



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:43 PM UTC

PDB ID : 3UHJ / pdb_00003uhj
Title : Crystal structure of a probable glycerol dehydrogenase from Sinorhizobium meliloti 1021
Authors : Agarwal, R.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRG)
Deposited on : 2011-11-03
Resolution : 2.34 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

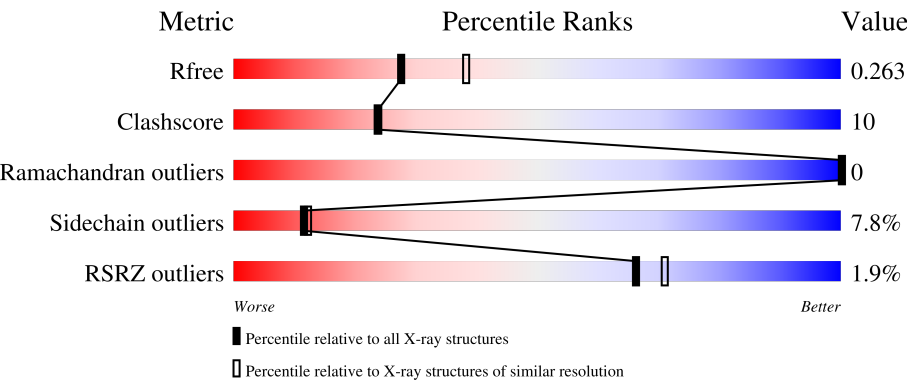
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	387	2% 72% 18% •• 8%
1	B	387	% 74% 15% •• 8%
1	C	387	2% 72% 18% • 8%
1	D	387	% 73% 17% •• 8%

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Mol	Chain	Length	Quality of chain
1	E	387	 % 71% 17% • 8%
1	F	387	 4% 73% 16% • 9%
1	G	387	 % 69% 19% • 8%
1	H	387	 2% 66% 22% • 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	487	-	-	X	-
2	GOL	D	487	-	-	-	X
2	GOL	E	487	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21320 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 Probable glycerol dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	Se	0	0	0
			2633	1660	468	492	9	4			
1	B	356	Total	C	N	O	S	Se	0	0	0
			2571	1621	455	483	9	3			
1	C	355	Total	C	N	O	S	Se	0	0	0
			2585	1632	453	488	9	3			
1	D	357	Total	C	N	O	S	Se	0	0	0
			2617	1647	467	491	9	3			
1	E	355	Total	C	N	O	S	Se	0	0	0
			2601	1638	462	489	9	3			
1	F	351	Total	C	N	O	S	Se	0	0	0
			2532	1591	452	477	9	3			
1	G	356	Total	C	N	O	S	Se	0	0	0
			2597	1639	459	487	9	3			
1	H	355	Total	C	N	O	S	Se	0	0	0
			2601	1641	459	489	9	3			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q92MR2
A	2	HIS	-	expression tag	UNP Q92MR2
A	3	HIS	-	expression tag	UNP Q92MR2
A	4	HIS	-	expression tag	UNP Q92MR2
A	5	HIS	-	expression tag	UNP Q92MR2
A	6	HIS	-	expression tag	UNP Q92MR2
A	7	HIS	-	expression tag	UNP Q92MR2
A	8	SER	-	expression tag	UNP Q92MR2
A	9	SER	-	expression tag	UNP Q92MR2
A	10	GLY	-	expression tag	UNP Q92MR2
A	11	VAL	-	expression tag	UNP Q92MR2
A	12	ASP	-	expression tag	UNP Q92MR2
A	13	LEU	-	expression tag	UNP Q92MR2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	14	GLY	-	expression tag	UNP Q92MR2
A	15	THR	-	expression tag	UNP Q92MR2
A	16	GLU	-	expression tag	UNP Q92MR2
A	17	ASN	-	expression tag	UNP Q92MR2
A	18	LEU	-	expression tag	UNP Q92MR2
A	19	TYR	-	expression tag	UNP Q92MR2
A	20	PHE	-	expression tag	UNP Q92MR2
A	21	GLN	-	expression tag	UNP Q92MR2
A	22	SER	-	expression tag	UNP Q92MR2
A	23	MSE	-	expression tag	UNP Q92MR2
B	1	MSE	-	expression tag	UNP Q92MR2
B	2	HIS	-	expression tag	UNP Q92MR2
B	3	HIS	-	expression tag	UNP Q92MR2
B	4	HIS	-	expression tag	UNP Q92MR2
B	5	HIS	-	expression tag	UNP Q92MR2
B	6	HIS	-	expression tag	UNP Q92MR2
B	7	HIS	-	expression tag	UNP Q92MR2
B	8	SER	-	expression tag	UNP Q92MR2
B	9	SER	-	expression tag	UNP Q92MR2
B	10	GLY	-	expression tag	UNP Q92MR2
B	11	VAL	-	expression tag	UNP Q92MR2
B	12	ASP	-	expression tag	UNP Q92MR2
B	13	LEU	-	expression tag	UNP Q92MR2
B	14	GLY	-	expression tag	UNP Q92MR2
B	15	THR	-	expression tag	UNP Q92MR2
B	16	GLU	-	expression tag	UNP Q92MR2
B	17	ASN	-	expression tag	UNP Q92MR2
B	18	LEU	-	expression tag	UNP Q92MR2
B	19	TYR	-	expression tag	UNP Q92MR2
B	20	PHE	-	expression tag	UNP Q92MR2
B	21	GLN	-	expression tag	UNP Q92MR2
B	22	SER	-	expression tag	UNP Q92MR2
B	23	MSE	-	expression tag	UNP Q92MR2
C	1	MSE	-	expression tag	UNP Q92MR2
C	2	HIS	-	expression tag	UNP Q92MR2
C	3	HIS	-	expression tag	UNP Q92MR2
C	4	HIS	-	expression tag	UNP Q92MR2
C	5	HIS	-	expression tag	UNP Q92MR2
C	6	HIS	-	expression tag	UNP Q92MR2
C	7	HIS	-	expression tag	UNP Q92MR2
C	8	SER	-	expression tag	UNP Q92MR2
C	9	SER	-	expression tag	UNP Q92MR2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	10	GLY	-	expression tag	UNP Q92MR2
C	11	VAL	-	expression tag	UNP Q92MR2
C	12	ASP	-	expression tag	UNP Q92MR2
C	13	LEU	-	expression tag	UNP Q92MR2
C	14	GLY	-	expression tag	UNP Q92MR2
C	15	THR	-	expression tag	UNP Q92MR2
C	16	GLU	-	expression tag	UNP Q92MR2
C	17	ASN	-	expression tag	UNP Q92MR2
C	18	LEU	-	expression tag	UNP Q92MR2
C	19	TYR	-	expression tag	UNP Q92MR2
C	20	PHE	-	expression tag	UNP Q92MR2
C	21	GLN	-	expression tag	UNP Q92MR2
C	22	SER	-	expression tag	UNP Q92MR2
C	23	MSE	-	expression tag	UNP Q92MR2
D	1	MSE	-	expression tag	UNP Q92MR2
D	2	HIS	-	expression tag	UNP Q92MR2
D	3	HIS	-	expression tag	UNP Q92MR2
D	4	HIS	-	expression tag	UNP Q92MR2
D	5	HIS	-	expression tag	UNP Q92MR2
D	6	HIS	-	expression tag	UNP Q92MR2
D	7	HIS	-	expression tag	UNP Q92MR2
D	8	SER	-	expression tag	UNP Q92MR2
D	9	SER	-	expression tag	UNP Q92MR2
D	10	GLY	-	expression tag	UNP Q92MR2
D	11	VAL	-	expression tag	UNP Q92MR2
D	12	ASP	-	expression tag	UNP Q92MR2
D	13	LEU	-	expression tag	UNP Q92MR2
D	14	GLY	-	expression tag	UNP Q92MR2
D	15	THR	-	expression tag	UNP Q92MR2
D	16	GLU	-	expression tag	UNP Q92MR2
D	17	ASN	-	expression tag	UNP Q92MR2
D	18	LEU	-	expression tag	UNP Q92MR2
D	19	TYR	-	expression tag	UNP Q92MR2
D	20	PHE	-	expression tag	UNP Q92MR2
D	21	GLN	-	expression tag	UNP Q92MR2
D	22	SER	-	expression tag	UNP Q92MR2
D	23	MSE	-	expression tag	UNP Q92MR2
E	1	MSE	-	expression tag	UNP Q92MR2
E	2	HIS	-	expression tag	UNP Q92MR2
E	3	HIS	-	expression tag	UNP Q92MR2
E	4	HIS	-	expression tag	UNP Q92MR2
E	5	HIS	-	expression tag	UNP Q92MR2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	6	HIS	-	expression tag	UNP Q92MR2
E	7	HIS	-	expression tag	UNP Q92MR2
E	8	SER	-	expression tag	UNP Q92MR2
E	9	SER	-	expression tag	UNP Q92MR2
E	10	GLY	-	expression tag	UNP Q92MR2
E	11	VAL	-	expression tag	UNP Q92MR2
E	12	ASP	-	expression tag	UNP Q92MR2
E	13	LEU	-	expression tag	UNP Q92MR2
E	14	GLY	-	expression tag	UNP Q92MR2
E	15	THR	-	expression tag	UNP Q92MR2
E	16	GLU	-	expression tag	UNP Q92MR2
E	17	ASN	-	expression tag	UNP Q92MR2
E	18	LEU	-	expression tag	UNP Q92MR2
E	19	TYR	-	expression tag	UNP Q92MR2
E	20	PHE	-	expression tag	UNP Q92MR2
E	21	GLN	-	expression tag	UNP Q92MR2
E	22	SER	-	expression tag	UNP Q92MR2
E	23	MSE	-	expression tag	UNP Q92MR2
F	1	MSE	-	expression tag	UNP Q92MR2
F	2	HIS	-	expression tag	UNP Q92MR2
F	3	HIS	-	expression tag	UNP Q92MR2
F	4	HIS	-	expression tag	UNP Q92MR2
F	5	HIS	-	expression tag	UNP Q92MR2
F	6	HIS	-	expression tag	UNP Q92MR2
F	7	HIS	-	expression tag	UNP Q92MR2
F	8	SER	-	expression tag	UNP Q92MR2
F	9	SER	-	expression tag	UNP Q92MR2
F	10	GLY	-	expression tag	UNP Q92MR2
F	11	VAL	-	expression tag	UNP Q92MR2
F	12	ASP	-	expression tag	UNP Q92MR2
F	13	LEU	-	expression tag	UNP Q92MR2
F	14	GLY	-	expression tag	UNP Q92MR2
F	15	THR	-	expression tag	UNP Q92MR2
F	16	GLU	-	expression tag	UNP Q92MR2
F	17	ASN	-	expression tag	UNP Q92MR2
F	18	LEU	-	expression tag	UNP Q92MR2
F	19	TYR	-	expression tag	UNP Q92MR2
F	20	PHE	-	expression tag	UNP Q92MR2
F	21	GLN	-	expression tag	UNP Q92MR2
F	22	SER	-	expression tag	UNP Q92MR2
F	23	MSE	-	expression tag	UNP Q92MR2
G	1	MSE	-	expression tag	UNP Q92MR2

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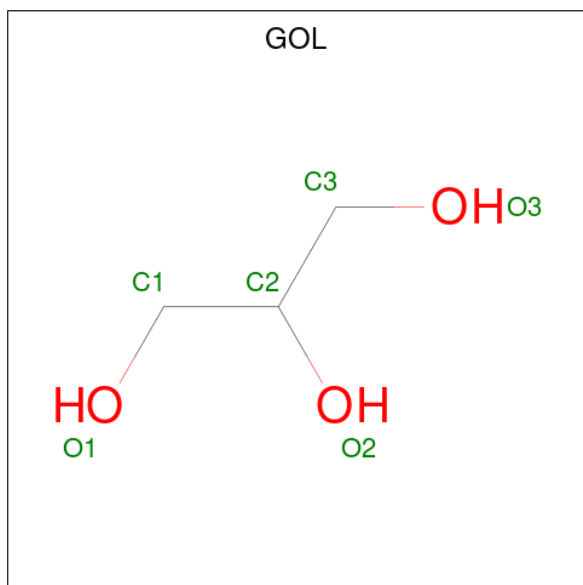
Chain	Residue	Modelled	Actual	Comment	Reference
G	2	HIS	-	expression tag	UNP Q92MR2
G	3	HIS	-	expression tag	UNP Q92MR2
G	4	HIS	-	expression tag	UNP Q92MR2
G	5	HIS	-	expression tag	UNP Q92MR2
G	6	HIS	-	expression tag	UNP Q92MR2
G	7	HIS	-	expression tag	UNP Q92MR2
G	8	SER	-	expression tag	UNP Q92MR2
G	9	SER	-	expression tag	UNP Q92MR2
G	10	GLY	-	expression tag	UNP Q92MR2
G	11	VAL	-	expression tag	UNP Q92MR2
G	12	ASP	-	expression tag	UNP Q92MR2
G	13	LEU	-	expression tag	UNP Q92MR2
G	14	GLY	-	expression tag	UNP Q92MR2
G	15	THR	-	expression tag	UNP Q92MR2
G	16	GLU	-	expression tag	UNP Q92MR2
G	17	ASN	-	expression tag	UNP Q92MR2
G	18	LEU	-	expression tag	UNP Q92MR2
G	19	TYR	-	expression tag	UNP Q92MR2
G	20	PHE	-	expression tag	UNP Q92MR2
G	21	GLN	-	expression tag	UNP Q92MR2
G	22	SER	-	expression tag	UNP Q92MR2
G	23	MSE	-	expression tag	UNP Q92MR2
H	1	MSE	-	expression tag	UNP Q92MR2
H	2	HIS	-	expression tag	UNP Q92MR2
H	3	HIS	-	expression tag	UNP Q92MR2
H	4	HIS	-	expression tag	UNP Q92MR2
H	5	HIS	-	expression tag	UNP Q92MR2
H	6	HIS	-	expression tag	UNP Q92MR2
H	7	HIS	-	expression tag	UNP Q92MR2
H	8	SER	-	expression tag	UNP Q92MR2
H	9	SER	-	expression tag	UNP Q92MR2
H	10	GLY	-	expression tag	UNP Q92MR2
H	11	VAL	-	expression tag	UNP Q92MR2
H	12	ASP	-	expression tag	UNP Q92MR2
H	13	LEU	-	expression tag	UNP Q92MR2
H	14	GLY	-	expression tag	UNP Q92MR2
H	15	THR	-	expression tag	UNP Q92MR2
H	16	GLU	-	expression tag	UNP Q92MR2
H	17	ASN	-	expression tag	UNP Q92MR2
H	18	LEU	-	expression tag	UNP Q92MR2
H	19	TYR	-	expression tag	UNP Q92MR2
H	20	PHE	-	expression tag	UNP Q92MR2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	21	GLN	-	expression tag	UNP Q92MR2
H	22	SER	-	expression tag	UNP Q92MR2
H	23	MSE	-	expression tag	UNP Q92MR2

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0
3	E	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0
3	G	1	Total 1	Zn 1	0	0
3	H	1	Total 1	Zn 1	0	0

- Molecule 4 is SELENIUM ATOM (CCD ID: SE) (formula: Se).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total 1	Se 1	0	0
4	H	1	Total 1	Se 1	0	0

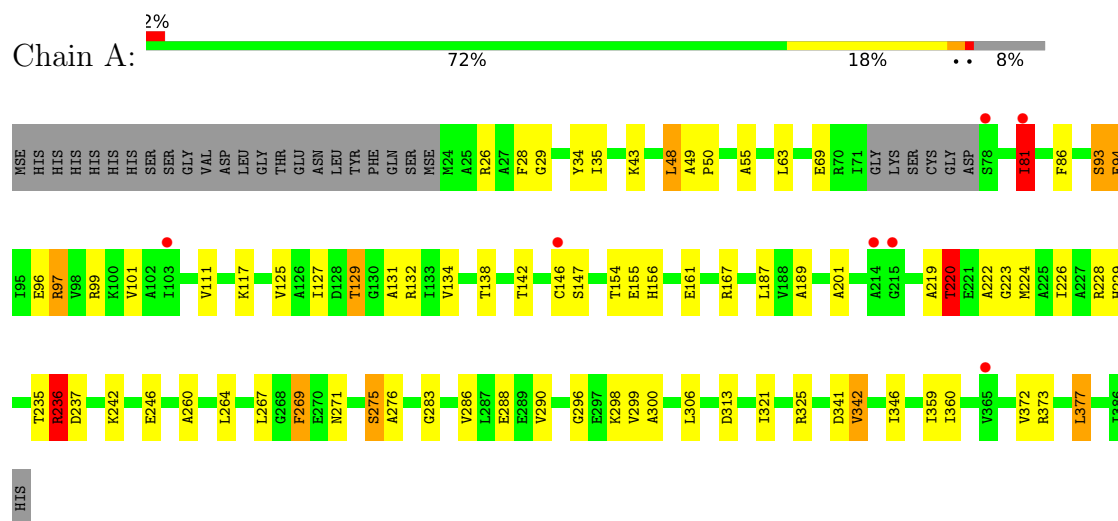
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total 79	O 79	0	0
5	B	80	Total 80	O 80	0	0
5	C	65	Total 65	O 65	0	0
5	D	54	Total 54	O 54	0	0
5	E	79	Total 79	O 79	0	0
5	F	55	Total 55	O 55	0	0
5	G	78	Total 78	O 78	0	0
5	H	47	Total 47	O 47	0	0

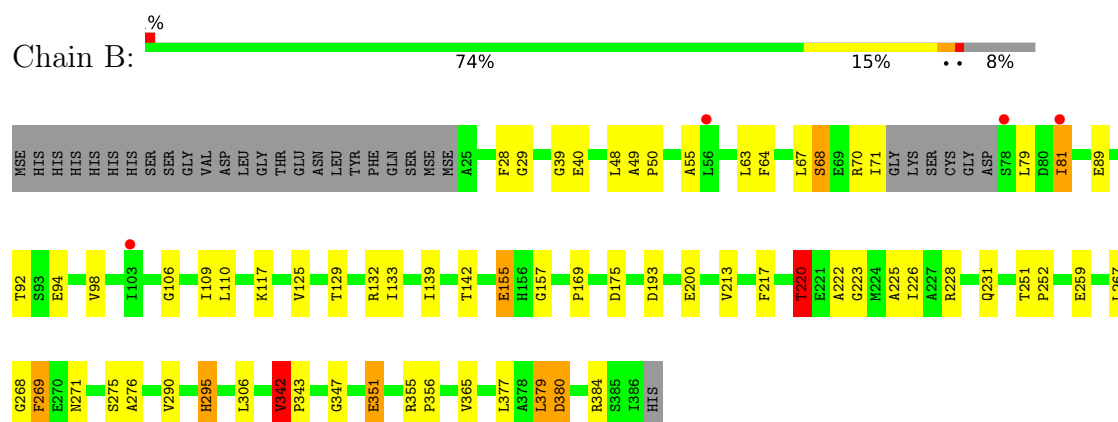
3 Residue-property plots

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.

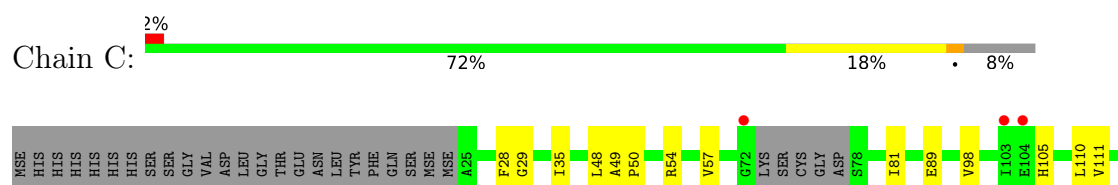
• Molecule 1: Probable glycerol dehydrogenase

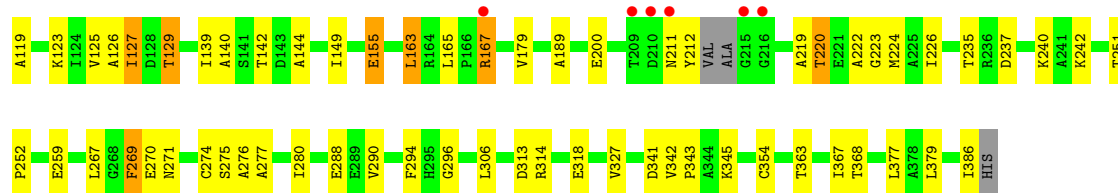


• Molecule 1: Probable glycerol dehydrogenase

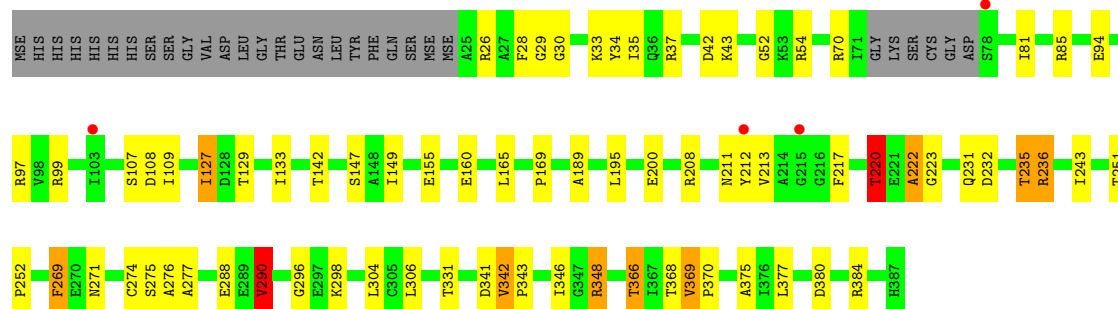


• Molecule 1: Probable glycerol dehydrogenase

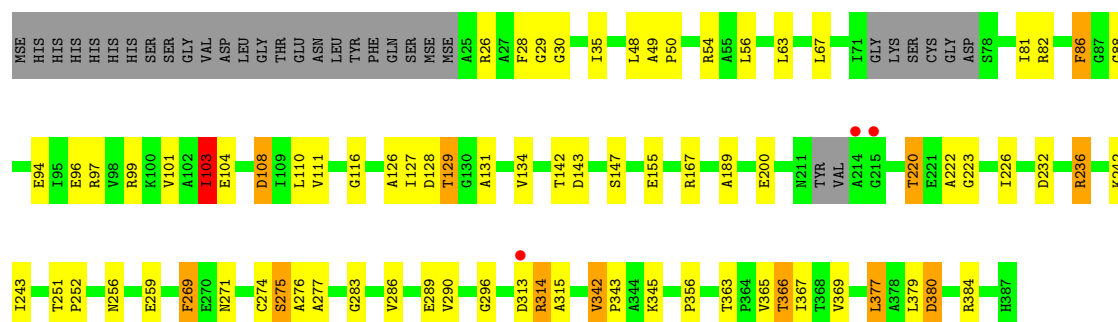




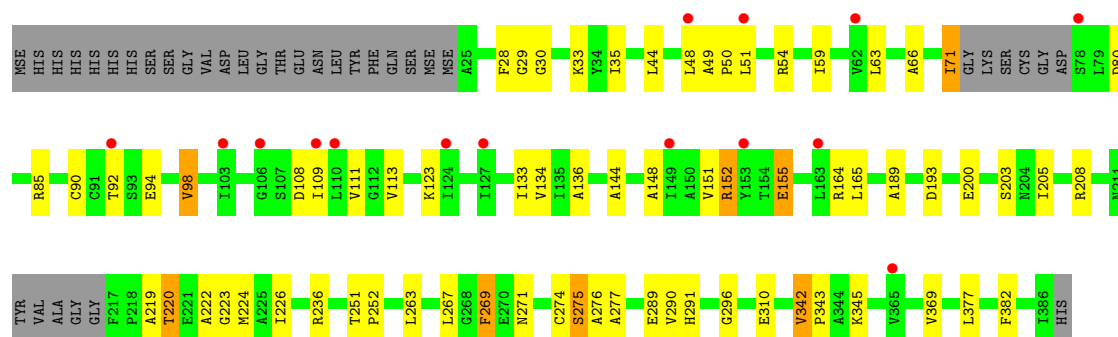
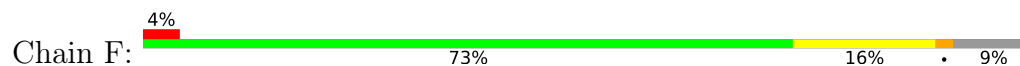
• Molecule 1: Probable glycerol dehydrogenase



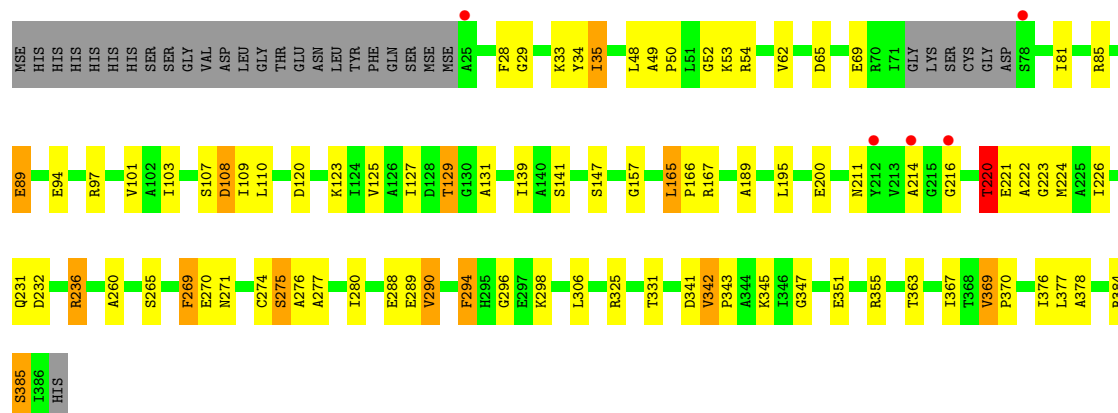
• Molecule 1: Probable glycerol dehydrogenase



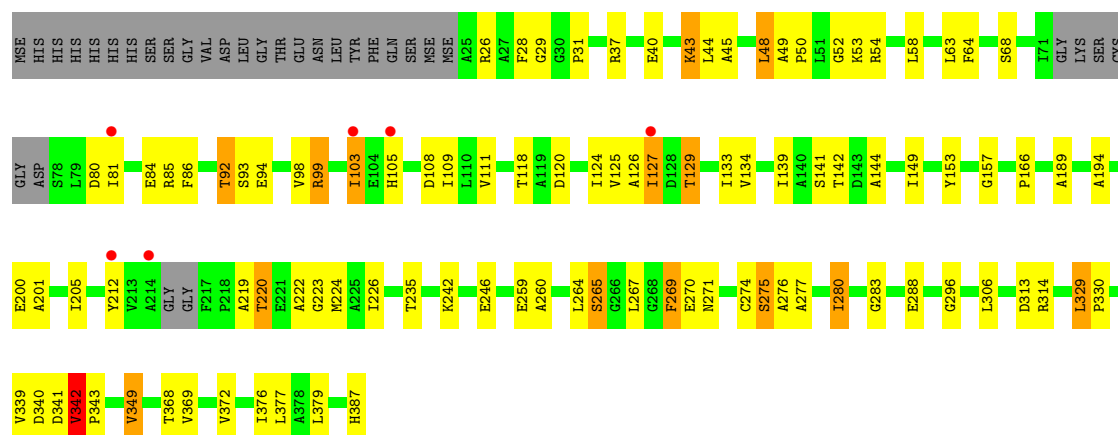
• Molecule 1: Probable glycerol dehydrogenase



• Molecule 1: Probable glycerol dehydrogenase



• Molecule 1: Probable glycerol dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.48Å 99.00Å 104.73Å 76.94° 83.38° 71.47°	Depositor
Resolution (Å)	45.98 – 2.34 45.98 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.2 (45.98-2.34) 98.2 (45.98-2.34)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.197 , 0.264 0.201 , 0.263	Depositor DCC
R_{free} test set	6116 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21320	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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, SE, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.36	8/2670 (0.3%)	1.21	14/3622 (0.4%)
1	B	1.27	3/2607 (0.1%)	1.19	11/3544 (0.3%)
1	C	1.19	2/2621 (0.1%)	1.15	5/3559 (0.1%)
1	D	1.18	4/2654 (0.2%)	1.24	13/3601 (0.4%)
1	E	1.24	7/2637 (0.3%)	1.17	7/3578 (0.2%)
1	F	1.11	2/2567 (0.1%)	1.15	9/3488 (0.3%)
1	G	1.28	7/2633 (0.3%)	1.19	8/3576 (0.2%)
1	H	1.15	2/2638 (0.1%)	1.15	11/3582 (0.3%)
All	All	1.23	35/21027 (0.2%)	1.18	78/28550 (0.3%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	342	VAL	CA-CB	14.39	1.62	1.54
1	E	369	VAL	CA-CB	8.00	1.58	1.54
1	H	342	VAL	CA-CB	7.76	1.58	1.54
1	A	342	VAL	C-O	-7.26	1.15	1.24
1	F	342	VAL	C-O	-6.44	1.19	1.24
1	B	380	ASP	C-O	-6.21	1.16	1.24
1	G	34	TYR	C-O	-6.14	1.17	1.24
1	B	379	LEU	C-O	-6.08	1.17	1.24
1	G	378	ALA	C-O	-6.07	1.17	1.24
1	D	369	VAL	CA-CB	5.96	1.57	1.54
1	A	96	GLU	C-O	-5.90	1.17	1.24
1	E	366	THR	CA-CB	5.89	1.60	1.53
1	G	385	SER	C-O	-5.88	1.17	1.24
1	D	342	VAL	CA-CB	-5.84	1.50	1.53
1	A	228	ARG	C-O	-5.74	1.17	1.24
1	E	315	ALA	C-O	-5.66	1.17	1.24
1	G	103	ILE	CA-CB	-5.62	1.47	1.54
1	G	369	VAL	C-O	-5.59	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	35	ILE	C-O	-5.57	1.18	1.24
1	D	217	PHE	C-O	-5.53	1.18	1.24
1	D	222	ALA	CA-CB	-5.52	1.44	1.53
1	F	382	PHE	C-O	-5.52	1.17	1.24
1	E	380	ASP	C-O	-5.48	1.17	1.24
1	A	235	THR	C-O	-5.47	1.17	1.24
1	A	236	ARG	C-O	-5.46	1.17	1.24
1	E	314	ARG	C-O	-5.45	1.17	1.24
1	C	235	THR	C-O	-5.43	1.17	1.24
1	A	237	ASP	C-O	-5.29	1.17	1.24
1	E	256	ASN	C-O	-5.28	1.18	1.24
1	E	377	LEU	C-O	-5.24	1.17	1.24
1	C	237	ASP	C-O	-5.13	1.17	1.24
1	H	376	ILE	C-O	-5.11	1.18	1.24
1	G	384	ARG	C-O	-5.03	1.18	1.24
1	A	93	SER	C-O	-5.02	1.18	1.24
1	A	101	VAL	CA-CB	-5.00	1.48	1.54

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	CYS	N-CA-C	10.01	122.27	111.36
1	H	53	LYS	N-CA-C	-9.49	103.81	114.62
1	F	30	GLY	CA-C-N	-8.31	111.46	119.85
1	F	30	GLY	C-N-CA	-8.31	111.46	119.85
1	A	147	SER	N-CA-C	7.42	120.32	110.53
1	C	144	ALA	CA-C-N	-7.32	112.09	119.56
1	C	144	ALA	C-N-CA	-7.32	112.09	119.56
1	D	147	SER	N-CA-C	7.29	119.38	110.41
1	A	237	ASP	N-CA-C	7.02	122.85	113.72
1	G	107	SER	CA-C-N	6.93	130.13	120.29
1	G	107	SER	C-N-CA	6.93	130.13	120.29
1	D	30	GLY	CA-C-N	-6.71	113.03	120.14
1	D	30	GLY	C-N-CA	-6.71	113.03	120.14
1	D	213	VAL	N-CA-C	-6.54	98.95	108.11
1	A	154	THR	N-CA-C	-6.48	102.44	110.41
1	A	86	PHE	CA-C-N	6.45	128.21	120.14
1	A	86	PHE	C-N-CA	6.45	128.21	120.14
1	D	290	VAL	N-CA-C	-6.43	106.42	113.43
1	B	217	PHE	CA-C-N	-6.30	113.30	119.78
1	B	217	PHE	C-N-CA	-6.30	113.30	119.78
1	A	341	ASP	CA-C-N	6.21	124.15	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ASP	C-N-CA	6.21	124.15	120.24
1	B	355	ARG	CA-C-N	6.09	126.45	119.93
1	B	355	ARG	C-N-CA	6.09	126.45	119.93
1	E	86	PHE	CA-C-N	6.07	127.73	120.14
1	E	86	PHE	C-N-CA	6.07	127.73	120.14
1	C	237	ASP	N-CA-C	6.05	121.59	113.72
1	H	201	ALA	N-CA-C	-6.00	103.91	111.11
1	B	295	HIS	CA-C-N	5.87	126.45	120.00
1	B	295	HIS	C-N-CA	5.87	126.45	120.00
1	D	220	THR	N-CA-CB	-5.78	101.54	110.56
1	A	220	THR	N-CA-CB	-5.78	101.85	110.17
1	G	165	LEU	CA-C-N	5.67	125.20	119.19
1	G	165	LEU	C-N-CA	5.67	125.20	119.19
1	D	375	ALA	N-CA-C	5.56	117.78	111.11
1	C	354	CYS	N-CA-C	5.55	119.67	113.02
1	G	81	ILE	CB-CA-C	-5.54	103.78	110.99
1	G	107	SER	N-CA-C	5.51	118.31	110.10
1	D	341	ASP	CA-C-N	5.51	123.71	120.24
1	D	341	ASP	C-N-CA	5.51	123.71	120.24
1	E	101	VAL	CB-CA-C	-5.48	104.74	112.14
1	H	329	LEU	CA-C-N	5.48	125.75	119.83
1	H	329	LEU	C-N-CA	5.48	125.75	119.83
1	B	40	GLU	N-CA-C	5.45	117.97	111.71
1	F	291	HIS	N-CA-C	5.44	117.91	111.33
1	H	144	ALA	N-CA-C	5.42	121.79	109.81
1	B	220	THR	N-CA-C	5.36	117.20	110.24
1	G	220	THR	N-CA-CB	-5.36	102.70	110.36
1	A	156	HIS	N-CA-C	5.34	119.79	113.16
1	A	201	ALA	N-CA-C	-5.33	105.54	111.36
1	H	92	THR	CB-CA-C	5.32	119.90	110.85
1	D	366	THR	CB-CA-C	5.30	119.07	110.22
1	H	103	ILE	CA-C-N	-5.28	113.21	120.28
1	H	103	ILE	C-N-CA	-5.28	113.21	120.28
1	D	235	THR	N-CA-C	-5.23	105.26	111.69
1	E	30	GLY	CA-C-N	5.20	125.10	119.85
1	E	30	GLY	C-N-CA	5.20	125.10	119.85
1	B	106	GLY	N-CA-C	-5.19	107.63	115.32
1	F	342	VAL	N-CA-C	5.19	118.58	112.35
1	F	144	ALA	N-CA-C	5.18	120.72	113.57
1	A	154	THR	N-CA-CB	5.13	117.40	110.38
1	F	369	VAL	CA-C-N	-5.13	113.75	119.19
1	F	369	VAL	C-N-CA	-5.13	113.75	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ILE	N-CA-C	5.12	115.28	108.11
1	H	369	VAL	CA-C-N	-5.11	113.37	119.05
1	H	369	VAL	C-N-CA	-5.11	113.37	119.05
1	A	138	THR	N-CA-C	-5.10	107.08	113.72
1	B	268	GLY	CA-C-N	5.10	127.38	120.65
1	B	268	GLY	C-N-CA	5.10	127.38	120.65
1	H	339	VAL	CB-CA-C	-5.09	102.93	111.29
1	F	208	ARG	N-CA-C	5.09	118.61	111.74
1	C	368	THR	N-CA-C	-5.06	101.61	109.14
1	E	103	ILE	CA-C-N	-5.05	113.51	120.28
1	E	103	ILE	C-N-CA	-5.05	113.51	120.28
1	D	107	SER	N-CA-C	5.04	117.65	110.24
1	F	276	ALA	N-CA-C	5.03	117.50	111.71
1	D	212	TYR	CA-C-O	-5.02	116.15	122.63
1	G	275	SER	CB-CA-C	-5.01	107.31	114.87

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	2633	0	2654	54	0
1	B	2571	0	2546	53	0
1	C	2585	0	2571	51	0
1	D	2617	0	2620	50	0
1	E	2601	0	2602	54	0
1	F	2532	0	2482	44	0
1	G	2597	0	2601	58	0
1	H	2601	0	2595	67	0
2	A	6	0	8	4	0
2	B	6	0	8	3	0
2	C	6	0	8	2	0
2	D	6	0	8	1	0
2	E	6	0	8	4	0
2	G	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
5	A	79	0	0	1	0
5	B	80	0	0	1	0
5	C	65	0	0	1	0
5	D	54	0	0	4	0
5	E	79	0	0	2	0
5	F	55	0	0	3	0
5	G	78	0	0	2	0
5	H	47	0	0	2	0
All	All	21320	0	20719	417	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 10.

All (417) 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:C:149:ILE:HD13	1:C:269:PHE:HE2	1.06	1.19
1:A:290:VAL:HG12	1:A:298:LYS:HE2	1.32	1.09
1:B:220:THR:HG22	1:B:223:GLY:H	1.17	1.05
1:G:29:GLY:H	1:G:271:ASN:HD21	1.05	1.02
1:C:149:ILE:HD13	1:C:269:PHE:CE2	1.95	1.01
1:F:220:THR:HG22	1:F:223:GLY:H	1.26	1.00
1:F:94:GLU:O	1:F:98:VAL:HG23	1.62	1.00
1:E:220:THR:HG22	1:E:223:GLY:H	1.21	1.00
1:C:29:GLY:H	1:C:271:ASN:HD21	1.09	0.94
1:A:220:THR:HG22	1:A:223:GLY:H	1.34	0.91
1:E:232:ASP:O	1:E:236:ARG:HG2	1.71	0.90
1:G:220:THR:HG22	1:G:223:GLY:H	1.37	0.90
1:H:205:ILE:HD11	1:H:224:MSE:HG2	1.55	0.89
1:G:269:PHE:CE1	1:G:274:CYS:SG	2.66	0.89
1:B:29:GLY:H	1:B:271:ASN:HD21	1.16	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:GLY:H	1:D:271:ASN:HD21	1.21	0.88
1:F:49:ALA:HB3	1:F:50:PRO:HD3	1.57	0.87
1:A:155:GLU:CD	1:A:155:GLU:H	1.84	0.85
1:H:29:GLY:H	1:H:271:ASN:HD21	1.22	0.85
1:F:155:GLU:H	1:F:155:GLU:CD	1.83	0.84
1:D:220:THR:HG22	1:D:223:GLY:H	1.41	0.84
1:H:99:ARG:O	1:H:103:ILE:HG13	1.77	0.84
1:G:269:PHE:CD1	1:G:274:CYS:SG	2.71	0.84
1:E:29:GLY:H	1:E:271:ASN:HD21	1.23	0.84
1:C:220:THR:HG22	1:C:223:GLY:H	1.44	0.83
1:B:67:LEU:O	1:B:71:ILE:HG13	1.79	0.82
1:C:155:GLU:CD	1:C:155:GLU:H	1.88	0.82
1:G:232:ASP:O	1:G:236:ARG:HG2	1.79	0.81
1:F:220:THR:CG2	1:F:223:GLY:H	1.93	0.81
1:A:290:VAL:CG1	1:A:298:LYS:HE2	2.10	0.80
1:H:269:PHE:CE1	1:H:274:CYS:SG	2.75	0.79
1:H:269:PHE:C	1:H:269:PHE:CD2	2.60	0.79
1:H:269:PHE:C	1:H:269:PHE:HD2	1.89	0.79
1:F:29:GLY:H	1:F:271:ASN:HD21	1.30	0.79
1:A:132:ARG:CZ	1:B:132:ARG:HH21	1.96	0.78
1:B:155:GLU:CD	1:B:155:GLU:H	1.91	0.78
1:B:220:THR:HG23	1:B:222:ALA:H	1.49	0.78
1:D:269:PHE:CD1	1:D:274:CYS:SG	2.77	0.78
1:D:269:PHE:HD1	1:D:274:CYS:SG	2.08	0.77
1:G:108:ASP:HB3	1:G:109:ILE:HG13	1.64	0.77
1:G:220:THR:CG2	1:G:223:GLY:H	1.97	0.77
1:A:269:PHE:C	1:A:269:PHE:HD2	1.93	0.76
1:F:200:GLU:HG2	1:F:275:SER:HB2	1.68	0.76
1:H:342:VAL:HG22	1:H:343:PRO:HD3	1.66	0.76
1:F:220:THR:HG23	1:F:222:ALA:N	2.02	0.75
1:A:49:ALA:HB3	1:A:50:PRO:HD3	1.69	0.75
1:A:125:VAL:O	1:A:129:THR:HB	1.86	0.75
1:B:220:THR:HG22	1:B:223:GLY:N	1.98	0.75
1:F:220:THR:HG23	1:F:222:ALA:H	1.50	0.75
1:B:193:ASP:OD2	1:B:295:HIS:HD2	1.70	0.74
1:A:142:THR:CG2	2:A:487:GOL:H32	2.17	0.74
1:B:342:VAL:HG22	1:B:343:PRO:HD3	1.69	0.74
1:G:29:GLY:N	1:G:271:ASN:HD21	1.83	0.73
1:G:28:PHE:HA	1:G:271:ASN:ND2	2.04	0.73
1:C:379:LEU:HD13	1:C:379:LEU:C	2.14	0.72
1:G:280:ILE:HD12	1:G:376:ILE:HD11	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:221:GLU:HA	1:G:224:MSE:HE3	1.72	0.71
1:E:220:THR:HG23	1:E:222:ALA:H	1.56	0.71
1:A:220:THR:HB	5:A:455:HOH:O	1.91	0.70
1:B:269:PHE:HD2	1:B:269:PHE:C	2.00	0.70
1:C:269:PHE:CE1	1:C:274:CYS:SG	2.84	0.70
1:B:49:ALA:HB3	1:B:50:PRO:HD3	1.73	0.70
1:G:276:ALA:O	1:G:280:ILE:HG12	1.92	0.70
1:A:226:ILE:HD11	1:B:226:ILE:HD11	1.74	0.69
1:D:127:ILE:HD13	1:D:165:LEU:HD13	1.74	0.69
1:E:155:GLU:CD	1:E:155:GLU:H	2.01	0.69
1:B:269:PHE:C	1:B:269:PHE:CD2	2.71	0.69
1:H:269:PHE:CD1	1:H:274:CYS:SG	2.86	0.69
1:A:29:GLY:H	1:A:271:ASN:HD21	1.39	0.69
1:A:276:ALA:HB3	1:A:306:LEU:HD13	1.75	0.69
1:E:142:THR:CG2	2:E:487:GOL:H31	2.22	0.69
1:G:342:VAL:HG22	1:G:343:PRO:HD3	1.75	0.69
1:A:269:PHE:C	1:A:269:PHE:CD2	2.68	0.68
1:H:28:PHE:HA	1:H:271:ASN:ND2	2.09	0.68
1:D:99:ARG:CD	5:D:597:HOH:O	2.39	0.68
1:G:139:ILE:HD12	1:G:141:SER:OG	1.93	0.68
1:B:63:LEU:HD12	1:B:67:LEU:HG	1.76	0.68
1:E:131:ALA:O	1:E:167:ARG:NH2	2.23	0.68
1:B:89:GLU:OE2	1:B:157:GLY:HA2	1.94	0.67
1:H:242:LYS:HE2	1:H:246:GLU:OE2	1.94	0.67
1:D:155:GLU:H	1:D:155:GLU:CD	2.03	0.67
1:E:363:THR:HB	1:E:367:ILE:HD11	1.77	0.66
1:E:99:ARG:HE	1:E:128:ASP:HB3	1.60	0.66
1:H:49:ALA:HB3	1:H:50:PRO:HD3	1.76	0.66
1:H:342:VAL:CG2	1:H:343:PRO:HD3	2.24	0.66
1:A:142:THR:HG23	2:A:487:GOL:H32	1.78	0.66
1:H:220:THR:HG22	1:H:223:GLY:H	1.60	0.66
1:G:290:VAL:HG13	1:G:298:LYS:HE2	1.76	0.66
1:B:28:PHE:HA	1:B:271:ASN:ND2	2.11	0.66
1:B:220:THR:HG23	1:B:222:ALA:N	2.10	0.65
1:E:342:VAL:HG22	1:E:343:PRO:HD3	1.79	0.65
1:C:29:GLY:N	1:C:271:ASN:HD21	1.90	0.65
1:D:99:ARG:HD2	5:D:597:HOH:O	1.97	0.65
1:D:232:ASP:O	1:D:236:ARG:HG3	1.97	0.64
1:G:52:GLY:HA3	1:G:108:ASP:OD2	1.97	0.64
1:H:220:THR:CG2	1:H:222:ALA:HB3	2.27	0.64
1:C:269:PHE:C	1:C:269:PHE:CD2	2.74	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:ARG:O	1:G:108:ASP:HB2	1.98	0.64
1:H:127:ILE:HG12	1:H:166:PRO:HD2	1.79	0.64
1:E:220:THR:HG22	1:E:223:GLY:N	2.05	0.63
1:C:220:THR:CG2	1:C:223:GLY:H	2.10	0.63
1:E:242:LYS:NZ	5:E:394:HOH:O	2.32	0.63
1:G:129:THR:HG22	1:G:131:ALA:H	1.64	0.63
1:D:342:VAL:HB	1:D:343:PRO:HD3	1.80	0.62
1:D:149:ILE:HD12	1:D:269:PHE:CZ	2.34	0.62
1:A:219:ALA:HB3	1:A:224:MSE:HE2	1.80	0.62
1:F:220:THR:HG22	1:F:223:GLY:N	2.07	0.62
1:C:28:PHE:HA	1:C:271:ASN:ND2	2.15	0.62
1:D:28:PHE:HA	1:D:271:ASN:ND2	2.15	0.62
1:E:142:THR:HG21	2:E:487:GOL:H31	1.82	0.61
1:A:131:ALA:O	1:A:167:ARG:NH2	2.26	0.61
1:B:29:GLY:N	1:B:271:ASN:HD21	1.95	0.61
1:C:212:TYR:OH	1:C:274:CYS:HB2	2.01	0.61
1:A:132:ARG:CZ	1:B:132:ARG:NH2	2.63	0.60
1:D:220:THR:CG2	1:D:223:GLY:H	2.14	0.60
1:F:113:VAL:HG22	1:F:136:ALA:HB3	1.83	0.60
1:G:276:ALA:HB3	1:G:306:LEU:HD13	1.82	0.60
1:B:142:THR:HG21	2:B:487:GOL:H31	1.83	0.60
1:B:129:THR:HG22	1:B:129:THR:O	2.01	0.60
1:B:379:LEU:O	1:B:379:LEU:HG	1.99	0.60
1:H:94:GLU:O	1:H:98:VAL:HG23	2.02	0.60
1:A:28:PHE:HA	1:A:271:ASN:ND2	2.17	0.59
1:B:142:THR:CG2	2:B:487:GOL:H31	2.32	0.59
1:A:142:THR:HG21	2:A:487:GOL:H32	1.83	0.59
1:C:219:ALA:HB3	1:C:224:MSE:HE3	1.84	0.59
1:E:220:THR:HG23	1:E:222:ALA:N	2.17	0.59
1:A:260:ALA:HA	1:A:264:LEU:HD12	1.85	0.58
1:B:193:ASP:OD2	1:B:295:HIS:CD2	2.53	0.58
1:C:220:THR:HG23	1:C:222:ALA:H	1.68	0.58
1:C:276:ALA:O	1:C:280:ILE:HG13	2.03	0.58
1:F:94:GLU:HG3	5:F:393:HOH:O	2.03	0.58
1:E:63:LEU:HB3	1:E:67:LEU:HD12	1.85	0.58
1:G:269:PHE:C	1:G:269:PHE:CD2	2.82	0.58
1:A:290:VAL:HG12	1:A:290:VAL:O	2.03	0.58
1:E:143:ASP:OD2	1:E:269:PHE:HD1	1.87	0.57
1:G:53:LYS:N	1:G:108:ASP:OD2	2.33	0.57
1:E:226:ILE:HD11	1:H:226:ILE:HD11	1.86	0.57
1:F:269:PHE:CE1	1:F:274:CYS:SG	2.98	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:GLY:O	1:B:351:GLU:HG2	2.05	0.56
1:A:132:ARG:NH2	1:B:132:ARG:HH21	2.02	0.56
1:H:149:ILE:HD11	1:H:212:TYR:CB	2.36	0.56
1:C:226:ILE:HD13	1:C:267:LEU:HD13	1.87	0.56
1:H:200:GLU:CD	1:H:277:ALA:HB3	2.31	0.56
1:D:290:VAL:HG13	1:D:298:LYS:HE2	1.86	0.56
1:E:269:PHE:C	1:E:269:PHE:CD2	2.83	0.56
1:H:45:ALA:HB3	5:H:483:HOH:O	2.05	0.56
1:H:276:ALA:O	1:H:280:ILE:HG12	2.06	0.56
1:C:119:ALA:O	1:C:123:LYS:HG3	2.06	0.55
1:C:269:PHE:C	1:C:269:PHE:HD2	2.15	0.55
1:F:94:GLU:O	1:F:98:VAL:CG2	2.47	0.55
1:B:155:GLU:CD	1:B:155:GLU:N	2.65	0.55
1:E:269:PHE:C	1:E:269:PHE:HD2	2.15	0.55
1:F:44:LEU:HD23	1:F:71:ILE:HG21	1.88	0.55
1:C:142:THR:HG21	2:C:487:GOL:H32	1.88	0.55
1:E:259:GLU:OE2	1:H:220:THR:HG23	2.06	0.55
1:F:49:ALA:CB	1:F:50:PRO:HD3	2.35	0.55
1:H:54:ARG:O	1:H:108:ASP:HB2	2.06	0.55
1:C:142:THR:CG2	2:C:487:GOL:H32	2.37	0.54
1:H:28:PHE:HA	1:H:271:ASN:HD22	1.72	0.54
1:H:314:ARG:HD2	5:H:592:HOH:O	2.07	0.54
1:B:133:ILE:HB	1:B:169:PRO:HA	1.89	0.54
1:B:380:ASP:OD2	1:B:384:ARG:NH1	2.40	0.54
1:F:90:CYS:O	1:F:152:ARG:HG2	2.08	0.54
1:B:231:GLN:NE2	5:B:402:HOH:O	2.37	0.54
1:D:220:THR:CG2	1:D:222:ALA:HB3	2.37	0.54
1:A:155:GLU:CD	1:A:155:GLU:N	2.61	0.54
1:B:142:THR:HG21	2:B:487:GOL:C3	2.38	0.54
1:H:189:ALA:O	1:H:296:GLY:HA3	2.07	0.54
1:C:379:LEU:HD13	1:C:379:LEU:O	2.07	0.54
1:G:189:ALA:O	1:G:296:GLY:HA3	2.07	0.54
1:B:55:ALA:HB3	1:B:81:ILE:HG22	1.90	0.53
1:C:342:VAL:HB	1:C:343:PRO:HD3	1.90	0.53
1:B:220:THR:CG2	1:B:222:ALA:HB3	2.39	0.53
1:E:220:THR:CG2	1:E:223:GLY:H	2.09	0.53
1:F:148:ALA:O	1:F:165:LEU:HB2	2.09	0.53
1:F:226:ILE:HD11	1:G:226:ILE:HD11	1.89	0.53
1:G:260:ALA:O	1:G:265:SER:HB2	2.08	0.53
1:F:33:LYS:HD3	1:G:214:ALA:HB2	1.89	0.53
1:H:219:ALA:HB3	1:H:224:MSE:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ARG:HG2	1:A:236:ARG:HH11	1.73	0.53
1:C:276:ALA:HB3	1:C:306:LEU:HD13	1.90	0.53
1:E:380:ASP:O	1:E:384:ARG:HG3	2.09	0.53
1:D:251:THR:HB	1:D:252:PRO:HD2	1.90	0.53
1:D:304:LEU:HD11	1:D:331:THR:HG22	1.90	0.53
1:B:129:THR:O	1:B:129:THR:CG2	2.57	0.53
1:E:56:LEU:HD12	1:E:82:ARG:O	2.08	0.52
1:D:348:ARG:HH11	1:D:348:ARG:HG2	1.74	0.52
1:F:203:SER:OG	1:F:310:GLU:OE2	2.26	0.52
1:C:220:THR:HG23	1:C:222:ALA:N	2.25	0.52
1:C:54:ARG:HB3	1:C:105:HIS:CE1	2.44	0.52
1:B:64:PHE:O	1:B:68:SER:OG	2.27	0.52
1:C:269:PHE:CD1	1:C:274:CYS:SG	3.03	0.52
1:G:89:GLU:OE2	1:G:157:GLY:HA2	2.10	0.52
1:D:220:THR:HG23	1:D:222:ALA:N	2.25	0.52
1:D:368:THR:HB	1:D:370:PRO:HD2	1.92	0.52
1:C:251:THR:HB	1:C:252:PRO:HD2	1.92	0.52
1:F:54:ARG:H	1:F:108:ASP:HB2	1.75	0.52
1:C:363:THR:HB	1:C:367:ILE:HD11	1.92	0.52
1:A:220:THR:CG2	1:A:222:ALA:HB3	2.39	0.52
1:E:232:ASP:O	1:E:236:ARG:CG	2.54	0.52
1:A:342:VAL:O	1:A:346:ILE:HG12	2.10	0.51
1:E:28:PHE:HA	1:E:271:ASN:ND2	2.25	0.51
1:H:194:ALA:HA	1:H:265:SER:OG	2.11	0.51
1:A:48:LEU:HD21	1:A:111:VAL:HG21	1.92	0.51
1:C:127:ILE:HD13	1:C:165:LEU:HD13	1.93	0.51
1:G:294:PHE:CD1	1:G:294:PHE:N	2.79	0.51
1:F:54:ARG:O	1:F:108:ASP:N	2.43	0.51
1:F:269:PHE:CZ	1:F:274:CYS:SG	3.04	0.51
1:C:259:GLU:OE1	1:D:26:ARG:NH1	2.38	0.50
1:G:52:GLY:N	1:G:109:ILE:HD11	2.26	0.50
1:G:347:GLY:O	1:G:351:GLU:HG2	2.10	0.50
1:A:229:HIS:CD2	1:B:225:ALA:HB2	2.47	0.50
1:A:321:ILE:O	1:A:325:ARG:HG3	2.12	0.50
1:B:276:ALA:HB3	1:B:306:LEU:HD13	1.92	0.50
1:E:200:GLU:CD	1:E:277:ALA:HB3	2.37	0.50
1:G:97:ARG:O	1:G:101:VAL:HG23	2.12	0.50
1:H:64:PHE:HE1	1:H:84:GLU:C	2.18	0.50
1:C:140:ALA:HB2	1:C:179:VAL:HG11	1.93	0.50
1:H:149:ILE:HG13	1:H:269:PHE:HE2	1.77	0.50
1:E:103:ILE:HG22	1:E:104:GLU:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:342:VAL:HB	1:F:343:PRO:HD3	1.94	0.50
1:G:294:PHE:N	1:G:294:PHE:HD1	2.09	0.50
1:A:129:THR:HG22	1:A:131:ALA:H	1.75	0.50
1:G:29:GLY:H	1:G:271:ASN:ND2	1.89	0.50
1:B:220:THR:HG21	1:B:222:ALA:HB3	1.94	0.50
1:B:365:VAL:HA	1:D:208:ARG:NH2	2.26	0.50
1:E:110:LEU:HB2	1:E:126:ALA:HB2	1.94	0.50
1:E:251:THR:HB	1:E:252:PRO:HD2	1.94	0.50
1:E:343:PRO:HD2	5:E:542:HOH:O	2.11	0.50
1:C:189:ALA:O	1:C:296:GLY:HA3	2.13	0.49
1:E:189:ALA:O	1:E:296:GLY:HA3	2.12	0.49
1:B:220:THR:CG2	1:B:223:GLY:H	2.06	0.49
1:F:251:THR:HB	1:F:252:PRO:CD	2.42	0.49
1:H:219:ALA:HB3	1:H:224:MSE:CE	2.43	0.49
1:E:142:THR:HG23	2:E:487:GOL:H31	1.94	0.49
1:H:276:ALA:HB3	1:H:306:LEU:HD13	1.95	0.49
1:C:211:ASN:OD1	1:C:211:ASN:C	2.56	0.49
1:C:155:GLU:CD	1:C:155:GLU:N	2.65	0.48
1:F:66:ALA:HB1	5:F:634:HOH:O	2.11	0.48
1:E:269:PHE:CZ	1:E:274:CYS:SG	3.07	0.48
1:A:26:ARG:NH1	1:B:259:GLU:OE1	2.41	0.48
1:D:42:ASP:OD2	1:D:70:ARG:NE	2.43	0.48
1:G:52:GLY:CA	1:G:108:ASP:OD2	2.60	0.48
1:C:242:LYS:HE3	1:C:327:VAL:O	2.13	0.48
1:D:29:GLY:N	1:D:271:ASN:HD21	2.01	0.48
1:D:195:LEU:HD12	1:D:231:GLN:HE22	1.78	0.48
1:H:313:ASP:OD1	1:H:314:ARG:N	2.47	0.48
1:D:189:ALA:O	1:D:296:GLY:HA3	2.14	0.48
1:E:143:ASP:OD2	1:E:269:PHE:CD1	2.66	0.48
1:E:313:ASP:OD1	1:E:314:ARG:N	2.47	0.48
1:F:28:PHE:HA	1:F:271:ASN:ND2	2.29	0.48
1:D:220:THR:HG23	1:D:222:ALA:H	1.79	0.47
1:E:220:THR:CG2	1:E:222:ALA:HB3	2.44	0.47
1:E:379:LEU:HD13	1:E:379:LEU:C	2.39	0.47
1:F:193:ASP:HB3	5:F:460:HOH:O	2.13	0.47
1:G:232:ASP:O	1:G:236:ARG:CG	2.58	0.47
1:A:242:LYS:CE	1:A:246:GLU:OE2	2.62	0.47
1:C:386:ILE:C	5:C:519:HOH:O	2.56	0.47
1:H:220:THR:HG23	1:H:222:ALA:H	1.79	0.47
1:D:220:THR:HG22	1:D:223:GLY:N	2.20	0.47
1:C:251:THR:HB	1:C:252:PRO:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:ALA:HB3	1:D:306:LEU:HD13	1.96	0.47
1:G:28:PHE:HA	1:G:271:ASN:HD22	1.76	0.47
1:A:55:ALA:O	1:A:81:ILE:HG22	2.15	0.46
1:C:98:VAL:HG12	1:C:125:VAL:HG21	1.96	0.46
1:H:129:THR:O	1:H:129:THR:CG2	2.62	0.46
1:A:142:THR:HG21	2:A:487:GOL:C3	2.45	0.46
1:B:290:VAL:HG12	1:B:290:VAL:O	2.15	0.46
1:C:125:VAL:O	1:C:129:THR:HB	2.15	0.46
1:E:86:PHE:CE2	1:E:88:GLY:HA2	2.49	0.46
1:E:259:GLU:OE1	1:H:26:ARG:NH1	2.42	0.46
1:C:379:LEU:C	1:C:379:LEU:CD1	2.84	0.46
1:D:220:THR:HG23	1:D:222:ALA:HB3	1.98	0.46
1:H:37:ARG:O	1:H:40:GLU:HB2	2.15	0.46
1:C:110:LEU:HB2	1:C:126:ALA:HB2	1.97	0.46
1:E:54:ARG:H	1:E:108:ASP:HB2	1.80	0.46
1:F:289:GLU:OE2	1:F:345:LYS:NZ	2.43	0.46
1:H:260:ALA:HA	1:H:264:LEU:HD12	1.97	0.46
1:A:55:ALA:HB3	1:A:81:ILE:CG2	2.46	0.46
1:A:346:ILE:HG21	1:A:377:LEU:HD13	1.98	0.46
1:A:220:THR:HG23	1:A:222:ALA:H	1.81	0.46
1:E:116:GLY:H	2:E:487:GOL:H32	1.81	0.46
1:E:129:THR:O	1:E:129:THR:CG2	2.64	0.46
1:H:153:TYR:HB3	1:H:157:GLY:HA2	1.98	0.46
1:G:28:PHE:CD2	1:G:28:PHE:C	2.94	0.45
1:G:220:THR:HG23	1:G:222:ALA:N	2.31	0.45
1:G:369:VAL:HB	1:G:370:PRO:HD3	1.98	0.45
1:A:34:TYR:C	1:A:35:ILE:HD12	2.41	0.45
1:B:98:VAL:HG12	1:B:125:VAL:HG21	1.98	0.45
1:D:28:PHE:HA	1:D:271:ASN:HD22	1.79	0.45
1:F:54:ARG:HG2	1:F:54:ARG:HH11	1.82	0.45
1:A:242:LYS:HE3	1:A:246:GLU:OE2	2.16	0.45
1:A:299:VAL:O	1:A:300:ALA:C	2.59	0.45
1:G:139:ILE:CD1	2:G:487:GOL:H31	2.47	0.45
1:H:111:VAL:HA	1:H:134:VAL:O	2.17	0.45
1:E:275:SER:HB3	1:E:276:ALA:H	1.37	0.45
1:F:251:THR:HB	1:F:252:PRO:HD2	1.98	0.45
1:G:129:THR:HG22	1:G:131:ALA:N	2.32	0.45
1:G:269:PHE:HD2	1:G:270:GLU:N	2.15	0.45
1:H:44:LEU:HD12	1:H:44:LEU:HA	1.69	0.45
1:D:34:TYR:C	1:D:35:ILE:HD12	2.42	0.45
1:E:220:THR:HG21	1:E:222:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:ALA:HB3	1:F:224:MSE:HE3	1.98	0.44
1:H:126:ALA:CB	1:H:133:ILE:HG12	2.47	0.44
1:F:44:LEU:HB3	1:F:71:ILE:HG23	1.99	0.44
1:F:269:PHE:C	1:F:269:PHE:CD2	2.96	0.44
1:G:200:GLU:CD	1:G:277:ALA:HB3	2.42	0.44
1:A:55:ALA:HB3	1:A:81:ILE:HG23	1.99	0.44
1:A:111:VAL:HA	1:A:134:VAL:O	2.17	0.44
1:H:48:LEU:N	1:H:48:LEU:CD1	2.80	0.44
1:A:219:ALA:HB3	1:A:224:MSE:CE	2.47	0.44
1:G:220:THR:HG22	1:G:223:GLY:N	2.18	0.44
1:H:340:ASP:O	1:H:341:ASP:HB3	2.18	0.44
1:B:28:PHE:CD2	1:B:28:PHE:C	2.95	0.44
1:G:54:ARG:HD3	5:G:452:HOH:O	2.16	0.44
1:H:44:LEU:O	1:H:45:ALA:C	2.61	0.44
1:H:329:LEU:HA	1:H:330:PRO:HD3	1.87	0.44
1:B:251:THR:HB	1:B:252:PRO:HD2	2.00	0.44
1:D:155:GLU:CD	1:D:155:GLU:N	2.72	0.44
1:G:125:VAL:O	1:G:129:THR:HB	2.18	0.44
1:H:220:THR:HG21	1:H:222:ALA:HB3	1.99	0.44
1:B:220:THR:CG2	1:B:222:ALA:N	2.80	0.44
1:E:111:VAL:HA	1:E:134:VAL:O	2.17	0.44
1:E:290:VAL:HG12	1:E:290:VAL:O	2.17	0.44
1:D:127:ILE:CD1	1:D:165:LEU:HD13	2.44	0.44
1:A:94:GLU:OE2	1:A:97:ARG:NH1	2.51	0.43
1:A:226:ILE:HG21	1:A:267:LEU:HB2	1.99	0.43
1:H:64:PHE:C	1:H:64:PHE:CD2	2.96	0.43
1:B:213:VAL:HG21	1:B:271:ASN:ND2	2.33	0.43
1:D:380:ASP:OD2	1:D:384:ARG:NH1	2.45	0.43
1:H:52:GLY:N	1:H:109:ILE:HD11	2.34	0.43
1:F:155:GLU:CD	1:F:155:GLU:N	2.64	0.43
1:E:155:GLU:CD	1:E:155:GLU:N	2.75	0.43
1:D:369:VAL:HB	1:D:370:PRO:HD3	2.00	0.43
1:A:220:THR:HG22	1:A:223:GLY:N	2.17	0.43
1:B:226:ILE:HG21	1:B:267:LEU:HB2	2.00	0.43
1:C:269:PHE:HD2	1:C:270:GLU:N	2.16	0.43
1:F:200:GLU:CD	1:F:277:ALA:HB3	2.43	0.43
1:G:231:GLN:NE2	1:G:231:GLN:HA	2.33	0.43
1:G:325:ARG:HG3	1:G:331:THR:HG21	2.01	0.43
1:H:120:ASP:O	1:H:124:ILE:HG13	2.19	0.43
1:H:283:GLY:O	1:H:349:VAL:HG22	2.19	0.43
1:D:133:ILE:HB	1:D:169:PRO:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:ALA:O	1:F:296:GLY:HA3	2.18	0.43
1:C:49:ALA:HB3	1:C:50:PRO:HD3	2.00	0.43
1:C:341:ASP:O	1:C:345:LYS:HG3	2.18	0.43
1:G:341:ASP:O	1:G:345:LYS:HG2	2.18	0.43
1:H:212:TYR:OH	1:H:274:CYS:HB2	2.19	0.43
1:A:275:SER:HB3	1:A:276:ALA:H	1.34	0.43
1:C:314:ARG:NH1	1:C:318:GLU:OE1	2.52	0.43
1:D:269:PHE:CE1	1:D:274:CYS:SG	3.11	0.43
1:H:125:VAL:O	1:H:126:ALA:C	2.62	0.43
1:H:139:ILE:HD12	1:H:141:SER:OG	2.18	0.43
1:A:189:ALA:O	1:A:296:GLY:HA3	2.19	0.43
1:C:200:GLU:CD	1:C:277:ALA:HB3	2.43	0.43
1:H:40:GLU:HA	1:H:43:LYS:HG3	2.00	0.43
1:H:379:LEU:C	1:H:379:LEU:HD13	2.44	0.43
1:F:111:VAL:HA	1:F:134:VAL:O	2.19	0.42
1:H:64:PHE:HE1	1:H:85:ARG:N	2.17	0.42
1:H:269:PHE:HD2	1:H:270:GLU:N	2.14	0.42
1:A:49:ALA:CB	1:A:50:PRO:HD3	2.45	0.42
1:B:55:ALA:HB3	1:B:81:ILE:CG2	2.49	0.42
1:B:117:LYS:H	1:B:117:LYS:HG2	1.68	0.42
1:D:200:GLU:HG2	1:D:275:SER:HB3	2.00	0.42
1:F:108:ASP:HB3	1:F:109:ILE:HG13	2.02	0.42
1:D:342:VAL:O	1:D:346:ILE:HG12	2.19	0.42
1:E:26:ARG:NH1	1:H:259:GLU:OE1	2.46	0.42
1:E:289:GLU:OE2	1:E:345:LYS:NZ	2.43	0.42
1:G:211:ASN:O	1:G:216:GLY:HA2	2.19	0.42
1:D:200:GLU:CD	1:D:277:ALA:HB3	2.43	0.42
1:B:200:GLU:HG2	1:B:275:SER:HB3	2.01	0.42
1:D:37:ARG:NH2	1:D:43:LYS:NZ	2.67	0.42
1:G:120:ASP:HA	1:G:123:LYS:HD2	2.01	0.42
1:F:123:LYS:HG2	1:F:133:ILE:HG21	2.02	0.42
1:G:54:ARG:HG2	1:G:54:ARG:HH11	1.83	0.42
1:D:211:ASN:OD1	1:D:211:ASN:C	2.62	0.42
1:F:205:ILE:HG12	1:F:224:MSE:HE2	2.01	0.42
1:H:29:GLY:N	1:H:271:ASN:HD21	2.02	0.42
1:E:269:PHE:CE2	1:E:274:CYS:SG	3.13	0.41
1:E:96:GLU:O	1:E:97:ARG:C	2.63	0.41
1:H:200:GLU:HG2	1:H:275:SER:HB2	2.02	0.41
1:B:39:GLY:H	1:B:175:ASP:CG	2.29	0.41
1:G:165:LEU:HB3	1:G:166:PRO:HD2	2.02	0.41
1:G:195:LEU:O	1:G:195:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:149:ILE:HG13	1:H:269:PHE:CE2	2.55	0.41
1:C:294:PHE:N	1:C:294:PHE:CD1	2.88	0.41
1:E:49:ALA:HB3	1:E:50:PRO:HD3	2.02	0.41
1:H:31:PRO:HD2	1:H:267:LEU:HD21	2.03	0.41
1:G:49:ALA:HB3	1:G:50:PRO:HD3	2.02	0.41
1:G:355:ARG:NH2	5:G:552:HOH:O	2.51	0.41
1:A:283:GLY:O	1:A:286:VAL:HG22	2.20	0.41
1:E:283:GLY:O	1:E:286:VAL:HG22	2.21	0.41
1:F:263:LEU:O	1:F:267:LEU:HB2	2.21	0.41
1:H:54:ARG:NH2	1:H:105:HIS:O	2.40	0.41
1:H:58:LEU:HG	1:H:86:PHE:HB2	2.02	0.41
1:C:163:LEU:HD12	1:C:163:LEU:N	2.35	0.41
1:D:231:GLN:O	1:D:235:THR:HG23	2.20	0.41
1:D:54:ARG:H	1:D:108:ASP:HB2	1.85	0.41
1:D:384:ARG:NH2	5:D:404:HOH:O	2.54	0.41
1:H:368:THR:O	1:H:372:VAL:HG23	2.21	0.41
1:C:149:ILE:HD11	1:C:212:TYR:HB2	2.03	0.41
1:D:195:LEU:O	1:D:195:LEU:HG	2.21	0.41
1:F:220:THR:CG2	1:F:223:GLY:N	2.73	0.41
1:G:363:THR:HB	1:G:367:ILE:HD11	2.02	0.41
1:E:363:THR:C	1:E:365:VAL:H	2.28	0.40
1:A:276:ALA:HB2	1:A:360:ILE:HG13	2.02	0.40
1:A:372:VAL:O	1:A:373:ARG:C	2.64	0.40
1:B:89:GLU:OE2	1:B:157:GLY:CA	2.68	0.40
1:C:127:ILE:HG13	1:C:167:ARG:CZ	2.51	0.40
1:D:52:GLY:N	1:D:109:ILE:HD11	2.35	0.40
1:A:220:THR:HG21	1:A:222:ALA:HB3	2.03	0.40
1:D:142:THR:HG21	2:D:487:GOL:H32	2.03	0.40
1:G:139:ILE:HD11	2:G:487:GOL:H31	2.03	0.40
1:H:99:ARG:HD2	1:H:103:ILE:HD11	2.03	0.40
1:D:384:ARG:NH1	5:D:398:HOH:O	2.46	0.40
1:C:57:VAL:HA	1:C:111:VAL:HB	2.04	0.40
1:G:65:ASP:O	1:G:69:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	353/387 (91%)	338 (96%)	15 (4%)	0	100	100
1	B	352/387 (91%)	341 (97%)	11 (3%)	0	100	100
1	C	349/387 (90%)	336 (96%)	13 (4%)	0	100	100
1	D	353/387 (91%)	342 (97%)	11 (3%)	0	100	100
1	E	349/387 (90%)	340 (97%)	9 (3%)	0	100	100
1	F	345/387 (89%)	329 (95%)	16 (5%)	0	100	100
1	G	352/387 (91%)	339 (96%)	13 (4%)	0	100	100
1	H	349/387 (90%)	332 (95%)	17 (5%)	0	100	100
All	All	2802/3096 (90%)	2697 (96%)	105 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	265/292 (91%)	243 (92%)	22 (8%)	10	11
1	B	251/292 (86%)	233 (93%)	18 (7%)	13	14
1	C	256/292 (88%)	238 (93%)	18 (7%)	14	15
1	D	262/292 (90%)	245 (94%)	17 (6%)	15	17
1	E	260/292 (89%)	242 (93%)	18 (7%)	14	15
1	F	245/292 (84%)	225 (92%)	20 (8%)	10	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	258/292 (88%)	234 (91%)	24 (9%)	8	8
1	H	260/292 (89%)	236 (91%)	24 (9%)	8	8
All	All	2057/2336 (88%)	1896 (92%)	161 (8%)	11	12

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
1	A	48	LEU
1	A	63	LEU
1	A	69	GLU
1	A	81	ILE
1	A	93	SER
1	A	94	GLU
1	A	97	ARG
1	A	99	ARG
1	A	117	LYS
1	A	127	ILE
1	A	129	THR
1	A	161	GLU
1	A	187	LEU
1	A	220	THR
1	A	236	ARG
1	A	269	PHE
1	A	275	SER
1	A	288	GLU
1	A	313	ASP
1	A	359	ILE
1	A	377	LEU
1	B	48	LEU
1	B	68	SER
1	B	70	ARG
1	B	79	LEU
1	B	81	ILE
1	B	92	THR
1	B	94	GLU
1	B	109	ILE
1	B	110	LEU
1	B	139	ILE
1	B	155	GLU
1	B	220	THR

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Mol	Chain	Res	Type
1	B	228	ARG
1	B	269	PHE
1	B	342	VAL
1	B	351	GLU
1	B	356	PRO
1	B	377	LEU
1	C	35	ILE
1	C	48	LEU
1	C	81	ILE
1	C	89	GLU
1	C	127	ILE
1	C	129	THR
1	C	139	ILE
1	C	155	GLU
1	C	163	LEU
1	C	167	ARG
1	C	220	THR
1	C	240	LYS
1	C	269	PHE
1	C	275	SER
1	C	288	GLU
1	C	290	VAL
1	C	313	ASP
1	C	377	LEU
1	D	33	LYS
1	D	81	ILE
1	D	85	ARG
1	D	94	GLU
1	D	97	ARG
1	D	127	ILE
1	D	129	THR
1	D	160	GLU
1	D	220	THR
1	D	236	ARG
1	D	243	ILE
1	D	269	PHE
1	D	288	GLU
1	D	290	VAL
1	D	348	ARG
1	D	366	THR
1	D	377	LEU
1	E	35	ILE

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Mol	Chain	Res	Type
1	E	48	LEU
1	E	81	ILE
1	E	94	GLU
1	E	103	ILE
1	E	108	ASP
1	E	127	ILE
1	E	129	THR
1	E	147	SER
1	E	220	THR
1	E	236	ARG
1	E	243	ILE
1	E	269	PHE
1	E	275	SER
1	E	342	VAL
1	E	356	PRO
1	E	366	THR
1	E	377	LEU
1	F	35	ILE
1	F	48	LEU
1	F	51	LEU
1	F	59	ILE
1	F	63	LEU
1	F	71	ILE
1	F	80	ASP
1	F	85	ARG
1	F	92	THR
1	F	98	VAL
1	F	151	VAL
1	F	152	ARG
1	F	155	GLU
1	F	164	ARG
1	F	220	THR
1	F	236	ARG
1	F	269	PHE
1	F	275	SER
1	F	290	VAL
1	F	377	LEU
1	G	33	LYS
1	G	35	ILE
1	G	48	LEU
1	G	62	VAL
1	G	85	ARG

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Mol	Chain	Res	Type
1	G	89	GLU
1	G	94	GLU
1	G	108	ASP
1	G	110	LEU
1	G	127	ILE
1	G	129	THR
1	G	147	SER
1	G	167	ARG
1	G	220	THR
1	G	236	ARG
1	G	269	PHE
1	G	275	SER
1	G	288	GLU
1	G	289	GLU
1	G	290	VAL
1	G	294	PHE
1	G	342	VAL
1	G	377	LEU
1	G	385	SER
1	H	43	LYS
1	H	48	LEU
1	H	63	LEU
1	H	68	SER
1	H	80	ASP
1	H	81	ILE
1	H	92	THR
1	H	93	SER
1	H	99	ARG
1	H	118	THR
1	H	127	ILE
1	H	129	THR
1	H	142	THR
1	H	220	THR
1	H	235	THR
1	H	265	SER
1	H	269	PHE
1	H	275	SER
1	H	280	ILE
1	H	288	GLU
1	H	342	VAL
1	H	349	VAL
1	H	377	LEU

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Mol	Chain	Res	Type
1	H	387	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	ASN
1	A	271	ASN
1	B	168	ASN
1	B	271	ASN
1	C	32	ASN
1	C	36	GLN
1	C	231	GLN
1	C	271	ASN
1	D	231	GLN
1	D	271	ASN
1	E	204	ASN
1	E	231	GLN
1	E	271	ASN
1	F	36	GLN
1	F	231	GLN
1	F	271	ASN
1	F	291	HIS
1	G	271	ASN
1	H	231	GLN
1	H	271	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	B	487	-	5,5,5	0.79	0	5,5,5	0.84	0
2	GOL	C	487	-	5,5,5	0.48	0	5,5,5	0.79	0
2	GOL	E	487	-	5,5,5	0.51	0	5,5,5	0.76	0
2	GOL	D	487	-	5,5,5	0.48	0	5,5,5	1.65	2 (40%)
2	GOL	A	487	-	5,5,5	0.51	0	5,5,5	0.39	0
2	GOL	G	487	-	5,5,5	0.50	0	5,5,5	1.24	1 (20%)

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	B	487	-	-	0/4/4/4	-
2	GOL	C	487	-	-	4/4/4/4	-
2	GOL	E	487	-	-	4/4/4/4	-
2	GOL	D	487	-	-	3/4/4/4	-
2	GOL	A	487	-	-	4/4/4/4	-
2	GOL	G	487	-	-	0/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	487	GOL	C3-C2-C1	-2.82	101.45	111.80
2	G	487	GOL	O1-C1-C2	-2.22	100.40	110.38
2	D	487	GOL	O1-C1-C2	-2.14	100.73	110.38

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	487	GOL	C1-C2-C3-O3
2	A	487	GOL	O2-C2-C3-O3
2	C	487	GOL	O1-C1-C2-C3
2	C	487	GOL	C1-C2-C3-O3
2	C	487	GOL	O2-C2-C3-O3
2	D	487	GOL	O1-C1-C2-O2
2	D	487	GOL	O1-C1-C2-C3
2	C	487	GOL	O1-C1-C2-O2
2	A	487	GOL	O1-C1-C2-C3
2	E	487	GOL	O1-C1-C2-C3
2	E	487	GOL	C1-C2-C3-O3
2	A	487	GOL	O1-C1-C2-O2
2	D	487	GOL	O2-C2-C3-O3
2	E	487	GOL	O1-C1-C2-O2
2	E	487	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	487	GOL	3	0
2	C	487	GOL	2	0
2	E	487	GOL	4	0
2	D	487	GOL	1	0
2	A	487	GOL	4	0
2	G	487	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	353/387 (91%)	-0.06	7 (1%) 65 70	19, 32, 50, 56	0
1	B	353/387 (91%)	0.07	4 (1%) 78 81	20, 34, 57, 72	0
1	C	352/387 (90%)	0.03	9 (2%) 57 63	20, 35, 51, 62	0
1	D	354/387 (91%)	0.01	4 (1%) 78 81	20, 35, 53, 64	0
1	E	352/387 (90%)	-0.03	3 (0%) 81 84	20, 35, 51, 61	0
1	F	348/387 (89%)	0.32	15 (4%) 40 46	25, 40, 66, 74	0
1	G	353/387 (91%)	-0.07	5 (1%) 73 77	22, 34, 50, 56	0
1	H	352/387 (90%)	0.22	6 (1%) 69 73	23, 40, 60, 70	0
All	All	2817/3096 (90%)	0.06	53 (1%) 66 71	19, 35, 57, 74	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	103	ILE	3.8
1	E	214	ALA	3.6
1	G	214	ALA	3.5
1	B	103	ILE	3.5
1	C	215	GLY	3.4
1	F	110	LEU	3.3
1	B	56	LEU	3.1
1	E	215	GLY	3.0
1	C	104	GLU	2.9
1	H	81	ILE	2.9
1	F	92	THR	2.8
1	B	78	SER	2.8
1	F	365	VAL	2.8
1	C	103	ILE	2.7
1	D	103	ILE	2.7
1	F	127	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	214	ALA	2.6
1	C	216	GLY	2.6
1	G	78	SER	2.6
1	C	209	THR	2.6
1	B	81	ILE	2.5
1	C	211	ASN	2.5
1	F	109	ILE	2.4
1	F	163	LEU	2.4
1	F	78	SER	2.4
1	A	214	ALA	2.4
1	D	78	SER	2.4
1	F	106	GLY	2.4
1	A	81	ILE	2.4
1	H	103	ILE	2.3
1	C	210	ASP	2.3
1	F	153	TYR	2.3
1	A	215	GLY	2.3
1	F	149	ILE	2.3
1	F	124	ILE	2.3
1	F	48	LEU	2.3
1	G	216	GLY	2.2
1	A	146	CYS	2.2
1	G	25	ALA	2.2
1	G	212	TYR	2.2
1	F	62	VAL	2.2
1	A	78	SER	2.2
1	C	72	GLY	2.1
1	F	51	LEU	2.1
1	D	215	GLY	2.1
1	E	313	ASP	2.1
1	H	127	ILE	2.1
1	H	212	TYR	2.1
1	C	167	ARG	2.1
1	H	105	HIS	2.0
1	A	103	ILE	2.0
1	D	212	TYR	2.0
1	A	365	VAL	2.0

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

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

6.3 Carbohydrates [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	GOL	G	487	6/6	0.70	0.33	24,26,27,28	6
2	GOL	D	487	6/6	0.74	0.45	34,37,38,39	6
2	GOL	E	487	6/6	0.79	0.31	29,35,38,40	6
2	GOL	C	487	6/6	0.80	0.26	34,35,36,40	6
2	GOL	B	487	6/6	0.81	0.25	27,33,35,37	6
3	ZN	F	388	1/1	0.87	0.06	37,37,37,37	1
2	GOL	A	487	6/6	0.90	0.21	34,36,40,40	6
3	ZN	E	389	1/1	0.95	0.07	39,39,39,39	1
3	ZN	G	388	1/1	0.95	0.08	36,36,36,36	1
3	ZN	B	388	1/1	0.96	0.04	47,47,47,47	1
3	ZN	A	388	1/1	0.96	0.05	38,38,38,38	1
3	ZN	H	389	1/1	0.96	0.08	44,44,44,44	1
3	ZN	C	388	1/1	0.97	0.04	41,41,41,41	1
4	SE	H	388	1/1	0.97	0.13	75,75,75,75	0
4	SE	E	388	1/1	0.98	0.14	69,69,69,69	0
3	ZN	D	388	1/1	0.98	0.04	42,42,42,42	1

6.5 Other polymers [i](#)

There are no such residues in this entry.