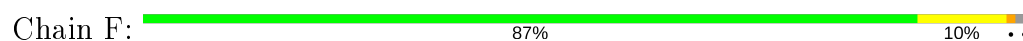
- Molecule 1: Trans-4-hydroxy-L-proline dehydratase




- Molecule 1: Trans-4-hydroxy-L-proline dehydratase



- Molecule 1: Trans-4-hydroxy-L-proline dehydratase




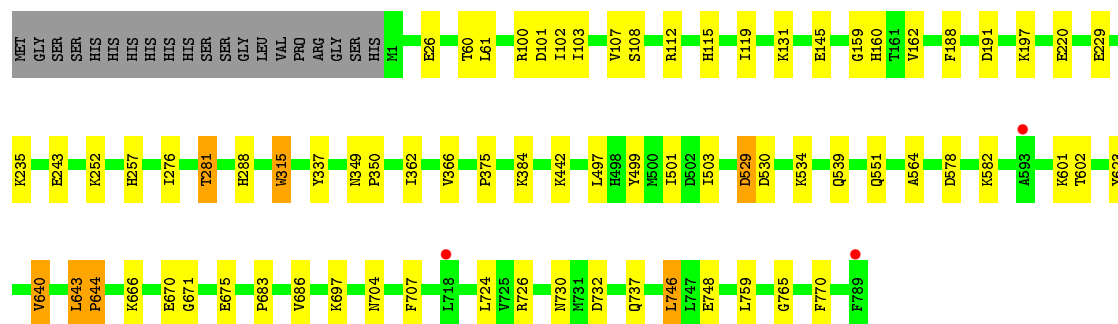
- Molecule 1: Trans-4-hydroxy-L-proline dehydratase

Chain G:  89% 8% ..



• Molecule 1: Trans-4-hydroxy-L-proline dehydratase

Chain H:  88% 8% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.35Å 341.65Å 122.61Å 90.00° 107.14° 90.00°	Depositor
Resolution (Å)	49.82 – 2.05 49.82 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.82-2.05) 98.8 (49.82-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.167 , 0.195 0.167 , 0.195	Depositor DCC
R_{free} test set	24248 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	54911	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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: GOL

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	0.42	0/6380	0.60	6/8616 (0.1%)
1	B	0.36	0/6380	0.55	4/8616 (0.0%)
1	C	0.39	0/6380	0.58	6/8616 (0.1%)
1	D	0.38	0/6380	0.58	4/8616 (0.0%)
1	E	0.40	0/6380	0.60	5/8616 (0.1%)
1	F	0.41	0/6380	0.61	7/8616 (0.1%)
1	G	0.41	0/6380	0.60	4/8616 (0.0%)
1	H	0.40	0/6380	0.59	4/8616 (0.0%)
All	All	0.40	0/51040	0.59	40/68928 (0.1%)

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	E	1	0
1	F	1	0
All	All	2	0

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	529	ASP	C-N-CA	12.99	154.17	121.70
1	G	529	ASP	C-N-CA	11.87	151.37	121.70
1	E	529	ASP	C-N-CA	11.18	149.66	121.70
1	A	529	ASP	C-N-CA	10.72	148.51	121.70
1	C	529	ASP	C-N-CA	10.38	147.65	121.70
1	H	529	ASP	C-N-CA	9.34	145.05	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	529	ASP	O-C-N	8.66	136.56	122.70
1	E	530	ASP	CB-CA-C	8.62	127.63	110.40
1	G	529	ASP	CA-C-N	-8.42	98.68	117.20
1	B	529	ASP	C-N-CA	8.38	142.65	121.70
1	F	529	ASP	O-C-N	8.16	135.75	122.70
1	A	529	ASP	CA-C-N	-8.11	99.36	117.20
1	C	529	ASP	CA-C-N	-7.97	99.67	117.20
1	A	529	ASP	O-C-N	7.88	135.31	122.70
1	D	643	LEU	CA-CB-CG	7.85	133.36	115.30
1	F	530	ASP	CB-CA-C	7.64	125.67	110.40
1	G	643	LEU	CA-CB-CG	7.58	132.72	115.30
1	H	529	ASP	CA-C-N	-7.56	100.56	117.20
1	H	529	ASP	O-C-N	7.32	134.40	122.70
1	C	529	ASP	O-C-N	7.28	134.34	122.70
1	E	529	ASP	O-C-N	7.28	134.34	122.70
1	F	529	ASP	CA-C-N	-7.18	101.41	117.20
1	B	529	ASP	CA-C-N	-7.00	101.79	117.20
1	D	529	ASP	C-N-CA	6.88	138.89	121.70
1	B	529	ASP	O-C-N	6.84	133.65	122.70
1	D	529	ASP	CA-C-N	-6.47	102.96	117.20
1	H	643	LEU	CA-CB-CG	6.14	129.43	115.30
1	E	643	LEU	CA-CB-CG	5.97	129.03	115.30
1	A	643	LEU	CA-CB-CG	5.93	128.95	115.30
1	C	643	LEU	CA-CB-CG	5.90	128.87	115.30
1	B	2	ALA	N-CA-C	-5.61	95.84	111.00
1	F	100	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	F	643	LEU	CA-CB-CG	5.45	127.83	115.30
1	C	530	ASP	CB-CA-C	5.41	121.21	110.40
1	E	529	ASP	CA-C-N	-5.34	105.44	117.20
1	D	530	ASP	CB-CA-C	5.25	120.90	110.40
1	F	530	ASP	N-CA-CB	5.25	120.04	110.60
1	A	100	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	530	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	530	ASP	CB-CA-C	5.01	120.41	110.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	530	ASP	CA
1	F	530	ASP	CA

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	6256	0	6151	41	0
1	B	6256	0	6152	44	0
1	C	6256	0	6151	38	0
1	D	6256	0	6152	52	0
1	E	6256	0	6151	46	0
1	F	6256	0	6151	53	0
1	G	6256	0	6151	44	0
1	H	6256	0	6151	51	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	1	0
2	E	6	0	8	2	0
2	F	6	0	8	1	0
2	G	6	0	8	0	0
2	H	6	0	8	0	0
3	A	657	0	0	12	1
3	B	427	0	0	11	1
3	C	612	0	0	11	1
3	D	516	0	0	10	0
3	E	646	0	0	13	0
3	F	664	0	0	12	1
3	G	676	0	0	15	0
3	H	617	0	0	18	0
All	All	54911	0	49274	366	2

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 (366) 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:E:758:ASP:HB2	3:E:1415:HOH:O	1.58	1.02
1:G:737:GLN:HE22	1:G:765:GLY:H	1.03	0.99
1:F:737:GLN:HE22	1:F:765:GLY:H	1.05	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:737:GLN:HE22	1:C:765:GLY:H	1.04	0.97
1:E:737:GLN:HE22	1:E:765:GLY:H	1.10	0.97
1:B:737:GLN:HE22	1:B:765:GLY:H	1.09	0.95
1:A:254:GLU:OE1	3:A:901:HOH:O	1.83	0.95
1:F:664:CYS:SG	3:F:1558:HOH:O	2.26	0.94
1:D:737:GLN:HE22	1:D:765:GLY:H	1.04	0.92
1:A:737:GLN:HE22	1:A:765:GLY:H	1.09	0.92
1:H:737:GLN:HE22	1:H:765:GLY:H	1.14	0.92
1:C:109:GLU:OE2	3:C:901:HOH:O	1.88	0.91
1:B:608:ASP:OD2	3:B:901:HOH:O	1.87	0.91
1:D:789:PHE:OXT	3:D:901:HOH:O	1.87	0.91
1:G:414:GLN:OE1	3:G:901:HOH:O	1.87	0.91
1:B:351:ASP:OD2	3:B:902:HOH:O	1.91	0.88
1:A:732:ASP:OD1	3:A:902:HOH:O	1.92	0.88
1:G:618:GLU:OE1	3:G:902:HOH:O	1.93	0.84
1:E:229:GLU:OE2	3:E:901:HOH:O	1.96	0.84
1:F:165:ASP:OD2	1:F:169:LYS:NZ	2.11	0.84
1:E:450:TYR:CD1	1:E:551:GLN:HG3	2.15	0.82
1:D:746:LEU:HD22	1:D:759:LEU:HD21	1.59	0.82
1:F:491:GLU:OE1	3:F:901:HOH:O	1.96	0.81
1:A:589:GLU:OE1	3:A:903:HOH:O	1.98	0.81
1:D:204:MET:CE	1:D:532:ILE:HG12	2.12	0.80
1:C:618:GLU:OE1	3:C:902:HOH:O	1.99	0.79
1:D:184:LYS:N	1:D:184:LYS:HD3	1.98	0.79
1:B:704:ASN:HD21	1:B:737:GLN:HE21	1.31	0.78
1:C:188:PHE:O	3:C:903:HOH:O	2.00	0.78
1:C:107:VAL:HG12	1:C:112:ARG:HG2	1.65	0.78
1:B:250:ALA:O	3:B:903:HOH:O	2.03	0.77
1:C:354:ASP:OD2	3:C:904:HOH:O	2.04	0.75
1:D:229:GLU:O	3:D:902:HOH:O	2.03	0.75
1:G:176:LYS:NZ	3:G:905:HOH:O	2.19	0.75
1:B:476:GLU:OE1	3:B:904:HOH:O	2.05	0.74
1:A:704:ASN:HD21	1:A:737:GLN:HE21	1.36	0.74
1:A:107:VAL:HG12	1:A:112:ARG:HG2	1.70	0.73
1:A:746:LEU:HD22	1:A:759:LEU:HD21	1.70	0.73
1:H:748:GLU:OE1	3:H:902:HOH:O	2.07	0.72
1:G:131:LYS:HE2	3:G:910:HOH:O	1.88	0.72
1:B:383:LYS:NZ	3:B:905:HOH:O	2.05	0.72
1:F:188:PHE:O	3:F:902:HOH:O	2.08	0.72
1:B:37:LYS:NZ	3:B:910:HOH:O	2.23	0.71
1:C:746:LEU:HD22	1:C:759:LEU:HD21	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:131:LYS:HE3	3:H:926:HOH:O	1.91	0.70
1:F:704:ASN:HD21	1:F:737:GLN:HE21	1.38	0.69
1:D:743:LYS:HE2	1:D:747:LEU:HD11	1.74	0.69
1:E:691:ALA:O	3:E:904:HOH:O	2.08	0.69
1:F:746:LEU:HD22	1:F:759:LEU:HD21	1.73	0.69
1:H:746:LEU:HD22	1:H:759:LEU:HD21	1.74	0.69
1:H:670:GLU:OE2	3:H:903:HOH:O	2.09	0.69
1:D:670:GLU:OE1	3:D:904:HOH:O	2.11	0.69
1:D:204:MET:HE1	1:D:532:ILE:CG1	2.23	0.69
1:E:746:LEU:HD22	1:E:759:LEU:HD21	1.74	0.69
1:H:697:LYS:NZ	3:H:911:HOH:O	2.25	0.69
3:E:1049:HOH:O	1:F:198:LYS:HE2	1.93	0.68
1:C:746:LEU:HD13	1:C:770:PHE:CE1	2.29	0.68
1:D:746:LEU:CD2	1:D:759:LEU:HD21	2.23	0.68
1:G:499:TYR:CZ	1:G:503:ILE:HD11	2.29	0.68
1:E:216:LYS:NZ	3:E:903:HOH:O	2.08	0.67
1:F:131:LYS:HE3	3:F:1004:HOH:O	1.95	0.67
1:D:26:GLU:OE1	1:D:60:THR:HG23	1.94	0.67
1:G:131:LYS:CE	3:G:910:HOH:O	2.43	0.67
1:G:131:LYS:NZ	3:G:910:HOH:O	2.27	0.67
1:D:204:MET:HE2	1:D:532:ILE:HG12	1.76	0.66
1:B:107:VAL:HG12	1:B:112:ARG:HG2	1.77	0.66
1:D:204:MET:HE1	1:D:532:ILE:HG12	1.78	0.65
1:H:188:PHE:O	3:H:904:HOH:O	2.14	0.65
1:A:358:GLU:OE2	3:A:904:HOH:O	2.13	0.65
1:H:107:VAL:HG12	1:H:112:ARG:HG2	1.79	0.65
1:A:131:LYS:HG3	3:A:965:HOH:O	1.97	0.64
1:H:26:GLU:OE2	1:H:60:THR:HG23	1.96	0.64
1:D:704:ASN:HD21	1:D:737:GLN:HE21	1.45	0.64
1:D:737:GLN:NE2	1:D:765:GLY:H	1.86	0.64
1:B:704:ASN:ND2	1:B:737:GLN:HE21	1.96	0.63
1:G:308:GLN:HG3	1:G:366:VAL:HG12	1.80	0.63
1:E:198:LYS:NZ	3:E:914:HOH:O	2.32	0.62
1:A:710:SER:O	3:A:905:HOH:O	2.16	0.62
1:F:107:VAL:HG12	1:F:112:ARG:HG2	1.80	0.62
1:G:683:PRO:HA	1:G:686:VAL:HG13	1.81	0.62
1:G:704:ASN:HD21	1:G:737:GLN:HE21	1.48	0.62
1:F:704:ASN:ND2	1:F:737:GLN:HE21	1.98	0.62
1:F:26:GLU:OE2	1:F:60:THR:HG23	1.99	0.61
1:H:197:LYS:HD3	1:H:534:LYS:O	2.00	0.61
1:H:732:ASP:OD2	3:H:905:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:LYS:HE2	3:D:1284:HOH:O	1.99	0.61
1:H:746:LEU:HD13	1:H:770:PHE:CE1	2.36	0.60
1:E:26:GLU:OE2	1:E:60:THR:HG23	2.01	0.60
1:F:96:VAL:O	1:F:100:ARG:HB2	2.02	0.60
1:D:548:ARG:HG3	3:D:1003:HOH:O	2.02	0.60
1:D:737:GLN:HE22	1:D:765:GLY:N	1.88	0.60
1:H:704:ASN:HD21	1:H:737:GLN:HE21	1.49	0.59
1:G:715:GLU:OE2	3:G:904:HOH:O	2.16	0.59
3:A:902:HOH:O	1:C:383:LYS:NZ	2.20	0.58
1:C:578:ASP:OD2	1:C:582:LYS:HE2	2.03	0.58
1:D:191:ASP:OD2	1:D:197:LYS:HE2	2.04	0.58
1:D:302:LEU:CD1	1:D:306:ARG:HG3	2.32	0.58
1:E:623:TYR:CE2	1:E:640:VAL:HG22	2.38	0.58
1:E:704:ASN:HD21	1:E:737:GLN:HE21	1.51	0.58
1:E:730:ASN:O	1:G:384:LYS:HE3	2.04	0.58
1:G:131:LYS:HE3	3:G:940:HOH:O	2.03	0.57
1:B:442:LYS:HG2	1:B:529:ASP:HB2	1.86	0.57
1:F:578:ASP:OD2	1:F:582:LYS:HE2	2.04	0.57
1:G:107:VAL:O	1:G:112:ARG:NH1	2.37	0.57
1:F:232:GLU:OE2	3:F:903:HOH:O	2.17	0.57
1:H:220:GLU:HG3	3:H:1121:HOH:O	2.05	0.57
1:C:107:VAL:CG1	1:C:112:ARG:HG2	2.33	0.56
1:G:704:ASN:ND2	1:G:737:GLN:HE21	2.03	0.56
1:H:103:ILE:HA	1:H:337:TYR:CZ	2.40	0.56
1:E:578:ASP:OD2	1:E:582:LYS:HE2	2.06	0.56
1:E:499:TYR:CZ	1:E:503:ILE:HD11	2.41	0.56
1:H:229:GLU:O	1:H:235:LYS:NZ	2.39	0.56
1:D:162:VAL:HG13	1:D:281:THR:HG23	1.88	0.56
1:D:204:MET:HE1	1:D:532:ILE:HG13	1.88	0.56
1:A:191:ASP:OD2	1:A:197:LYS:HE2	2.05	0.55
1:D:641:ASP:O	1:D:642:MET:HE2	2.06	0.55
1:E:257:HIS:HD2	3:E:1361:HOH:O	1.89	0.55
1:A:107:VAL:CG1	1:A:112:ARG:HG2	2.37	0.55
1:F:746:LEU:HD13	1:F:770:PHE:CE1	2.42	0.55
1:G:548:ARG:HG3	3:G:1161:HOH:O	2.05	0.55
1:H:145:GLU:OE1	3:H:907:HOH:O	2.18	0.55
1:G:362:ILE:O	1:G:366:VAL:HG13	2.07	0.55
1:F:491:GLU:HB3	3:F:901:HOH:O	2.07	0.55
1:H:704:ASN:ND2	1:H:737:GLN:HE21	2.05	0.55
1:B:198:LYS:HE3	1:B:202:GLU:OE1	2.06	0.55
1:D:489:LEU:CD2	1:D:565:ILE:HG21	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:752:ASN:HD22	1:F:754:GLN:HE22	1.53	0.55
1:G:442:LYS:HG2	1:G:529:ASP:HB2	1.89	0.55
1:H:257:HIS:HD2	3:H:1338:HOH:O	1.89	0.55
1:B:20:GLU:HB3	3:B:1113:HOH:O	2.07	0.54
1:G:218:TYR:OH	3:G:903:HOH:O	2.13	0.54
1:E:450:TYR:HA	1:E:551:GLN:HG2	1.89	0.54
1:E:198:LYS:NZ	3:E:910:HOH:O	2.28	0.54
1:F:362:ILE:O	1:F:366:VAL:HG13	2.08	0.54
1:E:442:LYS:HG2	1:E:529:ASP:HB2	1.90	0.54
1:E:737:GLN:NE2	1:E:765:GLY:H	1.93	0.53
1:A:131:LYS:HE3	3:A:965:HOH:O	2.07	0.53
1:B:191:ASP:OD2	1:B:197:LYS:HE2	2.08	0.53
1:D:302:LEU:HD12	1:D:306:ARG:HG3	1.88	0.53
1:D:383:LYS:NZ	3:D:906:HOH:O	2.31	0.53
1:F:191:ASP:OD2	1:F:197:LYS:HE2	2.08	0.53
1:B:713:GLN:OE1	3:B:906:HOH:O	2.18	0.53
1:D:623:TYR:CE2	1:D:642:MET:HE1	2.43	0.53
1:G:191:ASP:OD2	1:G:197:LYS:HE2	2.09	0.53
1:G:623:TYR:CE2	1:G:640:VAL:HG22	2.44	0.53
1:H:578:ASP:OD2	1:H:582:LYS:HE2	2.08	0.53
1:A:704:ASN:ND2	1:A:737:GLN:HE21	2.03	0.53
1:C:131:LYS:HE3	3:C:945:HOH:O	2.08	0.52
1:F:159:GLY:HA3	1:F:276:ILE:HB	1.90	0.52
1:A:746:LEU:HD13	1:A:770:PHE:CE1	2.45	0.52
1:F:730:ASN:O	1:H:384:LYS:HE3	2.08	0.52
1:A:159:GLY:HA3	1:A:276:ILE:HB	1.92	0.52
1:A:26:GLU:OE2	1:A:60:THR:HG23	2.10	0.52
1:H:160:HIS:O	3:H:906:HOH:O	2.18	0.52
1:H:288:HIS:HE1	3:H:1287:HOH:O	1.93	0.52
1:H:442:LYS:HG2	1:H:529:ASP:HB2	1.92	0.52
1:C:294:GLU:O	1:C:298:GLU:HG2	2.09	0.51
1:E:131:LYS:HE2	3:E:1426:HOH:O	2.09	0.51
1:G:159:GLY:HA3	1:G:276:ILE:HB	1.92	0.51
1:A:737:GLN:NE2	1:A:765:GLY:H	1.93	0.51
1:H:100:ARG:HD3	1:H:102:ILE:O	2.10	0.51
1:C:100:ARG:HD3	1:C:102:ILE:O	2.11	0.51
1:A:100:ARG:HD3	1:A:102:ILE:O	2.11	0.51
2:F:801:GOL:H32	3:F:954:HOH:O	2.09	0.50
1:G:26:GLU:OE2	1:G:60:THR:HG23	2.11	0.50
1:C:191:ASP:OD2	1:C:197:LYS:HE2	2.11	0.50
1:C:288:HIS:HD2	3:C:1439:HOH:O	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:107:VAL:CG1	1:H:112:ARG:HG2	2.41	0.50
1:D:746:LEU:HD13	1:D:770:PHE:CE1	2.47	0.50
1:F:737:GLN:NE2	1:F:765:GLY:H	1.89	0.50
1:A:362:ILE:O	1:A:366:VAL:HG13	2.11	0.50
1:E:575:PHE:CD2	1:E:594:ILE:HD12	2.46	0.50
1:G:103:ILE:HA	1:G:337:TYR:CZ	2.47	0.50
1:B:96:VAL:O	1:B:100:ARG:HB2	2.12	0.49
1:F:107:VAL:CG1	1:F:112:ARG:HG2	2.42	0.49
1:F:78:ASN:HA	1:F:322:PRO:HD3	1.94	0.49
1:C:26:GLU:OE2	1:C:60:THR:HG23	2.13	0.49
1:D:362:ILE:O	1:D:366:VAL:HG13	2.13	0.49
1:E:197:LYS:HD3	1:E:534:LYS:O	2.13	0.49
1:E:704:ASN:ND2	1:E:737:GLN:HE21	2.10	0.49
1:B:26:GLU:OE2	1:B:60:THR:HG23	2.13	0.49
1:B:644:PRO:HG3	1:B:671:GLY:H	1.77	0.49
1:D:726:ARG:HG3	3:D:1001:HOH:O	2.13	0.49
1:H:101:ASP:HB2	3:H:1290:HOH:O	2.12	0.48
1:B:78:ASN:HA	1:B:322:PRO:HD3	1.95	0.48
1:B:568:ASN:HB3	1:B:575:PHE:CE1	2.48	0.48
1:D:107:VAL:HG12	1:D:112:ARG:HG2	1.95	0.48
1:F:384:LYS:HE3	1:H:730:ASN:O	2.14	0.48
1:B:197:LYS:HD3	1:B:534:LYS:O	2.14	0.48
1:C:159:GLY:HA3	1:C:276:ILE:HB	1.96	0.48
1:C:169:LYS:CE	3:C:905:HOH:O	2.61	0.48
1:F:252:LYS:HD2	3:F:928:HOH:O	2.13	0.48
1:B:675:GLU:HG3	1:B:676:LYS:N	2.29	0.48
1:E:23:ILE:HD11	1:E:107:VAL:HG13	1.96	0.48
1:B:578:ASP:OD2	1:B:582:LYS:HE2	2.15	0.47
1:H:191:ASP:OD2	1:H:197:LYS:HE2	2.14	0.47
1:D:489:LEU:HD22	1:D:565:ILE:HG21	1.97	0.47
1:B:23:ILE:HD11	1:B:107:VAL:HG13	1.95	0.47
1:E:434:CYS:SG	2:E:801:GOL:H31	2.54	0.47
1:H:726:ARG:HG3	3:H:946:HOH:O	2.13	0.47
1:D:167:ILE:HG21	1:D:266:VAL:HG21	1.97	0.47
1:G:644:PRO:HG3	1:G:671:GLY:H	1.79	0.47
1:D:644:PRO:HG3	1:D:671:GLY:H	1.80	0.47
1:C:100:ARG:HD2	1:C:103:ILE:O	2.15	0.47
1:A:742:ASP:HB3	3:A:915:HOH:O	2.14	0.47
1:G:358:GLU:OE2	3:G:906:HOH:O	2.20	0.47
1:G:506:GLU:HG3	1:H:188:PHE:HB2	1.96	0.47
1:B:107:VAL:CG1	1:B:112:ARG:HG2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:LYS:O	1:B:239:LEU:HD13	2.15	0.46
1:H:683:PRO:HA	1:H:686:VAL:HG13	1.97	0.46
1:B:623:TYR:CE2	1:B:640:VAL:HG22	2.50	0.46
1:E:159:GLY:HA3	1:E:276:ILE:HB	1.96	0.46
1:F:471:LYS:HE2	3:F:1028:HOH:O	2.15	0.46
1:A:708:ALA:O	1:A:711:VAL:HG22	2.14	0.46
1:B:103:ILE:HA	1:B:337:TYR:CZ	2.50	0.46
1:A:288:HIS:HD2	3:A:1504:HOH:O	1.98	0.46
1:B:688:LYS:CD	3:B:901:HOH:O	2.62	0.46
1:D:204:MET:CE	1:D:532:ILE:CG1	2.84	0.46
1:D:704:ASN:ND2	1:D:737:GLN:HE21	2.10	0.46
1:F:103:ILE:HA	1:F:337:TYR:CZ	2.51	0.46
1:A:257:HIS:HD2	3:A:1397:HOH:O	1.97	0.46
1:F:131:LYS:HG3	3:F:1004:HOH:O	2.16	0.46
1:F:623:TYR:CE2	1:F:640:VAL:HG22	2.49	0.46
1:A:78:ASN:HA	1:A:322:PRO:HD3	1.96	0.46
1:B:362:ILE:O	1:B:366:VAL:HG13	2.14	0.46
1:A:564:ALA:HA	1:A:602:THR:HG21	1.98	0.46
1:E:562:LEU:HD12	1:E:619:ILE:HD11	1.98	0.46
1:G:499:TYR:CE2	1:G:503:ILE:HD11	2.50	0.46
1:B:83:TYR:CD1	1:B:275:ASN:HB2	2.51	0.46
1:C:103:ILE:HA	1:C:337:TYR:CZ	2.51	0.46
1:C:704:ASN:HD21	1:C:737:GLN:HE21	1.64	0.46
1:E:191:ASP:OD2	1:E:197:LYS:HE2	2.16	0.46
1:E:362:ILE:O	1:E:366:VAL:HG13	2.16	0.46
1:G:176:LYS:HE2	1:G:180:GLU:OE2	2.15	0.46
1:B:683:PRO:HA	1:B:686:VAL:HG13	1.96	0.46
1:C:704:ASN:ND2	1:C:737:GLN:HE21	2.13	0.46
1:G:23:ILE:HD11	1:G:107:VAL:HG13	1.98	0.46
1:H:362:ILE:O	1:H:366:VAL:HG13	2.16	0.46
1:B:83:TYR:CG	1:B:275:ASN:HB2	2.51	0.45
1:A:471:LYS:HE2	3:A:1169:HOH:O	2.14	0.45
1:A:752:ASN:HB3	1:A:754:GLN:NE2	2.32	0.45
1:C:442:LYS:HG2	1:C:529:ASP:HB2	1.98	0.45
1:E:481:ARG:CZ	1:E:581:LEU:HD12	2.47	0.45
1:A:162:VAL:HG21	1:A:432:SER:HB3	1.98	0.45
1:A:499:TYR:CZ	1:A:503:ILE:HD11	2.52	0.45
1:E:288:HIS:HE1	3:E:1239:HOH:O	1.99	0.45
1:A:578:ASP:OD2	1:A:582:LYS:HE2	2.17	0.45
1:C:644:PRO:HG3	1:C:671:GLY:H	1.81	0.45
1:C:696:ILE:HG12	3:C:1386:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:288:HIS:HD2	3:H:1461:HOH:O	1.99	0.45
1:H:499:TYR:CZ	1:H:503:ILE:HD11	2.51	0.45
1:D:361:TYR:OH	3:D:903:HOH:O	2.07	0.45
1:F:100:ARG:NH2	1:F:326:LYS:O	2.48	0.45
1:G:465:TYR:OH	1:G:470:LYS:HG2	2.17	0.45
1:B:100:ARG:NH2	1:B:326:LYS:O	2.47	0.45
1:A:442:LYS:HG2	1:A:529:ASP:HB2	1.98	0.45
1:G:38:TYR:OH	3:G:907:HOH:O	2.21	0.45
1:C:162:VAL:HG13	1:C:281:THR:HG23	1.99	0.44
1:F:705:GLN:O	1:F:738:PHE:HA	2.17	0.44
1:C:83:TYR:CG	1:C:275:ASN:HB2	2.52	0.44
1:F:288:HIS:HE1	3:F:1250:HOH:O	2.01	0.44
1:G:162:VAL:HG13	1:G:281:THR:HG23	1.99	0.44
1:H:159:GLY:HA3	1:H:276:ILE:HB	2.00	0.44
1:A:182:ARG:HD2	1:A:185:GLU:OE2	2.17	0.44
1:B:159:GLY:HA3	1:B:276:ILE:HB	1.99	0.44
1:B:254:GLU:O	3:B:908:HOH:O	2.21	0.44
1:F:100:ARG:CZ	1:F:331:LEU:HD22	2.48	0.44
1:D:263:TYR:CZ	1:D:282:PRO:HD3	2.53	0.44
1:F:23:ILE:HD11	1:F:107:VAL:HG13	1.98	0.44
1:F:517:LYS:NZ	3:F:921:HOH:O	2.44	0.44
1:F:564:ALA:HA	1:F:602:THR:HG21	1.99	0.44
1:D:688:LYS:NZ	3:D:924:HOH:O	2.51	0.44
1:A:103:ILE:HA	1:A:337:TYR:CZ	2.53	0.44
1:F:100:ARG:NH2	1:F:327:VAL:HG12	2.32	0.44
1:E:349:ASN:HB2	1:E:350:PRO:HD2	2.00	0.43
1:F:676:LYS:HE3	1:F:780:GLU:O	2.17	0.43
1:H:115:HIS:HA	1:H:119:ILE:HG12	2.00	0.43
1:H:349:ASN:HB2	1:H:350:PRO:CD	2.48	0.43
1:B:754:GLN:CD	1:B:754:GLN:H	2.21	0.43
1:D:159:GLY:HA3	1:D:276:ILE:HB	2.00	0.43
1:H:252:LYS:HG2	3:H:901:HOH:O	2.19	0.43
1:B:216:LYS:NZ	1:B:220:GLU:OE1	2.49	0.43
1:C:742:ASP:OD2	3:C:906:HOH:O	2.21	0.43
1:A:644:PRO:HG3	1:A:671:GLY:H	1.82	0.43
1:E:416:LEU:HD21	1:E:437:THR:HG22	1.99	0.43
1:D:683:PRO:HA	1:D:686:VAL:HG13	2.00	0.43
1:F:100:ARG:HD3	1:F:102:ILE:O	2.18	0.43
1:H:108:SER:O	1:H:112:ARG:HG3	2.19	0.43
1:H:497:LEU:O	1:H:501:ILE:HG12	2.19	0.43
1:B:362:ILE:O	1:B:366:VAL:CG1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:HIS:HE1	3:C:1192:HOH:O	2.00	0.43
1:D:278:ASP:HA	1:D:339:ASP:O	2.18	0.43
1:E:78:ASN:HA	1:E:322:PRO:HD3	2.01	0.43
1:A:683:PRO:HA	1:A:686:VAL:HG13	2.01	0.43
1:E:349:ASN:HB2	1:E:350:PRO:CD	2.49	0.42
1:E:697:LYS:HD2	3:E:1130:HOH:O	2.18	0.42
1:F:499:TYR:CZ	1:F:503:ILE:HD11	2.54	0.42
1:F:743:LYS:HD2	1:F:782:ILE:HG23	2.00	0.42
1:G:398:ARG:HD2	1:G:712:VAL:O	2.18	0.42
1:B:288:HIS:HE1	3:B:1163:HOH:O	2.02	0.42
1:G:707:PHE:HZ	1:G:724:LEU:HD22	1.84	0.42
1:A:450:TYR:HE1	1:A:643:LEU:HD22	1.85	0.42
1:H:644:PRO:HG3	1:H:671:GLY:H	1.84	0.42
1:B:266:VAL:O	1:B:270:VAL:HG22	2.20	0.42
1:E:436:GLU:OE2	2:E:801:GOL:O3	2.38	0.42
1:E:499:TYR:CE2	1:E:503:ILE:HD11	2.54	0.42
1:D:434:CYS:SG	2:D:801:GOL:H11	2.60	0.42
1:E:449:GLY:O	1:E:551:GLN:HG2	2.20	0.42
1:E:76:SER:HB2	1:E:77:PRO:HD2	2.02	0.42
1:G:16:SER:HB2	1:G:316:VAL:HG13	2.00	0.42
1:E:593:ALA:HB3	3:E:1421:HOH:O	2.20	0.42
1:F:110:GLU:H	1:F:110:GLU:CD	2.23	0.42
1:G:163:CYS:HB2	1:G:280:PHE:CE2	2.55	0.42
1:D:643:LEU:HA	1:D:644:PRO:HD3	1.89	0.42
1:H:243:GLU:OE1	3:H:908:HOH:O	2.21	0.42
1:H:623:TYR:CE2	1:H:640:VAL:HG22	2.55	0.42
1:H:666:LYS:HD2	3:H:1431:HOH:O	2.19	0.42
1:C:108:SER:O	1:C:112:ARG:HG3	2.20	0.41
1:E:220:GLU:HG3	3:E:1224:HOH:O	2.19	0.41
1:E:342:ASN:HB3	1:E:432:SER:HA	2.02	0.41
1:G:78:ASN:HA	1:G:322:PRO:HD3	2.02	0.41
1:B:602:THR:HG23	1:B:603:PRO:HD2	2.03	0.41
1:C:508:ASN:HB3	1:C:638:TYR:OH	2.21	0.41
1:F:349:ASN:HB2	1:F:350:PRO:CD	2.50	0.41
1:H:564:ALA:HA	1:H:602:THR:HG21	2.01	0.41
1:A:562:LEU:HD12	1:A:619:ILE:HD11	2.01	0.41
1:C:251:HIS:HD2	3:C:1416:HOH:O	2.03	0.41
1:C:683:PRO:HA	1:C:686:VAL:HG13	2.02	0.41
1:D:641:ASP:O	1:D:642:MET:CE	2.68	0.41
1:E:83:TYR:CG	1:E:275:ASN:HB2	2.56	0.41
1:F:308:GLN:HG3	1:F:366:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:414:GLN:NE2	3:G:939:HOH:O	2.52	0.41
1:H:499:TYR:CE2	1:H:503:ILE:HD11	2.56	0.41
1:H:707:PHE:HZ	1:H:724:LEU:HD22	1.86	0.41
1:F:198:LYS:HE3	1:F:202:GLU:OE1	2.21	0.41
1:C:708:ALA:O	1:C:711:VAL:HG22	2.21	0.41
1:D:171:GLY:HA3	3:D:931:HOH:O	2.21	0.41
1:A:648:HIS:CD2	1:A:670:GLU:HB3	2.56	0.41
1:E:746:LEU:HD13	1:E:770:PHE:CE1	2.56	0.41
1:F:424:GLU:CD	3:H:949:HOH:O	2.59	0.41
1:F:442:LYS:HG2	1:F:529:ASP:HB2	2.03	0.41
1:H:162:VAL:HG13	1:H:281:THR:HG23	2.03	0.41
1:H:601:LYS:HA	1:H:601:LYS:HD3	1.84	0.41
1:D:16:SER:HB2	1:D:316:VAL:HG13	2.03	0.41
1:D:63:ILE:HG12	1:D:70:VAL:CG2	2.51	0.41
1:A:278:ASP:HA	1:A:339:ASP:O	2.21	0.41
1:D:623:TYR:CD2	1:D:642:MET:HE1	2.56	0.41
1:F:229:GLU:HG2	1:F:234:LYS:HB2	2.03	0.41
1:F:16:SER:HB2	1:F:316:VAL:HG13	2.02	0.41
1:F:98:HIS:HA	1:F:105:PHE:O	2.21	0.40
1:G:705:GLN:O	1:G:738:PHE:HA	2.21	0.40
1:A:263:TYR:CD2	1:A:263:TYR:C	2.93	0.40
1:B:731:MET:O	1:B:732:ASP:HB2	2.22	0.40
1:D:78:ASN:HA	1:D:322:PRO:HD3	2.02	0.40
1:G:95:GLU:HG2	3:G:911:HOH:O	2.20	0.40
1:C:623:TYR:CE2	1:C:640:VAL:HG22	2.56	0.40
1:G:578:ASP:OD2	1:G:582:LYS:HE2	2.21	0.40
1:H:315:TRP:CD1	1:H:375:PRO:HD2	2.57	0.40
1:B:70:VAL:HG13	1:B:218:TYR:CE1	2.56	0.40
1:C:263:TYR:CZ	1:C:282:PRO:HD3	2.56	0.40
1:D:754:GLN:CD	1:D:754:GLN:H	2.25	0.40
1:G:26:GLU:OE1	3:G:908:HOH:O	2.22	0.40
1:C:737:GLN:NE2	1:C:765:GLY:H	1.89	0.40
1:D:519:MET:N	1:D:520:PRO:CD	2.85	0.40
1:E:132:ILE:O	1:E:136:MET:HG2	2.22	0.40
1:F:44:ILE:N	1:F:45:PRO:HD2	2.37	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1490:HOH:O	3:F:1481:HOH:O[2_557]	1.82	0.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1304:HOH:O	3:C:1305:HOH:O[1_554]	1.86	0.34

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	787/809 (97%)	773 (98%)	13 (2%)	1 (0%)	51	45
1	B	787/809 (97%)	773 (98%)	13 (2%)	1 (0%)	51	45
1	C	787/809 (97%)	773 (98%)	13 (2%)	1 (0%)	51	45
1	D	787/809 (97%)	772 (98%)	14 (2%)	1 (0%)	51	45
1	E	787/809 (97%)	772 (98%)	14 (2%)	1 (0%)	51	45
1	F	787/809 (97%)	771 (98%)	14 (2%)	2 (0%)	41	31
1	G	787/809 (97%)	773 (98%)	13 (2%)	1 (0%)	51	45
1	H	787/809 (97%)	773 (98%)	13 (2%)	1 (0%)	51	45
All	All	6296/6472 (97%)	6180 (98%)	107 (2%)	9 (0%)	51	45

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	644	PRO
1	F	530	ASP
1	A	644	PRO
1	B	644	PRO
1	C	644	PRO
1	E	644	PRO
1	F	644	PRO
1	G	644	PRO
1	H	644	PRO

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	676/694 (97%)	665 (98%)	11 (2%)	62	59
1	B	676/694 (97%)	668 (99%)	8 (1%)	71	70
1	C	676/694 (97%)	667 (99%)	9 (1%)	69	67
1	D	676/694 (97%)	663 (98%)	13 (2%)	57	53
1	E	676/694 (97%)	662 (98%)	14 (2%)	53	48
1	F	676/694 (97%)	663 (98%)	13 (2%)	57	53
1	G	676/694 (97%)	663 (98%)	13 (2%)	57	53
1	H	676/694 (97%)	666 (98%)	10 (2%)	65	63
All	All	5408/5552 (97%)	5317 (98%)	91 (2%)	60	57

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	315	TRP
1	A	530	ASP
1	A	539	GLN
1	A	551	GLN
1	A	601	LYS
1	A	643	LEU
1	A	670	GLU
1	A	675	GLU
1	A	742	ASP
1	A	746	LEU
1	B	70	VAL
1	B	315	TRP
1	B	530	ASP
1	B	539	GLN
1	B	551	GLN
1	B	631	PRO
1	B	640	VAL
1	B	643	LEU

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Mol	Chain	Res	Type
1	C	61	LEU
1	C	315	TRP
1	C	530	ASP
1	C	539	GLN
1	C	551	GLN
1	C	643	LEU
1	C	670	GLU
1	C	675	GLU
1	C	746	LEU
1	D	70	VAL
1	D	152	PHE
1	D	184	LYS
1	D	224	GLN
1	D	239	LEU
1	D	315	TRP
1	D	471	LYS
1	D	530	ASP
1	D	539	GLN
1	D	551	GLN
1	D	640	VAL
1	D	643	LEU
1	D	675	GLU
1	E	152	PHE
1	E	230	THR
1	E	281	THR
1	E	315	TRP
1	E	344	ASN
1	E	530	ASP
1	E	539	GLN
1	E	601	LYS
1	E	640	VAL
1	E	643	LEU
1	E	670	GLU
1	E	675	GLU
1	E	686	VAL
1	E	746	LEU
1	F	61	LEU
1	F	315	TRP
1	F	344	ASN
1	F	366	VAL
1	F	530	ASP
1	F	539	GLN

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Mol	Chain	Res	Type
1	F	551	GLN
1	F	601	LYS
1	F	640	VAL
1	F	643	LEU
1	F	670	GLU
1	F	675	GLU
1	F	746	LEU
1	G	45	PRO
1	G	61	LEU
1	G	152	PHE
1	G	315	TRP
1	G	366	VAL
1	G	530	ASP
1	G	539	GLN
1	G	551	GLN
1	G	640	VAL
1	G	643	LEU
1	G	670	GLU
1	G	675	GLU
1	G	686	VAL
1	H	61	LEU
1	H	281	THR
1	H	315	TRP
1	H	530	ASP
1	H	539	GLN
1	H	551	GLN
1	H	640	VAL
1	H	643	LEU
1	H	675	GLU
1	H	746	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	HIS
1	A	288	HIS
1	A	704	ASN
1	A	752	ASN
1	A	754	GLN
1	A	769	HIS
1	B	288	HIS
1	B	704	ASN

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Mol	Chain	Res	Type
1	C	251	HIS
1	C	288	HIS
1	C	414	GLN
1	C	704	ASN
1	C	752	ASN
1	D	190	ASN
1	D	224	GLN
1	D	288	HIS
1	D	704	ASN
1	D	752	ASN
1	E	251	HIS
1	E	257	HIS
1	E	288	HIS
1	E	704	ASN
1	E	752	ASN
1	F	18	ASN
1	F	251	HIS
1	F	288	HIS
1	F	704	ASN
1	F	730	ASN
1	F	752	ASN
1	G	596	ASN
1	G	600	ASN
1	G	704	ASN
1	H	251	HIS
1	H	257	HIS
1	H	288	HIS
1	H	704	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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	$\# Z > 2$
2	GOL	D	801	-	5,5,5	0.49	0	5,5,5	0.60	0
2	GOL	F	801	-	5,5,5	0.33	0	5,5,5	0.64	0
2	GOL	B	801	-	5,5,5	0.45	0	5,5,5	0.29	0
2	GOL	H	801	-	5,5,5	0.40	0	5,5,5	0.17	0
2	GOL	E	801	-	5,5,5	0.47	0	5,5,5	0.70	0
2	GOL	G	801	-	5,5,5	0.35	0	5,5,5	0.61	0
2	GOL	A	801	-	5,5,5	0.39	0	5,5,5	0.25	0
2	GOL	C	801	-	5,5,5	0.44	0	5,5,5	0.45	0

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
2	GOL	D	801	-	-	0/4/4/4	-
2	GOL	F	801	-	-	0/4/4/4	-
2	GOL	B	801	-	-	0/4/4/4	-
2	GOL	H	801	-	-	1/4/4/4	-
2	GOL	E	801	-	-	0/4/4/4	-
2	GOL	G	801	-	-	2/4/4/4	-
2	GOL	A	801	-	-	2/4/4/4	-
2	GOL	C	801	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	C1-C2-C3-O3
2	G	801	GOL	O1-C1-C2-C3
2	H	801	GOL	C1-C2-C3-O3
2	A	801	GOL	O2-C2-C3-O3
2	G	801	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	GOL	1	0
2	F	801	GOL	1	0
2	E	801	GOL	2	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	789/809 (97%)	-0.39	5 (0%) 89 91	9, 15, 29, 55	0
1	B	789/809 (97%)	-0.01	20 (2%) 57 61	14, 26, 42, 67	0
1	C	789/809 (97%)	-0.34	4 (0%) 91 92	11, 19, 35, 48	0
1	D	789/809 (97%)	-0.27	6 (0%) 86 88	12, 22, 39, 65	0
1	E	789/809 (97%)	-0.36	4 (0%) 91 92	9, 17, 34, 44	0
1	F	789/809 (97%)	-0.25	2 (0%) 94 94	9, 15, 31, 55	0
1	G	789/809 (97%)	-0.35	2 (0%) 94 94	9, 16, 28, 55	0
1	H	789/809 (97%)	-0.36	3 (0%) 92 93	9, 18, 35, 51	0
All	All	6312/6472 (97%)	-0.29	46 (0%) 87 89	9, 18, 36, 67	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	6.4
1	B	230	THR	4.3
1	H	789	PHE	3.8
1	B	301	ILE	3.5
1	D	230	THR	3.3
1	C	1	MET	3.3
1	D	1	MET	3.1
1	F	228	GLU	2.9
1	B	239	LEU	2.7
1	E	1	MET	2.7
1	B	236	LYS	2.6
1	B	7	GLU	2.5
1	D	297	VAL	2.5
1	F	230	THR	2.5
1	B	163	CYS	2.5
1	H	593	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	447	LEU	2.4
1	B	483	PHE	2.4
1	A	1	MET	2.4
1	D	7	GLU	2.4
1	B	573	LYS	2.3
1	A	647	CYS	2.3
1	D	227	GLU	2.3
1	H	718	LEU	2.2
1	B	487	GLU	2.2
1	D	184	LYS	2.2
1	B	157	ALA	2.2
1	C	590	GLY	2.2
1	A	230	THR	2.2
1	E	575	PHE	2.2
1	B	227	GLU	2.1
1	B	576	ASP	2.1
1	A	224	GLN	2.1
1	B	277	TRP	2.1
1	A	163	CYS	2.1
1	G	163	CYS	2.1
1	E	484	GLN	2.1
1	B	575	PHE	2.1
1	C	481	ARG	2.1
1	B	184	LYS	2.1
1	B	300	GLY	2.1
1	B	571	ASP	2.0
1	G	1	MET	2.0
1	E	586	ALA	2.0
1	C	479	ASP	2.0
1	B	484	GLN	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. 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(\AA^2)	Q<0.9
2	GOL	B	801	6/6	0.88	0.21	26,29,29,33	0
2	GOL	E	801	6/6	0.91	0.15	20,22,27,28	0
2	GOL	D	801	6/6	0.92	0.19	20,27,29,29	0
2	GOL	H	801	6/6	0.92	0.12	21,21,26,26	0
2	GOL	F	801	6/6	0.92	0.18	20,21,22,23	0
2	GOL	C	801	6/6	0.92	0.13	25,26,27,30	0
2	GOL	G	801	6/6	0.93	0.17	22,23,24,27	0
2	GOL	A	801	6/6	0.95	0.12	19,22,23,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.