



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:50 AM UTC

PDB ID : 5UHP / pdb_00005uhp
Title : Crystal structure of the core catalytic domain of human O-GlcNAcase
Authors : Klein, D.J.; Elsen, N.L.
Deposited on : 2017-01-11
Resolution : 2.79 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

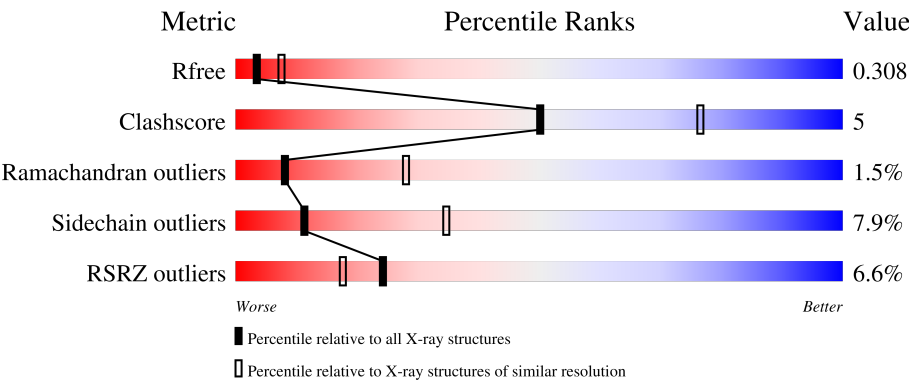
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	388	2% 62% 15% • 21%
1	B	388	2% 63% 15% • 21%
1	C	388	4% 61% 16% •• 20%
1	D	388	4% 56% 19% •• 20%
2	E	161	12% 50% 15% • 30%

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Mol	Chain	Length	Quality of chain
2	F	161	7%52%15%•32%
2	G	161	9%52%18%•29%
2	H	161	13%49%18%•30%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13813 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 O-GlcNAcase TIM-barrel domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2522	1634	414	460	14			
1	B	307	Total	C	N	O	S	0	0	0
			2518	1631	413	460	14			
1	C	310	Total	C	N	O	S	0	0	0
			2515	1626	416	459	14			
1	D	310	Total	C	N	O	S	0	0	0
			2512	1624	414	460	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	expression tag	UNP O60502
B	13	GLY	-	expression tag	UNP O60502
C	13	GLY	-	expression tag	UNP O60502
D	13	GLY	-	expression tag	UNP O60502

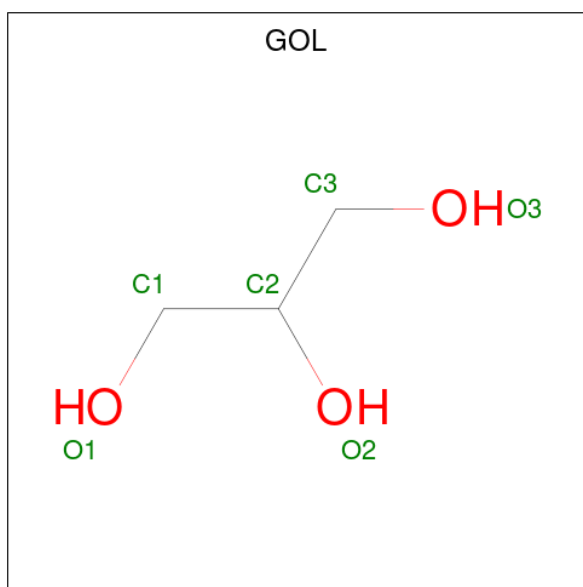
- Molecule 2 is a protein called O-GlcNAcase stalk domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	112	Total	C	N	O	S	0	0	0
			912	588	152	163	9			
2	F	109	Total	C	N	O	S	0	0	0
			896	580	149	158	9			
2	G	114	Total	C	N	O	S	0	0	0
			949	616	159	165	9			
2	H	112	Total	C	N	O	S	0	0	0
			928	600	156	163	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	553	MET	-	initiating methionine	UNP O60502
E	706	HIS	-	expression tag	UNP O60502
E	707	HIS	-	expression tag	UNP O60502
E	708	HIS	-	expression tag	UNP O60502
E	709	HIS	-	expression tag	UNP O60502
E	710	HIS	-	expression tag	UNP O60502
E	711	HIS	-	expression tag	UNP O60502
E	712	HIS	-	expression tag	UNP O60502
E	713	HIS	-	expression tag	UNP O60502
F	553	MET	-	initiating methionine	UNP O60502
F	706	HIS	-	expression tag	UNP O60502
F	707	HIS	-	expression tag	UNP O60502
F	708	HIS	-	expression tag	UNP O60502
F	709	HIS	-	expression tag	UNP O60502
F	710	HIS	-	expression tag	UNP O60502
F	711	HIS	-	expression tag	UNP O60502
F	712	HIS	-	expression tag	UNP O60502
F	713	HIS	-	expression tag	UNP O60502
G	553	MET	-	initiating methionine	UNP O60502
G	706	HIS	-	expression tag	UNP O60502
G	707	HIS	-	expression tag	UNP O60502
G	708	HIS	-	expression tag	UNP O60502
G	709	HIS	-	expression tag	UNP O60502
G	710	HIS	-	expression tag	UNP O60502
G	711	HIS	-	expression tag	UNP O60502
G	712	HIS	-	expression tag	UNP O60502
G	713	HIS	-	expression tag	UNP O60502
H	553	MET	-	initiating methionine	UNP O60502
H	706	HIS	-	expression tag	UNP O60502
H	707	HIS	-	expression tag	UNP O60502
H	708	HIS	-	expression tag	UNP O60502
H	709	HIS	-	expression tag	UNP O60502
H	710	HIS	-	expression tag	UNP O60502
H	711	HIS	-	expression tag	UNP O60502
H	712	HIS	-	expression tag	UNP O60502
H	713	HIS	-	expression tag	UNP O60502

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

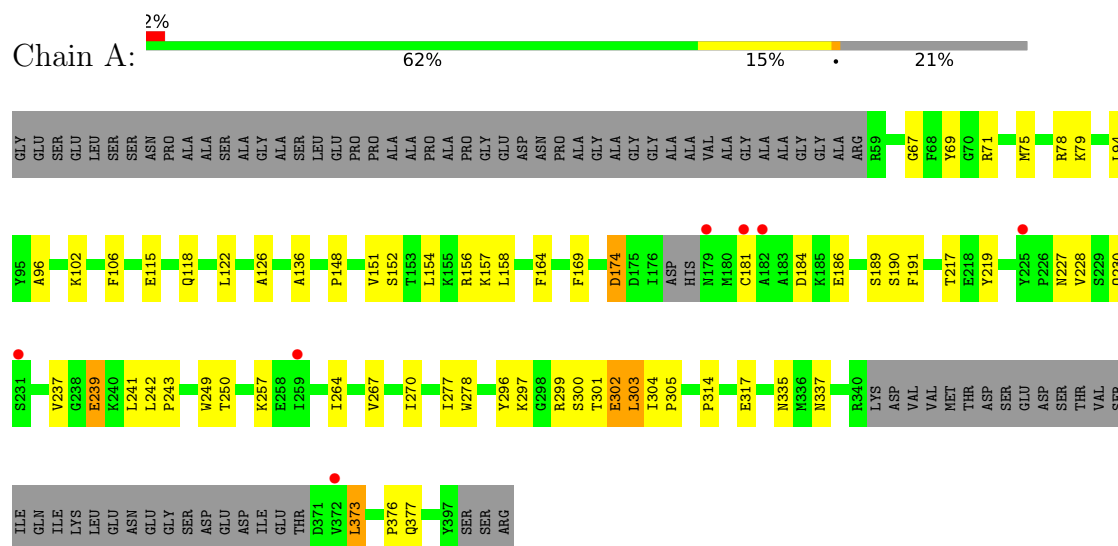
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	11	Total	O	0	0
			11	11		
4	C	8	Total	O	0	0
			8	8		
4	D	3	Total	O	0	0
			3	3		
4	E	3	Total	O	0	0
			3	3		
4	F	3	Total	O	0	0
			3	3		
4	H	4	Total	O	0	0
			4	4		

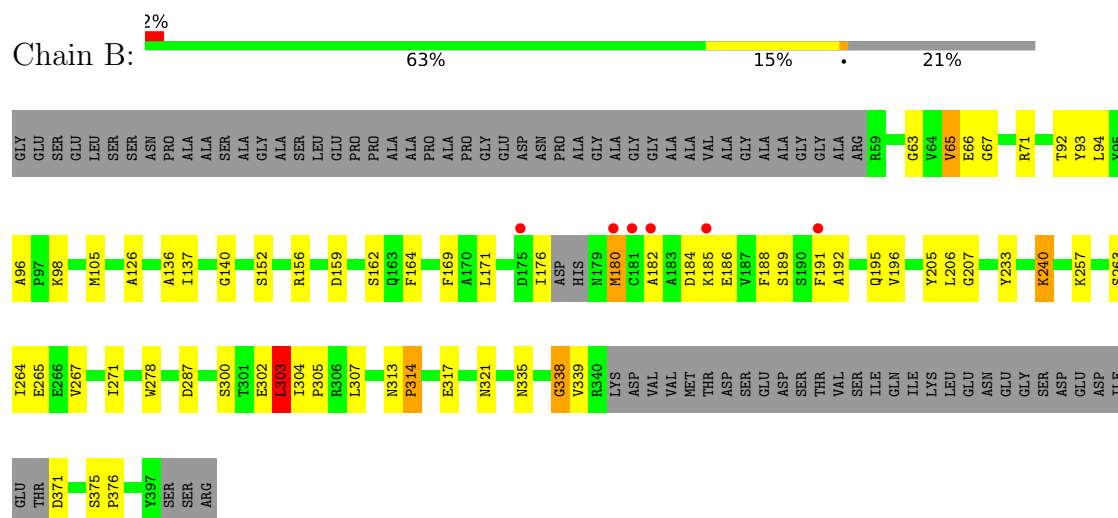
3 Residue-property plots

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: O-GlcNAcase TIM-barrel domain

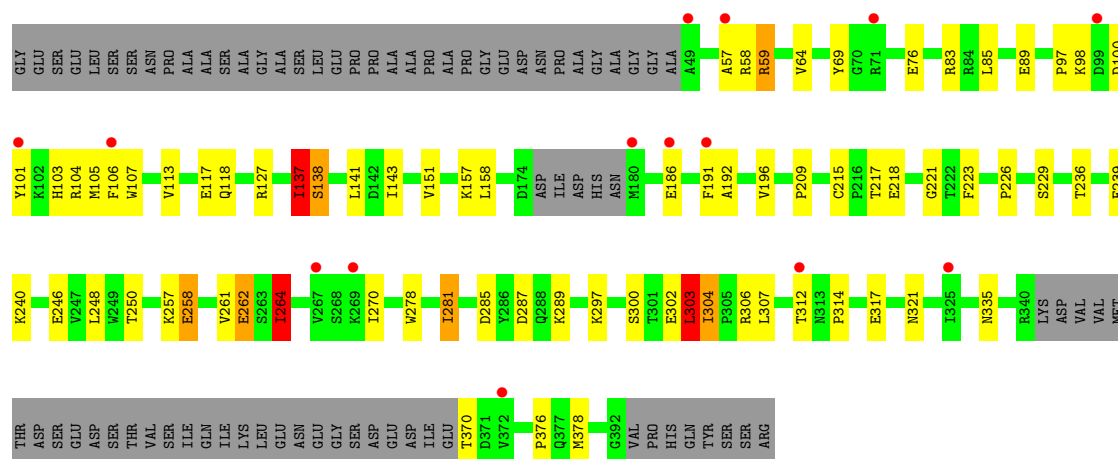


• Molecule 1: O-GlcNAcase TIM-barrel domain

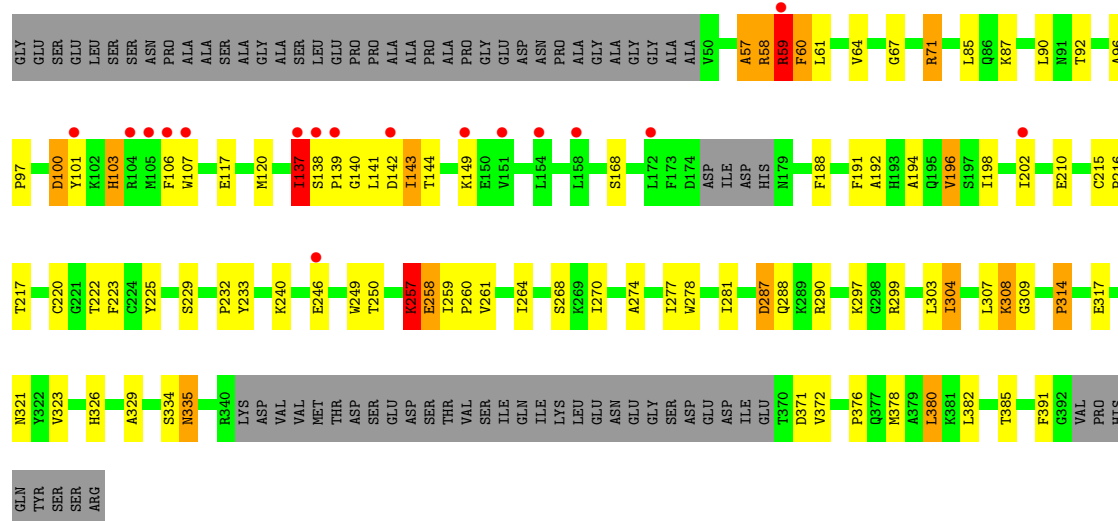


• Molecule 1: O-GlcNAcase TIM-barrel domain

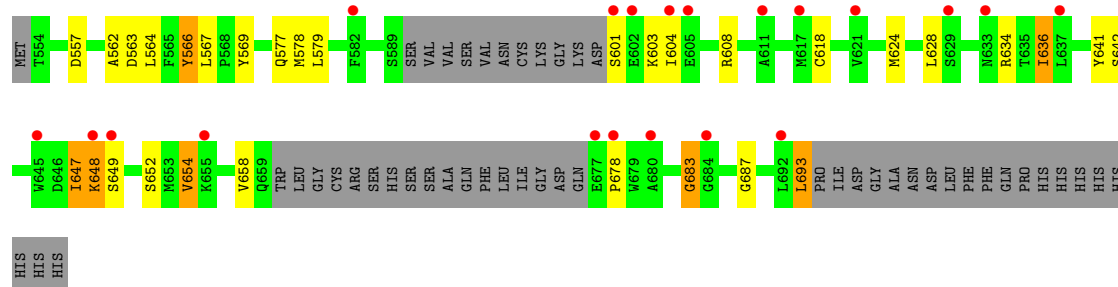




• Molecule 1: O-GlcNAcase TIM-barrel domain

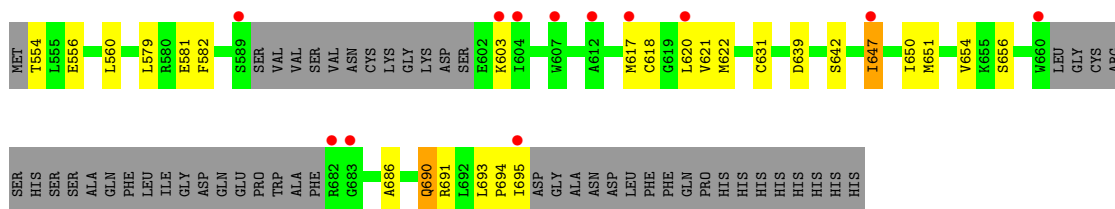


• Molecule 2: O-GlcNAcase stalk domain



• Molecule 2: O-GlcNAcase stalk domain





● Molecule 2: O-GlcNAcase stalk domain



● Molecule 2: O-GlcNAcase stalk domain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	89.72Å 91.53Å 94.52Å 77.27° 62.81° 63.03°	Depositor
Resolution (Å)	40.78 – 2.79 40.78 – 2.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.78-2.79) 100.0 (40.78-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.239 , 0.292 0.252 , 0.308	Depositor DCC
R_{free} test set	3077 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for h,l,h-k 0.000 for h,h-l,k 0.000 for h,h-k,h-l 0.000 for -h,-h+k,-l 0.000 for -h,-k,-h+l 0.000 for -h,-l,-k 0.022 for -h,-h+l,-h+k	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13813	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7936e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.84	0/2590	1.41	18/3510 (0.5%)
1	B	0.88	0/2586	1.44	23/3506 (0.7%)
1	C	0.92	2/2580 (0.1%)	1.49	24/3494 (0.7%)
1	D	0.88	0/2577	1.49	29/3491 (0.8%)
2	E	0.90	0/932	1.57	11/1251 (0.9%)
2	F	0.88	0/916	1.55	6/1230 (0.5%)
2	G	0.87	0/972	1.56	9/1305 (0.7%)
2	H	0.85	0/950	1.53	15/1276 (1.2%)
All	All	0.88	2/14103 (0.0%)	1.48	135/19063 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	264	ILE	CG1-CD1	-5.36	1.30	1.51
1	C	304	ILE	CA-CB	5.08	1.56	1.54

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	59	ARG	CA-C-N	11.29	138.66	120.94
1	D	59	ARG	C-N-CA	11.29	138.66	120.94
1	D	304	ILE	N-CA-CB	9.41	116.82	110.52
1	B	188	PHE	CA-C-N	8.02	131.83	120.28
1	B	188	PHE	C-N-CA	8.02	131.83	120.28
2	E	562	ALA	CA-C-N	7.99	130.99	120.28
2	E	562	ALA	C-N-CA	7.99	130.99	120.28
2	G	652	SER	N-CA-C	-7.81	101.16	111.24
1	C	217	THR	N-CA-C	-7.74	102.44	111.03
1	D	60	PHE	CA-CB-CG	7.61	121.41	113.80
2	H	605	GLU	N-CA-C	-7.40	103.71	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	GLU	CA-C-N	7.16	130.27	120.46
1	A	186	GLU	C-N-CA	7.16	130.27	120.46
2	H	603	LYS	N-CA-C	-6.90	102.92	112.30
1	C	127	ARG	CA-C-N	6.79	129.38	120.28
1	C	127	ARG	C-N-CA	6.79	129.38	120.28
2	E	683	GLY	N-CA-C	6.79	120.84	113.58
1	B	376	PRO	CA-C-N	6.68	129.23	120.28
1	B	376	PRO	C-N-CA	6.68	129.23	120.28
1	D	257	LYS	N-CA-C	-6.62	103.99	111.14
1	D	100	ASP	N-CA-C	-6.62	100.38	109.71
2	G	636	ILE	CA-C-N	6.56	128.97	120.44
2	G	636	ILE	C-N-CA	6.56	128.97	120.44
1	C	285	ASP	CA-CB-CG	6.54	119.14	112.60
2	H	601	SER	CA-C-N	6.50	133.96	121.54
2	H	601	SER	C-N-CA	6.50	133.96	121.54
1	C	302	GLU	CA-C-N	6.43	129.42	120.29
1	C	302	GLU	C-N-CA	6.43	129.42	120.29
2	F	603	LYS	N-CA-C	-6.38	105.80	113.97
1	B	159	ASP	CA-CB-CG	6.34	118.94	112.60
2	F	654	VAL	N-CA-C	-6.33	104.33	110.72
1	D	142	ASP	CA-CB-CG	6.24	118.84	112.60
1	B	126	ALA	CA-C-N	6.15	128.81	120.38
1	B	126	ALA	C-N-CA	6.15	128.81	120.38
1	A	304	ILE	N-CA-CB	6.08	115.19	110.45
1	B	303	LEU	CA-C-N	6.02	126.21	120.43
1	B	303	LEU	C-N-CA	6.02	126.21	120.43
1	B	287	ASP	CA-CB-CG	5.99	118.59	112.60
2	H	573	PRO	CA-C-N	5.97	128.29	120.28
2	H	573	PRO	C-N-CA	5.97	128.29	120.28
1	A	217	THR	N-CA-C	-5.91	104.92	111.36
1	D	308	LYS	N-CA-C	-5.89	106.14	113.38
1	C	239	GLU	N-CA-C	5.86	117.75	111.36
1	B	184	ASP	CA-CB-CG	5.85	118.45	112.60
2	G	604	ILE	N-CA-C	-5.83	103.62	111.44
1	C	137	ILE	CB-CA-C	5.80	118.01	110.12
1	D	223	PHE	CA-CB-CG	5.78	119.58	113.80
2	E	648	LYS	CA-C-N	5.71	128.51	120.28
2	E	648	LYS	C-N-CA	5.71	128.51	120.28
1	B	302	GLU	CA-C-N	5.70	128.39	120.29
1	B	302	GLU	C-N-CA	5.70	128.39	120.29
1	C	257	LYS	N-CA-C	-5.67	105.02	111.14
1	C	303	LEU	CA-C-N	5.66	125.86	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	303	LEU	C-N-CA	5.66	125.86	120.43
1	A	126	ALA	CA-C-N	5.64	127.83	120.28
1	A	126	ALA	C-N-CA	5.64	127.83	120.28
1	D	137	ILE	CB-CA-C	5.57	117.70	110.12
1	C	304	ILE	N-CA-CB	5.56	114.25	110.52
1	B	278	TRP	N-CA-C	-5.54	97.44	107.75
2	H	562	ALA	CA-C-N	5.51	127.66	120.28
2	H	562	ALA	C-N-CA	5.51	127.66	120.28
1	D	100	ASP	CA-C-N	5.50	132.05	121.54
1	D	100	ASP	C-N-CA	5.50	132.05	121.54
1	D	117	GLU	CA-C-N	5.50	127.58	120.44
1	D	117	GLU	C-N-CA	5.50	127.58	120.44
1	C	287	ASP	CA-CB-CG	5.49	118.09	112.60
2	E	563	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	164	PHE	CA-CB-CG	5.46	119.26	113.80
1	D	371	ASP	CA-C-N	5.45	129.67	120.29
1	D	371	ASP	C-N-CA	5.45	129.67	120.29
1	A	69	TYR	N-CA-C	-5.43	102.44	110.48
2	G	616	GLU	N-CA-C	-5.43	104.91	112.45
2	E	642	SER	N-CA-C	-5.42	105.02	111.03
2	G	603	LYS	N-CA-C	-5.40	105.50	113.61
1	C	209	PRO	CA-C-N	5.39	127.50	120.28
1	C	209	PRO	C-N-CA	5.39	127.50	120.28
1	B	338	GLY	N-CA-C	5.39	119.47	112.25
2	G	681	PHE	CA-C-N	5.36	131.78	121.54
2	G	681	PHE	C-N-CA	5.36	131.78	121.54
2	H	689	PHE	CA-C-N	5.36	128.00	120.28
2	H	689	PHE	C-N-CA	5.36	128.00	120.28
2	H	557	ASP	CA-CB-CG	5.36	117.96	112.60
1	C	58	ARG	CA-C-N	5.35	131.76	121.54
1	C	58	ARG	C-N-CA	5.35	131.76	121.54
2	G	609	SER	N-CA-C	-5.35	105.36	111.14
1	D	380	LEU	N-CA-C	-5.32	105.56	111.36
1	B	159	ASP	N-CA-C	-5.29	105.43	111.14
1	C	221	GLY	CA-C-N	5.29	127.67	120.54
1	C	221	GLY	C-N-CA	5.29	127.67	120.54
1	B	371	ASP	CA-C-N	5.28	127.92	120.42
1	B	371	ASP	C-N-CA	5.28	127.92	120.42
1	D	309	GLY	N-CA-C	5.28	118.28	110.63
1	A	106	PHE	CA-CB-CG	5.25	119.05	113.80
1	C	258	GLU	CB-CG-CD	5.25	121.52	112.60
1	D	217	THR	N-CA-C	-5.24	105.48	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	PHE	N-CA-C	5.20	117.45	109.07
1	A	174	ASP	CA-C-N	5.19	129.49	122.07
1	A	174	ASP	C-N-CA	5.19	129.49	122.07
1	A	239	GLU	CA-C-N	5.18	129.48	120.68
1	A	239	GLU	C-N-CA	5.18	129.48	120.68
1	D	57	ALA	CA-C-N	5.17	131.70	122.09
1	D	57	ALA	C-N-CA	5.17	131.70	122.09
1	D	188	PHE	CA-C-N	5.16	127.62	120.29
1	D	188	PHE	C-N-CA	5.16	127.62	120.29
2	E	578	MET	CA-C-N	5.13	127.16	120.28
2	E	578	MET	C-N-CA	5.13	127.16	120.28
1	D	287	ASP	CA-C-N	5.13	127.57	120.29
1	D	287	ASP	C-N-CA	5.13	127.57	120.29
1	A	302	GLU	CA-C-N	5.12	128.10	120.31
1	A	302	GLU	C-N-CA	5.12	128.10	120.31
1	D	268	SER	CA-C-N	5.12	127.14	120.28
1	D	268	SER	C-N-CA	5.12	127.14	120.28
2	F	603	LYS	CA-C-N	5.12	127.11	120.56
2	F	603	LYS	C-N-CA	5.12	127.11	120.56
2	H	652	SER	CA-C-N	5.12	127.13	120.28
2	H	652	SER	C-N-CA	5.12	127.13	120.28
1	D	194	ALA	CA-C-N	5.10	127.07	120.44
1	D	194	ALA	C-N-CA	5.10	127.07	120.44
1	A	164	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	184	ASP	CA-CB-CG	5.09	117.69	112.60
1	C	117	GLU	CA-C-N	5.08	127.05	120.44
1	C	117	GLU	C-N-CA	5.08	127.05	120.44
2	E	579	LEU	CA-C-N	5.07	127.08	120.28
2	E	579	LEU	C-N-CA	5.07	127.08	120.28
2	F	579	LEU	CA-C-N	5.04	126.99	120.44
2	F	579	LEU	C-N-CA	5.04	126.99	120.44
1	C	261	VAL	CA-C-N	5.04	127.34	120.54
1	C	261	VAL	C-N-CA	5.04	127.34	120.54
1	B	195	GLN	CA-C-N	5.03	127.09	120.60
1	B	195	GLN	C-N-CA	5.03	127.09	120.60
1	B	66	GLU	N-CA-C	-5.02	99.82	108.56
1	A	191	PHE	CA-C-N	5.01	127.25	120.38
1	A	191	PHE	C-N-CA	5.01	127.25	120.38
2	H	620	LEU	CA-C-N	5.01	126.83	120.72
2	H	620	LEU	C-N-CA	5.01	126.83	120.72

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	2522	0	2472	23	0
1	B	2518	0	2461	21	0
1	C	2515	0	2474	27	0
1	D	2512	0	2464	42	0
2	E	912	0	887	12	0
2	F	896	0	880	11	0
2	G	949	0	932	11	0
2	H	928	0	905	10	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	1	0
3	D	6	0	8	0	0
4	A	5	0	0	0	0
4	B	11	0	0	0	0
4	C	8	0	0	1	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
4	H	4	0	0	0	0
All	All	13813	0	13507	144	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 5.

All (144) 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:104:ARG:HG3	1:C:138:SER:HB2	1.64	0.79
1:D:58:ARG:O	1:D:59:ARG:HB2	1.82	0.76
1:C:97:PRO:HB2	1:C:100:ASP:HB2	1.74	0.69
1:D:71:ARG:HE	2:H:641:TYR:HD1	1.41	0.68
1:B:180:MET:HB3	1:B:185:LYS:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:TYR:O	1:D:232:PRO:HD2	1.96	0.65
2:F:617:MET:HA	2:F:620:LEU:HD23	1.79	0.63
2:G:657:PHE:O	2:G:660:TRP:HB2	1.99	0.63
1:C:98:LYS:HE2	3:C:501:GOL:O2	1.99	0.63
1:D:59:ARG:CG	1:D:59:ARG:HH21	2.12	0.62
1:C:300:SER:O	1:C:303:LEU:HB2	2.01	0.61
1:D:196:VAL:HG11	1:D:240:LYS:HB2	1.83	0.61
1:B:263:SER:O	1:B:267:VAL:HG23	2.00	0.60
1:A:71:ARG:HD3	1:B:71:ARG:HD2	1.84	0.60
1:D:229:SER:O	1:D:270:ILE:HD12	2.02	0.59
2:F:650:ILE:HD13	2:G:686:ALA:HB1	1.85	0.58
1:B:314:PRO:HB2	1:B:321:ASN:OD1	2.04	0.58
1:D:97:PRO:HB2	1:D:100:ASP:HB2	1.86	0.57
1:D:192:ALA:HB2	1:D:233:TYR:CD1	2.40	0.57
1:D:67:GLY:HA2	1:D:96:ALA:O	2.04	0.57
1:B:67:GLY:HA2	1:B:96:ALA:O	2.04	0.57
1:B:192:ALA:HB2	1:B:233:TYR:CD1	2.41	0.56
2:H:683:GLY:HA3	2:H:687:GLY:HA3	1.87	0.55
1:B:196:VAL:HG11	1:B:240:LYS:HB2	1.88	0.55
1:C:64:VAL:HG23	1:C:85:LEU:HD21	1.88	0.55
1:B:264:ILE:HD13	1:B:307:LEU:HD21	1.89	0.55
1:B:304:ILE:HD12	1:B:335:ASN:HB3	1.88	0.55
1:C:100:ASP:HB3	1:C:103:HIS:HD2	1.72	0.55
1:D:261:VAL:HG22	1:D:303:LEU:HD12	1.89	0.54
1:A:78:ARG:HB3	1:A:122:LEU:HD11	1.89	0.54
2:G:555:LEU:O	2:G:559:GLN:HG3	2.08	0.53
1:C:297:LYS:HG3	1:C:376:PRO:HG3	1.89	0.53
2:F:618:CYS:O	2:F:622:MET:HG2	2.09	0.53
2:H:656:SER:HA	2:H:659:GLN:HG2	1.90	0.53
1:B:140:GLY:HA3	1:B:176:ILE:HG21	1.91	0.52
1:C:312:THR:O	1:C:314:PRO:HD3	2.09	0.52
1:B:305:PRO:HB3	1:B:338:GLY:HA3	1.92	0.52
1:D:59:ARG:HH21	1:D:59:ARG:HG2	1.74	0.52
1:D:326:HIS:HE1	1:D:382:LEU:HD23	1.75	0.51
1:A:94:LEU:HD11	1:A:136:ALA:HB2	1.92	0.51
1:A:237:VAL:O	1:A:241:LEU:HB3	2.11	0.51
2:F:694:PRO:O	2:F:695:ILE:HG13	2.11	0.51
1:A:297:LYS:HG3	1:A:376:PRO:HG3	1.93	0.51
2:G:556:GLU:H	2:G:556:GLU:CD	2.19	0.51
2:E:683:GLY:HA3	2:E:687:GLY:HA3	1.93	0.50
2:E:601:SER:C	2:E:603:LYS:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:647:ILE:O	2:F:651:MET:HG2	2.10	0.50
1:C:229:SER:O	1:C:270:ILE:HD12	2.12	0.50
2:H:652:SER:HA	2:H:655:LYS:HE3	1.93	0.50
2:F:686:ALA:HB1	2:G:650:ILE:HD13	1.93	0.50
1:D:264:ILE:CD1	1:D:303:LEU:HG	2.42	0.49
1:D:304:ILE:HD12	1:D:335:ASN:HB3	1.94	0.49
2:H:621:VAL:HG11	2:H:651:MET:HG3	1.95	0.49
1:C:137:ILE:HG21	1:C:158:LEU:HD21	1.94	0.49
2:E:693:LEU:HD22	2:H:653:MET:HE3	1.94	0.49
1:D:314:PRO:HB2	1:D:321:ASN:OD1	2.13	0.49
2:G:650:ILE:O	2:G:654:VAL:HG23	2.13	0.49
1:B:63:GLY:HA3	1:B:92:THR:O	2.13	0.48
2:F:560:LEU:HD21	2:F:621:VAL:HG22	1.94	0.48
1:A:75:MET:HB3	1:A:79:LYS:NZ	2.28	0.48
1:A:67:GLY:HA2	1:A:96:ALA:O	2.14	0.48
1:D:257:LYS:HG3	2:E:569:TYR:CG	2.49	0.48
2:F:556:GLU:H	2:F:556:GLU:CD	2.23	0.47
1:D:277:ILE:HG12	1:D:307:LEU:HD22	1.97	0.47
2:E:557:ASP:HB3	2:E:624:MET:HG2	1.97	0.47
1:C:314:PRO:HB2	1:C:321:ASN:OD1	2.15	0.47
1:D:59:ARG:HG2	1:D:59:ARG:NH2	2.28	0.47
1:D:220:CYS:HB3	1:D:250:THR:OG1	2.15	0.47
1:D:64:VAL:HG23	1:D:85:LEU:HD21	1.96	0.47
1:C:304:ILE:HD12	1:C:335:ASN:HB3	1.97	0.47
1:C:101:TYR:HB3	1:C:106:PHE:HD2	1.80	0.47
1:D:323:VAL:HG11	1:D:380:LEU:HD12	1.97	0.47
1:A:249:TRP:O	1:A:277:ILE:HA	2.15	0.46
1:A:335:ASN:HB2	1:A:373:LEU:HD13	1.97	0.46
1:A:250:THR:HG22	1:A:278:TRP:HB3	1.96	0.46
2:H:603:LYS:O	2:H:606:GLU:HB3	2.16	0.46
1:A:296:TYR:CZ	1:A:299:ARG:HD3	2.51	0.46
1:D:287:ASP:HB3	1:D:290:ARG:HB2	1.97	0.46
2:F:690:GLN:HA	2:F:693:LEU:HD12	1.99	0.45
1:B:152:SER:O	1:B:156:ARG:HG3	2.17	0.45
1:C:218:GLU:HG2	1:C:223:PHE:O	2.16	0.45
1:A:300:SER:O	1:A:303:LEU:HB2	2.17	0.45
2:E:566:TYR:HB3	2:E:567:LEU:H	1.65	0.45
1:D:143:ILE:HG13	1:D:144:THR:N	2.31	0.45
1:D:198:ILE:O	1:D:202:ILE:HG12	2.16	0.45
1:B:300:SER:O	1:B:303:LEU:HB2	2.17	0.44
1:C:264:ILE:HD11	4:C:601:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:656:SER:O	2:H:660:TRP:HB3	2.18	0.44
1:D:249:TRP:O	1:D:277:ILE:HA	2.16	0.44
1:D:103:HIS:HD2	1:D:137:ILE:HA	1.82	0.44
2:G:625:PHE:CD1	2:G:644:VAL:HG13	2.52	0.44
1:D:250:THR:HG22	1:D:278:TRP:HB3	2.00	0.44
1:D:297:LYS:HG3	1:D:376:PRO:HG3	2.00	0.44
1:A:148:PRO:HA	1:A:151:VAL:HG22	2.00	0.44
1:B:162:SER:HB3	1:B:169:PHE:HZ	1.82	0.44
1:C:192:ALA:HB1	1:C:236:THR:HB	2.00	0.44
1:A:302:GLU:O	1:A:305:PRO:HD2	2.18	0.44
1:D:58:ARG:HD3	1:D:58:ARG:HA	1.79	0.44
2:F:693:LEU:HD21	2:G:654:VAL:HA	2.00	0.44
2:H:604:ILE:O	2:H:608:ARG:HB2	2.18	0.44
1:A:152:SER:O	1:A:156:ARG:HG3	2.18	0.43
1:B:65:VAL:O	1:B:313:ASN:HA	2.18	0.43
1:C:250:THR:HG22	1:C:278:TRP:HB3	2.00	0.43
2:E:564:LEU:HD13	2:E:647:ILE:HG12	2.00	0.43
1:B:94:LEU:HD11	1:B:136:ALA:HB2	2.00	0.43
1:C:107:TRP:HB2	1:C:137:ILE:HD11	2.00	0.43
1:D:71:ARG:NE	2:H:641:TYR:CD1	2.81	0.43
1:C:196:VAL:HG11	1:C:240:LYS:HB2	1.99	0.43
1:D:257:LYS:C	1:D:258:GLU:HG2	2.43	0.43
1:C:101:TYR:OH	2:E:649:SER:HA	2.18	0.43
1:B:92:THR:HG22	1:B:93:TYR:N	2.34	0.43
1:B:205:TYR:C	1:B:207:GLY:H	2.26	0.43
1:D:96:ALA:N	1:D:97:PRO:HD3	2.33	0.43
1:C:69:TYR:HE2	1:C:104:ARG:HH12	1.66	0.43
1:B:137:ILE:HG23	1:B:171:LEU:HD23	2.01	0.43
1:D:59:ARG:HB3	1:D:60:PHE:H	1.61	0.42
1:A:174:ASP:HB2	1:A:219:TYR:CE2	2.55	0.42
2:E:652:SER:C	2:E:654:VAL:H	2.27	0.42
1:C:157:LYS:HD2	1:C:157:LYS:HA	1.91	0.42
1:C:264:ILE:HD13	1:C:307:LEU:HD23	2.02	0.42
1:D:274:ALA:HB3	1:D:308:LYS:HG2	2.02	0.42
1:C:215:CYS:HA	1:C:248:LEU:HB2	2.02	0.42
2:G:625:PHE:CZ	2:G:647:ILE:HG23	2.55	0.42
1:A:102:LYS:HE2	2:G:638:TYR:OH	2.20	0.42
1:A:278:TRP:CD1	1:A:278:TRP:C	2.98	0.42
1:D:391:PHE:CE2	2:E:636:ILE:HD13	2.55	0.42
1:D:258:GLU:O	1:D:260:PRO:HD3	2.20	0.41
1:D:259:ILE:HD12	1:D:299:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ASN:OD1	1:A:230:GLN:HB2	2.20	0.41
1:C:262:GLU:H	1:C:262:GLU:CD	2.28	0.41
1:A:158:LEU:HD22	1:A:169:PHE:CD1	2.54	0.41
1:D:107:TRP:CE2	1:D:139:PRO:HB3	2.56	0.41
1:A:189:SER:O	1:A:190:SER:HB3	2.19	0.41
2:E:654:VAL:O	2:E:658:VAL:HG23	2.21	0.41
1:D:61:LEU:HG	1:D:92:THR:HG21	2.02	0.41
1:A:242:LEU:HD23	1:A:243:PRO:HD2	2.04	0.40
1:B:267:VAL:O	1:B:271:ILE:HG12	2.21	0.40
1:D:90:LEU:HD11	1:D:329:ALA:HB2	2.02	0.40
1:D:215:CYS:HA	1:D:216:PRO:HD3	1.98	0.40
1:D:288:GLN:CD	1:D:288:GLN:H	2.29	0.40
1:C:76:GLU:H	2:E:634:ARG:HH21	1.69	0.40
1:A:102:LYS:HE3	1:A:115:GLU:OE2	2.21	0.40
1:C:264:ILE:HD11	1:C:306:ARG:O	2.22	0.40
2:F:582:PHE:HE2	2:G:692:LEU:HB2	1.87	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	301/388 (78%)	280 (93%)	20 (7%)	1 (0%)	36	66
1	B	301/388 (78%)	281 (93%)	16 (5%)	4 (1%)	9	31
1	C	304/388 (78%)	279 (92%)	19 (6%)	6 (2%)	6	21
1	D	304/388 (78%)	273 (90%)	24 (8%)	7 (2%)	5	18
2	E	106/161 (66%)	94 (89%)	9 (8%)	3 (3%)	4	14
2	F	103/161 (64%)	100 (97%)	3 (3%)	0	100	100
2	G	108/161 (67%)	97 (90%)	9 (8%)	2 (2%)	6	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	106/161 (66%)	98 (92%)	7 (7%)	1 (1%)	14	41
All	All	1633/2196 (74%)	1502 (92%)	107 (7%)	24 (2%)	8	28

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	182	ALA
1	D	59	ARG
1	D	101	TYR
2	E	678	PRO
2	G	694	PRO
2	H	602	GLU
1	C	59	ARG
1	D	57	ALA
1	D	140	GLY
2	G	682	ARG
1	C	57	ALA
1	C	105	MET
2	E	566	TYR
1	B	105	MET
1	C	141	LEU
1	D	141	LEU
1	D	335	ASN
2	E	641	TYR
1	A	314	PRO
1	D	314	PRO
1	B	314	PRO
1	B	339	VAL
1	C	281	ILE
1	C	226	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	275/331 (83%)	259 (94%)	16 (6%)	18	49
1	B	274/331 (83%)	261 (95%)	13 (5%)	23	57
1	C	270/331 (82%)	249 (92%)	21 (8%)	11	35
1	D	270/331 (82%)	245 (91%)	25 (9%)	8	27
2	E	95/140 (68%)	85 (90%)	10 (10%)	6	22
2	F	94/140 (67%)	85 (90%)	9 (10%)	8	26
2	G	99/140 (71%)	88 (89%)	11 (11%)	6	20
2	H	96/140 (69%)	84 (88%)	12 (12%)	4	15
All	All	1473/1884 (78%)	1356 (92%)	117 (8%)	11	35

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	154	LEU
1	A	157	LYS
1	A	181	CYS
1	A	228	VAL
1	A	239	GLU
1	A	257	LYS
1	A	264	ILE
1	A	267	VAL
1	A	270	ILE
1	A	301	THR
1	A	303	LEU
1	A	317	GLU
1	A	337	ASN
1	A	373	LEU
1	A	377	GLN
1	B	65	VAL
1	B	98	LYS
1	B	180	MET
1	B	186	GLU
1	B	189	SER
1	B	191	PHE
1	B	206	LEU
1	B	240	LYS
1	B	257	LYS
1	B	265	GLU
1	B	303	LEU

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Mol	Chain	Res	Type
1	B	317	GLU
1	B	375	SER
1	C	59	ARG
1	C	83	ARG
1	C	89	GLU
1	C	113	VAL
1	C	118	GLN
1	C	137	ILE
1	C	138	SER
1	C	143	ILE
1	C	151	VAL
1	C	186	GLU
1	C	191	PHE
1	C	246	GLU
1	C	258	GLU
1	C	262	GLU
1	C	264	ILE
1	C	281	ILE
1	C	289	LYS
1	C	303	LEU
1	C	317	GLU
1	C	370	THR
1	C	378	MET
1	D	58	ARG
1	D	59	ARG
1	D	71	ARG
1	D	87	LYS
1	D	103	HIS
1	D	106	PHE
1	D	120	MET
1	D	137	ILE
1	D	138	SER
1	D	143	ILE
1	D	149	LYS
1	D	168	SER
1	D	191	PHE
1	D	196	VAL
1	D	210	GLU
1	D	222	THR
1	D	246	GLU
1	D	257	LYS
1	D	258	GLU

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Mol	Chain	Res	Type
1	D	281	ILE
1	D	317	GLU
1	D	334	SER
1	D	372	VAL
1	D	378	MET
1	D	385	THR
2	E	577	GLN
2	E	604	ILE
2	E	608	ARG
2	E	618	CYS
2	E	628	LEU
2	E	636	ILE
2	E	647	ILE
2	E	648	LYS
2	E	654	VAL
2	E	693	LEU
2	F	554	THR
2	F	581	GLU
2	F	631	CYS
2	F	639	ASP
2	F	642	SER
2	F	647	ILE
2	F	656	SER
2	F	690	GLN
2	F	691	ARG
2	G	613	LYS
2	G	640	MET
2	G	647	ILE
2	G	651	MET
2	G	653	MET
2	G	658	VAL
2	G	682	ARG
2	G	688	GLU
2	G	690	GLN
2	G	693	LEU
2	G	695	ILE
2	H	559	GLN
2	H	563	ASP
2	H	570	GLU
2	H	602	GLU
2	H	609	SER
2	H	616	GLU

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Mol	Chain	Res	Type
2	H	620	LEU
2	H	639	ASP
2	H	644	VAL
2	H	646	ASP
2	H	676	GLN
2	H	681	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	389	GLN
1	A	395	HIS
1	B	395	HIS
1	C	77	GLN
1	C	118	GLN
1	C	204	GLN
1	C	389	GLN
1	D	86	GLN
1	D	118	GLN
1	D	147	ASN
1	D	313	ASN
2	E	577	GLN
2	F	659	GLN
2	H	630	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 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	$\# Z > 2$
3	GOL	C	501	-	5,5,5	0.20	0	5,5,5	0.40	0
3	GOL	D	501	-	5,5,5	0.12	0	5,5,5	0.47	0
3	GOL	B	501	-	5,5,5	0.13	0	5,5,5	0.31	0
3	GOL	A	501	-	5,5,5	0.14	0	5,5,5	0.57	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
3	GOL	C	501	-	-	1/4/4/4	-
3	GOL	D	501	-	-	0/4/4/4	-
3	GOL	B	501	-	-	0/4/4/4	-
3	GOL	A	501	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	501	GOL	O2-C2-C3-O3
3	A	501	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	307/388 (79%)	0.19	7 (2%) 61 51	35, 49, 67, 80	0
1	B	307/388 (79%)	-0.01	6 (1%) 65 56	32, 45, 61, 74	0
1	C	310/388 (79%)	0.39	14 (4%) 38 30	26, 52, 77, 100	0
1	D	310/388 (79%)	0.69	17 (5%) 30 23	32, 63, 96, 115	0
2	E	112/161 (69%)	1.28	20 (17%) 3 3	49, 79, 104, 118	0
2	F	109/161 (67%)	0.74	12 (11%) 10 8	35, 57, 78, 91	0
2	G	114/161 (70%)	0.81	14 (12%) 8 6	34, 58, 86, 108	0
2	H	112/161 (69%)	1.35	21 (18%) 3 2	46, 78, 109, 121	0
All	All	1681/2196 (76%)	0.51	111 (6%) 24 18	26, 54, 93, 121	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	680	ALA	4.2
2	E	645	TRP	4.1
1	D	104	ARG	4.1
1	D	151	VAL	4.1
2	H	641	TYR	3.8
1	A	372	VAL	3.7
1	D	154	LEU	3.6
2	G	682	ARG	3.6
1	D	139	PRO	3.5
2	G	681	PHE	3.4
2	H	625	PHE	3.4
2	H	604	ILE	3.3
2	G	601	SER	3.3
1	D	138	SER	3.3
2	F	589	SER	3.3
2	F	603	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	106	PHE	3.2
2	G	604	ILE	3.2
1	C	99	ASP	3.2
2	H	645	TRP	3.2
2	H	637	LEU	3.1
2	G	695	ILE	3.1
2	E	604	ILE	3.1
1	B	185	LYS	3.0
2	F	612	ALA	3.0
1	C	49	ALA	3.0
1	C	191	PHE	3.0
2	E	637	LEU	2.9
2	E	649	SER	2.9
1	D	101	TYR	2.9
1	C	57	ALA	2.9
2	F	620	LEU	2.8
1	D	158	LEU	2.8
2	H	686	ALA	2.8
1	D	246	GLU	2.7
2	F	695	ILE	2.7
2	F	683	GLY	2.7
2	H	652	SER	2.7
2	E	678	PRO	2.7
1	B	180	MET	2.7
1	A	179	ASN	2.7
2	E	601	SER	2.7
2	G	656	SER	2.7
2	H	649	SER	2.7
2	H	554	THR	2.7
2	E	677	GLU	2.6
2	E	680	ALA	2.6
2	H	658	VAL	2.6
2	E	617	MET	2.6
2	E	621	VAL	2.6
2	F	617	MET	2.6
2	H	601	SER	2.6
2	H	607	TRP	2.6
1	C	267	VAL	2.6
2	H	660	TRP	2.5
2	G	599	LYS	2.5
1	C	372	VAL	2.5
2	G	617	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	202	ILE	2.5
1	A	231	SER	2.4
2	F	607	TRP	2.4
2	E	633	ASN	2.4
2	E	648	LYS	2.4
1	C	186	GLU	2.4
2	E	602	GLU	2.4
2	E	629	SER	2.4
2	G	652	SER	2.4
2	F	682	ARG	2.4
2	G	620	LEU	2.3
2	F	604	ILE	2.3
2	E	684	GLY	2.3
2	E	692	LEU	2.3
1	D	107	TRP	2.3
2	E	582	PHE	2.3
1	A	225	TYR	2.3
1	B	181	CYS	2.2
2	E	611	ALA	2.2
2	F	660	TRP	2.2
2	G	693	LEU	2.2
2	H	685	LEU	2.2
2	H	657	PHE	2.2
1	C	180	MET	2.2
1	D	59	ARG	2.2
1	C	269	LYS	2.2
2	E	655	LYS	2.2
1	D	137	ILE	2.2
1	B	175	ASP	2.2
2	H	587	ALA	2.2
2	H	575	GLY	2.2
1	D	142	ASP	2.2
1	C	106	PHE	2.2
1	A	182	ALA	2.1
1	B	182	ALA	2.1
2	H	611	ALA	2.1
1	C	71	ARG	2.1
1	A	181	CYS	2.1
1	C	101	TYR	2.1
2	H	638	TYR	2.1
1	C	325	ILE	2.1
1	A	259	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	657	PHE	2.1
1	D	149	LYS	2.1
2	H	693	LEU	2.1
2	F	647	ILE	2.1
1	C	312	THR	2.1
2	G	683	GLY	2.1
2	E	605	GLU	2.0
1	D	172	LEU	2.0
1	B	191	PHE	2.0
2	H	615	GLU	2.0
1	D	105	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	D	501	6/6	0.77	0.14	46,51,51,52	0
3	GOL	B	501	6/6	0.90	0.13	58,60,62,63	0
3	GOL	A	501	6/6	0.91	0.13	52,54,55,56	0
3	GOL	C	501	6/6	0.93	0.11	53,55,56,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.