

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	8WKO
Title	:	Crystal structure of O-acetylhomoserine sulfhydrylase from Lactobacillus plan-
		tarum 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 (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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (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 <=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	А	448	3% 64%	29%	• 5%		
1	В	448	57%	34%	•• 5%		



2 Entry composition (i)

There are 4 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	Δ	425	Total	С	Ν	0	\mathbf{S}	0	1	0
	A		3224	2053	543	627	1	0		
1	р	494	Total	С	Ν	0	S	0	0	0
ГВ	424	3209	2041	542	625	1		0		

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A0G9F7S9
А	-18	GLY	-	expression tag	UNP A0A0G9F7S9
A	-17	SER	-	expression tag	UNP A0A0G9F7S9
А	-16	SER	-	expression tag	UNP A0A0G9F7S9
А	-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
А	-10	HIS	-	expression tag	UNP A0A0G9F7S9
A	-9	SER	-	expression tag	UNP A0A0G9F7S9
А	-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
В	-19	MET	-	initiating methionine	UNP A0A0G9F7S9
В	-18	GLY	-	expression tag	UNP A0A0G9F7S9
В	-17	SER	-	expression tag	UNP A0A0G9F7S9
В	-16	SER	-	expression tag	UNP A0A0G9F7S9
В	-15	HIS	-	expression tag	UNP A0A0G9F7S9

There are 40 discrepancies between the modelled and reference sequences:



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

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total O S	0	0
2	А	1	Total O S	0	0
	11	1	5 4 1		
0	D	1	Total O S	0	0
	D	1	$5 \ 4 \ 1$	0	0
0	D	1	Total O S	0	0
	В		5 4 1	0	U



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Mol	Chain	Residues	Atom	IS	ZeroOcc	AltConf
2	В	1	Total C 5 4) S 1	0	0

• Molecule 3 is (2S)-2-amino-6-[[3-hydroxy-2-methyl-5-(phosphonooxymethyl)pyridin-4-yl]me thylideneamino]hexanoic acid (three-letter code: LLP) (formula: C₁₄H₂₂N₃O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Δ	1	Total C N O P	0	0
D A	1	24 14 3 6 1	0	0	
9	9 D	1	Total C N O P	0	0
3	D	1	24 14 3 6 1	0	

• Molecule 4 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	В	1	Total 8	$\begin{array}{c} \mathrm{C} \\ 5 \end{array}$	N 1	O 2	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: L-methionine gamma-lyase

1418 L310 A419 H313 A419 H313 A425 H313 A426 H313 P322 B327 P323 F334 P322 B327 P323 F334 P326 F336 P323 F337 P326 F336 P327 F337 P328 F337 P329 F336 P329 F337 P329 F339 P329 F339 P329</



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants	155.82Å 155.82Å 259.26Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Bosolution(A)	48.40 - 2.91	Depositor
Resolution (A)	48.40 - 2.91	EDS
% Data completeness	98.4 (48.40-2.91)	Depositor
(in resolution range)	98.4 (48.40-2.91)	EDS
R_{merge}	0.11	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.26 (at 2.91 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
B B.	0.203 , 0.262	Depositor
n, n_{free}	0.203 , 0.262	DCC
R_{free} test set	1308 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, 51.5	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.

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.



¹Intensities estimated from amplitudes.

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, 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	Bo	nd lengths	Bond angles		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.53	0/3297	0.90	7/4501~(0.2%)	
1	В	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	А	0	1
1	В	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	В	106	GLU	CG-CD	-6.37	1.42	1.51
1	В	128	LEU	CG-CD2	5.33	1.71	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	396	LEU	CA-CB-CG	14.71	149.13	115.30
1	В	128	LEU	CB-CG-CD2	-10.22	93.62	111.00
1	В	347	LEU	CB-CG-CD2	-9.81	94.33	111.00
1	А	24	GLU	CA-CB-CG	-9.04	93.52	113.40
1	В	128	LEU	N-CA-CB	-8.41	93.59	110.40
1	В	106	GLU	CA-CB-CG	-7.83	96.17	113.40
1	В	44	LYS	CB-CG-CD	7.66	131.52	111.60



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	347	LEU	CA-CB-CG	7.19	131.85	115.30
1	В	298	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	В	44	LYS	CA-CB-CG	6.50	127.70	113.40
1	В	256	LEU	CA-CB-CG	-5.76	102.05	115.30
1	В	128	LEU	CA-CB-CG	-5.63	102.35	115.30
1	А	44	LYS	CA-CB-CG	5.62	125.77	113.40
1	В	131	THR	OG1-CB-CG2	5.42	122.48	110.00
1	А	63	THR	OG1-CB-CG2	-5.40	97.59	110.00
1	В	368	LEU	CA-CB-CG	5.31	127.52	115.30
1	В	357	LYS	CA-CB-CG	5.21	124.86	113.40
1	В	44	LYS	N-CA-CB	5.17	119.91	110.60
1	А	378	LEU	CB-CG-CD2	-5.15	102.24	111.00
1	В	396	LEU	CA-CB-CG	5.12	127.09	115.30
1	В	126	LYS	CA-CB-CG	-5.12	102.14	113.40
1	А	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	А	391	ASN	Peptide
1	В	128	LEU	Mainchain

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	А	3224	0	3163	105	0
1	В	3209	0	3147	133	0
2	А	10	0	0	0	0
2	В	15	0	0	0	0
3	А	24	0	18	0	0
3	В	24	0	17	0	0
4	В	8	0	7	1	0
All	All	6514	0	6352	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	Clash
Atom-1	Atom-2	distance (\AA)	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:271:ARG:HG3	1.49	0.95
1:B:24:GLU:CD	1:B:24:GLU:H	1.71	0.93
1:B:368:LEU:HD12	1:B:380:ILE:HD13	1.50	0.92
1:B:168:ASP:O	1:B:172:ILE:HD12	1.72	0.89
1:A:425:LEU:O	1:A:428: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:322: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:223:VAL:HG11	1.68	0.74
1:A:62:LEU:HD11	1:A:271:ARG:HG3	1.68	0.74
1:B:269:THR:O	1:B:273:THR:OG1	2.04	0.74
1:A:24:GLU:OE1	1:A:24:GLU:N	2.16	0.73
1:B:381:HIS:HD2	1:B:384:SER:HB3	1.52	0.73
1:A:362:HIS:HD2	1:A:427:GLN:NE2	1.87	0.72
1:A:315:LYS:HE3	1:A:428: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:322: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:293: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:362:HIS:CD2	1:A:427: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:322: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:387:HIS:CE1	2.32	0.65
1:A:362:HIS:HD2	1:A:427: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



	A L C	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:102:GLN:HG3	1:A:103:GLN:H	1.62	0.64	
1:A:315:LYS:HE3	1:A:428:VAL:HG12	1.80	0.63	
1:A:18:ALA:HB3	1:A:73:ARG:HG3	1.79	0.63	
1:B:107:ILE:HG23	1:B:153:ALA:O	1.99	0.62	
1:B:381:HIS:CD2	1:B:384: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:337:PHE:HB3	1:B:340:GLY:O	2.01	0.61	
1:B:184:ILE:HG12	1:B:204:VAL:HB	1.81	0.61	
1:A:347:LEU:HD21	1:A:349:LEU:HD21	1.82	0.60	
1:B:369:LEU:HD11	1:B:378: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:414:ALA:O	1:B:418:ILE:HG13	2.03	0.59	
1:A:143:PHE:O	1:A:147:ILE:HG13	2.01	0.59	
1:A:360:ILE:HG21	1:A:368:LEU:HD13	1.85	0.58	
1:A:168:ASP:O	1:A:172:ILE:HD12	2.02	0.58	
1:A:251:LEU:HD12	1:A:252:VAL:N	2.18	0.58	
1:A:15:GLN:NE2	1:A:293: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:310:LEU:HD13	1:B:347: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:348:GLY:O	1:A:349: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:224: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:326:ASP:OD2	1:B:326:ASP:N	2.40	0.55	
1:B:184:ILE:HG23	1:B:204:VAL:HG12	1.89	0.55	
1:A:392:GLU:HA	1:A:395:LEU:HB3	1.88	0.54	
1:A:313:HIS:CE1	1:A:315:LYS:HB2	2.42	0.54	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:92:ALA:O	1:B:224: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
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:237:LYS:HB3	2.23	0.53
1:A:199:GLU:O	1:A:200:HIS:ND1	2.41	0.53
1:A:231:ASP:HB3	1:A:234:ALA:HB3	1.90	0.52
1:B:368:LEU:HD12	1:B:380:ILE:CD1	2.32	0.52
1:B:118:TYR:OH	1:B:394:GLU:OE1	2.14	0.52
1:B:160:GLY:HA3	1:B:165:ASN:OD1	2.10	0.52
1:A:320:ASN:O	1:A:345:PHE:HB2	2.10	0.52
1:B:79:HIS:ND1	1:B:196:ARG:HD3	2.24	0.52
1:B:313:HIS:HE1	1:B:315:LYS:HD2	1.73	0.52
1:A:174:LYS:HE2	1:A:178:ASP:OD2	2.10	0.51
1:B:377:SER:O	1:B:378:LEU:HD23	2.10	0.51
1:B:391:ASN:O	1:B:393:GLN:N	2.43	0.51
1:A:74:VAL:HG23	1:A:289:LEU:HD11	1.92	0.51
1:B:33:TYR:CE2	1:B:65:PRO:HB2	2.46	0.51
1:A:244:PRO:HB3	1:A:250: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:223:VAL:HG11	2.41	0.50
1:B:152:LYS:HB3	1:B:238:TYR:HE1	1.76	0.50
1:B:219:THR:HG23	1:B:281:ASN:ND2	2.27	0.50
1:A:414:ALA:O	1:A:418:ILE:HG13	2.11	0.50
1:B:95:ALA:HA	1:B:269: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:335:LYS:HD3	1:A:336:TYR:CZ	2.46	0.50
1:B:327:SER:O	1:B:329:TYR:N	2.45	0.50
1:B:192:PRO:HD3	1:B:207:HIS:CE1	2.47	0.49
1:B:330:HIS:O	1:B:334:THR:HG23	2.11	0.49
1:B:425:LEU:C	1:B:427:GLN:H	2.16	0.49
1:B:109:ALA:HA	1:B:155:TYR:O	2.13	0.49
1:B:238:TYR:O	1:B:242:THR:HG23	2.12	0.49
1:A:7:GLU:H	1:A:7:GLU:CD	2.10	0.49
1:A:392:GLU:O	1:A:396:LEU:HB2	2.13	0.49



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:390:LEU:HB3	1:B:394:GLU:HB2	1.94	0.49	
1:B:393:GLN:OE1	1:B:394:GLU:HG3	2.12	0.49	
1:B:74:VAL:HG11	1:B:223:VAL:HG11	1.94	0.49	
1:B:259:ALA:O	1:B:263:THR:HG23	2.13	0.49	
1:B:152:LYS:O	1:B:238:TYR:OH	2.15	0.49	
1:B:242:THR:OG1	1:B:243:THR:HG23	2.13	0.49	
1:A:261:PHE:O	1:A:265:VAL:HG23	2.12	0.49	
1:B:179:HIS:O	1:B:237: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:382:PRO:HG2	1:A:404: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:224:ILE:HG12	1.95	0.48	
1:B:318:TRP:NE1	1:B:348:GLY:HA3	2.28	0.48	
1:A:107:ILE:O	1:A:132:THR:HA	2.13	0.47	
1:B:253:PHE:CE1	1:B:264:LYS:HG3	2.49	0.47	
1:A:412:GLU:HB2	1:A:417:LEU:HD21	1.96	0.47	
1:A:362:HIS:CD2	1:A:427:GLN:NE2	2.74	0.47	
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.64	0.47	
1:A:283:PHE:O	1:A:287:GLN:HG2	2.14	0.47	
1:A:164:ILE:HG13	1:A:345:PHE:HA	1.96	0.47	
1:B:84:VAL:HG11	1:B:265: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:404:LEU:HD23	1:A:405:ILE:N	2.29	0.46	
1:B:320:ASN:HB2	1:B:346: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:252:VAL:O	1:A:255: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:253:PHE:CD1	1:B:264:LYS:HG3	2.51	0.46	
1:B:231:ASP:HB3	1:B:234:ALA:HB3	1.98	0.46	
1:B:363:LEU:HD13	1:B:366:PHE:HB2	1.98	0.46	
1:A:164:ILE:CG2	1:A:322:PRO:CD	2.91	0.46	
1:A:284:LEU:HD21	1:B:284: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	



	,	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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
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:377:SER:O	1:A:378: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:337:PHE:HB3	1:A:340:GLY:O	2.17	0.45
1:A:198:LEU:HD23	1:A:198:LEU:HA	1.79	0.44
1:A:351:GLY:HA3	1:A:355: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:225:VAL:HG21	2.00	0.44
1:A:78:GLU:HG2	1:A:205:VAL:HG11	2.00	0.44
1:A:313:HIS:HE1	1:A:315: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:310:LEU:HD23	1:B:310:LEU:HA	1.70	0.43
1:A:219:THR:HG21	1:A:284:LEU:CB	2.48	0.43
1:A:363:LEU:CD1	1:A:379:ILE:HD13	2.48	0.43
1:B:108:VAL:HB	1:B:154:LEU:HD22	2.00	0.43
1:B:420:ASP:O	1:B:423:GLN:HG3	2.17	0.43
1:B:287:GLN:HB2	4:B:504:PRO:HG2	1.99	0.43
1:A:152:LYS:HZ2	1:A:237:LYS:HB3	1.84	0.43
1:A:335:LYS:HD3	1:A:336:TYR:CE2	2.53	0.43
1:B:391:ASN:O	1:B:392:GLU:C	2.57	0.43
1:A:297:GLU:O	1:A:301:THR:HG23	2.19	0.43
1:A:327:SER:O	1:A:329:TYR:N	2.51	0.42
1:B:252:VAL:HG23	1:B:255:ASP:CG	2.40	0.42
1:B:304:ARG:NH2	1:B:323: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



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:297:GLU:O	1:B:300:VAL:HG22	2.20	0.42	
1:B:88:THR:O	1:B:222:GLY:HA3	2.19	0.42	
1:B:41:LYS:NZ	1:B:44:LYS:NZ	2.68	0.42	
1:B:347:LEU:HD23	1:B:347:LEU:N	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:420:ASP:O	1:A:423: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:336:TYR:O	1:A:338:PRO:HD2	2.20	0.41	
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.90	0.41	
1:A:60:THR:HA	1:A:63:THR:O	2.20	0.41	
1:A:381:HIS:CE1	1:A:384:SER:HB3	2.55	0.41	
1:B:380:ILE:O	1:B:382:PRO:HD3	2.21	0.41	
1:A:289:LEU:HA	1:A:289:LEU:HD23	1.86	0.41	
1:B:20:GLN:NE2	1:B:28:ARG:HH11	2.18	0.41	
1:A:212:PHE:HA	1:A:373:ALA:HB1	2.02	0.41	
1:A:251:LEU:HD12	1:A:252:VAL:H	1.85	0.41	
1:A:385:THR:OG1	1:A:386:THR:N	2.53	0.41	
1:A:187:ASN:HB2	1:A:205:VAL:CG2	2.51	0.41	
1:B:391:ASN:C	1:B:393:GLN:N	2.72	0.41	
1:B:298:ARG:HH21	1:B:298:ARG:HD3	1.57	0.41	
1:A:392:GLU:HA	1:A:395: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:323:GLU:HB2	1:B:341:VAL:HG22	2.03	0.40	
1:B:164:ILE:HG22	1:B:322:PRO:HD2	2.03	0.40	
1:B:79:HIS:ND1	1:B:196:ARG:CD	2.84	0.40	
1:B:368:LEU:CD1	1:B:380:ILE:HD13	2.35	0.40	
1:A:310:LEU:HD13	1:A:347:LEU:HD11	2.03	0.40	
1:A:327:SER:C	1:A:329: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 (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	А	422/448~(94%)	374 (89%)	41 (10%)	7 (2%)	9 29
1	В	420/448~(94%)	353 (84%)	57 (14%)	10 (2%)	6 21
All	All	842/896~(94%)	727 (86%)	98 (12%)	17 (2%)	7 26

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	42	ASP
1	А	234	ALA
1	А	392	GLU
1	В	234	ALA
1	В	392	GLU
1	А	6	PRO
1	А	8	ASN
1	А	325	GLU
1	В	6	PRO
1	В	127	LYS
1	В	8	ASN
1	В	426	ALA
1	А	328	PRO
1	В	328	PRO
1	В	244	PRO
1	В	236	GLY
1	В	322	PRO

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	338/357~(95%)	335~(99%)	3(1%)	78 92
1	В	336/357~(94%)	327~(97%)	9~(3%)	44 75
All	All	674/714~(94%)	662 (98%)	12 (2%)	59 83

analysed, and the total number of residues.

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

Mol	Chain	\mathbf{Res}	Type
1	А	102	GLN
1	А	126	LYS
1	А	247	GLN
1	В	42	ASP
1	В	44	LYS
1	В	122	SER
1	В	251	LEU
1	В	266	ARG
1	В	272	ASP
1	В	293	SER
1	В	298	ARG
1	В	327	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	А	111	ASN
1	А	362	HIS
1	А	393	GLN
1	А	427	GLN
1	В	111	ASN
1	В	281	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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).

Mal	Turne	Chain	Dec	Tiple	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	А	501	-	4,4,4	0.21	0	6,6,6	0.12	0
4	PRO	В	504	-	8,8,8	1.16	0	10,10,10	1.97	3 (30%)
2	SO4	В	503	-	4,4,4	0.28	0	6,6,6	0.31	0
2	SO4	А	502	-	4,4,4	0.28	0	6,6,6	0.30	0
2	SO4	В	501	-	4,4,4	0.30	0	6,6,6	0.28	0
2	SO4	В	502	-	4,4,4	0.19	0	6,6,6	0.35	0
3	LLP	В	505	1	23,24,25	1.03	1 (4%)	25,32,34	1.19	2 (8%)
3	LLP	А	503	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
3	LLP	В	505	1	-	2/16/17/19	0/1/1/1
3	LLP	А	503	1	-	2/16/17/19	0/1/1/1
4	PRO	В	504	-	-	2/4/11/11	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
3	В	505	LLP	C3-C2	-2.66	1.38	1.40
3	А	503	LLP	C3-C2	-2.28	1.38	1.40
3	A	503	LLP	C4-C5	-2.26	1.39	1.42



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	503	LLP	C4-C4'	2.04	1.50	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
4	В	504	PRO	OXT-C-O	-3.66	115.79	124.09
3	В	505	LLP	OP4-C5'-C5	3.38	115.79	109.35
4	В	504	PRO	C-CA-N	3.22	119.44	106.73
4	В	504	PRO	OXT-C-CA	3.09	123.69	113.40
3	А	503	LLP	OP4-C5'-C5	2.57	114.24	109.35
3	А	503	LLP	C5-C4-C4'	-2.41	117.59	121.56
3	В	505	LLP	OP4-P-OP1	2.32	112.97	106.47
3	А	503	LLP	OP2-P-OP4	2.26	112.75	106.73
3	A	503	LLP	C3-C4-C4'	2.20	124.51	120.41

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	503	LLP	O-C-CA-CB
3	В	505	LLP	O-C-CA-CB
3	А	503	LLP	CG-CD-CE-NZ
3	В	505	LLP	CG-CD-CE-NZ
4	В	504	PRO	O-C-CA-CB
4	В	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
4	В	504	PRO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and



any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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		$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	А	425/448~(94%)	0.20	14 (3%) 46 4	42	42, 71, 95, 126	0
1	В	424/448~(94%)	0.45	38 (8%) 9 7	7	46, 80, 111, 124	0
All	All	849/896~(94%)	0.32	52 (6%) 21 1	18	42, 75, 107, 126	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	169	PHE	4.6
1	В	173	GLY	4.2
1	В	147	ILE	3.9
1	В	428	VAL	3.8
1	В	54	ASP	3.6
1	В	90	SER	3.6
1	А	324	LEU	3.6
1	В	108	VAL	3.5
1	А	428	VAL	3.5
1	В	143	PHE	3.4
1	В	4	THR	3.3
1	В	42	ASP	3.3
1	В	137	PRO	3.2
1	В	426	ALA	3.1
1	В	232	TRP	3.0
1	В	336	TYR	2.9
1	В	274	GLY	2.9
1	В	276	THR	2.9
1	В	273	THR	2.8
1	В	175	ILE	2.7
1	В	238	TYR	2.7
1	В	141	ALA	2.6
1	A	4	THR	2.6
1	В	178	ASP	2.6



Mol	Chain	Res	Type	RSRZ
1	В	154	LEU	2.5
1	А	181	ILE	2.5
1	В	94	THR	2.5
1	В	145	THR	2.5
1	А	175	ILE	2.5
1	А	221	GLY	2.4
1	В	149	ASP	2.3
1	В	92	ALA	2.3
1	А	208	SER	2.3
1	В	230	PHE	2.3
1	В	182	ILE	2.3
1	В	109	ALA	2.2
1	В	251	LEU	2.2
1	А	237	LYS	2.2
1	В	134	PHE	2.2
1	В	151	THR	2.2
1	В	393	GLN	2.2
1	А	232	TRP	2.2
1	В	228	GLY	2.1
1	В	135	VAL	2.1
1	А	278	SER	2.1
1	А	90	SER	2.1
1	В	174	LYS	2.1
1	А	235	SER	2.1
1	А	219	THR	2.0
1	В	144	GLU	2.0
1	В	200	HIS	2.0
1	А	310	LEU	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 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,



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	SO4	В	503	5/5	0.83	0.30	91,91,112,118	0
2	SO4	В	501	5/5	0.88	0.28	81,90,112,115	0
2	SO4	А	502	5/5	0.91	0.36	88,95,97,106	0
2	SO4	В	502	5/5	0.92	0.33	87,90,106,110	0
3	LLP	В	505	24/25	0.94	0.28	52,71,80,83	0
2	SO4	А	501	5/5	0.95	0.14	67,83,92,98	0
3	LLP	А	503	24/25	0.96	0.26	50,64,70,71	0
4	PRO	В	504	8/8	0.96	0.26	42,53,57,58	0

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.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.









6.5 Other polymers (i)

There are no such residues in this entry.

