



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:16 AM UTC

PDB ID : 3SIM / pdb\_00003sim  
Title : Crystallographic structure analysis of family 18 Chitinase from *Crocus vernus*  
Authors : Akrem, A.; Iqbal, S.; Buck, F.; Negm, A.; Perbandt, M.; Betzel, C.  
Deposited on : 2011-06-19  
Resolution : 2.10 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](mailto: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>.

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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

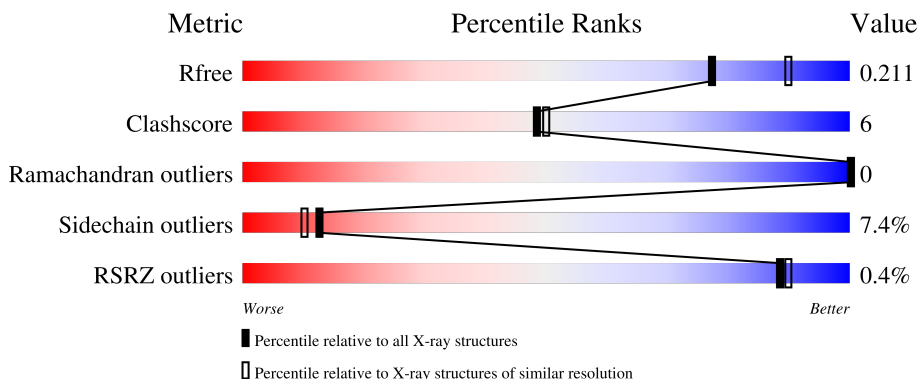
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

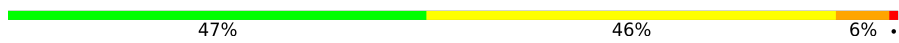

The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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  $\geq 3$ , 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	275	 47% 46% 6% .
1	B	275	 % 50% 44% . .

## 2 Entry composition [i](#)

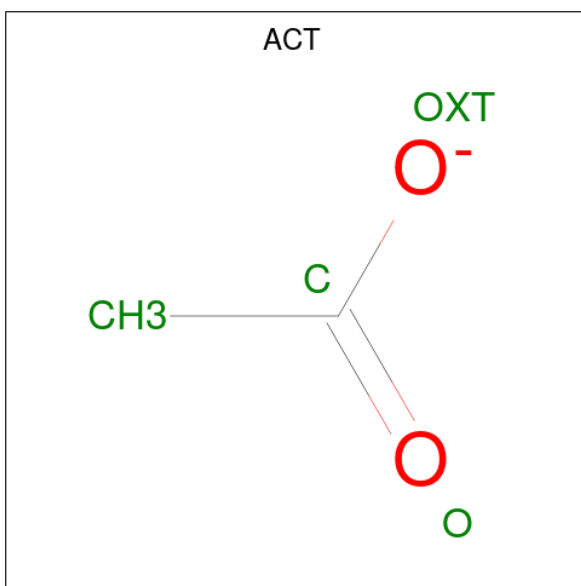
There are 4 unique types of molecules in this entry. The entry contains 4713 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Protein, Family 18 Chitinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	Total 2147	C 1381	N 350	O 415	S 1	14	1	0
1	B	275	Total 2144	C 1379	N 350	O 414	S 1	29	0	0

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 4	C 2	O 2	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

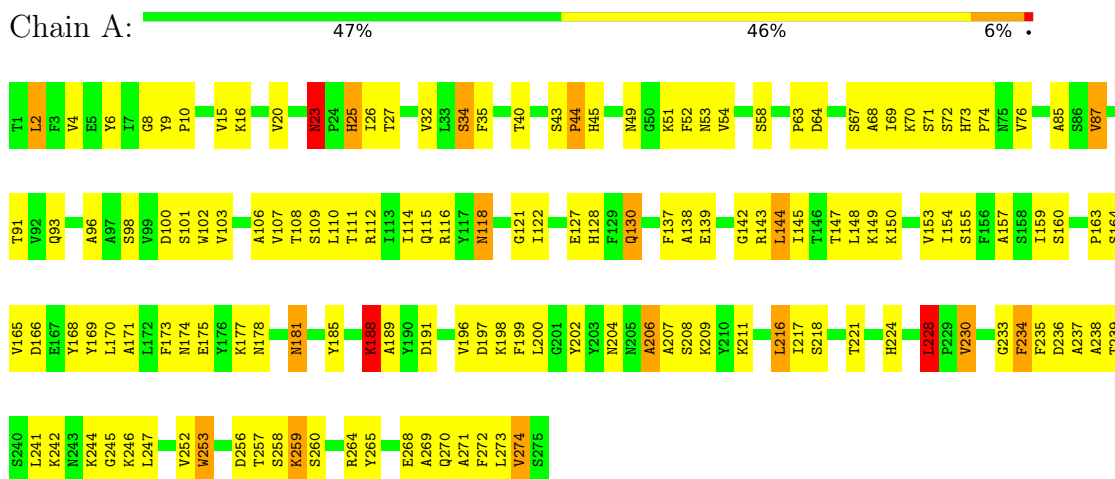
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	208	Total O 208 208	0	0
4	B	198	Total O 198 198	0	0

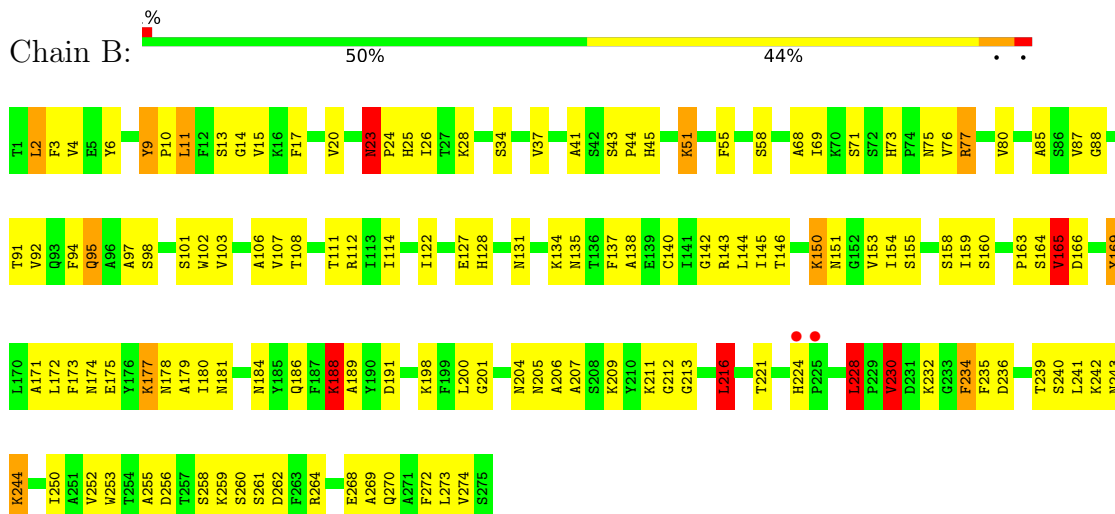
### 3 Residue-property plots

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: Protein, Family 18 Chitinase



- Molecule 1: Protein, Family 18 Chitinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.27Å 37.08Å 126.37Å 90.00° 127.01° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (30.00-2.10) 95.9 (30.00-2.10)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	0.01	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.08 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.155 , 0.213 (Not available) , 0.211	Depositor DCC
$R_{free}$ test set	1831 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.1	Xtrriage
Anisotropy	0.144	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4713	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, ACT

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	2.27	126/2208 (5.7%)	1.51	19/3001 (0.6%)
1	B	2.23	109/2202 (5.0%)	1.48	19/2993 (0.6%)
All	All	2.25	235/4410 (5.3%)	1.49	38/5994 (0.6%)

All (235) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	224	HIS	C-O	-12.98	1.17	1.23
1	A	15	VAL	C-O	-8.27	1.15	1.24
1	A	272	PHE	C-O	-8.23	1.14	1.24
1	A	109	SER	C-O	-7.93	1.15	1.24
1	A	265	TYR	C-O	-7.90	1.14	1.24
1	B	174	ASN	C-O	-7.90	1.14	1.24
1	A	171	ALA	C-O	-7.73	1.15	1.24
1	B	137	PHE	C-O	-7.70	1.15	1.24
1	B	242	LYS	C-O	-7.63	1.15	1.24
1	A	150	LYS	C-O	-7.58	1.15	1.24
1	A	107	VAL	C-O	-7.51	1.15	1.24
1	A	137	PHE	C-O	-7.44	1.15	1.24
1	B	273	LEU	C-O	-7.28	1.15	1.24
1	B	68	ALA	CA-CB	-7.26	1.42	1.53
1	A	54	VAL	C-O	-7.25	1.15	1.23
1	A	143	ARG	C-O	-7.22	1.15	1.24
1	B	160	SER	C-O	-7.18	1.15	1.24
1	B	234	PHE	C-O	-7.15	1.15	1.24
1	A	259	LYS	C-O	-7.15	1.15	1.24
1	A	69	ILE	C-O	-7.12	1.15	1.24
1	A	115	GLN	C-O	-7.11	1.16	1.24
1	B	92	VAL	CA-CB	7.11	1.60	1.53
1	A	145	ILE	C-O	-7.06	1.16	1.24
1	A	102	TRP	C-O	-7.05	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	107	VAL	C-O	-7.04	1.16	1.24
1	A	160	SER	C-O	-7.04	1.15	1.23
1	B	269	ALA	C-O	-6.92	1.16	1.24
1	A	27	THR	C-O	-6.88	1.16	1.24
1	A	58	SER	C-O	-6.88	1.15	1.24
1	A	257	THR	C-O	-6.85	1.16	1.24
1	A	185	TYR	C-O	-6.84	1.15	1.23
1	A	238	ALA	CA-CB	-6.83	1.42	1.53
1	A	139	GLU	C-O	-6.79	1.16	1.24
1	A	74	PRO	C-O	-6.79	1.15	1.24
1	B	41	ALA	C-O	-6.79	1.15	1.24
1	B	111	THR	C-O	-6.79	1.16	1.24
1	A	164	SER	C-O	-6.75	1.15	1.24
1	A	230	VAL	C-O	-6.75	1.16	1.24
1	A	271	ALA	C-O	-6.70	1.16	1.24
1	B	207	ALA	C-O	-6.70	1.16	1.24
1	A	154	ILE	C-O	-6.69	1.17	1.24
1	B	97	ALA	C-O	-6.68	1.16	1.24
1	B	259	LYS	C-O	-6.65	1.16	1.24
1	A	274	VAL	C-O	-6.61	1.16	1.24
1	A	110	LEU	C-O	-6.60	1.16	1.24
1	A	73	HIS	C-O	-6.58	1.18	1.24
1	A	111	THR	C-O	-6.57	1.16	1.24
1	A	239	THR	C-O	-6.55	1.16	1.24
1	B	272	PHE	C-O	-6.53	1.16	1.24
1	B	98	SER	C-O	-6.53	1.15	1.23
1	A	70	LYS	C-O	-6.52	1.16	1.24
1	B	200	LEU	C-O	-6.51	1.16	1.24
1	B	164	SER	C-O	-6.47	1.15	1.24
1	B	239	THR	C-O	-6.46	1.16	1.24
1	A	163	PRO	C-O	-6.45	1.16	1.24
1	A	197	ASP	C-O	-6.42	1.16	1.24
1	B	260	SER	C-O	-6.39	1.16	1.24
1	A	208[A]	SER	N-CA	-6.34	1.38	1.46
1	A	208[B]	SER	N-CA	-6.34	1.38	1.46
1	B	108	THR	C-O	-6.33	1.16	1.24
1	A	173	PHE	C-O	-6.32	1.16	1.24
1	A	45	HIS	C-O	-6.32	1.16	1.24
1	A	244	LYS	C-O	-6.31	1.15	1.24
1	B	179	ALA	C-O	-6.30	1.15	1.24
1	A	199	PHE	C-O	-6.29	1.16	1.24
1	A	170	LEU	C-O	-6.29	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	ILE	C-O	-6.27	1.17	1.24
1	A	207	ALA	C-O	-6.27	1.16	1.24
1	B	135	ASN	C-O	-6.27	1.16	1.24
1	A	16	LYS	C-O	-6.23	1.15	1.23
1	A	118	ASN	C-O	-6.22	1.15	1.23
1	A	181	ASN	C-O	-6.22	1.16	1.24
1	A	253	TRP	C-O	-6.21	1.16	1.23
1	B	230	VAL	C-O	-6.20	1.16	1.24
1	B	228	LEU	C-O	-6.20	1.16	1.24
1	B	201	GLY	C-O	-6.19	1.16	1.23
1	A	144	LEU	C-O	-6.18	1.17	1.24
1	B	106	ALA	C-O	-6.18	1.17	1.24
1	A	63	PRO	C-O	-6.18	1.16	1.24
1	B	102	TRP	C-O	-6.18	1.17	1.24
1	A	101	SER	C-O	-6.17	1.16	1.24
1	B	236	ASP	C-O	-6.17	1.17	1.24
1	B	88	GLY	C-O	-6.16	1.16	1.24
1	B	154	ILE	C-O	-6.15	1.18	1.24
1	A	114	ILE	C-O	-6.15	1.17	1.24
1	A	189	ALA	C-O	-6.14	1.16	1.24
1	B	241	LEU	C-O	-6.12	1.17	1.24
1	B	142	GLY	C-O	-6.11	1.16	1.23
1	B	181	ASN	C-O	-6.09	1.17	1.24
1	B	76	VAL	CA-CB	6.08	1.61	1.54
1	B	171	ALA	CA-CB	-6.06	1.44	1.53
1	A	20	VAL	C-O	-6.06	1.16	1.24
1	A	67	SER	C-O	-6.06	1.17	1.24
1	B	24	PRO	C-O	-6.06	1.16	1.24
1	B	243	ASN	C-O	-6.05	1.16	1.24
1	A	166	ASP	C-O	-6.04	1.16	1.24
1	B	17	PHE	C-O	-6.02	1.17	1.24
1	A	233	GLY	C-O	-6.01	1.17	1.24
1	A	196	VAL	C-O	-5.99	1.17	1.24
1	A	236	ASP	C-O	-5.98	1.17	1.24
1	A	85	ALA	C-O	-5.98	1.17	1.24
1	A	100	ASP	C-O	-5.97	1.17	1.24
1	A	138	ALA	C-O	-5.96	1.17	1.24
1	B	270	GLN	C-O	-5.96	1.17	1.24
1	B	13	SER	C-O	-5.92	1.17	1.24
1	A	218	SER	C-O	-5.91	1.16	1.23
1	B	166	ASP	C-O	-5.90	1.16	1.24
1	A	256	ASP	C-O	-5.90	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	THR	C-O	-5.88	1.17	1.24
1	A	71	SER	C-O	-5.88	1.17	1.24
1	B	20	VAL	C-O	-5.87	1.16	1.24
1	B	94	PHE	C-O	-5.87	1.17	1.24
1	A	234	PHE	C-O	-5.85	1.17	1.24
1	B	258	SER	C-O	-5.85	1.16	1.24
1	A	206	ALA	CA-CB	-5.85	1.44	1.53
1	A	235	PHE	C-O	-5.85	1.16	1.24
1	B	184	ASN	C-O	-5.84	1.17	1.23
1	B	209	LYS	C-O	-5.84	1.17	1.24
1	B	73	HIS	C-O	-5.80	1.19	1.24
1	A	221	THR	C-O	-5.80	1.16	1.24
1	B	171	ALA	C-O	-5.80	1.17	1.24
1	B	76	VAL	C-O	-5.80	1.17	1.24
1	A	40	THR	C-O	-5.78	1.17	1.23
1	B	26	ILE	C-O	-5.78	1.18	1.24
1	B	221	THR	C-O	-5.78	1.16	1.24
1	A	26	ILE	C-O	-5.77	1.18	1.24
1	B	138	ALA	C-O	-5.76	1.17	1.24
1	B	189	ALA	C-O	-5.76	1.16	1.24
1	A	174	ASN	C-O	-5.75	1.17	1.24
1	B	256	ASP	C-O	-5.74	1.17	1.24
1	B	3	PHE	C-O	-5.69	1.17	1.24
1	B	15	VAL	C-O	-5.69	1.18	1.24
1	B	206	ALA	CA-CB	-5.68	1.44	1.53
1	B	250	ILE	C-O	-5.67	1.18	1.24
1	A	130	GLN	C-O	-5.67	1.16	1.24
1	B	143	ARG	C-O	-5.65	1.17	1.24
1	A	4	VAL	C-O	-5.64	1.18	1.24
1	A	269	ALA	C-O	-5.64	1.17	1.24
1	B	114	ILE	C-O	-5.63	1.17	1.24
1	A	258	SER	C-O	-5.63	1.16	1.24
1	B	206	ALA	C-O	-5.62	1.17	1.24
1	B	6	TYR	C-O	-5.61	1.17	1.23
1	B	150	LYS	C-O	-5.60	1.17	1.24
1	B	71	SER	C-O	-5.59	1.17	1.24
1	B	198	LYS	C-O	-5.59	1.17	1.24
1	A	121	GLY	C-O	-5.58	1.18	1.23
1	A	112	ARG	C-O	-5.57	1.17	1.24
1	A	159	ILE	C-O	-5.57	1.18	1.24
1	A	217	ILE	C-O	-5.56	1.17	1.24
1	A	49	ASN	C-O	-5.55	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	ALA	C-O	-5.55	1.17	1.24
1	A	116	ARG	C-O	-5.55	1.17	1.24
1	B	23	ASN	C-O	-5.54	1.17	1.24
1	A	72	SER	C-O	-5.54	1.17	1.24
1	A	147	THR	C-O	-5.53	1.17	1.24
1	A	188	LYS	C-O	-5.53	1.17	1.24
1	A	268	GLU	C-O	-5.52	1.17	1.24
1	A	245	GLY	C-O	-5.52	1.15	1.23
1	B	75	ASN	C-O	-5.52	1.16	1.24
1	B	255	ALA	C-O	-5.52	1.17	1.24
1	B	9	TYR	C-O	-5.51	1.17	1.24
1	A	202	TYR	C-O	-5.51	1.17	1.24
1	A	191	ASP	C-O	-5.51	1.17	1.23
1	B	212	GLY	C-O	-5.50	1.17	1.24
1	A	228	LEU	C-O	-5.49	1.17	1.24
1	A	224	HIS	C-O	-5.48	1.17	1.24
1	A	264	ARG	C-O	-5.48	1.17	1.24
1	A	91	THR	C-O	-5.48	1.17	1.23
1	A	103	VAL	C-O	-5.47	1.18	1.24
1	A	247	LEU	C-O	-5.47	1.17	1.23
1	B	69	ILE	C-O	-5.47	1.17	1.24
1	A	98	SER	C-O	-5.47	1.17	1.23
1	B	244	LYS	C-O	-5.44	1.16	1.24
1	A	6	TYR	C-O	-5.43	1.17	1.23
1	B	188	LYS	C-O	-5.40	1.17	1.24
1	B	204	ASN	C-O	-5.40	1.17	1.24
1	B	103	VAL	C-O	-5.39	1.17	1.24
1	B	158	SER	C-O	-5.38	1.17	1.23
1	B	155	SER	C-O	-5.38	1.17	1.24
1	B	191	ASP	C-O	-5.38	1.17	1.23
1	A	168	TYR	C-O	-5.37	1.18	1.24
1	B	205	ASN	C-O	-5.36	1.18	1.24
1	B	4	VAL	C-O	-5.36	1.18	1.24
1	A	52	PHE	C-O	-5.33	1.17	1.23
1	B	128	HIS	C-O	-5.33	1.17	1.24
1	B	37	VAL	C-O	-5.32	1.18	1.24
1	B	179	ALA	CA-CB	-5.32	1.44	1.53
1	B	268	GLU	C-O	-5.29	1.17	1.24
1	B	14	GLY	C-O	-5.27	1.17	1.24
1	B	146	THR	C-O	-5.25	1.18	1.24
1	A	51	LYS	C-O	-5.24	1.17	1.23
1	A	166	ASP	CG-OD2	-5.22	1.15	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	HIS	C-O	-5.22	1.17	1.24
1	B	262	ASP	C-O	-5.22	1.15	1.24
1	A	142	GLY	C-O	-5.20	1.17	1.23
1	A	198	LYS	C-O	-5.20	1.18	1.24
1	B	101	SER	C-O	-5.20	1.18	1.24
1	B	235	PHE	C-O	-5.19	1.17	1.24
1	B	151	ASN	C-O	-5.19	1.17	1.24
1	A	211	LYS	C-O	-5.17	1.17	1.24
1	A	23	ASN	C-O	-5.16	1.17	1.24
1	B	80	VAL	C-O	-5.16	1.18	1.24
1	A	273	LEU	C-O	-5.16	1.18	1.24
1	B	177	LYS	C-O	-5.16	1.18	1.24
1	A	106	ALA	C-O	-5.16	1.18	1.24
1	A	8	GLY	C-O	-5.15	1.17	1.24
1	A	169	TYR	C-O	-5.15	1.18	1.24
1	A	269	ALA	CA-CB	-5.15	1.45	1.53
1	A	53	ASN	C-O	-5.14	1.17	1.23
1	B	95	GLN	C-O	-5.13	1.18	1.23
1	B	134	LYS	C-O	-5.13	1.18	1.24
1	B	173	PHE	C-O	-5.12	1.18	1.24
1	B	58	SER	C-O	-5.12	1.17	1.24
1	A	178	ASN	C-O	-5.12	1.17	1.24
1	B	264	ARG	C-O	-5.10	1.18	1.24
1	A	128	HIS	C-O	-5.10	1.18	1.23
1	A	64	ASP	C-O	-5.09	1.18	1.24
1	B	216	LEU	C-O	-5.08	1.17	1.23
1	B	127	GLU	C-O	-5.07	1.17	1.24
1	A	68	ALA	C-O	-5.07	1.18	1.24
1	A	148	LEU	C-O	-5.07	1.18	1.24
1	A	204	ASN	C-O	-5.06	1.18	1.24
1	B	213	GLY	C-O	-5.05	1.16	1.23
1	B	145	ILE	C-O	-5.05	1.18	1.24
1	A	241	LEU	C-O	-5.04	1.18	1.24
1	A	127	GLU	CA-C	5.03	1.59	1.52
1	A	32	VAL	CA-CB	5.02	1.60	1.53
1	B	11	LEU	C-O	-5.02	1.17	1.23
1	B	180	ILE	C-O	-5.02	1.18	1.24
1	A	200	LEU	C-O	-5.02	1.18	1.24
1	B	140	CYS	C-O	-5.02	1.18	1.24
1	A	188	LYS	CE-NZ	-5.01	1.34	1.49
1	A	252	VAL	CA-C	5.01	1.58	1.52
1	B	261	SER	C-O	-5.01	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	LYS	C-O	-5.00	1.18	1.24

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	VAL	CB-CA-C	-10.84	97.51	112.14
1	A	181	ASN	N-CA-C	9.56	121.78	111.36
1	A	155	SER	N-CA-C	9.02	120.88	111.14
1	B	181	ASN	N-CA-C	8.99	120.84	111.14
1	B	85	ALA	N-CA-C	8.59	120.72	111.36
1	A	208[A]	SER	CA-C-O	-8.36	112.09	120.70
1	A	208[B]	SER	CA-C-O	-8.36	112.09	120.70
1	B	165	VAL	N-CA-CB	-8.30	101.57	112.36
1	B	155	SER	N-CA-C	8.29	120.10	111.14
1	A	175	GLU	N-CA-C	7.29	120.28	111.82
1	A	85	ALA	N-CA-C	7.19	118.91	111.14
1	B	153	VAL	N-CA-C	6.72	117.50	110.72
1	A	87	VAL	CB-CA-C	6.68	119.43	110.42
1	A	153	VAL	N-CA-C	6.48	117.26	110.72
1	B	13	SER	N-CA-C	6.48	118.42	111.36
1	B	175	GLU	N-CA-C	6.47	119.33	111.82
1	B	252	VAL	N-CA-C	6.29	117.18	108.12
1	A	8	GLY	N-CA-C	6.21	123.89	115.32
1	B	230	VAL	CB-CA-C	-6.16	102.61	112.16
1	A	20	VAL	N-CA-C	6.08	113.90	107.76
1	B	20	VAL	N-CA-C	5.99	113.81	107.76
1	B	68	ALA	N-CA-C	5.96	117.44	111.07
1	B	58	SER	N-CA-C	5.75	118.48	111.82
1	B	23	ASN	CA-C-N	5.70	125.38	119.56
1	B	23	ASN	C-N-CA	5.70	125.38	119.56
1	A	260	SER	N-CA-C	5.68	118.41	111.82
1	A	87	VAL	N-CA-CB	-5.67	104.11	111.82
1	B	165	VAL	CG1-CB-CG2	5.62	123.17	110.80
1	B	216	LEU	CA-CB-CG	5.48	135.48	116.30
1	A	165	VAL	N-CA-C	5.42	117.38	112.29
1	A	76	VAL	N-CA-C	5.41	116.37	108.58
1	A	169	TYR	N-CA-C	5.33	117.09	111.28
1	A	246	LYS	N-CA-C	5.21	119.60	112.88
1	A	118	ASN	CB-CA-C	-5.16	104.40	111.73
1	B	55	PHE	N-CA-C	5.14	120.40	113.72
1	A	32	VAL	N-CA-C	5.12	115.43	107.28
1	B	169	TYR	N-CA-C	5.07	116.81	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	PHE	N-CA-C	-5.00	105.83	111.28

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	2147	0	2073	21	0
1	B	2144	0	2068	24	0
2	A	4	0	3	0	0
3	A	6	0	8	1	0
3	B	6	0	8	1	0
4	A	208	0	0	3	0
4	B	198	0	0	4	0
All	All	4713	0	4160	46	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (46) 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:259:LYS:HE3	4:A:687:HOH:O	1.57	1.04
1:A:188:LYS:HE2	1:A:253:TRP:CE3	2.17	0.79
1:B:228:LEU:HD13	1:B:234:PHE:HA	1.61	0.79
1:B:2:LEU:HD13	1:B:216:LEU:HD11	1.69	0.74
1:A:2:LEU:HD13	1:A:216:LEU:HD11	1.71	0.71
3:B:276:GOL:O3	3:B:276:GOL:O1	2.03	0.71
1:A:157:ALA:H	1:A:181:ASN:HD22	1.39	0.70
1:A:259:LYS:CE	4:A:687:HOH:O	2.26	0.66
1:A:188:LYS:H	1:A:188:LYS:HD3	1.63	0.64
1:A:228:LEU:HD13	1:A:234:PHE:HA	1.82	0.62
1:B:23:ASN:HD22	1:B:25:HIS:H	1.51	0.59
1:B:45:HIS:CD2	1:B:87:VAL:HG12	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLN:HB3	1:B:188:LYS:HE3	1.85	0.58
1:B:95:GLN:HE21	1:B:131:ASN:HD22	1.53	0.57
1:A:23:ASN:HD22	1:A:25:HIS:H	1.52	0.56
1:A:118:ASN:HB3	4:A:730:HOH:O	2.05	0.55
1:A:23:ASN:HD22	1:A:23:ASN:C	2.14	0.55
1:B:112:ARG:HD3	4:B:805:HOH:O	2.06	0.54
1:B:230:VAL:HG22	4:B:347:HOH:O	2.08	0.53
1:A:206:ALA:HA	1:A:209:LYS:HE3	1.90	0.53
1:B:95:GLN:NE2	1:B:131:ASN:HD22	2.07	0.52
1:B:188:LYS:HE2	1:B:253:TRP:CE3	2.45	0.52
1:A:43:SER:HA	1:A:44:PRO:C	2.34	0.51
1:A:96:ALA:O	3:A:277:GOL:H12	2.11	0.51
1:A:23:ASN:ND2	1:A:25:HIS:H	2.09	0.50
1:B:244:LYS:HE2	4:B:327:HOH:O	2.11	0.50
1:A:23:ASN:H	1:A:270:GLN:NE2	2.10	0.50
1:B:165:VAL:HG13	1:B:169:TYR:HD2	1.75	0.50
1:A:149:LYS:NZ	1:A:181:ASN:HD21	2.12	0.48
1:A:9:TYR:HA	1:A:10:PRO:C	2.37	0.48
1:B:165:VAL:HG13	1:B:169:TYR:CD2	2.47	0.48
1:B:240:SER:O	1:B:244:LYS:HD3	2.14	0.47
1:A:93:GLN:HE22	1:A:130:GLN:H	1.62	0.47
1:B:2:LEU:HD13	1:B:216:LEU:CD1	2.42	0.46
1:B:45:HIS:CG	1:B:87:VAL:HG12	2.51	0.46
1:A:188:LYS:CE	1:A:253:TRP:CE3	2.94	0.46
1:B:77:ARG:HG3	4:B:580:HOH:O	2.15	0.45
1:B:43:SER:HA	1:B:44:PRO:C	2.40	0.45
1:B:23:ASN:ND2	1:B:25:HIS:H	2.15	0.44
1:B:51:LYS:H	1:B:51:LYS:HG2	1.62	0.44
1:B:9:TYR:HA	1:B:10:PRO:C	2.44	0.43
1:A:34:SER:HA	1:A:35:PHE:HA	1.80	0.43
1:A:23:ASN:H	1:A:270:GLN:HE22	1.67	0.42
1:B:9:TYR:CG	1:B:10:PRO:HA	2.55	0.42
1:B:122:ILE:HD13	1:B:122:ILE:HG21	1.76	0.41
1:B:23:ASN:HD22	1:B:23:ASN:C	2.29	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	274/275 (100%)	273 (100%)	1 (0%)	0	100	100
1	B	273/275 (99%)	272 (100%)	1 (0%)	0	100	100
All	All	547/550 (100%)	545 (100%)	2 (0%)	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	236/235 (100%)	223 (94%)	13 (6%)	19	18
1	B	235/235 (100%)	213 (91%)	22 (9%)	8	6
All	All	471/470 (100%)	436 (93%)	35 (7%)	13	10

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	23	ASN
1	A	34	SER
1	A	44	PRO
1	A	87	VAL
1	A	122	ILE
1	A	144	LEU
1	A	177	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	188	LYS
1	A	216	LEU
1	A	228	LEU
1	A	230	VAL
1	A	274	VAL
1	B	2	LEU
1	B	11	LEU
1	B	23	ASN
1	B	28	LYS
1	B	34	SER
1	B	51	LYS
1	B	77	ARG
1	B	91	THR
1	B	144	LEU
1	B	150	LYS
1	B	163	PRO
1	B	165	VAL
1	B	172	LEU
1	B	177	LYS
1	B	178	ASN
1	B	188	LYS
1	B	211	LYS
1	B	216	LEU
1	B	228	LEU
1	B	230	VAL
1	B	232	LYS
1	B	274	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	23	ASN
1	A	93	GLN
1	A	118	ASN
1	A	130	GLN
1	A	181	ASN
1	A	186	GLN
1	A	224	HIS
1	A	270	GLN
1	B	23	ASN
1	B	25	HIS
1	B	95	GLN

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Mol	Chain	Res	Type
1	B	130	GLN
1	B	131	ASN
1	B	182	HIS
1	B	186	GLN
1	B	205	ASN
1	B	270	GLN

### 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 [i](#)

3 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	B	276	-	5,5,5	0.37	0	5,5,5	0.84	0
2	ACT	A	276	-	3,3,3	0.88	0	3,3,3	1.59	0
3	GOL	A	277	-	5,5,5	0.72	0	5,5,5	1.22	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	B	276	-	-	1/4/4/4	-
3	GOL	A	277	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	277	GOL	O1-C1-C2-C3
3	A	277	GOL	C1-C2-C3-O3
3	A	277	GOL	O1-C1-C2-O2
3	A	277	GOL	O2-C2-C3-O3
3	B	276	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	276	GOL	1	0
3	A	277	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	275/275 (100%)	-0.32	0 <b>100</b>   <b>100</b>	7, 13, 21, 26	11 (4%)
1	B	275/275 (100%)	-0.24	2 (0%) <b>84</b>   <b>86</b>	7, 14, 23, 31	15 (5%)
All	All	550/550 (100%)	-0.28	2 (0%) <b>88</b>   <b>90</b>	7, 13, 23, 31	26 (4%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	PRO	8.9
1	B	224	HIS	3.1

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	ACT	A	276	4/4	0.79	0.15	33,33,33,34	0
3	GOL	A	277	6/6	0.81	0.14	34,37,39,40	0
3	GOL	B	276	6/6	0.83	0.15	39,42,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.