



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:15 PM UTC

PDB ID : 1GOI / pdb_00001goi
Title : Crystal structure of the D140N mutant of chitinase B from *Serratia marcescens* at 1.45 Å resolution
Authors : Kolstad, G.; Synstad, B.; Eijsink, V.G.H.; Van Aalten, D.M.F.
Deposited on : 2001-10-21
Resolution : 1.45 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

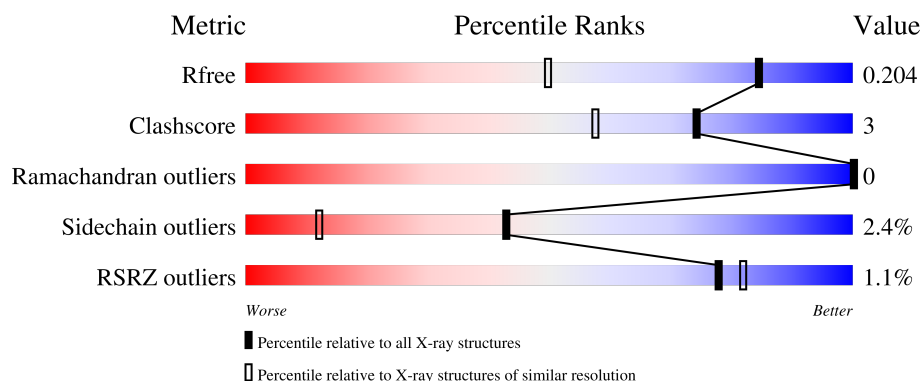
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	499	81%17%.
1	B	499	83%15%.

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	1500	-	X	-	-
2	GOL	B	1501	-	X	-	-
2	GOL	B	1502	-	X	-	-
2	GOL	B	1505	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8990 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 CHITINASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	10	1
			3926	2511	660	741	14			
1	B	497	Total	C	N	O	S	0	14	0
			3972	2536	677	745	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	ASN	ASP	engineered mutation	UNP Q54276
B	140	ASN	ASP	engineered mutation	UNP Q54276

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

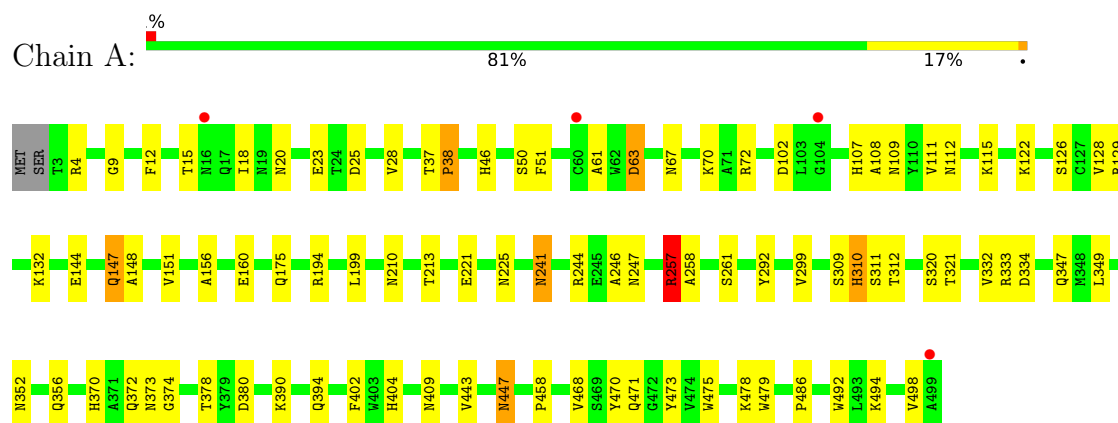
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	446	Total O 446 446	0	0
4	B	554	Total O 554 554	0	0

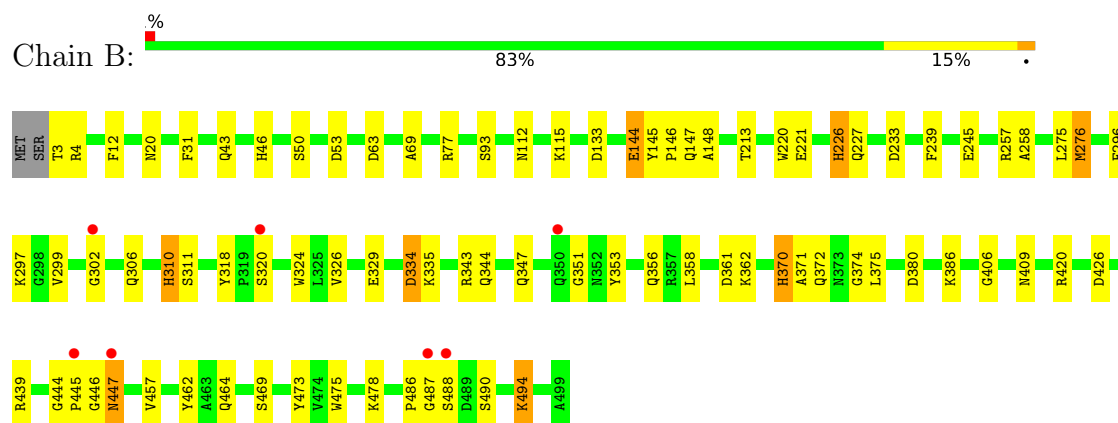
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CHITINASE B



• Molecule 1: CHITINASE B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.90Å 104.02Å 186.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 1.45 17.00 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.3 (17.00-1.45) 94.0 (17.00-1.45)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 1.45Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.160 , 0.220 0.157 , 0.204	Depositor DCC
R_{free} test set	1921 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 61.9	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	0.97	EDS
Total number of atoms	8990	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	0.87	1/4076 (0.0%)	1.79	73/5558 (1.3%)
1	B	0.89	0/4142	1.68	77/5638 (1.4%)
All	All	0.88	1/8218 (0.0%)	1.73	150/11196 (1.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	498	VAL	C-N	-5.47	1.25	1.33

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	ASN	OD1-CG-ND2	-18.92	103.68	122.60
1	A	311	SER	CA-C-N	16.32	144.30	121.61
1	A	311	SER	C-N-CA	16.32	144.30	121.61
1	A	443	VAL	CA-C-N	12.20	141.03	121.87
1	A	443	VAL	C-N-CA	12.20	141.03	121.87
1	A	447	ASN	CB-CG-OD1	11.82	144.44	120.80
1	B	257	ARG	NE-CZ-NH2	11.00	129.10	119.20
1	B	370	HIS	CG-CD2-NE2	10.29	117.49	107.20
1	A	447	ASN	CA-CB-CG	10.19	122.79	112.60
1	B	311	SER	CA-C-N	9.96	135.15	121.20
1	B	311	SER	C-N-CA	9.96	135.15	121.20
1	A	310	HIS	CG-CD2-NE2	9.02	116.22	107.20
1	A	241	ASN	OD1-CG-ND2	-8.81	113.79	122.60
1	B	227	GLN	OE1-CD-NE2	-8.75	113.85	122.60
1	B	318	TYR	O-C-N	8.65	128.22	121.47
1	A	311	SER	O-C-N	-8.57	110.25	121.83
1	B	43	GLN	OE1-CD-NE2	-8.45	114.16	122.60
1	A	63	ASP	CA-CB-CG	8.35	120.95	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ARG	NE-CZ-NH2	8.25	126.62	119.20
1	B	115	LYS	N-CA-C	8.13	120.22	111.36
1	B	343	ARG	NE-CZ-NH1	-8.10	113.40	121.50
1	A	352	ASN	OD1-CG-ND2	-7.96	114.64	122.60
1	B	351	GLY	O-C-N	7.77	129.35	121.97
1	B	144	GLU	CA-C-N	7.74	135.62	121.70
1	B	144	GLU	C-N-CA	7.74	135.62	121.70
1	A	247	ASN	OD1-CG-ND2	-7.70	114.90	122.60
1	B	457	VAL	CB-CA-C	-7.67	103.79	111.08
1	B	310	HIS	CG-CD2-NE2	7.60	114.80	107.20
1	B	112	ASN	OD1-CG-ND2	-7.58	115.02	122.60
1	A	129	ARG	CD-NE-CZ	7.36	134.70	124.40
1	B	488	SER	O-C-N	7.35	131.31	122.27
1	A	50	SER	CA-C-O	-7.32	111.81	120.60
1	B	426	ASP	CA-CB-CG	7.30	119.90	112.60
1	A	102	ASP	CA-CB-CG	7.19	119.79	112.60
1	A	311	SER	CA-C-O	7.18	129.65	121.32
1	B	311	SER	CA-C-O	7.18	129.48	120.65
1	B	370	HIS	CE1-NE2-CD2	-7.10	101.90	109.00
1	B	347	GLN	CB-CG-CD	7.07	124.63	112.60
1	B	361	ASP	CA-CB-CG	-6.97	105.63	112.60
1	B	370	HIS	CB-CG-ND1	6.86	132.98	122.70
1	B	347	GLN	OE1-CD-NE2	-6.84	115.76	122.60
1	B	302	GLY	O-C-N	-6.83	115.03	122.54
1	A	210	ASN	CA-CB-CG	6.80	119.40	112.60
1	A	309	SER	O-C-N	-6.76	114.70	122.68
1	B	334	ASP	CA-C-O	6.76	127.26	119.35
1	A	4	ARG	NE-CZ-NH2	6.76	125.28	119.20
1	A	112	ASN	OD1-CG-ND2	-6.74	115.86	122.60
1	A	108	ALA	CA-C-O	6.71	127.68	120.10
1	A	46	HIS	CA-CB-CG	6.64	120.44	113.80
1	A	310	HIS	CE1-NE2-CD2	-6.63	102.37	109.00
1	A	148	ALA	CA-C-N	6.57	129.08	120.28
1	A	148	ALA	C-N-CA	6.57	129.08	120.28
1	A	225	ASN	OD1-CG-ND2	-6.55	116.05	122.60
1	A	109	ASN	O-C-N	6.53	130.30	122.27
1	B	296	PHE	CA-CB-CG	6.52	120.32	113.80
1	B	302	GLY	N-CA-C	6.51	122.32	113.99
1	B	372	GLN	CA-C-N	6.50	132.60	122.26
1	B	372	GLN	C-N-CA	6.50	132.60	122.26
1	A	15	THR	CA-CB-OG1	-6.46	99.91	109.60
1	A	144	GLU	CA-C-N	6.42	133.26	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	GLU	C-N-CA	6.42	133.26	121.70
1	A	312	THR	N-CA-CB	6.41	118.63	110.23
1	A	20	ASN	CA-CB-CG	-6.40	106.20	112.60
1	A	23	GLU	CA-C-N	-6.40	111.91	122.08
1	A	23	GLU	C-N-CA	-6.40	111.91	122.08
1	B	372	GLN	O-C-N	-6.36	115.38	122.12
1	B	444	GLY	CA-C-O	-6.31	112.50	121.52
1	B	146	PRO	CA-C-N	-6.29	112.30	122.36
1	B	146	PRO	C-N-CA	-6.29	112.30	122.36
1	A	210	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	A	12	PHE	CA-CB-CG	-6.26	107.54	113.80
1	B	420[A]	ARG	CD-NE-CZ	6.25	133.15	124.40
1	B	420[B]	ARG	CD-NE-CZ	6.25	133.15	124.40
1	B	133	ASP	CA-CB-CG	6.24	118.84	112.60
1	A	458	PRO	CA-C-O	6.17	128.38	121.34
1	B	370	HIS	ND1-CG-CD2	-6.11	99.99	106.10
1	B	329	GLU	CA-C-N	6.06	128.40	120.28
1	B	329	GLU	C-N-CA	6.06	128.40	120.28
1	A	15	THR	N-CA-C	6.05	119.49	111.75
1	A	108	ALA	O-C-N	-6.04	115.15	122.22
1	B	276	MET	CA-CB-CG	6.02	126.14	114.10
1	A	257	ARG	NE-CZ-NH2	-6.00	113.80	119.20
1	B	409	ASN	CA-CB-CG	6.00	118.60	112.60
1	B	77	ARG	CG-CD-NE	-5.96	98.88	112.00
1	A	404	HIS	ND1-CE1-NE2	-5.90	102.50	108.40
1	B	488	SER	N-CA-CB	5.89	119.41	110.28
1	B	344	GLN	CG-CD-OE1	5.88	132.57	120.80
1	A	370	HIS	ND1-CE1-NE2	-5.86	102.54	108.40
1	A	347	GLN	CB-CG-CD	5.86	122.56	112.60
1	B	310	HIS	CE1-NE2-CD2	-5.85	103.15	109.00
1	B	226	HIS	CB-CG-CD2	-5.80	123.65	131.20
1	B	344	GLN	OE1-CD-NE2	-5.80	116.80	122.60
1	B	488	SER	N-CA-C	-5.79	105.10	111.82
1	B	486	PRO	O-C-N	-5.76	116.06	123.03
1	A	25	ASP	CA-C-O	5.74	128.18	120.89
1	A	372	GLN	CA-C-O	5.73	126.56	119.97
1	A	402	PHE	CA-CB-CG	5.71	119.52	113.80
1	A	404	HIS	CA-CB-CG	5.71	119.51	113.80
1	B	69	ALA	O-C-N	5.68	128.14	122.12
1	A	332	VAL	N-CA-C	-5.64	104.85	111.00
1	A	28	VAL	CA-C-O	5.63	125.59	120.30
1	B	93	SER	O-C-N	5.63	129.63	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	HIS	ND1-CG-CD2	-5.62	100.48	106.10
1	A	370	HIS	ND1-CG-CD2	-5.59	100.51	106.10
1	B	239	PHE	CA-CB-CG	-5.57	108.23	113.80
1	A	175	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	A	194	ARG	CD-NE-CZ	5.51	132.11	124.40
1	A	409	ASN	CA-CB-CG	5.50	118.10	112.60
1	B	275	LEU	CA-C-N	5.48	128.64	120.31
1	B	275	LEU	C-N-CA	5.48	128.64	120.31
1	B	50	SER	CA-C-N	5.45	131.50	121.70
1	B	50	SER	C-N-CA	5.45	131.50	121.70
1	A	352	ASN	CB-CG-ND2	5.43	124.54	116.40
1	B	464	GLN	O-C-N	5.40	129.51	122.87
1	B	446	GLY	CA-C-N	-5.38	113.87	121.83
1	B	446	GLY	C-N-CA	-5.38	113.87	121.83
1	A	373	ASN	CA-C-O	-5.35	113.25	118.97
1	A	9	GLY	CA-C-O	5.34	125.77	120.75
1	A	128	VAL	O-C-N	5.34	127.33	121.83
1	A	107	HIS	O-C-N	5.33	127.77	122.12
1	A	61	ALA	N-CA-C	5.33	116.61	108.52
1	B	12	PHE	CA-CB-CG	-5.33	108.47	113.80
1	B	457	VAL	N-CA-C	5.33	113.42	108.15
1	B	233	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	326	VAL	O-C-N	5.30	127.93	122.79
1	B	439	ARG	NE-CZ-NH1	-5.30	116.20	121.50
1	B	494	LYS	CA-C-O	-5.27	114.47	120.58
1	B	53	ASP	CA-CB-CG	5.25	117.85	112.60
1	B	386	LYS	CA-C-O	5.25	126.11	120.55
1	A	147	GLN	OE1-CD-NE2	5.21	127.81	122.60
1	B	371	ALA	CA-C-N	-5.19	113.33	120.28
1	B	371	ALA	C-N-CA	-5.19	113.33	120.28
1	B	311	SER	O-C-N	-5.18	115.25	122.20
1	A	311	SER	N-CA-C	5.17	117.50	110.88
1	A	246	ALA	CA-C-O	-5.17	115.88	121.87
1	B	462	TYR	O-C-N	5.14	129.74	123.21
1	A	244	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	A	72	ARG	N-CA-C	-5.09	105.81	111.36
1	B	63	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	334	ASP	CA-C-N	5.08	129.58	122.36
1	A	334	ASP	C-N-CA	5.08	129.58	122.36
1	B	310	HIS	CA-C-O	-5.07	116.01	121.38
1	A	404	HIS	ND1-CG-CD2	-5.06	101.04	106.10
1	B	46	HIS	CA-CB-CG	5.06	118.86	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	SER	O-C-N	5.05	128.49	122.27
1	A	28	VAL	O-C-N	-5.05	116.82	122.07
1	B	469	SER	O-C-N	-5.04	117.30	123.19
1	A	292	TYR	CA-C-O	-5.03	115.72	121.40
1	B	310	HIS	ND1-CG-CD2	-5.01	101.08	106.10
1	B	20	ASN	CA-CB-CG	-5.00	107.60	112.60

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	3926	0	3748	26	0
1	B	3972	0	3795	23	0
2	A	36	0	48	4	0
2	B	36	0	47	4	0
3	A	5	0	0	0	0
3	B	15	0	0	0	0
4	A	446	0	0	4	0
4	B	554	0	0	5	0
All	All	8990	0	7638	49	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 3.

All (49) 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:A:479:TRP:HE1	2:B:1505:GOL:H2	1.42	0.85
1:A:261:SER:H	2:A:1501:GOL:H31	1.41	0.84
2:B:1500:GOL:H31	4:B:2536:HOH:O	1.89	0.72
1:A:111:VAL:O	1:A:115:LYS:HG3	1.95	0.66
1:B:4:ARG:HD3	2:B:1504:GOL:O2	1.95	0.66
1:A:261:SER:N	2:A:1501:GOL:H31	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356[A]:GLN:NE2	1:B:358:LEU:HD21	2.17	0.58
1:A:221:GLU:O	1:A:310:HIS:HE1	1.86	0.58
1:B:221:GLU:O	1:B:310:HIS:HE1	1.87	0.57
1:B:147[B]:GLN:HG3	1:B:148:ALA:N	2.20	0.57
1:B:258:ALA:O	1:B:276:MET:HE1	2.06	0.56
1:B:475:TRP:CZ3	1:B:487:GLY:HA3	2.41	0.55
1:B:356[B]:GLN:HG3	4:B:2401:HOH:O	2.05	0.55
1:B:226:HIS:HD2	4:B:2418:HOH:O	1.88	0.55
1:B:478:LYS:HE3	1:B:490:SER:O	2.08	0.54
1:B:226:HIS:HE1	1:B:306:GLN:OE1	1.90	0.54
1:B:297:LYS:HD3	1:B:324:TRP:CE2	2.43	0.53
1:A:122[B]:LYS:HE2	4:A:2114:HOH:O	2.11	0.51
1:B:445:PRO:HD3	4:B:2487:HOH:O	2.11	0.50
1:B:299:VAL:HG22	1:B:374:GLY:C	2.36	0.50
1:B:353:TYR:O	1:B:370:HIS:HE1	1.95	0.49
1:B:362[B]:LYS:HD2	4:B:2309:HOH:O	2.12	0.49
1:A:122[B]:LYS:HE2	1:A:122[B]:LYS:HB3	1.53	0.48
1:B:276:MET:O	1:B:447:ASN:ND2	2.45	0.48
1:A:37[B]:THR:OG1	1:A:38:PRO:HD2	2.13	0.48
1:B:221:GLU:OE2	2:B:1501:GOL:O2	2.30	0.48
1:A:18:ILE:O	1:A:70:LYS:HE3	2.15	0.46
1:A:147:GLN:O	1:A:151:VAL:HG23	2.16	0.45
1:A:475:TRP:CD2	1:A:486:PRO:HB3	2.51	0.45
1:A:51:PHE:HZ	2:A:1504:GOL:O2	1.99	0.45
1:A:390:LYS:O	1:A:394:GLN:HG3	2.16	0.45
1:A:473:TYR:CD1	1:A:494:LYS:HD3	2.52	0.45
1:A:478:LYS:NZ	1:B:245:GLU:OE1	2.50	0.44
1:A:257:ARG:NH2	4:A:2235:HOH:O	2.50	0.44
1:A:356:GLN:HG3	4:A:2309:HOH:O	2.18	0.44
1:B:220:TRP:CD1	1:B:221:GLU:HG2	2.53	0.43
1:A:67:ASN:OD1	1:A:70:LYS:HG2	2.19	0.43
1:A:470:TYR:CD2	1:A:471:GLN:HG3	2.54	0.43
1:A:156:ALA:O	1:A:160:GLU:HG2	2.19	0.42
1:B:144:GLU:HA	1:B:145:TYR:CG	2.54	0.42
1:A:241:ASN:HD22	1:A:241:ASN:C	2.28	0.42
1:B:31:PHE:CG	1:B:406:GLY:HA2	2.54	0.42
1:B:473:TYR:CE2	1:B:494:LYS:HD3	2.54	0.42
1:A:257:ARG:HG3	1:A:258:ALA:N	2.33	0.42
1:A:299:VAL:HG22	1:A:374:GLY:C	2.45	0.42
1:B:334:ASP:O	1:B:335:LYS:HB2	2.20	0.42
1:A:468:VAL:HG22	1:A:492:TRP:CZ3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:GLN:NE2	4:A:2309:HOH:O	2.51	0.41
1:A:261:SER:H	2:A:1501:GOL:C3	2.23	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	505/499 (101%)	493 (98%)	12 (2%)	0	100	100
1	B	509/499 (102%)	502 (99%)	7 (1%)	0	100	100
All	All	1014/998 (102%)	995 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	411/405 (102%)	397 (97%)	14 (3%)	32	5
1	B	414/405 (102%)	408 (99%)	6 (1%)	59	28
All	All	825/810 (102%)	805 (98%)	20 (2%)	43	12

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	PRO
1	A	63	ASP
1	A	132	LYS
1	A	199	LEU
1	A	213	THR
1	A	257	ARG
1	A	320	SER
1	A	321[A]	THR
1	A	321[B]	THR
1	A	333	ARG
1	A	349	LEU
1	A	378	THR
1	A	380	ASP
1	A	447	ASN
1	B	3	THR
1	B	213	THR
1	B	320	SER
1	B	375	LEU
1	B	380	ASP
1	B	447	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	241	ASN
1	A	310	HIS
1	A	447	ASN
1	B	112	ASN
1	B	167	GLN
1	B	180	GLN
1	B	226	HIS
1	B	227	GLN
1	B	272	GLN
1	B	273	GLN
1	B	310	HIS
1	B	344	GLN
1	B	370	HIS
1	B	372	GLN
1	B	431	GLN

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 ⓘ

16 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	B	1504	-	5,5,5	0.56	0	5,5,5	3.89	3 (60%)
3	SO4	A	1505	-	4,4,4	0.60	0	6,6,6	0.55	0
2	GOL	A	1502	-	5,5,5	0.77	0	5,5,5	3.81	3 (60%)
2	GOL	B	1503	-	5,5,5	0.70	0	5,5,5	4.32	4 (80%)
2	GOL	A	1503	-	5,5,5	0.36	0	5,5,5	3.60	3 (60%)
3	SO4	B	1507	-	4,4,4	0.63	0	6,6,6	0.42	0
2	GOL	A	1500	-	5,5,5	0.59	0	5,5,5	3.50	4 (80%)
2	GOL	A	1499	-	5,5,5	0.59	0	5,5,5	2.21	2 (40%)
2	GOL	A	1501	-	5,5,5	0.42	0	5,5,5	4.79	4 (80%)
2	GOL	B	1500	-	5,5,5	0.92	0	5,5,5	5.81	3 (60%)
2	GOL	B	1502	-	5,5,5	0.71	0	5,5,5	3.19	4 (80%)
3	SO4	B	1508	-	4,4,4	0.64	0	6,6,6	0.30	0
2	GOL	A	1504	-	5,5,5	0.36	0	5,5,5	4.37	3 (60%)
2	GOL	B	1505	-	5,5,5	0.30	0	5,5,5	4.62	4 (80%)
3	SO4	B	1506	-	4,4,4	0.63	0	6,6,6	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	1501	-	5,5,5	0.37	0	5,5,5	4.24	2 (40%)

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	1504	-	-	2/4/4/4	-
2	GOL	A	1502	-	-	1/4/4/4	-
2	GOL	B	1503	-	-	1/4/4/4	-
2	GOL	A	1503	-	-	2/4/4/4	-
2	GOL	A	1500	-	-	4/4/4/4	-
2	GOL	A	1499	-	-	0/4/4/4	-
2	GOL	A	1501	-	-	0/4/4/4	-
2	GOL	B	1500	-	-	2/4/4/4	-
2	GOL	B	1502	-	-	2/4/4/4	-
2	GOL	A	1504	-	-	0/4/4/4	-
2	GOL	B	1505	-	-	2/4/4/4	-
2	GOL	B	1501	-	-	4/4/4/4	-

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1500	GOL	O3-C3-C2	11.55	162.39	110.38
2	A	1501	GOL	O3-C3-C2	8.90	150.45	110.38
2	B	1505	GOL	O3-C3-C2	8.02	146.48	110.38
2	B	1503	GOL	O3-C3-C2	7.98	146.29	110.38
2	B	1501	GOL	O3-C3-C2	7.25	143.04	110.38
2	A	1504	GOL	O3-C3-C2	6.59	140.06	110.38
2	B	1504	GOL	O3-C3-C2	6.40	139.20	110.38
2	A	1503	GOL	O3-C3-C2	6.27	138.62	110.38
2	B	1501	GOL	O2-C2-C3	5.80	133.19	109.18
2	A	1504	GOL	O2-C2-C3	5.66	132.60	109.18
2	A	1502	GOL	O3-C3-C2	5.43	134.80	110.38
2	A	1500	GOL	O3-C3-C2	5.27	134.09	110.38
2	B	1500	GOL	C3-C2-C1	-5.06	93.25	111.80
2	B	1504	GOL	O2-C2-C3	4.74	128.80	109.18
2	A	1502	GOL	C3-C2-C1	-4.65	94.75	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1502	GOL	O2-C2-C3	4.59	128.17	109.18
2	B	1502	GOL	O3-C3-C2	4.39	130.12	110.38
2	A	1501	GOL	O1-C1-C2	4.34	129.90	110.38
2	B	1505	GOL	O1-C1-C2	4.13	128.95	110.38
2	A	1504	GOL	C3-C2-C1	-4.07	96.86	111.80
2	B	1502	GOL	C3-C2-C1	-4.01	97.10	111.80
2	B	1505	GOL	O2-C2-C3	3.95	125.54	109.18
2	A	1499	GOL	O3-C3-C2	3.93	128.08	110.38
2	A	1500	GOL	C3-C2-C1	-3.93	97.38	111.80
2	A	1503	GOL	O2-C2-C3	3.71	124.56	109.18
2	B	1503	GOL	C3-C2-C1	-3.66	98.39	111.80
2	A	1500	GOL	O2-C2-C3	3.38	123.16	109.18
2	B	1502	GOL	O2-C2-C3	3.23	122.56	109.18
2	B	1504	GOL	C3-C2-C1	-3.21	100.01	111.80
2	B	1505	GOL	C3-C2-C1	-3.13	100.33	111.80
2	A	1503	GOL	C3-C2-C1	-3.10	100.44	111.80
2	A	1501	GOL	O2-C2-C3	2.94	121.33	109.18
2	B	1503	GOL	O2-C2-C1	-2.88	97.24	109.18
2	B	1503	GOL	O2-C2-C3	2.83	120.90	109.18
2	A	1501	GOL	C3-C2-C1	-2.80	101.52	111.80
2	A	1500	GOL	O1-C1-C2	2.50	121.65	110.38
2	B	1500	GOL	O2-C2-C3	2.34	118.88	109.18
2	A	1499	GOL	O2-C2-C1	-2.29	99.70	109.18
2	B	1502	GOL	O1-C1-C2	2.10	119.82	110.38

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1500	GOL	C1-C2-C3-O3
2	B	1501	GOL	O1-C1-C2-C3
2	B	1504	GOL	C1-C2-C3-O3
2	B	1505	GOL	O1-C1-C2-C3
2	A	1500	GOL	O1-C1-C2-C3
2	A	1500	GOL	C1-C2-C3-O3
2	B	1501	GOL	C1-C2-C3-O3
2	B	1502	GOL	C1-C2-C3-O3
2	B	1501	GOL	O2-C2-C3-O3
2	B	1503	GOL	O2-C2-C3-O3
2	B	1504	GOL	O2-C2-C3-O3
2	A	1500	GOL	O1-C1-C2-O2
2	A	1503	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	1500	GOL	O2-C2-C3-O3
2	B	1501	GOL	O1-C1-C2-O2
2	B	1505	GOL	O1-C1-C2-O2
2	A	1502	GOL	C1-C2-C3-O3
2	B	1502	GOL	O2-C2-C3-O3
2	A	1500	GOL	O2-C2-C3-O3
2	A	1503	GOL	O1-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1504	GOL	1	0
2	A	1501	GOL	3	0
2	B	1500	GOL	1	0
2	A	1504	GOL	1	0
2	B	1505	GOL	1	0
2	B	1501	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	497/499 (99%)	-0.13	4 (0%) 82 86	11, 22, 37, 48	10 (2%)
1	B	497/499 (99%)	-0.32	7 (1%) 73 77	11, 18, 31, 47	14 (2%)
All	All	994/998 (99%)	-0.22	11 (1%) 78 82	11, 20, 36, 48	24 (2%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	SER	5.4
1	B	487	GLY	3.6
1	B	445	PRO	3.0
1	A	499	ALA	2.9
1	A	16	ASN	2.6
1	A	104	GLY	2.5
1	B	447	ASN	2.5
1	B	320	SER	2.3
1	B	302	GLY	2.1
1	B	350	GLN	2.1
1	A	60	CYS	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($\text{\AA}^2$)	Q<0.9
2	GOL	A	1504	6/6	0.68	0.23	61,65,67,68	0
2	GOL	B	1505	6/6	0.79	0.26	69,69,70,72	0
2	GOL	A	1503	6/6	0.80	0.15	50,54,54,59	0
2	GOL	A	1501	6/6	0.84	0.14	38,45,49,53	0
2	GOL	B	1500	6/6	0.85	0.18	55,58,59,59	0
2	GOL	B	1503	6/6	0.86	0.12	30,35,38,39	0
2	GOL	A	1502	6/6	0.88	0.10	38,40,43,51	0
2	GOL	B	1501	6/6	0.88	0.11	31,37,39,40	0
2	GOL	B	1504	6/6	0.90	0.11	23,36,38,43	0
2	GOL	B	1502	6/6	0.90	0.11	23,33,37,40	0
2	GOL	A	1499	6/6	0.92	0.08	31,33,35,40	0
2	GOL	A	1500	6/6	0.92	0.10	22,31,34,35	0
3	SO4	B	1508	5/5	0.93	0.09	61,66,67,67	0
3	SO4	B	1507	5/5	0.94	0.07	48,52,54,57	0
3	SO4	B	1506	5/5	0.96	0.07	35,36,37,40	0
3	SO4	A	1505	5/5	0.97	0.06	36,39,43,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.