



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2024 – 02:08 PM JST

PDB ID : 8WKO
Title : Crystal structure of O-acetylhomoserine sulfhydrylase from *Lactobacillus plantarum* in the closed form
Authors : Oda, K.; Matoba, Y.
Deposited on : 2023-09-28
Resolution : 2.91 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

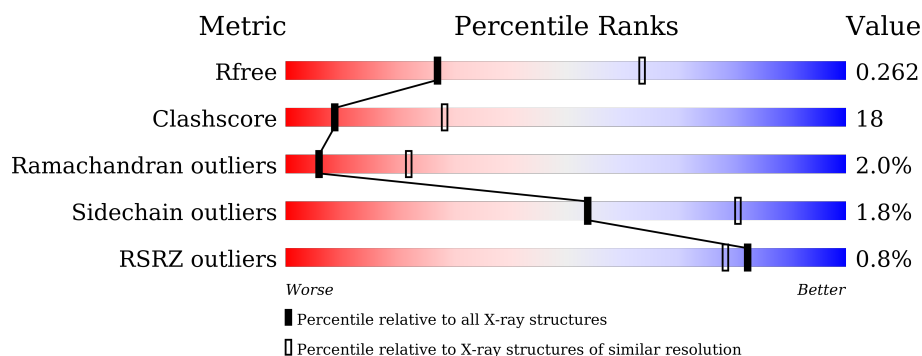
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.91 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	2797 (2.94-2.90)
Clashscore	180529	3049 (2.94-2.90)
Ramachandran outliers	177936	2981 (2.94-2.90)
Sidechain outliers	177891	2983 (2.94-2.90)
RSRZ outliers	164620	2799 (2.94-2.90)

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	448	 64% 29% • 5%
1	B	448	 2% 57% 34% • • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6514 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 L-methionine gamma-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	P	S	0	1	0
			3248	2067	546	633	1	1			
1	B	425	Total	C	N	O	P	S	0	0	0
			3233	2055	545	631	1	1			

There are 40 discrepancies between the modelled and reference sequences:

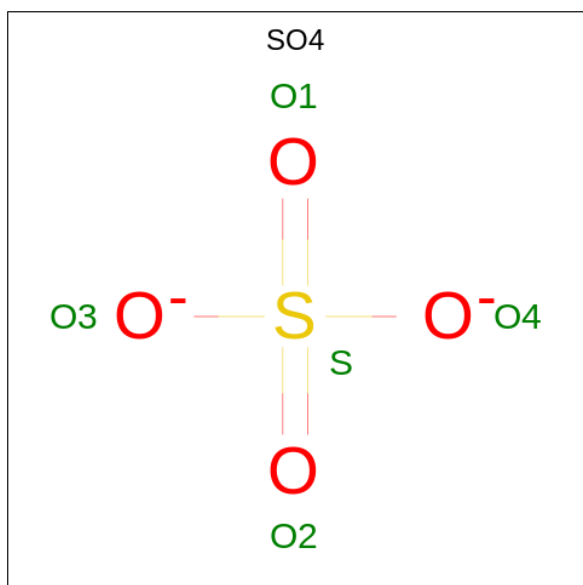
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A0G9F7S9
A	-18	GLY	-	expression tag	UNP A0A0G9F7S9
A	-17	SER	-	expression tag	UNP A0A0G9F7S9
A	-16	SER	-	expression tag	UNP A0A0G9F7S9
A	-15	HIS	-	expression tag	UNP A0A0G9F7S9
A	-14	HIS	-	expression tag	UNP A0A0G9F7S9
A	-13	HIS	-	expression tag	UNP A0A0G9F7S9
A	-12	HIS	-	expression tag	UNP A0A0G9F7S9
A	-11	HIS	-	expression tag	UNP A0A0G9F7S9
A	-10	HIS	-	expression tag	UNP A0A0G9F7S9
A	-9	SER	-	expression tag	UNP A0A0G9F7S9
A	-8	SER	-	expression tag	UNP A0A0G9F7S9
A	-7	GLY	-	expression tag	UNP A0A0G9F7S9
A	-6	LEU	-	expression tag	UNP A0A0G9F7S9
A	-5	VAL	-	expression tag	UNP A0A0G9F7S9
A	-4	PRO	-	expression tag	UNP A0A0G9F7S9
A	-3	ARG	-	expression tag	UNP A0A0G9F7S9
A	-2	GLY	-	expression tag	UNP A0A0G9F7S9
A	-1	SER	-	expression tag	UNP A0A0G9F7S9
A	0	HIS	-	expression tag	UNP A0A0G9F7S9
B	-19	MET	-	initiating methionine	UNP A0A0G9F7S9
B	-18	GLY	-	expression tag	UNP A0A0G9F7S9
B	-17	SER	-	expression tag	UNP A0A0G9F7S9
B	-16	SER	-	expression tag	UNP A0A0G9F7S9
B	-15	HIS	-	expression tag	UNP A0A0G9F7S9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP A0A0G9F7S9
B	-13	HIS	-	expression tag	UNP A0A0G9F7S9
B	-12	HIS	-	expression tag	UNP A0A0G9F7S9
B	-11	HIS	-	expression tag	UNP A0A0G9F7S9
B	-10	HIS	-	expression tag	UNP A0A0G9F7S9
B	-9	SER	-	expression tag	UNP A0A0G9F7S9
B	-8	SER	-	expression tag	UNP A0A0G9F7S9
B	-7	GLY	-	expression tag	UNP A0A0G9F7S9
B	-6	LEU	-	expression tag	UNP A0A0G9F7S9
B	-5	VAL	-	expression tag	UNP A0A0G9F7S9
B	-4	PRO	-	expression tag	UNP A0A0G9F7S9
B	-3	ARG	-	expression tag	UNP A0A0G9F7S9
B	-2	GLY	-	expression tag	UNP A0A0G9F7S9
B	-1	SER	-	expression tag	UNP A0A0G9F7S9
B	0	HIS	-	expression tag	UNP A0A0G9F7S9

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



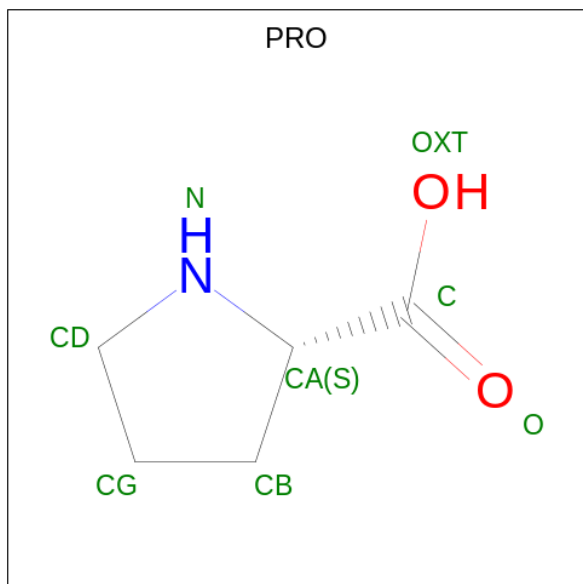
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).

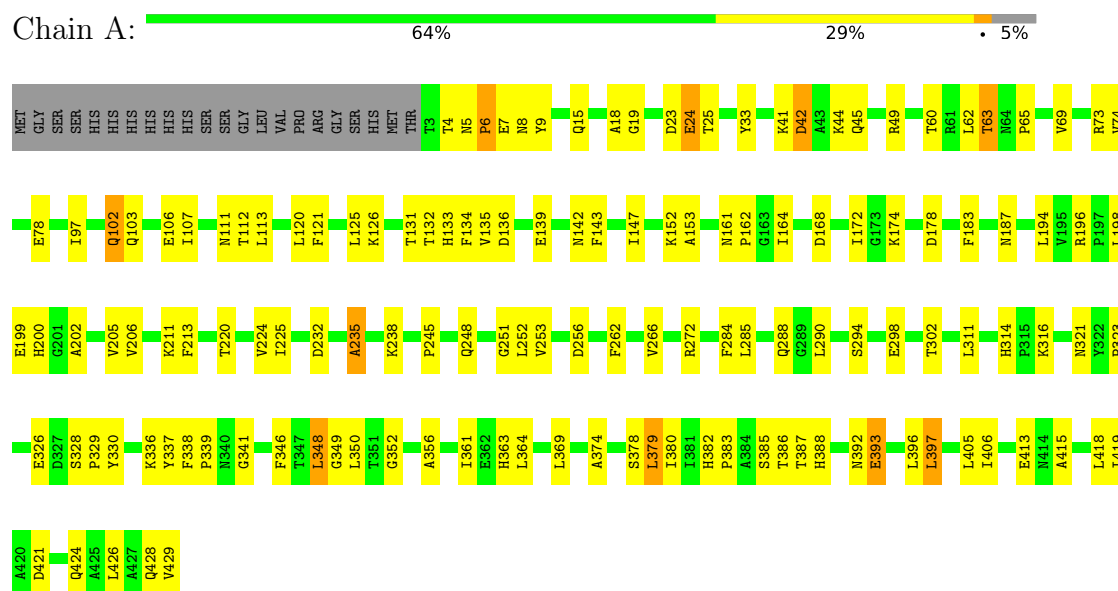


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			8	5	1	2		

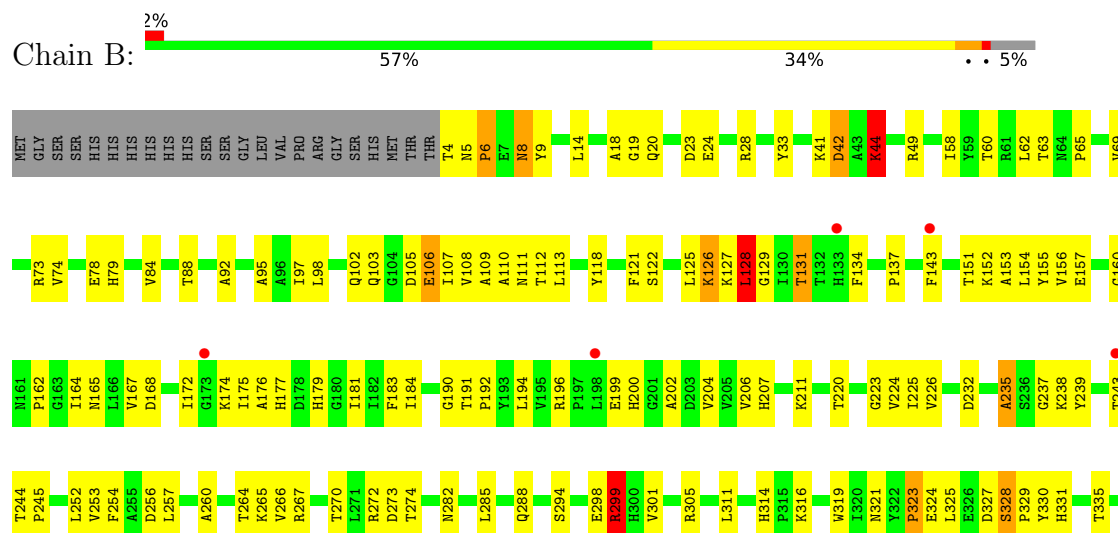
3 Residue-property plots

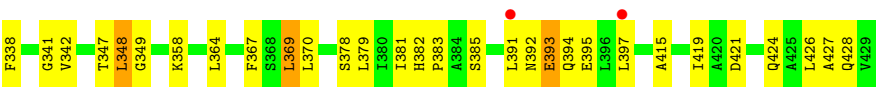
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: L-methionine gamma-lyase



• Molecule 1: L-methionine gamma-lyase





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	155.82Å 155.82Å 259.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.40 – 2.91 48.40 – 2.91	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.40-2.91) 98.3 (48.40-2.91)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.203 , 0.262 0.203 , 0.262	Depositor DCC
R_{free} test set	1323 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	73.3	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6514	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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, LLP

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	0.53	0/3297	0.90	7/4501 (0.2%)
1	B	0.58	2/3278 (0.1%)	0.95	15/4475 (0.3%)
All	All	0.56	2/6575 (0.0%)	0.93	22/8976 (0.2%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	106	GLU	CG-CD	-6.37	1.42	1.51
1	B	128	LEU	CG-CD2	5.33	1.71	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	LEU	CA-CB-CG	14.71	149.13	115.30
1	B	128	LEU	CB-CG-CD2	-10.22	93.62	111.00
1	B	348	LEU	CB-CG-CD2	-9.81	94.33	111.00
1	A	24	GLU	CA-CB-CG	-9.04	93.52	113.40
1	B	128	LEU	N-CA-CB	-8.41	93.59	110.40
1	B	106	GLU	CA-CB-CG	-7.83	96.17	113.40
1	B	44	LYS	CB-CG-CD	7.66	131.52	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	LEU	CA-CB-CG	7.19	131.85	115.30
1	B	299	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	B	44	LYS	CA-CB-CG	6.50	127.70	113.40
1	B	257	LEU	CA-CB-CG	-5.76	102.05	115.30
1	B	128	LEU	CA-CB-CG	-5.63	102.35	115.30
1	A	44	LYS	CA-CB-CG	5.62	125.77	113.40
1	B	131	THR	OG1-CB-CG2	5.42	122.48	110.00
1	A	63	THR	OG1-CB-CG2	-5.40	97.59	110.00
1	B	369	LEU	CA-CB-CG	5.31	127.52	115.30
1	B	358	LYS	CA-CB-CG	5.21	124.86	113.40
1	B	44	LYS	N-CA-CB	5.17	119.91	110.60
1	A	379	LEU	CB-CG-CD2	-5.15	102.24	111.00
1	B	397	LEU	CA-CB-CG	5.12	127.09	115.30
1	B	126	LYS	CA-CB-CG	-5.12	102.14	113.40
1	A	24	GLU	OE1-CD-OE2	-5.08	117.20	123.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	392	ASN	Peptide
1	B	128	LEU	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3248	0	3182	105	0
1	B	3233	0	3165	133	0
2	A	10	0	0	0	0
2	B	15	0	0	0	0
3	B	8	0	7	1	0
All	All	6514	0	6354	237	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 18.

All (237) 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:B:126:LYS:HG3	1:B:131:THR:HG23	1.34	1.06
1:B:126:LYS:O	1:B:129:GLY:N	1.93	1.00
1:B:62:LEU:HD11	1:B:272:ARG:HG3	1.49	0.95
1:B:24:GLU:CD	1:B:24:GLU:H	1.71	0.93
1:B:369:LEU:HD12	1:B:381:ILE:HD13	1.50	0.92
1:B:168:ASP:O	1:B:172:ILE:HD12	1.72	0.89
1:A:426:LEU:O	1:A:429:VAL:HG12	1.76	0.85
1:B:106:GLU:HG2	1:B:131:THR:O	1.77	0.84
1:B:110:ALA:HB2	1:B:156:VAL:HG12	1.58	0.83
1:A:164:ILE:HG22	1:A:323:PRO:HD3	1.60	0.82
1:B:42:ASP:OD1	1:B:44:LYS:HD3	1.80	0.81
1:B:41:LYS:HE2	1:B:44:LYS:NZ	1.96	0.80
1:B:126:LYS:HG3	1:B:131:THR:CG2	2.14	0.76
1:A:74:VAL:HG11	1:A:224:VAL:HG11	1.68	0.74
1:A:62:LEU:HD11	1:A:272:ARG:HG3	1.68	0.74
1:B:270:THR:O	1:B:274:THR:OG1	2.04	0.74
1:A:24:GLU:OE1	1:A:24:GLU:N	2.16	0.73
1:B:382:HIS:HD2	1:B:385:SER:HB3	1.52	0.73
1:A:363:HIS:HD2	1:A:428:GLN:NE2	1.87	0.72
1:A:316:LYS:HE3	1:A:429:VAL:CG1	2.20	0.72
1:B:126:LYS:C	1:B:128:LEU:H	1.93	0.71
1:B:60:THR:HA	1:B:63:THR:O	1.91	0.71
1:A:164:ILE:CG2	1:A:323:PRO:HD3	2.21	0.70
1:B:18:ALA:HB3	1:B:73:ARG:HG3	1.73	0.69
1:A:15:GLN:HE22	1:A:294:SER:HB3	1.58	0.69
1:A:106:GLU:OE2	1:A:133:HIS:NE2	2.25	0.69
1:B:172:ILE:HA	1:B:175:ILE:HD12	1.74	0.69
1:B:154:LEU:HD12	1:B:176:ALA:HB2	1.73	0.68
1:B:105:ASP:O	1:B:106:GLU:HG3	1.93	0.68
1:B:126:LYS:C	1:B:128:LEU:N	2.48	0.68
1:A:363:HIS:CD2	1:A:428:GLN:HE21	2.11	0.68
1:B:97:ILE:HG13	1:B:121:PHE:HE1	1.58	0.67
1:A:164:ILE:HG22	1:A:323:PRO:CD	2.24	0.67
1:A:107:ILE:HD12	1:A:153:ALA:HB3	1.78	0.65
1:A:162:PRO:HD3	1:A:388:HIS:CE1	2.32	0.65
1:A:363:HIS:HD2	1:A:428:GLN:HE21	1.41	0.65
1:A:135:VAL:HG13	1:A:142:ASN:HB3	1.78	0.65
1:B:112:THR:O	1:B:113:LEU:HD23	1.97	0.64
1:A:102:GLN:HG3	1:A:103:GLN:H	1.62	0.64
1:A:316:LYS:HE3	1:A:429:VAL:HG12	1.80	0.63
1:A:18:ALA:HB3	1:A:73:ARG:HG3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ILE:HG23	1:B:153:ALA:O	1.99	0.62
1:B:382:HIS:CD2	1:B:385:SER:HB3	2.32	0.62
1:B:33:TYR:CD2	1:B:65:PRO:HB2	2.34	0.62
1:A:33:TYR:CD2	1:A:65:PRO:HB2	2.35	0.62
1:A:6:PRO:HB2	1:A:7:GLU:OE2	1.99	0.61
1:B:105:ASP:C	1:B:106:GLU:HG3	2.20	0.61
1:B:338:PHE:HB3	1:B:341:GLY:O	2.01	0.61
1:B:184:ILE:HG12	1:B:204:VAL:HB	1.81	0.61
1:A:348:LEU:HD21	1:A:350:LEU:HD21	1.82	0.60
1:B:370:LEU:HD11	1:B:379:LEU:HD13	1.83	0.60
1:A:111:ASN:ND2	1:A:134:PHE:HB3	2.16	0.60
1:B:41:LYS:HE2	1:B:44:LYS:HZ2	1.65	0.60
1:B:41:LYS:CE	1:B:44:LYS:NZ	2.64	0.60
1:A:107:ILE:CD1	1:A:153:ALA:HB3	2.31	0.59
1:B:415:ALA:O	1:B:419:ILE:HG13	2.03	0.59
1:A:143:PHE:O	1:A:147:ILE:HG13	2.01	0.59
1:A:361:ILE:HG21	1:A:369:LEU:HD13	1.85	0.58
1:A:168:ASP:O	1:A:172:ILE:HD12	2.02	0.58
1:A:252:LEU:HD12	1:A:253:VAL:N	2.18	0.58
1:A:15:GLN:NE2	1:A:294:SER:HB3	2.18	0.57
1:B:174:LYS:HE3	1:B:177:HIS:ND1	2.19	0.57
1:B:199:GLU:O	1:B:200:HIS:ND1	2.36	0.57
1:B:311:LEU:HD13	1:B:348:LEU:HD13	1.86	0.57
1:A:23:ASP:HB2	1:A:24:GLU:OE1	2.05	0.57
1:B:79:HIS:CE1	1:B:196:ARG:HH11	2.23	0.57
1:B:79:HIS:CE1	1:B:196:ARG:NH1	2.73	0.57
1:B:106:GLU:O	1:B:151:THR:HA	2.05	0.56
1:A:349:GLY:O	1:A:350:LEU:HD23	2.05	0.56
1:B:143:PHE:CE1	1:B:172:ILE:HG12	2.40	0.56
1:B:190:GLY:O	1:B:194:LEU:HB2	2.06	0.56
1:B:78:GLU:OE1	1:B:207:HIS:NE2	2.33	0.56
1:A:206:VAL:HG12	1:A:225:ILE:HG12	1.88	0.55
1:A:139:GLU:O	1:A:142:ASN:HB2	2.07	0.55
1:B:151:THR:HG22	1:B:181:ILE:HD13	1.88	0.55
1:B:327:ASP:OD2	1:B:327:ASP:N	2.40	0.55
1:B:184:ILE:HG23	1:B:204:VAL:HG12	1.89	0.55
1:A:393:GLU:HA	1:A:396:LEU:HB3	1.88	0.54
1:A:314:HIS:CE1	1:A:316:LYS:HB2	2.42	0.54
1:B:92:ALA:O	1:B:225:ILE:HD11	2.07	0.54
1:A:5:ASN:HD21	1:A:9:TYR:H	1.55	0.54
1:A:135:VAL:CG1	1:A:142:ASN:HB3	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:GLU:OE2	1:B:131:THR:OG1	2.24	0.54
1:A:97:ILE:HG13	1:A:121:PHE:HE1	1.73	0.54
1:B:125:LEU:O	1:B:128:LEU:HB3	2.08	0.53
1:B:41:LYS:HE2	1:B:44:LYS:HZ3	1.70	0.53
1:A:152:LYS:NZ	1:A:238:LYS:HB3	2.23	0.53
1:A:199:GLU:O	1:A:200:HIS:ND1	2.41	0.53
1:A:232:ASP:HB3	1:A:235:ALA:HB3	1.90	0.52
1:B:369:LEU:HD12	1:B:381:ILE:CD1	2.32	0.52
1:B:118:TYR:OH	1:B:395:GLU:OE1	2.14	0.52
1:B:160:GLY:HA3	1:B:165:ASN:OD1	2.10	0.52
1:A:321:ASN:O	1:A:346:PHE:HB2	2.10	0.52
1:B:79:HIS:ND1	1:B:196:ARG:HD3	2.24	0.52
1:B:314:HIS:HE1	1:B:316:LYS:HD2	1.73	0.52
1:A:174:LYS:HE2	1:A:178:ASP:OD2	2.10	0.51
1:B:378:SER:O	1:B:379:LEU:HD23	2.10	0.51
1:B:392:ASN:O	1:B:394:GLN:N	2.43	0.51
1:A:74:VAL:HG23	1:A:290:LEU:HD11	1.92	0.51
1:B:33:TYR:CE2	1:B:65:PRO:HB2	2.46	0.51
1:A:245:PRO:HB3	1:A:251:GLY:O	2.11	0.51
1:B:126:LYS:O	1:B:128:LEU:N	2.44	0.51
1:A:23:ASP:OD2	1:A:25:THR:OG1	2.27	0.51
1:B:109:ALA:O	1:B:134:PHE:HA	2.11	0.51
1:A:74:VAL:CG1	1:A:224:VAL:HG11	2.41	0.50
1:B:152:LYS:HB3	1:B:239:TYR:HE1	1.76	0.50
1:B:220:THR:HG23	1:B:282:ASN:ND2	2.27	0.50
1:A:415:ALA:O	1:A:419:ILE:HG13	2.11	0.50
1:B:95:ALA:HA	1:B:270:THR:HG21	1.93	0.50
1:B:107:ILE:HD12	1:B:153:ALA:N	2.27	0.50
1:B:113:LEU:HD22	1:B:157:GLU:HG3	1.93	0.50
1:A:336:LYS:HD3	1:A:337:TYR:CZ	2.46	0.50
1:B:328:SER:O	1:B:330:TYR:N	2.45	0.50
1:B:192:PRO:HD3	1:B:207:HIS:CE1	2.47	0.49
1:B:331:HIS:O	1:B:335:THR:HG23	2.11	0.49
1:B:426:LEU:C	1:B:428:GLN:H	2.16	0.49
1:B:109:ALA:HA	1:B:155:TYR:O	2.13	0.49
1:B:239:TYR:O	1:B:243:THR:HG23	2.12	0.49
1:A:7:GLU:H	1:A:7:GLU:CD	2.10	0.49
1:A:393:GLU:O	1:A:397:LEU:HB2	2.13	0.49
1:B:391:LEU:HB3	1:B:395:GLU:HB2	1.94	0.49
1:B:394:GLN:OE1	1:B:395:GLU:HG3	2.12	0.49
1:B:74:VAL:HG11	1:B:224:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ALA:O	1:B:264:THR:HG23	2.13	0.49
1:B:152:LYS:O	1:B:239:TYR:OH	2.15	0.49
1:B:243:THR:OG1	1:B:244:THR:HG23	2.13	0.49
1:A:262:PHE:O	1:A:266:VAL:HG23	2.12	0.49
1:B:179:HIS:O	1:B:238:LYS:HE2	2.13	0.49
1:B:143:PHE:HE1	1:B:172:ILE:HG12	1.75	0.48
1:B:162:PRO:O	1:B:164:ILE:HD12	2.12	0.48
1:A:383:PRO:HG2	1:A:405:LEU:HD22	1.93	0.48
1:A:112:THR:O	1:A:113:LEU:HD23	2.13	0.48
1:B:126:LYS:CG	1:B:131:THR:HG23	2.24	0.48
1:B:206:VAL:HG12	1:B:225:ILE:HG12	1.95	0.48
1:B:319:TRP:NE1	1:B:349:GLY:HA3	2.28	0.48
1:A:107:ILE:O	1:A:132:THR:HA	2.13	0.47
1:B:254:PHE:CE1	1:B:265:LYS:HG3	2.49	0.47
1:A:413:GLU:HB2	1:A:418:LEU:HD21	1.96	0.47
1:A:363:HIS:CD2	1:A:428:GLN:NE2	2.74	0.47
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.64	0.47
1:A:284:PHE:O	1:A:288:GLN:HG2	2.14	0.47
1:A:164:ILE:HG13	1:A:346:PHE:HA	1.96	0.47
1:B:84:VAL:HG11	1:B:266:VAL:HG11	1.97	0.47
1:A:4:THR:O	1:A:6:PRO:HD3	2.15	0.47
1:A:6:PRO:HB2	1:A:7:GLU:CD	2.35	0.47
1:A:405:LEU:HD23	1:A:406:ILE:N	2.29	0.46
1:B:321:ASN:HB2	1:B:347:THR:HG22	1.97	0.46
1:B:5:ASN:HD21	1:B:9:TYR:H	1.63	0.46
1:A:139:GLU:HB2	1:A:142:ASN:OD1	2.16	0.46
1:A:253:VAL:O	1:A:256:ASP:HB2	2.15	0.46
1:A:106:GLU:HB3	1:A:131:THR:OG1	2.16	0.46
1:B:19:GLY:O	1:B:69:VAL:HG13	2.15	0.46
1:B:254:PHE:CD1	1:B:265:LYS:HG3	2.51	0.46
1:B:232:ASP:HB3	1:B:235:ALA:HB3	1.98	0.46
1:B:364:LEU:HD13	1:B:367:PHE:HB2	1.98	0.46
1:A:164:ILE:CG2	1:A:323:PRO:CD	2.91	0.46
1:A:285:LEU:HD21	1:B:285:LEU:HD21	1.97	0.46
1:B:113:LEU:CD2	1:B:157:GLU:HG3	2.46	0.46
1:A:120:LEU:HG	1:A:125:LEU:HD13	1.98	0.45
1:A:164:ILE:HD13	1:A:164:ILE:H	1.81	0.45
1:B:102:GLN:HG3	1:B:103:GLN:H	1.81	0.45
1:B:98:LEU:HD23	1:B:98:LEU:HA	1.66	0.45
1:A:78:GLU:CG	1:A:205:VAL:HG11	2.46	0.45
1:B:107:ILE:CD1	1:B:153:ALA:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLN:CD	1:A:49:ARG:NH2	2.70	0.45
1:A:164:ILE:HD13	1:A:164:ILE:N	2.32	0.45
1:A:161:ASN:HA	1:A:162:PRO:HA	1.72	0.45
1:A:378:SER:O	1:A:379:LEU:HD23	2.16	0.45
1:B:49:ARG:HB3	1:B:58:ILE:HG12	1.98	0.45
1:A:5:ASN:HD21	1:A:9:TYR:N	2.15	0.45
1:A:338:PHE:HB3	1:A:341:GLY:O	2.17	0.45
1:A:198:LEU:HD23	1:A:198:LEU:HA	1.79	0.44
1:A:352:GLY:HA3	1:A:356:ALA:HB2	1.99	0.44
1:B:174:LYS:HA	1:B:174:LYS:HD3	1.69	0.44
1:B:9:TYR:HB2	1:B:14:LEU:HD21	1.99	0.44
1:B:111:ASN:ND2	1:B:134:PHE:HB3	2.32	0.44
1:A:183:PHE:HB3	1:A:202:ALA:HA	2.00	0.44
1:B:74:VAL:HG12	1:B:226:VAL:HG21	2.00	0.44
1:A:78:GLU:HG2	1:A:205:VAL:HG11	2.00	0.44
1:A:314:HIS:HE1	1:A:316:LYS:HB2	1.83	0.44
1:B:183:PHE:HB3	1:B:202:ALA:HA	2.00	0.43
1:B:191:THR:HA	1:B:207:HIS:HE1	1.83	0.43
1:A:41:LYS:O	1:A:42:ASP:O	2.36	0.43
1:B:108:VAL:HB	1:B:154:LEU:CD2	2.48	0.43
1:B:311:LEU:HD23	1:B:311:LEU:HA	1.70	0.43
1:A:220:THR:HG21	1:A:285:LEU:CB	2.48	0.43
1:A:364:LEU:CD1	1:A:380:ILE:HD13	2.48	0.43
1:B:108:VAL:HB	1:B:154:LEU:HD22	2.00	0.43
1:B:421:ASP:O	1:B:424:GLN:HG3	2.17	0.43
1:B:288:GLN:HB2	3:B:504:PRO:HG2	1.99	0.43
1:A:152:LYS:HZ2	1:A:238:LYS:HB3	1.84	0.43
1:A:336:LYS:HD3	1:A:337:TYR:CE2	2.53	0.43
1:B:392:ASN:O	1:B:393:GLU:C	2.57	0.43
1:A:298:GLU:O	1:A:302:THR:HG23	2.19	0.43
1:A:328:SER:O	1:A:330:TYR:N	2.51	0.42
1:B:253:VAL:HG23	1:B:256:ASP:CG	2.40	0.42
1:B:305:ARG:NH2	1:B:324:GLU:OE1	2.46	0.42
1:B:23:ASP:HB2	1:B:24:GLU:CD	2.40	0.42
1:B:106:GLU:CD	1:B:131:THR:OG1	2.58	0.42
1:B:111:ASN:HD22	1:B:134:PHE:HB3	1.83	0.42
1:A:196:ARG:HG3	1:A:196:ARG:HH11	1.83	0.42
1:B:107:ILE:HD13	1:B:107:ILE:HA	1.66	0.42
1:B:298:GLU:O	1:B:301:VAL:HG22	2.20	0.42
1:B:88:THR:O	1:B:223:GLY:HA3	2.19	0.42
1:B:41:LYS:NZ	1:B:44:LYS:NZ	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:LEU:N	1:B:348:LEU:HD23	2.35	0.42
1:B:5:ASN:ND2	1:B:8:ASN:HA	2.33	0.42
1:A:194:LEU:HD23	1:A:194:LEU:HA	1.83	0.42
1:A:421:ASP:O	1:A:424:GLN:HG3	2.19	0.42
1:B:128:LEU:C	1:B:128:LEU:HD23	2.40	0.42
1:B:137:PRO:HB2	1:B:167:VAL:HG12	2.01	0.42
1:A:19:GLY:O	1:A:69:VAL:HG22	2.20	0.41
1:A:135:VAL:CG1	1:A:136:ASP:N	2.82	0.41
1:A:337:TYR:O	1:A:339:PRO:HD2	2.20	0.41
1:B:325:LEU:HD23	1:B:325:LEU:HA	1.90	0.41
1:A:60:THR:HA	1:A:63:THR:O	2.20	0.41
1:A:382:HIS:CE1	1:A:385:SER:HB3	2.55	0.41
1:B:381:ILE:O	1:B:383:PRO:HD3	2.21	0.41
1:A:290:LEU:HA	1:A:290:LEU:HD23	1.86	0.41
1:B:20:GLN:NE2	1:B:28:ARG:HH11	2.18	0.41
1:A:213:PHE:HA	1:A:374:ALA:HB1	2.02	0.41
1:A:252:LEU:HD12	1:A:253:VAL:H	1.85	0.41
1:A:386:THR:OG1	1:A:387:THR:N	2.53	0.41
1:A:187:ASN:HB2	1:A:205:VAL:CG2	2.51	0.41
1:B:392:ASN:C	1:B:394:GLN:N	2.72	0.41
1:B:299:ARG:HH21	1:B:299:ARG:HD3	1.57	0.41
1:A:393:GLU:HA	1:A:396:LEU:CB	2.51	0.40
1:B:4:THR:O	1:B:6:PRO:HD3	2.22	0.40
1:B:107:ILE:HD12	1:B:153:ALA:H	1.86	0.40
1:B:324:GLU:HB2	1:B:342:VAL:HG22	2.03	0.40
1:B:164:ILE:HG22	1:B:323:PRO:HD2	2.03	0.40
1:B:79:HIS:ND1	1:B:196:ARG:CD	2.84	0.40
1:B:369:LEU:CD1	1:B:381:ILE:HD13	2.35	0.40
1:A:311:LEU:HD13	1:A:348:LEU:HD11	2.03	0.40
1:A:328:SER:C	1:A:330:TYR:H	2.24	0.40
1:B:102:GLN:CG	1:B:103:GLN:H	2.34	0.40
1:B:107:ILE:HD12	1:B:153:ALA:O	2.22	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	424/448 (95%)	376 (89%)	41 (10%)	7 (2%)	7	25
1	B	422/448 (94%)	355 (84%)	57 (14%)	10 (2%)	5	18
All	All	846/896 (94%)	731 (86%)	98 (12%)	17 (2%)	6	22

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	235	ALA
1	A	393	GLU
1	B	235	ALA
1	B	393	GLU
1	A	6	PRO
1	A	8	ASN
1	A	326	GLU
1	B	6	PRO
1	B	127	LYS
1	B	8	ASN
1	B	427	ALA
1	A	329	PRO
1	B	329	PRO
1	B	245	PRO
1	B	237	GLY
1	B	323	PRO

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	338/356 (95%)	335 (99%)	3 (1%)	75	91
1	B	336/356 (94%)	327 (97%)	9 (3%)	40	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	674/712 (95%)	662 (98%)	12 (2%)	54 81

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	126	LYS
1	A	248	GLN
1	B	42	ASP
1	B	44	LYS
1	B	122	SER
1	B	252	LEU
1	B	267	ARG
1	B	273	ASP
1	B	294	SER
1	B	299	ARG
1	B	328	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	363	HIS
1	A	394	GLN
1	A	428	GLN
1	B	111	ASN
1	B	282	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
1	LLP	B	211	1	23,24,25	1.03	1 (4%)	25,32,34	1.19	2 (8%)
1	LLP	A	211	1	23,24,25	1.02	3 (13%)	25,32,34	1.26	4 (16%)

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
1	LLP	B	211	1	-	2/16/17/19	0/1/1/1
1	LLP	A	211	1	-	2/16/17/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	211	LLP	C3-C2	-2.66	1.38	1.40
1	A	211	LLP	C3-C2	-2.28	1.38	1.40
1	A	211	LLP	C4-C5	-2.26	1.39	1.42
1	A	211	LLP	C4-C4'	2.04	1.50	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	LLP	OP4-C5'-C5	3.38	115.79	109.35
1	A	211	LLP	OP4-C5'-C5	2.57	114.24	109.35
1	A	211	LLP	C5-C4-C4'	-2.41	117.59	121.56
1	B	211	LLP	OP4-P-OP1	2.32	112.97	106.47
1	A	211	LLP	OP2-P-OP4	2.26	112.75	106.73
1	A	211	LLP	C3-C4-C4'	2.20	124.51	120.41

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	211	LLP	O-C-CA-CB
1	B	211	LLP	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	A	211	LLP	CG-CD-CE-NZ
1	B	211	LLP	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	503	-	4,4,4	0.28	0	6,6,6	0.31	0
2	SO4	A	502	-	4,4,4	0.28	0	6,6,6	0.30	0
2	SO4	A	501	-	4,4,4	0.21	0	6,6,6	0.12	0
3	PRO	B	504	-	8,8,8	1.16	0	10,10,10	1.97	3 (30%)
2	SO4	B	501	-	4,4,4	0.30	0	6,6,6	0.28	0
2	SO4	B	502	-	4,4,4	0.19	0	6,6,6	0.35	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	PRO	B	504	-	-	2/4/11/11	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	504	PRO	OXT-C-O	-3.66	115.79	124.09
3	B	504	PRO	C-CA-N	3.22	119.44	106.73
3	B	504	PRO	OXT-C-CA	3.09	123.69	113.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	504	PRO	O-C-CA-CB
3	B	504	PRO	OXT-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	504	PRO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	425/448 (94%)	-0.27	0 100 100	26, 71, 95, 126	1 (0%)
1	B	424/448 (94%)	0.01	7 (1%) 69 63	46, 80, 111, 124	0
All	All	849/896 (94%)	-0.13	7 (0%) 82 78	26, 75, 107, 126	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	173	GLY	3.1
1	B	243	THR	2.7
1	B	198	LEU	2.4
1	B	397	LEU	2.3
1	B	143	PHE	2.1
1	B	391	LEU	2.0
1	B	133	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	LLP	B	211	24/25	0.93	0.10	52,71,80,83	0
1	LLP	A	211	24/25	0.95	0.10	50,64,70,71	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å ²)	Q<0.9
2	SO4	B	503	5/5	0.72	0.19	91,91,112,118	0
2	SO4	A	502	5/5	0.87	0.28	88,95,97,106	0
2	SO4	B	501	5/5	0.89	0.17	81,90,112,115	0
2	SO4	B	502	5/5	0.90	0.30	87,90,106,110	0
2	SO4	A	501	5/5	0.92	0.16	67,83,92,98	0
3	PRO	B	504	8/8	0.96	0.10	42,53,57,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.