wwPDB X-ray Structure Validation Summary Report (i)

Nov 3, 2024 – 01:10 am GMT

PDB ID	:	2WNI
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 wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

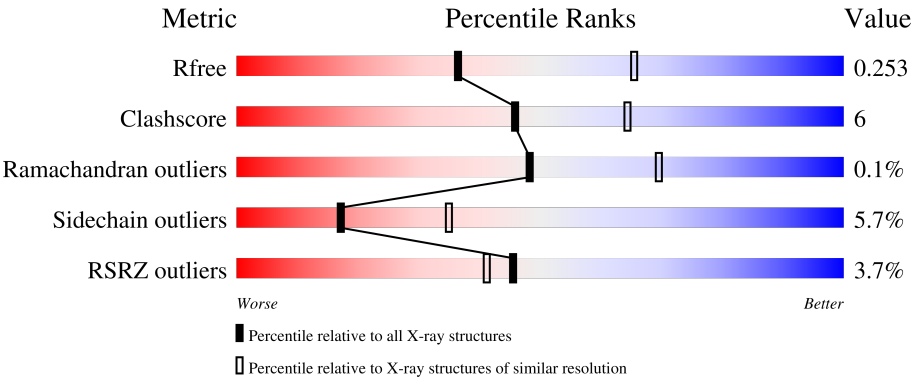
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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}	164625	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (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 <=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	3% 75% 17% • 6%
1	B	418	3% 74% 17% • 6%
1	C	418	4% 75% 18% • 6%
1	D	418	4% 75% 16% •• 6%

2 Entry composition (i)

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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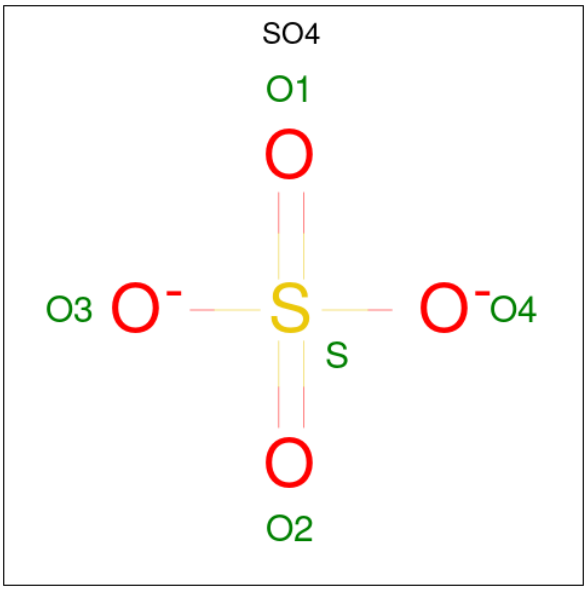
Chain	Residue	Modelled	Actual	Comment	Reference
D	408	ALA	-	expression tag	UNP Q84CN9
D	409	ALA	-	expression tag	UNP Q84CN9
D	410	ALA	-	expression tag	UNP Q84CN9
D	411	LEU	-	expression tag	UNP Q84CN9
D	412	GLU	-	expression tag	UNP Q84CN9
D	413	HIS	-	expression tag	UNP Q84CN9
D	414	HIS	-	expression tag	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 (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 3 is water.

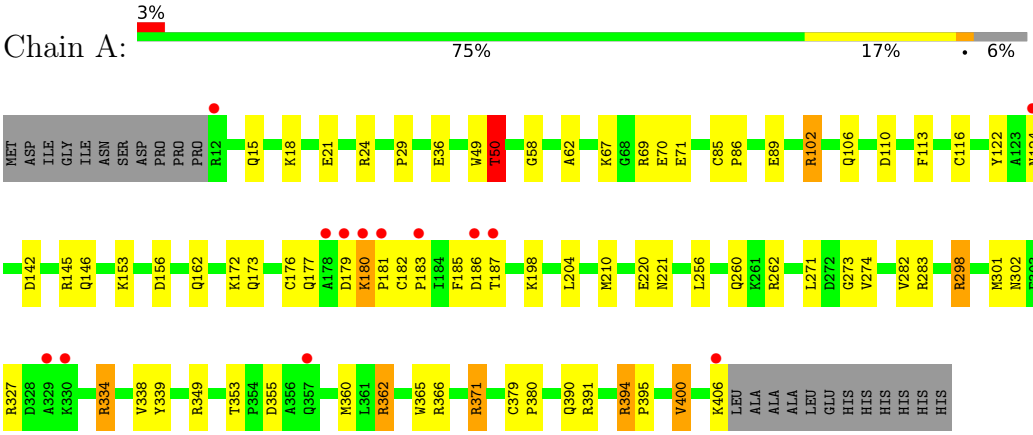
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	33	Total O 33 33	0	0
3	B	43	Total O 43 43	0	0
3	C	25	Total O 25 25	0	0
3	D	27	Total O 27 27	0	0

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.

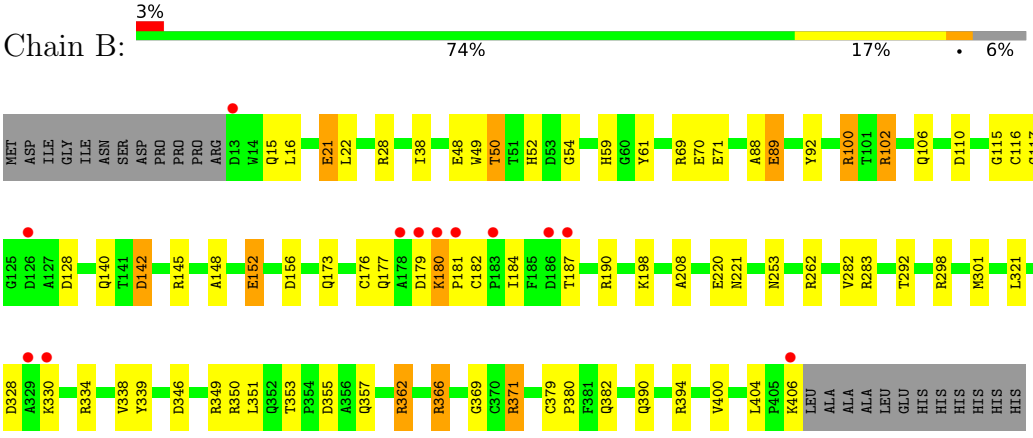
• Molecule 1: 3-PHYTASE

Chain A:



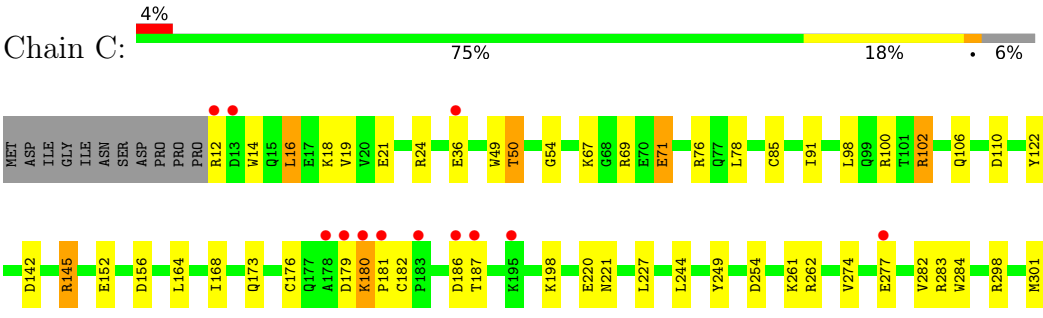
• Molecule 1: 3-PHYTASE

Chain B:

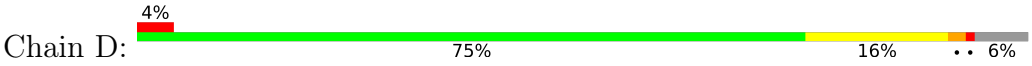


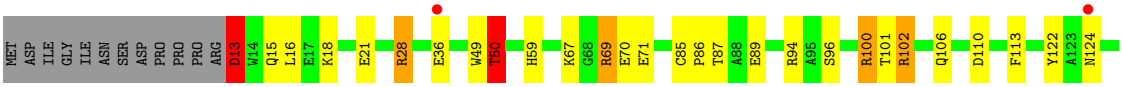
• Molecule 1: 3-PHYTASE

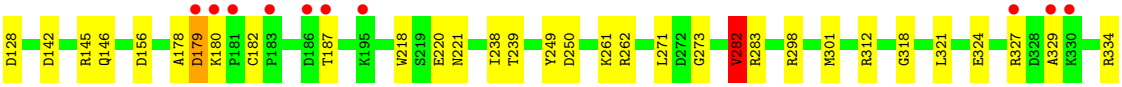
Chain C:

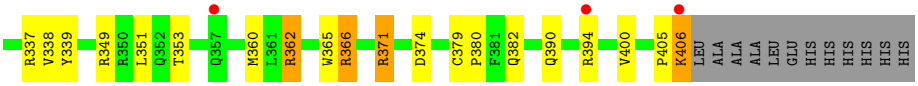


• Molecule 1: 3-PHYTASE









4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	1.34	10/3125 (0.3%)	1.18	21/4254 (0.5%)
1	B	1.35	17/3114 (0.5%)	1.19	25/4240 (0.6%)
1	C	1.40	13/3125 (0.4%)	1.20	21/4254 (0.5%)
1	D	1.36	10/3114 (0.3%)	1.17	24/4240 (0.6%)
All	All	1.37	50/12478 (0.4%)	1.19	91/16988 (0.5%)

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

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	277	GLU	CB-CG	9.30	1.69	1.52
1	C	36	GLU	CG-CD	9.07	1.65	1.51
1	D	36	GLU	CG-CD	7.99	1.64	1.51
1	D	218	TRP	CB-CG	-7.50	1.36	1.50
1	A	36	GLU	CG-CD	7.07	1.62	1.51

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	102	ARG	NE-CZ-NH2	-11.37	114.62	120.30
1	A	362	ARG	NE-CZ-NH2	-10.67	114.96	120.30
1	B	362	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	A	262	ARG	NE-CZ-NH2	-9.80	115.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	102	ARG	NE-CZ-NH2	-9.56	115.52	120.30

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	36	0
1	B	3047	0	3038	28	0
1	C	3058	0	3051	40	0
1	D	3047	0	3038	37	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	1	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	139	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.

The worst 5 of 139 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

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%)	37	57
1	C	393/418 (94%)	379 (96%)	13 (3%)	1 (0%)	37	57
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%)	300 (94%)	19 (6%)	16	33
1	B	318/338 (94%)	298 (94%)	20 (6%)	15	31
1	C	319/338 (94%)	303 (95%)	16 (5%)	20	41
1	D	318/338 (94%)	301 (95%)	17 (5%)	19	38
All	All	1274/1352 (94%)	1202 (94%)	72 (6%)	17	35

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	146	GLN
1	D	406	LYS
1	D	180	LYS
1	D	353	THR
1	B	179	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	106	GLN
1	C	302	ASN
1	C	248	ASN
1	D	15	GLN
1	A	390	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)

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	B	1410	-	4,4,4	0.58	0	6,6,6	1.10	0
2	SO4	A	1409	-	4,4,4	0.38	0	6,6,6	0.61	0
2	SO4	A	1407	-	4,4,4	0.15	0	6,6,6	0.90	0
2	SO4	B	1409	-	4,4,4	0.78	0	6,6,6	0.97	0
2	SO4	D	1408	-	4,4,4	0.60	0	6,6,6	0.89	0
2	SO4	B	1412	-	4,4,4	0.36	0	6,6,6	0.30	0
2	SO4	A	1410	-	4,4,4	0.55	0	6,6,6	1.47	1 (16%)
2	SO4	C	1408	-	4,4,4	0.47	0	6,6,6	1.03	0
2	SO4	D	1410	-	4,4,4	0.70	0	6,6,6	1.23	0
2	SO4	C	1407	-	4,4,4	0.69	0	6,6,6	1.65	2 (33%)
2	SO4	A	1408	-	4,4,4	0.52	0	6,6,6	0.77	0
2	SO4	B	1408	-	4,4,4	0.17	0	6,6,6	0.88	0
2	SO4	B	1411	-	4,4,4	0.40	0	6,6,6	0.87	0
2	SO4	B	1407	-	4,4,4	0.36	0	6,6,6	0.94	1 (16%)
2	SO4	C	1409	-	4,4,4	0.60	0	6,6,6	0.81	0
2	SO4	D	1407	-	4,4,4	0.21	0	6,6,6	1.55	2 (33%)
2	SO4	D	1409	-	4,4,4	0.70	0	6,6,6	0.76	0

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1407	SO4	O3-S-O1	-2.96	93.85	109.31
2	C	1407	SO4	O4-S-O3	2.55	119.95	109.06
2	C	1407	SO4	O4-S-O2	-2.55	96.03	109.31
2	A	1410	SO4	O3-S-O1	-2.39	96.83	109.31
2	B	1407	SO4	O3-S-O1	-2.05	98.63	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1409	SO4	1	0
2	D	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, 95^{th} 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%)	-0.16	14 (3%)	47	43	22, 32, 55, 75	0
1	B	394/418 (94%)	-0.14	13 (3%)	49	45	21, 32, 55, 75	0
1	C	395/418 (94%)	-0.12	16 (4%)	42	37	21, 33, 55, 76	0
1	D	394/418 (94%)	-0.18	15 (3%)	44	40	22, 33, 55, 75	0
All	All	1578/1672 (94%)	-0.15	58 (3%)	45	41	21, 33, 55, 76	0

The worst 5 of 58 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	4.3
1	C	330	LYS	4.2
1	B	183	PRO	3.9

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	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.