



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:15 PM UTC

PDB ID : 2WNI / pdb_00002wni
Title : Crystal Structure Analysis of Klebsiella sp ASR1 Phytase
Authors : Bohm, K.; Mueller, J.J.; Heinemann, U.
Deposited on : 2009-07-09
Resolution : 2.57 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

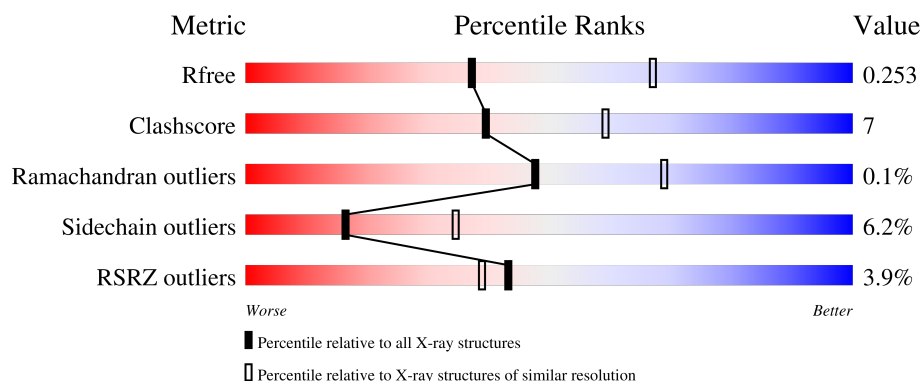
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

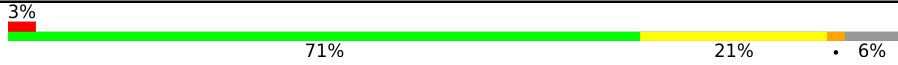
The reported resolution of this entry is 2.57 Å.

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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	418	
1	B	418	
1	C	418	
1	D	418	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12423 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 3-PHYTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3058	1917	562	566	13			
1	B	394	Total	C	N	O	S	0	0	0
			3047	1911	558	565	13			
1	C	395	Total	C	N	O	S	0	0	0
			3058	1917	562	566	13			
1	D	394	Total	C	N	O	S	0	0	0
			3047	1911	558	565	13			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q84CN9
A	2	ASP	-	expression tag	UNP Q84CN9
A	3	ILE	-	expression tag	UNP Q84CN9
A	4	GLY	-	expression tag	UNP Q84CN9
A	5	ILE	-	expression tag	UNP Q84CN9
A	6	ASN	-	expression tag	UNP Q84CN9
A	7	SER	-	expression tag	UNP Q84CN9
A	8	ASP	-	expression tag	UNP Q84CN9
A	9	PRO	-	expression tag	UNP Q84CN9
A	10	PRO	-	expression tag	UNP Q84CN9
A	11	PRO	-	expression tag	UNP Q84CN9
A	12	ARG	-	expression tag	UNP Q84CN9
A	25	ALA	HIS	engineered mutation	UNP Q84CN9
A	123	ALA	VAL	engineered mutation	UNP Q84CN9
A	279	SER	ASN	engineered mutation	UNP Q84CN9
A	397	ALA	THR	engineered mutation	UNP Q84CN9
A	406	LYS	-	expression tag	UNP Q84CN9
A	407	LEU	-	expression tag	UNP Q84CN9
A	408	ALA	-	expression tag	UNP Q84CN9
A	409	ALA	-	expression tag	UNP Q84CN9
A	410	ALA	-	expression tag	UNP Q84CN9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	411	LEU	-	expression tag	UNP Q84CN9
A	412	GLU	-	expression tag	UNP Q84CN9
A	413	HIS	-	expression tag	UNP Q84CN9
A	414	HIS	-	expression tag	UNP Q84CN9
A	415	HIS	-	expression tag	UNP Q84CN9
A	416	HIS	-	expression tag	UNP Q84CN9
A	417	HIS	-	expression tag	UNP Q84CN9
A	418	HIS	-	expression tag	UNP Q84CN9
B	1	MET	-	expression tag	UNP Q84CN9
B	2	ASP	-	expression tag	UNP Q84CN9
B	3	ILE	-	expression tag	UNP Q84CN9
B	4	GLY	-	expression tag	UNP Q84CN9
B	5	ILE	-	expression tag	UNP Q84CN9
B	6	ASN	-	expression tag	UNP Q84CN9
B	7	SER	-	expression tag	UNP Q84CN9
B	8	ASP	-	expression tag	UNP Q84CN9
B	9	PRO	-	expression tag	UNP Q84CN9
B	10	PRO	-	expression tag	UNP Q84CN9
B	11	PRO	-	expression tag	UNP Q84CN9
B	12	ARG	-	expression tag	UNP Q84CN9
B	25	ALA	HIS	engineered mutation	UNP Q84CN9
B	123	ALA	VAL	engineered mutation	UNP Q84CN9
B	279	SER	ASN	engineered mutation	UNP Q84CN9
B	397	ALA	THR	engineered mutation	UNP Q84CN9
B	406	LYS	-	expression tag	UNP Q84CN9
B	407	LEU	-	expression tag	UNP Q84CN9
B	408	ALA	-	expression tag	UNP Q84CN9
B	409	ALA	-	expression tag	UNP Q84CN9
B	410	ALA	-	expression tag	UNP Q84CN9
B	411	LEU	-	expression tag	UNP Q84CN9
B	412	GLU	-	expression tag	UNP Q84CN9
B	413	HIS	-	expression tag	UNP Q84CN9
B	414	HIS	-	expression tag	UNP Q84CN9
B	415	HIS	-	expression tag	UNP Q84CN9
B	416	HIS	-	expression tag	UNP Q84CN9
B	417	HIS	-	expression tag	UNP Q84CN9
B	418	HIS	-	expression tag	UNP Q84CN9
C	1	MET	-	expression tag	UNP Q84CN9
C	2	ASP	-	expression tag	UNP Q84CN9
C	3	ILE	-	expression tag	UNP Q84CN9
C	4	GLY	-	expression tag	UNP Q84CN9
C	5	ILE	-	expression tag	UNP Q84CN9

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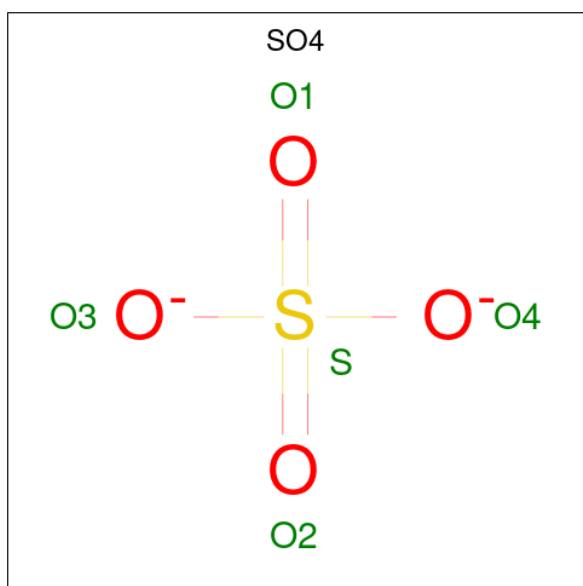
Chain	Residue	Modelled	Actual	Comment	Reference
C	6	ASN	-	expression tag	UNP Q84CN9
C	7	SER	-	expression tag	UNP Q84CN9
C	8	ASP	-	expression tag	UNP Q84CN9
C	9	PRO	-	expression tag	UNP Q84CN9
C	10	PRO	-	expression tag	UNP Q84CN9
C	11	PRO	-	expression tag	UNP Q84CN9
C	12	ARG	-	expression tag	UNP Q84CN9
C	25	ALA	HIS	engineered mutation	UNP Q84CN9
C	123	ALA	VAL	engineered mutation	UNP Q84CN9
C	279	SER	ASN	engineered mutation	UNP Q84CN9
C	397	ALA	THR	engineered mutation	UNP Q84CN9
C	406	LYS	-	expression tag	UNP Q84CN9
C	407	LEU	-	expression tag	UNP Q84CN9
C	408	ALA	-	expression tag	UNP Q84CN9
C	409	ALA	-	expression tag	UNP Q84CN9
C	410	ALA	-	expression tag	UNP Q84CN9
C	411	LEU	-	expression tag	UNP Q84CN9
C	412	GLU	-	expression tag	UNP Q84CN9
C	413	HIS	-	expression tag	UNP Q84CN9
C	414	HIS	-	expression tag	UNP Q84CN9
C	415	HIS	-	expression tag	UNP Q84CN9
C	416	HIS	-	expression tag	UNP Q84CN9
C	417	HIS	-	expression tag	UNP Q84CN9
C	418	HIS	-	expression tag	UNP Q84CN9
D	1	MET	-	expression tag	UNP Q84CN9
D	2	ASP	-	expression tag	UNP Q84CN9
D	3	ILE	-	expression tag	UNP Q84CN9
D	4	GLY	-	expression tag	UNP Q84CN9
D	5	ILE	-	expression tag	UNP Q84CN9
D	6	ASN	-	expression tag	UNP Q84CN9
D	7	SER	-	expression tag	UNP Q84CN9
D	8	ASP	-	expression tag	UNP Q84CN9
D	9	PRO	-	expression tag	UNP Q84CN9
D	10	PRO	-	expression tag	UNP Q84CN9
D	11	PRO	-	expression tag	UNP Q84CN9
D	12	ARG	-	expression tag	UNP Q84CN9
D	25	ALA	HIS	engineered mutation	UNP Q84CN9
D	123	ALA	VAL	engineered mutation	UNP Q84CN9
D	279	SER	ASN	engineered mutation	UNP Q84CN9
D	397	ALA	THR	engineered mutation	UNP Q84CN9
D	406	LYS	-	expression tag	UNP Q84CN9
D	407	LEU	-	expression tag	UNP Q84CN9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	408	ALA	-	expression tag	UNP Q84CN9
D	409	ALA	-	expression tag	UNP Q84CN9
D	410	ALA	-	expression tag	UNP Q84CN9
D	411	LEU	-	expression tag	UNP Q84CN9
D	412	GLU	-	expression tag	UNP Q84CN9
D	413	HIS	-	expression tag	UNP Q84CN9
D	414	HIS	-	expression tag	UNP Q84CN9
D	415	HIS	-	expression tag	UNP Q84CN9
D	416	HIS	-	expression tag	UNP Q84CN9
D	417	HIS	-	expression tag	UNP Q84CN9
D	418	HIS	-	expression tag	UNP Q84CN9

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

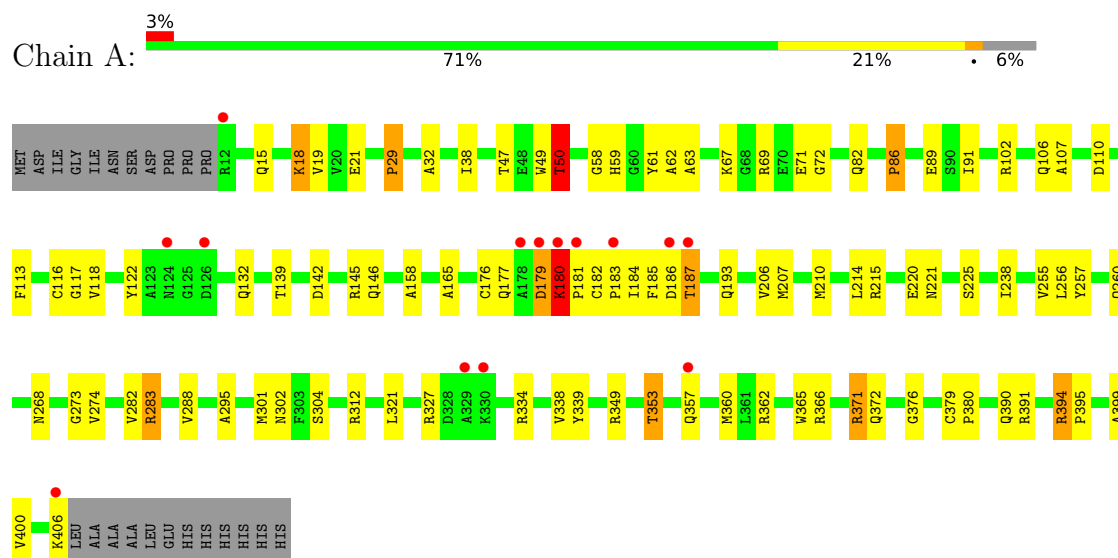
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	43	Total	O	0	0
			43	43		
3	C	25	Total	O	0	0
			25	25		
3	D	27	Total	O	0	0
			27	27		

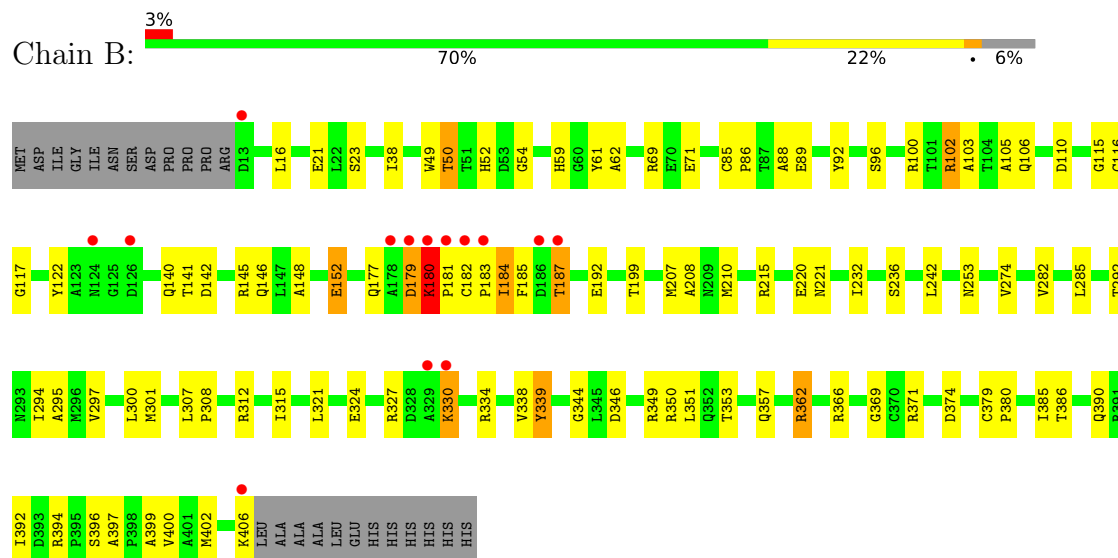
3 Residue-property plots [i](#)

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: 3-PHYTASE

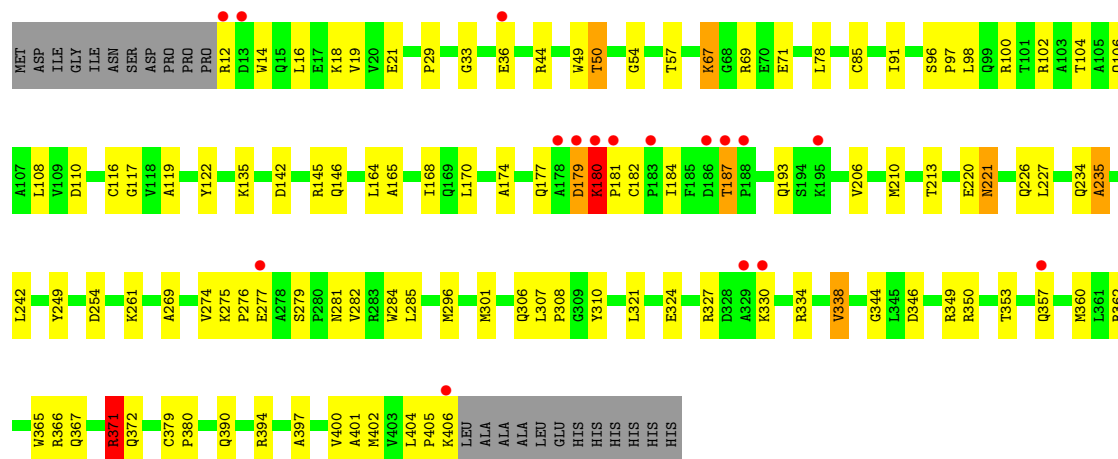


• Molecule 1: 3-PHYTASE

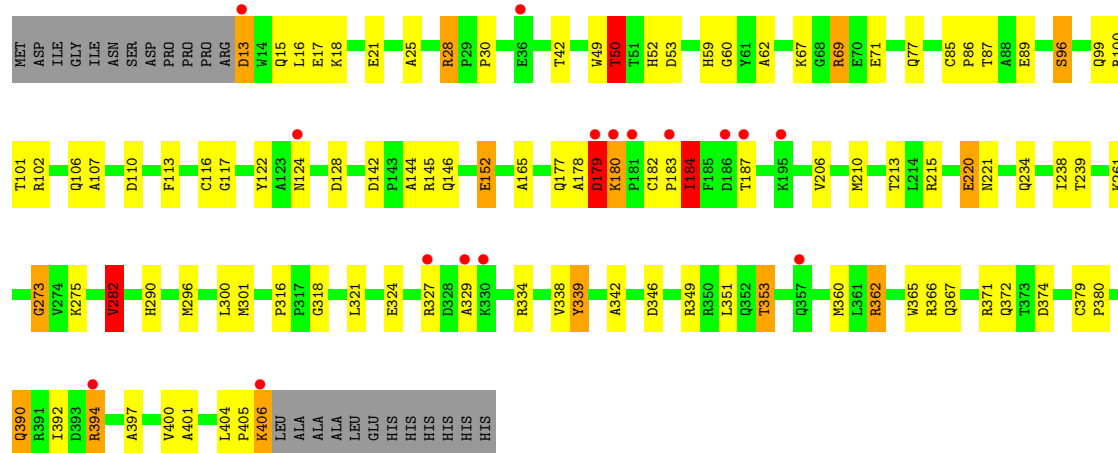


• Molecule 1: 3-PHYTASE





• Molecule 1: 3-PHYTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.71Å 122.93Å 205.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.41 – 2.57 105.41 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.2 (105.41-2.57) 99.2 (105.41-2.57)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.39 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.251 0.203 , 0.253	Depositor DCC
R_{free} test set	3356 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 24.0	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	0.92	EDS
Total number of atoms	12423	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: 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	1.67	29/3125 (0.9%)	1.44	20/4254 (0.5%)
1	B	1.68	23/3114 (0.7%)	1.44	28/4240 (0.7%)
1	C	1.71	29/3125 (0.9%)	1.50	31/4254 (0.7%)
1	D	1.68	28/3114 (0.9%)	1.43	33/4240 (0.8%)
All	All	1.69	109/12478 (0.9%)	1.45	112/16988 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	ALA	CA-CB	-8.85	1.39	1.53
1	C	401	ALA	CA-CB	8.09	1.63	1.53
1	D	282	VAL	CA-C	-7.95	1.43	1.52
1	B	208	ALA	CA-CB	-7.87	1.40	1.53
1	C	213	THR	CA-CB	-7.55	1.41	1.53
1	B	232	ILE	CA-CB	-7.52	1.45	1.54
1	A	312	ARG	N-CA	-7.37	1.36	1.46
1	C	276	PRO	C-O	7.11	1.32	1.23
1	C	338	VAL	C-O	7.05	1.31	1.24
1	C	344	GLY	N-CA	7.04	1.54	1.45
1	A	29	PRO	C-O	-6.97	1.16	1.24
1	C	279	SER	CA-C	6.79	1.59	1.52
1	B	199	THR	C-O	-6.66	1.16	1.23
1	C	174	ALA	CA-CB	-6.63	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	107	ALA	CA-CB	-6.57	1.43	1.53
1	C	372	GLN	CA-C	6.47	1.61	1.52
1	B	274	VAL	C-O	-6.42	1.17	1.24
1	A	238	ILE	CA-CB	-6.42	1.46	1.54
1	B	103	ALA	N-CA	-6.40	1.38	1.46
1	B	386	THR	C-O	-6.37	1.16	1.24
1	B	62	ALA	CA-CB	-6.33	1.43	1.53
1	D	390	GLN	C-O	-6.29	1.16	1.24
1	D	220	GLU	C-O	-6.28	1.16	1.24
1	D	30	PRO	C-O	-6.20	1.16	1.23
1	A	61	TYR	N-CA	-6.17	1.39	1.46
1	A	82	GLN	C-O	-6.16	1.15	1.23
1	D	316	PRO	CA-C	-6.12	1.48	1.52
1	A	193	GLN	N-CA	-6.12	1.38	1.46
1	D	397	ALA	C-O	-6.11	1.16	1.23
1	C	29	PRO	CA-C	6.10	1.57	1.52
1	C	281	ASN	N-CA	-6.05	1.39	1.46
1	C	14	TRP	CA-C	-6.05	1.45	1.52
1	B	397	ALA	C-O	-6.02	1.17	1.24
1	A	107	ALA	CA-CB	-5.97	1.43	1.53
1	C	372	GLN	N-CA	-5.96	1.38	1.46
1	A	225	SER	C-O	-5.94	1.16	1.24
1	A	59	HIS	N-CA	-5.94	1.39	1.46
1	A	63	ALA	CA-CB	-5.92	1.43	1.53
1	C	310	TYR	CA-C	-5.91	1.45	1.52
1	A	86	PRO	C-O	-5.89	1.16	1.23
1	C	344	GLY	C-O	5.88	1.31	1.23
1	D	290	HIS	C-O	-5.86	1.16	1.23
1	D	15	GLN	CG-CD	5.85	1.66	1.52
1	B	369	GLY	C-O	-5.84	1.15	1.24
1	C	193	GLN	CA-C	-5.84	1.45	1.52
1	D	25	ALA	C-O	5.82	1.31	1.24
1	D	392	ILE	C-O	-5.82	1.17	1.24
1	A	371	ARG	CA-C	-5.80	1.45	1.52
1	C	277	GLU	CB-CG	5.79	1.69	1.52
1	B	397	ALA	CA-C	-5.79	1.46	1.53
1	B	88	ALA	CA-CB	5.76	1.63	1.53
1	B	392	ILE	CA-CB	-5.71	1.48	1.54
1	A	118	VAL	CA-CB	-5.71	1.47	1.54
1	C	269	ALA	CA-CB	-5.69	1.44	1.53
1	D	406	LYS	CG-CD	5.61	1.69	1.52
1	B	315	ILE	C-O	-5.60	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	213	THR	CA-CB	-5.59	1.44	1.53
1	D	342	ALA	CA-CB	-5.55	1.44	1.53
1	A	158	ALA	CA-CB	5.54	1.62	1.53
1	D	372	GLN	N-CA	-5.54	1.39	1.46
1	A	295	ALA	CA-CB	-5.51	1.44	1.53
1	A	257	TYR	C-O	-5.50	1.17	1.24
1	D	152	GLU	N-CA	-5.49	1.39	1.46
1	B	105	ALA	CA-CB	-5.47	1.44	1.53
1	D	165	ALA	N-CA	5.44	1.51	1.46
1	C	36	GLU	CG-CD	5.40	1.65	1.52
1	A	50	THR	CA-CB	-5.39	1.43	1.53
1	A	372	GLN	CA-C	5.39	1.59	1.52
1	A	139	THR	CA-CB	5.39	1.60	1.53
1	D	183	PRO	CA-C	5.38	1.60	1.52
1	C	119	ALA	C-O	-5.36	1.17	1.23
1	C	296	MET	CA-C	-5.36	1.45	1.52
1	B	300	LEU	C-O	-5.35	1.17	1.24
1	D	406	LYS	N-CA	5.34	1.56	1.46
1	D	367	GLN	C-O	-5.32	1.19	1.24
1	C	346	ASP	C-O	5.31	1.30	1.24
1	A	50	THR	CA-C	5.31	1.60	1.52
1	C	306	GLN	C-O	-5.30	1.17	1.23
1	D	124	ASN	CB-CG	5.29	1.65	1.52
1	D	99	GLN	N-CA	-5.29	1.40	1.46
1	B	183	PRO	CA-C	5.28	1.59	1.52
1	C	50	THR	CA-C	5.28	1.60	1.52
1	A	288	VAL	CA-CB	-5.26	1.47	1.54
1	C	242	LEU	CA-C	5.23	1.59	1.52
1	C	170	LEU	N-CA	5.23	1.52	1.46
1	C	371	ARG	CA-C	-5.18	1.46	1.52
1	A	15	GLN	CG-CD	5.17	1.65	1.52
1	C	108	LEU	N-CA	5.15	1.52	1.46
1	D	85	CYS	CA-C	-5.15	1.47	1.53
1	A	91	ILE	C-O	-5.15	1.18	1.23
1	D	144	ALA	CA-CB	5.11	1.61	1.53
1	D	60	GLY	C-O	5.11	1.29	1.23
1	B	297	VAL	CA-CB	-5.11	1.48	1.54
1	D	300	LEU	C-O	-5.11	1.18	1.24
1	A	268	ASN	N-CA	-5.11	1.40	1.46
1	D	234	GLN	CA-C	-5.10	1.46	1.52
1	B	192	GLU	CA-C	-5.09	1.46	1.52
1	B	295	ALA	CA-CB	-5.08	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	33	GLY	C-O	5.06	1.29	1.23
1	B	312	ARG	CA-C	5.06	1.59	1.52
1	B	339	TYR	CA-C	-5.05	1.46	1.52
1	A	19	VAL	N-CA	-5.04	1.40	1.46
1	A	165	ALA	N-CA	5.04	1.51	1.46
1	B	23	SER	C-O	-5.04	1.17	1.23
1	D	339	TYR	CA-C	-5.04	1.46	1.52
1	A	214	LEU	N-CA	-5.04	1.40	1.46
1	B	141	THR	CA-CB	-5.03	1.45	1.53
1	A	391	ARG	CA-C	5.02	1.59	1.52
1	C	104	THR	C-O	5.02	1.29	1.24

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	404	LEU	CA-C-N	10.22	132.62	119.84
1	C	404	LEU	C-N-CA	10.22	132.62	119.84
1	A	180	LYS	CA-C-N	-9.06	111.55	120.52
1	A	180	LYS	C-N-CA	-9.06	111.55	120.52
1	B	180	LYS	CA-C-N	-8.05	112.42	120.31
1	B	180	LYS	C-N-CA	-8.05	112.42	120.31
1	A	283	ARG	N-CA-C	-7.82	103.87	113.41
1	C	50	THR	N-CA-CB	-7.52	97.90	110.39
1	C	44	ARG	CA-C-N	-7.27	112.50	119.85
1	C	44	ARG	C-N-CA	-7.27	112.50	119.85
1	B	96	SER	CA-C-N	-7.23	112.43	120.45
1	B	96	SER	C-N-CA	-7.23	112.43	120.45
1	A	59	HIS	N-CA-C	-7.21	103.42	111.28
1	D	96	SER	CA-C-N	-6.78	112.60	120.12
1	D	96	SER	C-N-CA	-6.78	112.60	120.12
1	D	50	THR	N-CA-CB	-6.68	99.51	110.40
1	A	47	THR	N-CA-C	6.67	120.15	110.42
1	A	132	GLN	N-CA-C	-6.60	101.51	110.68
1	C	242	LEU	CA-C-N	-6.59	112.83	119.56
1	C	242	LEU	C-N-CA	-6.59	112.83	119.56
1	B	50	THR	N-CA-CB	-6.59	99.45	110.39
1	D	180	LYS	N-CA-C	-6.58	100.63	110.24
1	B	374	ASP	CA-C-N	-6.56	112.97	122.28
1	B	374	ASP	C-N-CA	-6.56	112.97	122.28
1	C	397	ALA	CA-C-N	-6.52	113.26	119.85
1	C	397	ALA	C-N-CA	-6.52	113.26	119.85
1	B	50	THR	OG1-CB-CG2	6.45	122.19	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	235	ALA	N-CA-C	-6.36	104.34	111.28
1	B	397	ALA	CA-C-N	-6.33	113.26	119.78
1	B	397	ALA	C-N-CA	-6.33	113.26	119.78
1	C	165	ALA	CA-C-N	-6.30	112.06	119.05
1	C	165	ALA	C-N-CA	-6.30	112.06	119.05
1	D	397	ALA	CA-C-N	-6.30	113.29	119.78
1	D	397	ALA	C-N-CA	-6.30	113.29	119.78
1	B	242	LEU	CA-C-N	-6.28	112.37	119.28
1	B	242	LEU	C-N-CA	-6.28	112.37	119.28
1	A	50	THR	N-CA-CB	-6.22	99.75	110.32
1	D	404	LEU	CA-C-N	-6.20	114.25	120.21
1	D	404	LEU	C-N-CA	-6.20	114.25	120.21
1	B	396	SER	CA-C-N	-6.15	115.40	123.34
1	B	396	SER	C-N-CA	-6.15	115.40	123.34
1	C	85	CYS	N-CA-C	6.09	117.57	109.83
1	D	273	GLY	N-CA-C	-6.09	107.11	114.66
1	D	17	GLU	N-CA-C	6.06	120.80	113.41
1	A	391	ARG	CG-CD-NE	-5.91	98.99	112.00
1	D	28	ARG	CA-C-N	-5.91	114.29	120.38
1	D	28	ARG	C-N-CA	-5.91	114.29	120.38
1	B	86	PRO	CA-C-O	-5.90	114.47	121.67
1	D	282	VAL	CB-CA-C	-5.84	100.66	111.18
1	D	401	ALA	N-CA-C	-5.82	100.35	109.25
1	D	184	ILE	N-CA-C	5.76	117.18	110.62
1	B	85	CYS	N-CA-C	5.75	117.06	109.93
1	C	180	LYS	CA-C-N	-5.74	114.69	120.31
1	C	180	LYS	C-N-CA	-5.74	114.69	120.31
1	D	62	ALA	N-CA-C	-5.70	105.20	111.82
1	A	187	THR	CA-C-N	-5.69	114.88	120.52
1	A	187	THR	C-N-CA	-5.69	114.88	120.52
1	D	394	ARG	CA-C-N	-5.66	113.79	119.56
1	D	394	ARG	C-N-CA	-5.66	113.79	119.56
1	B	236	SER	N-CA-C	-5.60	105.70	112.54
1	C	97	PRO	N-CA-C	5.59	120.91	114.20
1	C	350	ARG	NE-CZ-NH2	5.55	124.19	119.20
1	D	353	THR	CB-CA-C	5.54	118.37	109.51
1	C	85	CYS	CA-CB-SG	-5.51	101.72	114.40
1	C	275	LYS	CA-C-N	-5.49	114.12	119.78
1	C	275	LYS	C-N-CA	-5.49	114.12	119.78
1	D	296	MET	N-CA-C	-5.47	105.39	111.36
1	D	179	ASP	N-CA-C	5.43	122.37	110.80
1	A	179	ASP	N-CA-C	5.43	122.36	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	179	ASP	N-CA-C	5.35	122.20	110.80
1	D	275	LYS	CA-C-N	-5.33	114.21	119.92
1	D	275	LYS	C-N-CA	-5.33	114.21	119.92
1	B	385	ILE	N-CA-C	-5.33	105.33	110.72
1	D	316	PRO	O-C-N	5.31	123.65	121.15
1	D	206	VAL	N-CA-C	-5.31	104.46	111.09
1	C	296	MET	N-CA-C	-5.30	105.58	111.36
1	A	376	GLY	N-CA-C	-5.28	105.56	111.63
1	B	294	ILE	N-CA-C	-5.28	105.39	110.72
1	A	371	ARG	CA-CB-CG	5.27	124.64	114.10
1	C	221	ASN	CB-CA-C	-5.27	103.19	111.51
1	D	69	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	C	96	SER	CA-C-N	-5.25	114.29	120.12
1	C	96	SER	C-N-CA	-5.25	114.29	120.12
1	B	187	THR	CA-C-N	-5.24	115.33	120.52
1	B	187	THR	C-N-CA	-5.24	115.33	120.52
1	B	399	ALA	CA-C-N	-5.24	115.66	122.94
1	B	399	ALA	C-N-CA	-5.24	115.66	122.94
1	D	42	THR	N-CA-C	-5.24	105.75	113.61
1	C	187	THR	CA-C-N	-5.23	115.20	120.85
1	C	187	THR	C-N-CA	-5.23	115.20	120.85
1	C	187	THR	N-CA-C	5.21	115.98	109.57
1	C	57	THR	N-CA-C	-5.18	103.56	110.55
1	C	226	GLN	N-CA-C	-5.17	106.37	113.30
1	A	61	TYR	N-CA-C	-5.17	105.56	111.14
1	D	50	THR	N-CA-C	-5.17	106.48	112.89
1	D	374	ASP	CB-CA-C	-5.15	99.46	110.32
1	A	72	GLY	N-CA-C	-5.10	106.24	112.77
1	D	77	GLN	N-CA-C	-5.10	105.91	111.82
1	B	102	ARG	NE-CZ-NH2	-5.09	114.62	119.20
1	B	362	ARG	NH1-CZ-NH2	5.07	125.89	119.30
1	D	362	ARG	NH1-CZ-NH2	5.04	125.86	119.30
1	B	179	ASP	N-CA-C	5.04	121.54	110.80
1	B	344	GLY	N-CA-C	-5.04	104.73	112.85
1	A	353	THR	CB-CA-C	5.04	117.57	109.51
1	B	208	ALA	N-CA-C	-5.04	105.87	111.36
1	A	399	ALA	CA-C-N	-5.01	116.14	123.06
1	A	399	ALA	C-N-CA	-5.01	116.14	123.06
1	C	67	LYS	N-CA-C	-5.01	105.53	111.69
1	D	346	ASP	N-CA-C	5.01	116.82	111.36
1	A	32	ALA	CA-C-N	5.01	125.50	119.94
1	A	32	ALA	C-N-CA	5.01	125.50	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	406	LYS	CA-CB-CG	5.00	124.10	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	405	PRO	Peptide

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	3058	0	3051	42	0
1	B	3047	0	3038	34	0
1	C	3058	0	3051	47	0
1	D	3047	0	3038	42	0
2	A	20	0	0	0	0
2	B	30	0	0	1	0
2	C	15	0	0	0	0
2	D	20	0	0	0	0
3	A	33	0	0	3	0
3	B	43	0	0	0	0
3	C	25	0	0	0	0
3	D	27	0	0	2	0
All	All	12423	0	12178	163	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 7.

All (163) 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:D:50:THR:HG22	3:D:2003:HOH:O	1.46	1.15
1:C:12:ARG:HE	1:C:371:ARG:NH2	1.54	1.05
1:C:220:GLU:HG3	1:C:220:GLU:O	1.63	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ARG:HE	1:C:371:ARG:HH22	0.96	0.95
1:A:18:LYS:HE3	1:A:282:VAL:O	1.68	0.92
1:A:69:ARG:HG3	1:A:69:ARG:HH11	1.37	0.89
1:C:12:ARG:NE	1:C:371:ARG:HH22	1.75	0.84
1:D:18:LYS:NZ	1:D:273:GLY:O	2.15	0.79
1:B:69:ARG:HH11	1:B:69:ARG:HG3	1.49	0.78
1:D:327:ARG:HH12	1:D:334:ARG:NH2	1.86	0.73
1:C:327:ARG:HH12	1:C:334:ARG:NH2	1.86	0.72
1:A:220:GLU:O	1:A:220:GLU:HG3	1.88	0.71
1:C:21:GLU:OE1	1:C:71:GLU:OE2	2.09	0.70
1:C:180:LYS:HG3	1:C:181:PRO:HD2	1.78	0.66
1:A:69:ARG:HG3	1:A:69:ARG:NH1	2.10	0.64
1:A:180:LYS:HG3	1:A:181:PRO:HD2	1.82	0.62
1:B:301:MET:HE1	1:B:338:VAL:HG11	1.81	0.62
1:A:379:CYS:HB3	3:A:2033:HOH:O	1.98	0.62
1:D:18:LYS:CE	1:D:282:VAL:O	2.49	0.61
1:B:21:GLU:OE1	1:B:71:GLU:OE2	2.20	0.59
1:C:142:ASP:OD2	1:C:145:ARG:HG2	2.02	0.59
1:C:220:GLU:O	1:C:220:GLU:CG	2.46	0.59
1:A:50:THR:HG22	3:A:2012:HOH:O	2.02	0.58
1:A:142:ASP:OD2	1:A:145:ARG:HG2	2.04	0.58
1:D:221:ASN:HA	1:D:349:ARG:NH1	2.18	0.58
1:B:184:ILE:HG21	1:B:210:MET:HE1	1.87	0.57
1:D:18:LYS:HE2	1:D:282:VAL:O	2.04	0.57
1:A:379:CYS:O	1:A:380:PRO:C	2.48	0.57
1:B:220:GLU:O	1:B:220:GLU:HG3	2.05	0.57
1:B:185:PHE:CD2	1:B:207:MET:HE2	2.39	0.56
1:B:301:MET:CE	1:B:338:VAL:HG11	2.36	0.56
1:D:339:TYR:CD2	1:D:362:ARG:HD2	2.40	0.56
1:B:379:CYS:O	1:B:380:PRO:C	2.44	0.56
1:C:54:GLY:O	1:C:100:ARG:HD3	2.06	0.56
1:C:301:MET:HE1	1:C:338:VAL:HG11	1.88	0.55
1:B:69:ARG:HG3	1:B:69:ARG:NH1	2.19	0.55
1:C:206:VAL:HG12	1:C:210:MET:HE3	1.88	0.55
1:D:96:SER:HB3	1:D:101:THR:OG1	2.07	0.55
1:A:304:SER:HA	3:A:2023:HOH:O	2.07	0.54
1:A:221:ASN:HA	1:A:349:ARG:NH1	2.22	0.54
1:B:327:ARG:HH12	1:B:334:ARG:NH2	2.05	0.53
1:C:164:LEU:O	1:C:168:ILE:HG13	2.09	0.53
1:D:49:TRP:CD1	1:D:49:TRP:N	2.76	0.53
1:C:67:LYS:HG3	1:C:360:MET:CE	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ARG:HG3	1:D:69:ARG:HH11	1.73	0.53
1:C:16:LEU:CD1	1:C:324:GLU:HB3	2.38	0.52
1:D:220:GLU:O	1:D:220:GLU:HG3	2.09	0.52
1:A:69:ARG:HH11	1:A:69:ARG:CG	2.15	0.52
1:D:338:VAL:HB	1:D:365:TRP:HB3	1.92	0.52
1:A:102:ARG:HD3	1:A:122:TYR:CG	2.44	0.52
1:C:102:ARG:HD3	1:C:122:TYR:CG	2.45	0.51
1:B:339:TYR:CD2	1:B:362:ARG:HD2	2.45	0.51
1:A:18:LYS:NZ	1:A:273:GLY:O	2.39	0.51
1:C:327:ARG:HH12	1:C:334:ARG:CZ	2.24	0.51
1:D:301:MET:HE1	1:D:338:VAL:HG11	1.92	0.51
1:C:379:CYS:O	1:C:380:PRO:C	2.53	0.50
1:A:86:PRO:HD3	1:A:113:PHE:CD1	2.46	0.50
1:A:184:ILE:HG21	1:A:210:MET:HE1	1.93	0.50
1:B:253:ASN:OD1	1:B:292:THR:HG22	2.10	0.50
1:B:106:GLN:O	1:B:110:ASP:HB2	2.11	0.50
1:C:69:ARG:HH11	1:C:69:ARG:HG3	1.76	0.50
1:D:102:ARG:HD3	1:D:122:TYR:CG	2.46	0.50
1:A:327:ARG:HH12	1:A:334:ARG:NH2	2.09	0.50
1:B:89:GLU:O	1:B:282:VAL:HA	2.12	0.50
1:C:12:ARG:NE	1:C:371:ARG:NH2	2.39	0.50
1:C:227:LEU:C	1:C:227:LEU:HD12	2.37	0.50
1:C:285:LEU:HD21	1:C:402:MET:HE3	1.92	0.49
1:C:301:MET:CE	1:C:338:VAL:HG11	2.42	0.49
1:D:87:THR:OG1	1:D:89:GLU:HB2	2.12	0.49
1:B:102:ARG:HD3	1:B:122:TYR:CG	2.48	0.49
1:D:184:ILE:HG21	1:D:210:MET:HE1	1.94	0.49
1:A:206:VAL:HG12	1:A:210:MET:HE3	1.95	0.49
1:B:221:ASN:HA	1:B:349:ARG:NH1	2.27	0.49
1:D:142:ASP:OD2	1:D:145:ARG:HG2	2.12	0.49
1:D:301:MET:CE	1:D:338:VAL:HG11	2.43	0.49
1:B:116:CYS:O	1:B:117:GLY:C	2.53	0.49
1:C:67:LYS:HG3	1:C:360:MET:HE2	1.95	0.48
1:D:178:ALA:O	1:D:179:ASP:HB2	2.12	0.48
1:A:220:GLU:O	1:A:220:GLU:CG	2.59	0.48
1:D:379:CYS:O	1:D:380:PRO:C	2.52	0.48
1:D:59:HIS:CE1	1:D:351:LEU:HG	2.50	0.47
1:B:52:HIS:ND1	2:B:1409:SO4:O4	2.47	0.47
1:C:106:GLN:O	1:C:110:ASP:HB2	2.15	0.47
1:D:351:LEU:HD23	1:D:351:LEU:HA	1.71	0.47
1:A:69:ARG:NH1	1:A:69:ARG:CG	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:GLN:O	1:D:110:ASP:HB2	2.14	0.46
1:A:185:PHE:CD2	1:A:207:MET:HE2	2.51	0.46
1:D:28:ARG:HD3	1:D:100:ARG:CD	2.46	0.46
1:A:29:PRO:HB3	1:A:49:TRP:CD2	2.50	0.46
1:C:221:ASN:CG	1:C:221:ASN:O	2.58	0.46
1:A:21:GLU:OE1	1:A:71:GLU:OE2	2.34	0.46
1:D:16:LEU:CD1	1:D:324:GLU:HB3	2.45	0.46
1:B:59:HIS:CE1	1:B:351:LEU:HG	2.51	0.46
1:B:180:LYS:HG3	1:B:181:PRO:HD2	1.97	0.46
1:B:301:MET:HE1	1:B:338:VAL:CG1	2.44	0.46
1:D:21:GLU:OE1	1:D:71:GLU:OE2	2.33	0.46
1:C:18:LYS:HE3	1:C:282:VAL:HG23	1.98	0.46
1:B:346:ASP:O	1:B:350:ARG:HG3	2.16	0.46
1:B:54:GLY:O	1:B:100:ARG:HD3	2.16	0.45
1:D:102:ARG:HD3	1:D:122:TYR:CD1	2.52	0.45
1:C:91:ILE:HD12	1:C:284:TRP:CE3	2.51	0.45
1:D:128:ASP:OD1	1:D:128:ASP:C	2.59	0.45
1:D:238:ILE:O	1:D:239:THR:C	2.58	0.45
1:D:261:LYS:HB3	1:D:261:LYS:HE3	1.79	0.45
1:A:106:GLN:O	1:A:110:ASP:HB2	2.15	0.45
1:B:148:ALA:O	1:B:152:GLU:HB3	2.17	0.45
1:D:18:LYS:HE3	1:D:282:VAL:O	2.17	0.45
1:A:338:VAL:HB	1:A:365:TRP:HB3	1.98	0.45
1:B:285:LEU:HD21	1:B:402:MET:HE3	1.97	0.45
1:D:116:CYS:O	1:D:117:GLY:C	2.59	0.44
1:A:215:ARG:HD2	1:A:215:ARG:C	2.42	0.44
1:D:86:PRO:HD3	1:D:113:PHE:CD1	2.52	0.44
1:D:13:ASP:OD1	1:D:329:ALA:CB	2.65	0.44
1:C:184:ILE:HG21	1:C:210:MET:HE1	1.98	0.44
1:A:301:MET:CE	1:A:338:VAL:HG11	2.48	0.44
1:C:301:MET:HE1	1:C:338:VAL:CG1	2.47	0.44
1:B:16:LEU:CD1	1:B:324:GLU:HB3	2.48	0.43
1:B:215:ARG:HD2	1:B:215:ARG:C	2.43	0.43
1:B:307:LEU:O	1:B:308:PRO:C	2.58	0.43
1:D:318:GLY:HA3	3:D:2019:HOH:O	2.17	0.43
1:C:16:LEU:HD13	1:C:324:GLU:HB3	2.00	0.43
1:D:67:LYS:HG3	1:D:360:MET:CE	2.48	0.43
1:C:98:LEU:N	1:C:98:LEU:HD12	2.34	0.43
1:A:339:TYR:CD2	1:A:362:ARG:HD2	2.53	0.43
1:A:302:ASN:HD22	1:A:302:ASN:HA	1.63	0.43
1:A:301:MET:HE1	1:A:338:VAL:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:CYS:O	1:A:117:GLY:C	2.61	0.42
1:B:142:ASP:OD2	1:B:145:ARG:HG2	2.19	0.42
1:C:78:LEU:HD23	1:C:78:LEU:HA	1.90	0.42
1:C:102:ARG:HD3	1:C:122:TYR:CD1	2.54	0.42
1:A:176:CYS:SG	1:A:185:PHE:CE1	3.13	0.42
1:C:261:LYS:HB3	1:C:261:LYS:HE3	1.87	0.42
1:A:349:ARG:HG2	1:B:115:GLY:HA2	2.01	0.42
1:C:249:TYR:HB3	1:C:254:ASP:OD2	2.20	0.42
1:A:183:PRO:O	1:A:186:ASP:HB2	2.20	0.42
1:D:327:ARG:HH12	1:D:334:ARG:HH21	1.65	0.42
1:C:135:LYS:HA	1:C:135:LYS:HD3	1.85	0.42
1:A:67:LYS:HG3	1:A:360:MET:CE	2.50	0.41
1:B:92:TYR:HB2	1:B:282:VAL:HG11	2.02	0.41
1:C:234:GLN:O	1:C:235:ALA:C	2.62	0.41
1:A:49:TRP:N	1:A:49:TRP:CD1	2.89	0.41
1:A:394:ARG:N	1:A:395:PRO:CD	2.83	0.41
1:B:69:ARG:NH1	1:B:69:ARG:CG	2.82	0.41
1:A:102:ARG:HD3	1:A:122:TYR:CD1	2.56	0.41
1:A:256:LEU:O	1:A:260:GLN:HG3	2.20	0.41
1:B:49:TRP:CD1	1:B:49:TRP:N	2.88	0.41
1:C:221:ASN:HA	1:C:349:ARG:NH1	2.35	0.41
1:A:255:VAL:O	1:A:256:LEU:C	2.64	0.41
1:C:307:LEU:O	1:C:308:PRO:C	2.62	0.41
1:C:19:VAL:HG22	1:C:324:GLU:HG2	2.02	0.41
1:C:362:ARG:HH11	1:C:362:ARG:HD3	1.73	0.41
1:A:58:GLY:HA3	1:B:61:TYR:CG	2.56	0.41
1:C:116:CYS:O	1:C:117:GLY:C	2.61	0.41
1:C:338:VAL:HB	1:C:365:TRP:HB3	2.03	0.41
1:D:28:ARG:HH11	1:D:28:ARG:HG3	1.86	0.41
1:D:52:HIS:O	1:D:53:ASP:C	2.63	0.41
1:C:365:TRP:CH2	1:C:367:GLN:HG2	2.56	0.41
1:C:49:TRP:CD1	1:C:49:TRP:N	2.89	0.40
1:D:301:MET:HE1	1:D:338:VAL:CG1	2.51	0.40
1:C:180:LYS:HB2	1:C:180:LYS:NZ	2.36	0.40
1:D:215:ARG:HD2	1:D:215:ARG:C	2.46	0.40
1:A:67:LYS:O	1:A:67:LYS:HG2	2.18	0.40
1:D:67:LYS:HG3	1:D:360:MET:HE2	2.03	0.40

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	393/418 (94%)	380 (97%)	13 (3%)	0	100	100
1	B	392/418 (94%)	381 (97%)	10 (3%)	1 (0%)	36	56
1	C	393/418 (94%)	379 (96%)	13 (3%)	1 (0%)	36	56
1	D	392/418 (94%)	380 (97%)	12 (3%)	0	100	100
All	All	1570/1672 (94%)	1520 (97%)	48 (3%)	2 (0%)	48	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	405	PRO
1	B	330	LYS

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	319/338 (94%)	298 (93%)	21 (7%)	15	32
1	B	318/338 (94%)	297 (93%)	21 (7%)	15	32
1	C	319/338 (94%)	301 (94%)	18 (6%)	19	38
1	D	318/338 (94%)	299 (94%)	19 (6%)	17	36
All	All	1274/1352 (94%)	1195 (94%)	79 (6%)	16	34

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	38	ILE
1	A	50	THR
1	A	89	GLU
1	A	146	GLN
1	A	177	GLN
1	A	179	ASP
1	A	180	LYS
1	A	182	CYS
1	A	187	THR
1	A	274	VAL
1	A	283	ARG
1	A	321	LEU
1	A	353	THR
1	A	357	GLN
1	A	366	ARG
1	A	371	ARG
1	A	390	GLN
1	A	394	ARG
1	A	400	VAL
1	A	406	LYS
1	B	38	ILE
1	B	50	THR
1	B	140	GLN
1	B	146	GLN
1	B	152	GLU
1	B	177	GLN
1	B	179	ASP
1	B	180	LYS
1	B	182	CYS
1	B	184	ILE
1	B	187	THR
1	B	321	LEU
1	B	330	LYS
1	B	353	THR
1	B	357	GLN
1	B	366	ARG
1	B	371	ARG
1	B	390	GLN
1	B	394	ARG
1	B	400	VAL
1	B	406	LYS
1	C	50	THR

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Mol	Chain	Res	Type
1	C	146	GLN
1	C	177	GLN
1	C	179	ASP
1	C	180	LYS
1	C	182	CYS
1	C	187	THR
1	C	274	VAL
1	C	321	LEU
1	C	330	LYS
1	C	353	THR
1	C	357	GLN
1	C	366	ARG
1	C	371	ARG
1	C	390	GLN
1	C	394	ARG
1	C	400	VAL
1	C	406	LYS
1	D	13	ASP
1	D	50	THR
1	D	146	GLN
1	D	152	GLU
1	D	177	GLN
1	D	179	ASP
1	D	180	LYS
1	D	182	CYS
1	D	184	ILE
1	D	187	THR
1	D	282	VAL
1	D	321	LEU
1	D	353	THR
1	D	366	ARG
1	D	371	ARG
1	D	390	GLN
1	D	394	ARG
1	D	400	VAL
1	D	406	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	34	ASN

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Mol	Chain	Res	Type
1	A	73	GLN
1	A	124	ASN
1	A	209	ASN
1	A	226	GLN
1	A	260	GLN
1	A	302	ASN
1	A	358	HIS
1	A	382	GLN
1	B	15	GLN
1	B	34	ASN
1	B	73	GLN
1	B	209	ASN
1	B	226	GLN
1	B	302	ASN
1	B	382	GLN
1	C	34	ASN
1	C	73	GLN
1	C	82	GLN
1	C	106	GLN
1	C	209	ASN
1	C	260	GLN
1	C	302	ASN
1	C	358	HIS
1	C	382	GLN
1	D	15	GLN
1	D	73	GLN
1	D	106	GLN
1	D	159	GLN
1	D	209	ASN
1	D	226	GLN
1	D	302	ASN
1	D	358	HIS
1	D	382	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 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	SO4	D	1410	-	4,4,4	0.58	0	6,6,6	1.23	0
2	SO4	C	1408	-	4,4,4	0.56	0	6,6,6	0.97	0
2	SO4	A	1409	-	4,4,4	0.46	0	6,6,6	0.57	0
2	SO4	C	1409	-	4,4,4	0.47	0	6,6,6	0.77	0
2	SO4	B	1408	-	4,4,4	0.27	0	6,6,6	0.85	0
2	SO4	B	1409	-	4,4,4	0.84	0	6,6,6	0.89	0
2	SO4	B	1410	-	4,4,4	0.64	0	6,6,6	1.08	0
2	SO4	B	1411	-	4,4,4	0.48	0	6,6,6	0.86	0
2	SO4	B	1412	-	4,4,4	0.46	0	6,6,6	0.30	0
2	SO4	D	1408	-	4,4,4	0.66	0	6,6,6	0.88	0
2	SO4	A	1407	-	4,4,4	0.23	0	6,6,6	0.89	0
2	SO4	B	1407	-	4,4,4	0.46	0	6,6,6	0.95	1 (16%)
2	SO4	A	1408	-	4,4,4	0.60	0	6,6,6	0.82	0
2	SO4	A	1410	-	4,4,4	0.48	0	6,6,6	1.45	1 (16%)
2	SO4	D	1409	-	4,4,4	0.76	0	6,6,6	0.60	0
2	SO4	D	1407	-	4,4,4	0.15	0	6,6,6	1.54	1 (16%)
2	SO4	C	1407	-	4,4,4	0.73	0	6,6,6	1.55	2 (33%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1407	SO4	O3-S-O1	-3.01	93.85	109.56
2	C	1407	SO4	O4-S-O2	-2.59	96.03	109.56
2	A	1410	SO4	O3-S-O1	-2.44	96.83	109.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1407	SO4	O3-S-O1	-2.09	98.63	109.56
2	C	1407	SO4	O4-S-O3	2.07	119.95	108.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1409	SO4	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	395/418 (94%)	-0.06	14 (3%) 47 42	22, 32, 55, 75	0
1	B	394/418 (94%)	-0.04	14 (3%) 46 41	21, 32, 55, 75	0
1	C	395/418 (94%)	-0.02	17 (4%) 40 35	21, 33, 55, 76	0
1	D	394/418 (94%)	-0.08	16 (4%) 41 37	22, 33, 55, 75	0
All	All	1578/1672 (94%)	-0.05	61 (3%) 43 39	21, 33, 55, 76	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	ASP	4.9
1	B	180	LYS	4.4
1	D	180	LYS	4.2
1	C	330	LYS	4.2
1	B	183	PRO	4.0
1	C	329	ALA	3.8
1	B	181	PRO	3.8
1	B	330	LYS	3.8
1	A	186	ASP	3.8
1	A	180	LYS	3.8
1	C	12	ARG	3.8
1	C	178	ALA	3.8
1	A	181	PRO	3.7
1	D	183	PRO	3.6
1	B	179	ASP	3.6
1	D	195	LYS	3.5
1	D	187	THR	3.5
1	B	124	ASN	3.5
1	C	179	ASP	3.5
1	A	406	LYS	3.5
1	C	406	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	180	LYS	3.3
1	D	124	ASN	3.3
1	A	183	PRO	3.3
1	A	329	ALA	3.3
1	B	329	ALA	3.1
1	C	181	PRO	3.0
1	C	277	GLU	3.0
1	D	181	PRO	3.0
1	C	195	LYS	3.0
1	A	187	THR	2.9
1	C	187	THR	2.9
1	A	178	ALA	2.9
1	A	124	ASN	2.9
1	B	178	ALA	2.9
1	A	126	ASP	2.8
1	C	186	ASP	2.8
1	D	330	LYS	2.8
1	A	330	LYS	2.7
1	C	357	GLN	2.7
1	D	179	ASP	2.7
1	D	36	GLU	2.7
1	D	406	LYS	2.6
1	C	36	GLU	2.6
1	B	126	ASP	2.6
1	C	183	PRO	2.5
1	B	187	THR	2.5
1	D	186	ASP	2.4
1	D	329	ALA	2.4
1	A	179	ASP	2.4
1	B	406	LYS	2.4
1	D	327	ARG	2.2
1	A	12	ARG	2.2
1	D	357	GLN	2.2
1	A	357	GLN	2.2
1	C	13	ASP	2.2
1	B	13	ASP	2.1
1	D	394	ARG	2.1
1	B	182	CYS	2.1
1	C	188	PRO	2.1
1	D	13	ASP	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	SO4	A	1408	5/5	0.70	0.26	94,96,99,99	0
2	SO4	B	1411	5/5	0.75	0.25	89,90,91,93	0
2	SO4	A	1409	5/5	0.78	0.24	101,102,105,106	0
2	SO4	C	1408	5/5	0.84	0.17	62,63,67,69	0
2	SO4	C	1407	5/5	0.85	0.17	58,59,71,72	0
2	SO4	D	1409	5/5	0.87	0.17	56,58,64,69	0
2	SO4	D	1408	5/5	0.89	0.19	55,60,65,65	0
2	SO4	B	1410	5/5	0.89	0.19	60,64,69,73	0
2	SO4	B	1409	5/5	0.95	0.11	41,57,60,64	0
2	SO4	B	1408	5/5	0.98	0.08	31,32,36,42	0
2	SO4	A	1410	5/5	0.99	0.06	26,28,30,32	0
2	SO4	B	1407	5/5	0.99	0.05	21,26,29,29	0
2	SO4	C	1409	5/5	0.99	0.05	28,31,35,42	0
2	SO4	D	1407	5/5	0.99	0.07	24,27,33,37	0
2	SO4	A	1407	5/5	0.99	0.07	28,30,33,37	0
2	SO4	B	1412	5/5	0.99	0.04	23,25,30,30	0
2	SO4	D	1410	5/5	0.99	0.04	31,33,34,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.