



# Full wwPDB X-ray Structure Validation Report

Sep 22, 2014 – 12:14 AM EDT

PDB ID : 4LXC  
Title : The antimicrobial peptidase lysostaphin from *Staphylococcus simulans*  
Authors : Sabala, I.; Jagielska, E.; Bardelang, P.T.; Czapinska, H.; Dahms, S.O.; Sharpe, J.A.; James, R.; Than, M.E.; Thomas, N.R.; Bochtler, M.  
Deposited on : 2013-07-29  
Resolution : 3.50 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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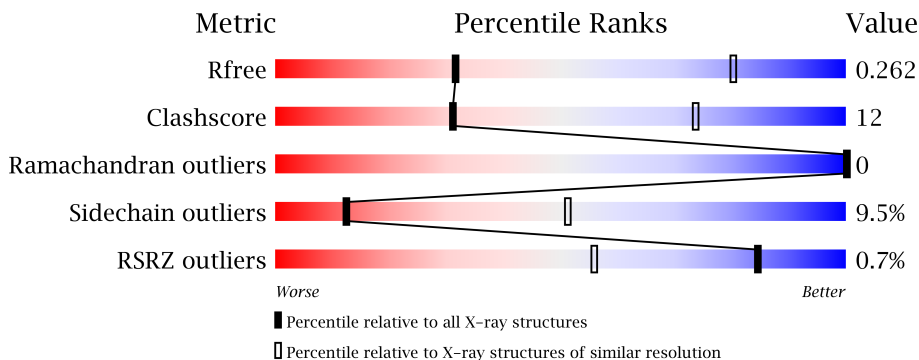
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23489  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 3.50 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))
$R_{free}$	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	255	
1	B	255	
1	C	255	
1	D	255	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	D	604	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7589 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Lysostaphin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1905	1213	332	353	7			
1	B	240	Total	C	N	O	S	0	0	0
			1855	1183	321	344	7			
1	C	240	Total	C	N	O	S	0	0	0
			1872	1194	325	346	7			
1	D	246	Total	C	N	O	S	0	0	0
			1908	1216	332	353	7			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	247	MET	-	INITIATING METHIONINE	UNP P10547
A	494	LEU	-	EXPRESSION TAG	UNP P10547
A	495	GLU	-	EXPRESSION TAG	UNP P10547
A	496	HIS	-	EXPRESSION TAG	UNP P10547
A	497	HIS	-	EXPRESSION TAG	UNP P10547
A	498	HIS	-	EXPRESSION TAG	UNP P10547
A	499	HIS	-	EXPRESSION TAG	UNP P10547
A	500	HIS	-	EXPRESSION TAG	UNP P10547
A	501	HIS	-	EXPRESSION TAG	UNP P10547
B	247	MET	-	INITIATING METHIONINE	UNP P10547
B	494	LEU	-	EXPRESSION TAG	UNP P10547
B	495	GLU	-	EXPRESSION TAG	UNP P10547
B	496	HIS	-	EXPRESSION TAG	UNP P10547
B	497	HIS	-	EXPRESSION TAG	UNP P10547
B	498	HIS	-	EXPRESSION TAG	UNP P10547
B	499	HIS	-	EXPRESSION TAG	UNP P10547
B	500	HIS	-	EXPRESSION TAG	UNP P10547
B	501	HIS	-	EXPRESSION TAG	UNP P10547
C	247	MET	-	INITIATING METHIONINE	UNP P10547
C	494	LEU	-	EXPRESSION TAG	UNP P10547
C	495	GLU	-	EXPRESSION TAG	UNP P10547

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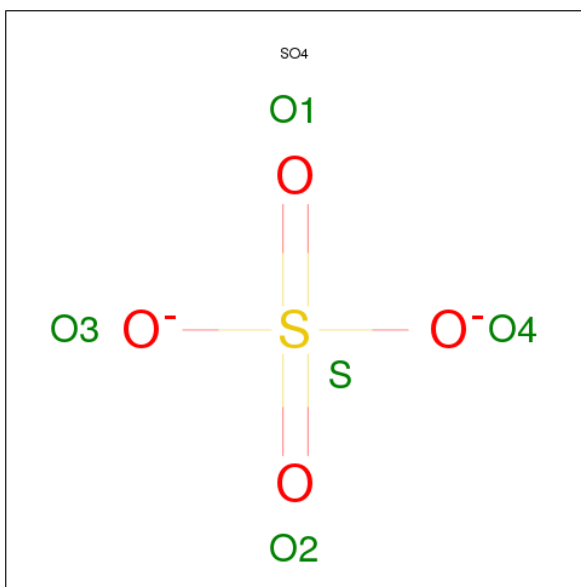
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Chain	Residue	Modelled	Actual	Comment	Reference
C	496	HIS	-	EXPRESSION TAG	UNP P10547
C	497	HIS	-	EXPRESSION TAG	UNP P10547
C	498	HIS	-	EXPRESSION TAG	UNP P10547
C	499	HIS	-	EXPRESSION TAG	UNP P10547
C	500	HIS	-	EXPRESSION TAG	UNP P10547
C	501	HIS	-	EXPRESSION TAG	UNP P10547
D	247	MET	-	INITIATING METHIONINE	UNP P10547
D	494	LEU	-	EXPRESSION TAG	UNP P10547
D	495	GLU	-	EXPRESSION TAG	UNP P10547
D	496	HIS	-	EXPRESSION TAG	UNP P10547
D	497	HIS	-	EXPRESSION TAG	UNP P10547
D	498	HIS	-	EXPRESSION TAG	UNP P10547
D	499	HIS	-	EXPRESSION TAG	UNP P10547
D	500	HIS	-	EXPRESSION TAG	UNP P10547
D	501	HIS	-	EXPRESSION TAG	UNP P10547

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



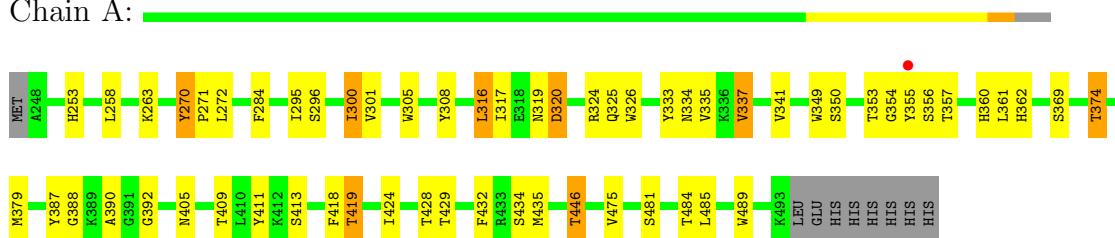
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

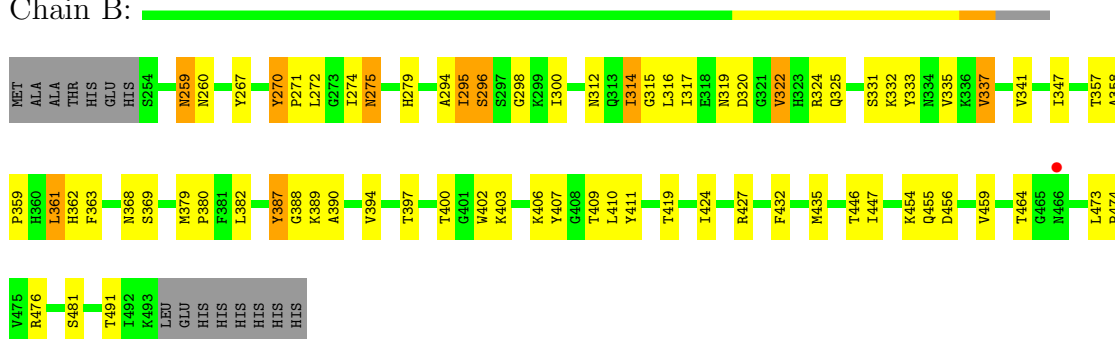
#### • Molecule 1: Lysostaphin

Chain A:



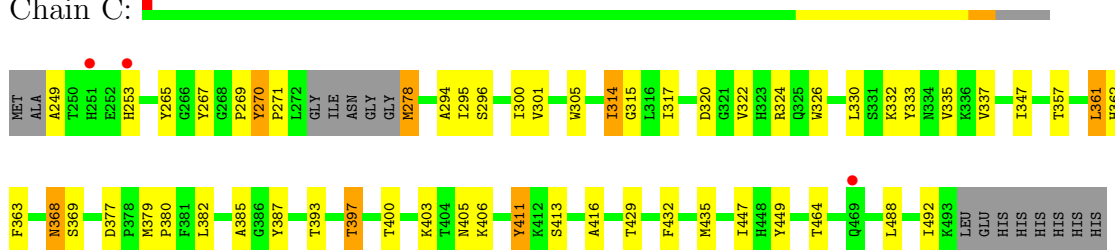
#### • Molecule 1: Lysostaphin

Chain B:



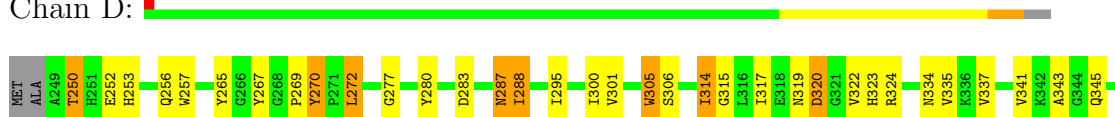
#### • Molecule 1: Lysostaphin

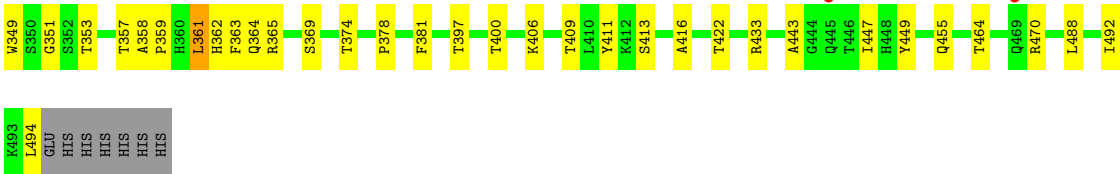
Chain C:



#### • Molecule 1: Lysostaphin

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	282.01 Å   282.01 Å   282.01 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	47.67 – 3.50 48.36 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.67-3.50) 100.0 (48.36-3.50)	Depositor EDS
$R_{merge}$	0.29	Depositor
$R_{sym}$	0.29	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.94 (at 3.48 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.268   ,   0.287 0.249   ,   0.262	Depositor DCC
$R_{free}$ test set	2435 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 7.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 48691 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	7589	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.45	0/1964	0.62	0/2668
1	B	0.48	0/1912	0.63	0/2598
1	C	0.46	0/1930	0.61	0/2621
1	D	0.46	0/1967	0.62	0/2672
All	All	0.46	0/7773	0.62	0/10559

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	316	LEU	Peptide
1	B	387	TYR	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1905	0	1829	49	0
1	B	1855	0	1781	55	0
1	C	1872	0	1797	32	0
1	D	1908	0	1835	47	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	0	0	0
3	B	15	0	0	0	0
3	D	20	0	0	1	0
All	All	7589	0	7242	173	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (173) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:353:THR:HG23	1:A:354:GLY:O	1.64	0.97
1:C:317:ILE:HG22	1:C:324:ARG:HG2	1.60	0.81
1:D:301:VAL:HG21	1:D:317:ILE:HG23	1.64	0.78
1:D:409:THR:HG22	1:D:455:GLN:HE21	1.49	0.77
1:A:361:LEU:HD23	1:A:362:HIS:N	2.01	0.76
1:B:274:ILE:HG23	1:B:275:ASN:N	2.07	0.70
1:B:314:ILE:HD12	1:B:315:GLY:N	2.06	0.69
1:D:272:LEU:HD23	1:D:272:LEU:H	1.61	0.66
1:C:314:ILE:HD12	1:C:315:GLY:N	2.11	0.65
1:A:424:ILE:HG23	1:B:390:ALA:HB3	1.77	0.65
1:A:369:SER:HB3	1:A:374:THR:HG21	1.79	0.65
1:D:314:ILE:HD12	1:D:315:GLY:N	2.12	0.64
1:A:489:TRP:CZ3	1:B:390:ALA:HB1	2.32	0.64
1:B:322:VAL:HG22	1:B:368:ASN:HA	1.80	0.62
1:D:295:ILE:HD11	1:D:363:PHE:CE1	2.35	0.61
1:B:409:THR:HG23	1:B:455:GLN:HB2	1.84	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:300:ILE:HD13	1:D:335:VAL:HB	1.84	0.60
1:B:419:THR:OG1	1:B:446:THR:HG23	2.02	0.59
1:A:301:VAL:HG21	1:A:317:ILE:HG23	1.84	0.59
1:C:447:ILE:HD12	1:C:447:ILE:O	2.03	0.59
1:C:322:VAL:HG22	1:C:368:ASN:HA	1.85	0.58
1:A:300:ILE:HG22	1:A:337:VAL:HA	1.85	0.58
1:A:405:ASN:HB3	1:A:409:THR:HG23	1.83	0.58
1:D:300:ILE:HD13	1:D:335:VAL:CB	2.34	0.57
1:D:317:ILE:HG22	1:D:324:ARG:HG2	1.85	0.57
1:B:270:TYR:CD2	1:B:279:HIS:HB2	2.38	0.57
1:A:300:ILE:HD13	1:A:335:VAL:HG21	1.86	0.57
1:B:387:TYR:CD2	1:B:388:GLY:HA2	2.40	0.57
1:B:300:ILE:HD13	1:B:335:VAL:HG21	1.87	0.56
1:C:416:ALA:HB3	1:C:449:TYR:CZ	2.41	0.56
1:D:409:THR:CG2	1:D:455:GLN:HE21	2.18	0.56
1:D:464:THR:HG23	1:D:470:ARG:HH11	1.71	0.55
1:D:250:THR:HG23	1:D:253:HIS:HD2	1.70	0.55
1:D:409:THR:HG22	1:D:455:GLN:NE2	2.19	0.55
1:A:392:GLY:HA3	1:B:427:ARG:HH21	1.72	0.55
1:A:263:LYS:HE3	1:A:379:MET:HE1	1.89	0.55
1:D:447:ILE:HD12	1:D:447:ILE:O	2.06	0.54
1:A:295:ILE:O	1:A:295:ILE:HG22	2.06	0.54
1:A:392:GLY:HA3	1:B:427:ARG:NH2	2.23	0.54
1:D:300:ILE:HD13	1:D:335:VAL:HG21	1.89	0.54
1:B:274:ILE:CG2	1:B:275:ASN:N	2.71	0.53
1:B:296:SER:HB2	1:B:325:GLN:HE22	1.74	0.53
1:C:295:ILE:HD11	1:C:363:PHE:CE2	2.42	0.53
1:B:294:ALA:HB2	1:B:347:ILE:HG21	1.89	0.53
1:D:300:ILE:HD13	1:D:335:VAL:CG2	2.38	0.53
1:A:316:LEU:HD21	1:A:341:VAL:HG21	1.89	0.53
1:B:294:ALA:HB2	1:B:347:ILE:CG2	2.38	0.53
1:C:332:LYS:NZ	1:C:332:LYS:HB2	2.24	0.53
1:B:432:PHE:HB2	1:B:435:MET:HG2	1.91	0.53
1:C:361:LEU:HD23	1:C:362:HIS:N	2.24	0.53
1:A:387:TYR:CD2	1:A:388:GLY:N	2.77	0.52
1:B:259:ASN:ND2	1:B:387:TYR:O	2.38	0.52
1:B:295:ILE:HD11	1:B:363:PHE:CE1	2.44	0.52
1:D:272:LEU:H	1:D:272:LEU:CD2	2.22	0.52
1:C:300:ILE:HD13	1:C:335:VAL:HB	1.91	0.52
1:C:300:ILE:HD13	1:C:335:VAL:CB	2.40	0.52
1:A:390:ALA:HB3	1:B:424:ILE:HA	1.92	0.52
1:D:406:LYS:N	3:D:605:SO4:O2	2.41	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:379:MET:N	1:C:380:PRO:HD2	2.24	0.51
1:C:393:THR:HG22	1:D:433:ARG:O	2.10	0.51
1:B:270:TYR:CE1	1:B:272:LEU:HB2	2.46	0.51
1:D:488:LEU:HD21	1:D:492:ILE:HG13	1.92	0.51
1:B:361:LEU:HD23	1:B:362:HIS:N	2.26	0.50
1:D:409:THR:HG22	1:D:455:GLN:HG2	1.92	0.50
1:A:300:ILE:CD1	1:A:335:VAL:HG21	2.40	0.50
1:B:260:ASN:ND2	1:B:394:VAL:HG13	2.25	0.50
1:D:252:GLU:O	1:D:343:ALA:HB2	2.11	0.50
1:D:320:ASP:C	1:D:320:ASP:OD1	2.50	0.50
1:A:258:LEU:HD13	1:A:284:PHE:CE2	2.47	0.49
1:B:312:ASN:ND2	1:B:333:TYR:OH	2.27	0.49
1:C:295:ILE:HD11	1:C:363:PHE:CZ	2.47	0.49
1:A:353:THR:HG21	1:A:357:THR:HB	1.94	0.48
1:C:447:ILE:C	1:C:447:ILE:HD12	2.33	0.48
1:A:296:SER:HB2	1:A:325:GLN:HE22	1.78	0.48
1:D:416:ALA:HB3	1:D:449:TYR:CZ	2.48	0.48
1:B:274:ILE:HG23	1:B:275:ASN:CG	2.34	0.48
1:B:447:ILE:HD12	1:B:447:ILE:C	2.35	0.48
1:A:272:LEU:HD11	1:A:357:THR:HG23	1.95	0.47
1:C:253:HIS:HB3	1:C:296:SER:HA	1.96	0.47
1:B:389:LYS:O	1:B:390:ALA:C	2.53	0.47
1:D:305:TRP:C	1:D:305:TRP:CD1	2.87	0.47
1:B:400:THR:HG22	1:B:402:TRP:HD1	1.79	0.47
1:D:358:ALA:HB1	1:D:359:PRO:HD2	1.95	0.47
1:A:355:TYR:O	1:A:356:SER:HB2	2.15	0.47
1:D:361:LEU:HD23	1:D:362:HIS:N	2.30	0.47
1:C:294:ALA:HB2	1:C:347:ILE:CG2	2.46	0.46
1:B:316:LEU:HD21	1:B:341:VAL:CG2	2.45	0.46
1:A:300:ILE:O	1:A:300:ILE:HG22	2.16	0.46
1:B:379:MET:N	1:B:380:PRO:HD2	2.31	0.46
1:B:455:GLN:O	1:B:456:ASP:C	2.54	0.46
1:A:253:HIS:CE1	1:A:296:SER:HG	2.33	0.46
1:A:484:THR:O	1:A:485:LEU:HD23	2.15	0.45
1:A:296:SER:CB	1:A:325:GLN:HE22	2.29	0.45
1:A:320:ASP:C	1:A:320:ASP:OD1	2.54	0.45
1:B:274:ILE:HG23	1:B:275:ASN:ND2	2.31	0.45
1:D:265:TYR:H	1:D:283:ASP:HB2	1.82	0.45
1:D:369:SER:HB3	1:D:374:THR:HG21	1.97	0.45
1:C:269:PRO:HA	1:C:278:MET:HG2	1.99	0.45
1:D:272:LEU:N	1:D:272:LEU:HD23	2.28	0.45
1:A:317:ILE:HG22	1:A:324:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:432:PHE:HB2	1:A:435:MET:HG2	1.98	0.45
1:B:317:ILE:HD11	1:B:324:ARG:NH2	2.31	0.45
1:B:403:LYS:O	1:B:410:LEU:HA	2.17	0.45
1:D:267:TYR:CD2	1:D:267:TYR:C	2.90	0.45
1:D:334:ASN:HB2	1:D:349:TRP:CZ3	2.52	0.44
1:C:305:TRP:C	1:C:305:TRP:CD1	2.91	0.44
1:C:403:LYS:HB2	1:C:411:TYR:CE1	2.52	0.44
1:A:435:MET:CE	1:B:407:TYR:CD1	3.00	0.44
1:B:298:GLY:HA3	1:B:316:LEU:HD22	1.99	0.44
1:C:322:VAL:CG2	1:C:368:ASN:HA	2.46	0.44
1:D:270:TYR:CE1	1:D:272:LEU:HD21	2.53	0.44
1:B:270:TYR:OH	1:B:274:ILE:HG21	2.18	0.44
1:C:249:ALA:N	1:C:385:ALA:O	2.51	0.44
1:A:353:THR:O	1:A:354:GLY:C	2.56	0.44
1:A:258:LEU:HD22	1:A:284:PHE:CD2	2.53	0.44
1:A:301:VAL:CG2	1:A:317:ILE:HG23	2.46	0.44
1:B:331:SER:C	1:B:332:LYS:HG2	2.38	0.44
1:C:267:TYR:CD1	1:C:377:ASP:HA	2.53	0.44
1:C:270:TYR:HB2	1:C:271:PRO:CD	2.48	0.44
1:C:397:THR:O	1:C:400:THR:OG1	2.36	0.44
1:C:432:PHE:HB2	1:C:435:MET:HG2	2.00	0.43
1:A:300:ILE:HD13	1:A:335:VAL:CB	2.48	0.43
1:B:300:ILE:HG22	1:B:337:VAL:HA	2.00	0.43
1:A:300:ILE:HD13	1:A:335:VAL:CG2	2.47	0.43
1:A:300:ILE:HG13	1:A:316:LEU:HD23	2.00	0.43
1:A:418:PHE:CZ	1:A:475:VAL:HG12	2.52	0.43
1:C:488:LEU:HD21	1:C:492:ILE:HG13	2.00	0.43
1:A:355:TYR:CG	1:A:356:SER:N	2.86	0.43
1:B:300:ILE:HD13	1:B:335:VAL:CG2	2.48	0.43
1:D:288:ILE:HG22	1:D:351:GLY:HA2	2.01	0.43
1:D:269:PRO:HA	1:D:277:GLY:O	2.19	0.43
1:D:409:THR:HG22	1:D:455:GLN:CG	2.49	0.43
1:C:330:LEU:HD12	1:C:330:LEU:N	2.34	0.43
1:C:294:ALA:HB2	1:C:347:ILE:HG21	2.00	0.43
1:D:301:VAL:CG2	1:D:317:ILE:HG23	2.44	0.43
1:B:271:PRO:O	1:B:272:LEU:C	2.57	0.43
1:D:361:LEU:CD2	1:D:362:HIS:N	2.82	0.42
1:A:419:THR:OG1	1:A:446:THR:HG23	2.19	0.42
1:B:267:TYR:C	1:B:267:TYR:CD2	2.93	0.42
1:C:301:VAL:HG21	1:C:317:ILE:HG23	2.02	0.42
1:D:287:ASN:OD1	1:D:287:ASN:N	2.53	0.42
1:D:257:TRP:HE1	1:D:295:ILE:HG23	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:435:MET:CE	1:B:407:TYR:CE1	3.03	0.42
1:B:459:VAL:HB	1:B:476:ARG:HG2	2.01	0.42
1:C:382:LEU:O	1:C:385:ALA:HB3	2.19	0.42
1:B:473:LEU:HD12	1:B:474:PRO:HD2	2.02	0.42
1:B:387:TYR:CD2	1:B:388:GLY:CA	3.02	0.42
1:B:447:ILE:O	1:B:447:ILE:HD12	2.20	0.42
1:B:402:TRP:CZ2	1:B:454:LYS:HE3	2.55	0.41
1:A:435:MET:HE1	1:B:407:TYR:CE1	2.56	0.41
1:D:378:PRO:O	1:D:381:PHE:HB3	2.20	0.41
1:A:353:THR:HG21	1:A:360:HIS:HE1	1.85	0.41
1:C:314:ILE:CG2	1:C:330:LEU:HD22	2.51	0.41
1:A:424:ILE:HG23	1:B:390:ALA:CB	2.48	0.41
1:D:447:ILE:C	1:D:447:ILE:HD12	2.40	0.41
1:A:334:ASN:HB2	1:A:349:TRP:CZ3	2.56	0.41
1:D:295:ILE:HD11	1:D:363:PHE:CD1	2.55	0.41
1:A:428:THR:HG22	1:A:429:THR:OG1	2.21	0.41
1:B:300:ILE:HD13	1:B:335:VAL:CB	2.50	0.41
1:D:422:THR:C	1:D:443:ALA:HB2	2.41	0.41
1:B:315:GLY:HA2	1:B:325:GLN:O	2.20	0.41
1:C:406:LYS:HD3	1:C:406:LYS:N	2.35	0.41
1:B:295:ILE:HD12	1:B:382:LEU:HD21	2.03	0.41
1:D:341:VAL:HG12	1:D:345:GLN:NE2	2.35	0.41
1:A:300:ILE:HD12	1:A:341:VAL:HG13	2.02	0.41
1:A:361:LEU:C	1:A:361:LEU:HD23	2.41	0.41
1:B:260:ASN:CG	1:B:394:VAL:HG13	2.41	0.41
1:D:280:TYR:O	1:D:364:GLN:HG3	2.21	0.41
1:A:353:THR:CG2	1:A:357:THR:HB	2.51	0.40
1:D:323:HIS:CG	1:D:365:ARG:NH2	2.89	0.40
1:B:358:ALA:HB1	1:B:359:PRO:HD2	2.04	0.40
1:D:256:GLN:OE1	1:D:257:TRP:HA	2.20	0.40
1:A:270:TYR:HB2	1:A:271:PRO:CD	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	244/255 (96%)	224 (92%)	20 (8%)	0	100	100
1	B	238/255 (93%)	223 (94%)	15 (6%)	0	100	100
1	C	236/255 (92%)	222 (94%)	14 (6%)	0	100	100
1	D	244/255 (96%)	231 (95%)	13 (5%)	0	100	100
All	All	962/1020 (94%)	900 (94%)	62 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/208 (96%)	182 (92%)	17 (8%)	15	58
1	B	194/208 (93%)	175 (90%)	19 (10%)	12	50
1	C	197/208 (95%)	178 (90%)	19 (10%)	12	51
1	D	200/208 (96%)	180 (90%)	20 (10%)	11	49
All	All	790/832 (95%)	715 (90%)	75 (10%)	12	51

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	TYR
1	A	300	ILE
1	A	305	TRP
1	A	308	TYR
1	A	319	ASN
1	A	320	ASP
1	A	326	TRP
1	A	333	TYR
1	A	337	VAL
1	A	350	SER
1	A	374	THR

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Mol	Chain	Res	Type
1	A	411	TYR
1	A	413	SER
1	A	419	THR
1	A	434	SER
1	A	446	THR
1	A	481	SER
1	B	259	ASN
1	B	270	TYR
1	B	275	ASN
1	B	295	ILE
1	B	296	SER
1	B	314	ILE
1	B	319	ASN
1	B	320	ASP
1	B	322	VAL
1	B	337	VAL
1	B	357	THR
1	B	361	LEU
1	B	369	SER
1	B	397	THR
1	B	406	LYS
1	B	411	TYR
1	B	464	THR
1	B	481	SER
1	B	491	THR
1	C	265	TYR
1	C	270	TYR
1	C	278	MET
1	C	314	ILE
1	C	320	ASP
1	C	326	TRP
1	C	333	TYR
1	C	337	VAL
1	C	357	THR
1	C	361	LEU
1	C	368	ASN
1	C	369	SER
1	C	387	TYR
1	C	397	THR
1	C	405	ASN
1	C	411	TYR
1	C	413	SER

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Mol	Chain	Res	Type
1	C	429	THR
1	C	464	THR
1	D	250	THR
1	D	270	TYR
1	D	272	LEU
1	D	287	ASN
1	D	288	ILE
1	D	305	TRP
1	D	306	SER
1	D	314	ILE
1	D	319	ASN
1	D	320	ASP
1	D	322	VAL
1	D	337	VAL
1	D	353	THR
1	D	357	THR
1	D	361	LEU
1	D	397	THR
1	D	400	THR
1	D	411	TYR
1	D	413	SER
1	D	494	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	253	HIS
1	D	319	ASN
1	D	345	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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	SO4	A	602	2	4,4,4	0.09	0	6,6,6	0.31	0
3	SO4	A	603	-	4,4,4	0.26	0	6,6,6	0.23	0
3	SO4	B	602	-	4,4,4	0.12	0	6,6,6	0.10	0
3	SO4	B	603	-	4,4,4	0.12	0	6,6,6	0.53	0
3	SO4	B	604	-	4,4,4	0.30	0	6,6,6	0.23	0
3	SO4	D	602	-	4,4,4	0.11	0	6,6,6	0.22	0
3	SO4	D	603	-	4,4,4	0.17	0	6,6,6	0.32	0
3	SO4	D	604	-	4,4,4	0.19	0	6,6,6	0.14	0
3	SO4	D	605	-	4,4,4	0.15	0	6,6,6	0.23	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	SO4	A	602	2	-	0/0/0/0	0/0/0/0
3	SO4	A	603	-	-	0/0/0/0	0/0/0/0
3	SO4	B	602	-	-	0/0/0/0	0/0/0/0
3	SO4	B	603	-	-	0/0/0/0	0/0/0/0
3	SO4	B	604	-	-	0/0/0/0	0/0/0/0
3	SO4	D	602	-	-	0/0/0/0	0/0/0/0
3	SO4	D	603	-	-	0/0/0/0	0/0/0/0
3	SO4	D	604	-	-	0/0/0/0	0/0/0/0
3	SO4	D	605	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<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	246/255 (96%)	0.17	1 (0%) 90 71	24, 47, 71, 123	0
1	B	240/255 (94%)	0.15	1 (0%) 90 71	15, 39, 68, 99	0
1	C	240/255 (94%)	0.26	3 (1%) 74 40	22, 48, 110, 134	0
1	D	246/255 (96%)	0.18	2 (0%) 83 53	15, 43, 75, 115	0
All	All	972/1020 (95%)	0.19	7 (0%) 84 56	15, 47, 83, 134	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	253	HIS	2.6
1	D	469	GLN	2.6
1	B	466	ASN	2.2
1	D	445	GLN	2.1
1	C	251	HIS	2.1
1	A	355	TYR	2.1
1	C	469	GLN	2.0

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	D	604	5/5	0.34	2.30	47,47,47,47	0
3	SO4	B	604	5/5	0.35	1.08	47,47,47,47	0
3	SO4	A	603	5/5	0.32	0.82	47,47,47,47	0
3	SO4	D	603	5/5	0.29	0.28	47,47,47,47	0
2	ZN	D	601	1/1	0.17	0.18	16,16,16,16	0
3	SO4	B	602	5/5	0.27	0.17	47,47,47,47	0
3	SO4	B	603	5/5	0.20	-0.45	47,47,47,47	0
2	ZN	C	601	1/1	0.15	-1.06	62,62,62,62	0
3	SO4	D	605	5/5	0.17	-1.17	47,47,47,47	0
3	SO4	A	602	5/5	0.17	-1.17	47,47,47,47	0
2	ZN	B	601	1/1	0.12	-1.74	19,19,19,19	0
3	SO4	D	602	5/5	0.18	-3.25	47,47,47,47	0
2	ZN	A	601	1/1	0.09	-3.70	36,36,36,36	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.