

Full wwPDB X-ray Structure Validation Report (i)

Jan 16, 2024 - 03:16 am GMT

PDB ID	:	80QP
Title	:	Structure of Mycobacterium tuberculosis beta-oxidation trifunctional enzyme
		in complex with Fragment-M-76
Authors	:	Dalwani, S.; Wierenga, R.K.; Venkatesan, R.
Deposited on	:	2023-04-12
Resolution	:	2.18 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	:	1.8.4, 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 2.18 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	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	736	^{2%} 91%	7% •
1	В	736	2% 92%	6% •
2	С	403	4% 92%	8%
2	D	403	91%	9%



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17691 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	723	Total 5371	C 3399	N 922	O 1030	S 20	0	0	0
1	В	726	Total 5383	C 3406	N 925	0 1031	S 21	0	0	0

• Molecule 1 is a protein called 3-hydroxyacyl-CoA dehydrogenase.

Residue	Modelled	Actual Comment		Reference
-15	MET	-	initiating methionine	UNP O53872
-14	GLY	-	expression tag	UNP O53872
-13	SER	-	expression tag	UNP O53872
-12	SER	-	expression tag	UNP O53872
-11	HIS	-	expression tag	UNP O53872
-10	HIS	-	expression tag	UNP O53872
-9	HIS	-	expression tag	UNP O53872
-8	HIS	-	expression tag	UNP O53872
-7	HIS	-	expression tag	UNP O53872
-6	HIS	-	expression tag	UNP O53872
-5	SER	-	expression tag	UNP O53872
-4	GLN	-	expression tag	UNP O53872
-3	ASP	-	expression tag	UNP O53872
-2	PRO	-	expression tag	UNP O53872
-1	ASN	-	expression tag	UNP O53872
0	SER	-	expression tag	UNP O53872
-15	MET	-	initiating methionine	UNP O53872
-14	GLY	-	expression tag	UNP O53872
-13	SER	-	expression tag	UNP O53872
-12	SER	-	expression tag	UNP O53872
-11	HIS	-	expression tag	UNP O53872
-10	HIS	-	expression tag	UNP O53872
-9	HIS	-	expression tag	UNP O53872
-8	HIS	-	expression tag	UNP O53872
-7	HIS	-	expression tag	UNP 053872
	Residue -15 -14 -13 -12 -11 -0 -9 -8 -7 -6 -5 -4 -3 -2 -1 0 -15 -14 -3 -2 -1 0 -15 -14 -13 -12 -11 -10 -9 -8 -7	Residue Modelled -15 MET -14 GLY -13 SER -12 SER -11 HIS -10 HIS -9 HIS -9 HIS -7 HIS -7 HIS -6 HIS -5 SER -4 GLN -3 ASP -2 PRO -1 ASN 0 SER -15 MET -14 GLY -15 MET -14 GLY -15 SER -14 GLY -13 SER -12 SER -13 SER -12 SER -11 HIS -10 HIS -9 HIS -8 HIS -7 HIS	Residue Modelled Actual -15 MET - -14 GLY - -13 SER - -12 SER - -12 SER - -11 HIS - -10 HIS - -10 HIS - -9 HIS - -9 HIS - -9 HIS - -9 HIS - -10 HIS - -10 HIS - -11 HIS - -5 SER - -6 HIS - -14 GLN - -15 MET - -14 GLY - -15 MET - -13 SER - -12 SER - -11 HIS - <tr tbl=""> -1</tr>	ResidueModelledActualComment-15MET-initiating methionine-14GLY-expression tag-13SER-expression tag-12SER-expression tag-11HIS-expression tag-10HIS-expression tag-10HIS-expression tag-9HIS-expression tag-9HIS-expression tag-7HIS-expression tag-6HIS-expression tag-5SER-expression tag-4GLN-expression tag-3ASP-expression tag-1ASN-expression tag-1GLY-expression tag-1ASN-expression tag-1SER-expression tag-1HIS-expression tag-11HIS-expression tag-12SER-expression tag-13SER-expression tag-14GLY-expression tag-15MET-expression tag-16HIS-expression tag-17HIS-expression tag-18HIS-expression tag-19HIS-expression tag-10HIS-expression tag-9HIS-expression tag<

There are 32 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
В	-6	HIS	-	expression tag	UNP O53872
В	-5	SER	-	expression tag	UNP O53872
В	-4	GLN	-	expression tag	UNP O53872
В	-3	ASP	-	expression tag	UNP O53872
В	-2	PRO	-	expression tag	UNP O53872
В	-1	ASN	-	expression tag	UNP O53872
В	0	SER	-	expression tag	UNP O53872

• Molecule 2 is a protein called Putative acyltransferase Rv0859.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	С	402	Total 2963	C 1852	N 524	0 572	S 15	0	1	0
2	D	402	Total 2965	C 1853	N 525	O 572	S 15	0	1	0

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf		
3	А	1	Total O S	0	0		
		_	5 4 1				
3	В	1	Total O S	0	0		
			5 4 1				
3	В	1	Total O S	0	0		
			5 4 1				
3	В	1	Total O S	0	0		
			5 4 1				
3	В	1	Total O S	0	0		
			5 4 1				
3	В	В	В	1	Total O S	0	0
					$\begin{array}{ccc} 0 & 4 & 1 \\ \hline \end{array}$		
3	С	1	$\begin{array}{ccc} 10tal & O & S \\ 5 & 4 & 1 \end{array}$	0	0		
3	С	1	$\begin{array}{ccc} 10tal & 0 & 5 \\ 5 & 4 & 1 \end{array}$	0	0		
			$\frac{5}{\text{Total}}$				
3	С	1	$\begin{array}{ccc} 10tal & O & S \\ 5 & 4 & 1 \end{array}$	0	0		
			$\begin{array}{ccc} \mathbf{J} & \mathbf{\bar{4}} & \mathbf{\bar{1}} \\ \mathbf{Total} & \mathbf{O} & \mathbf{S} \end{array}$				
3	С	1	5 4 1	0	0		
			$\begin{array}{ccc} \mathbf{J} & \mathbf{I} \\ \mathbf{T} \\ $				
3	D	1	5 4 1	0	0		
			$\begin{array}{c c} \mathbf{J} & \mathbf{T} \\ \hline \mathbf{Total} & \mathbf{O} & \mathbf{S} \\ \end{array}$				
3	D	1		0	0		
			Total O S				
3	D	1	5 4 1	0	0		

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0

• Molecule 5 is 2-azanyl-5-sulfo-benzoic acid (three-letter code: VXZ) (formula: C₇H₇NO₅S) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
-	٨	1	Total	С	Ν	Ο	S	0	0
6	А	1	14	7	1	5	1	0	0
5	٨	1	Total	С	Ν	0	S	0	0
5	A	1	14	7	1	5	1	0	0
5	Δ	1	Total	С	Ν	Ο	S	0	0
5	A	1	14	7	1	5	1	0	0
5	Δ	1	Total	С	Ν	Ο	S	0	0
5	A	1	14	7	1	5	1	0	0
Б	Δ	1	Total	С	Ν	0	S	0	0
5	A	1	14	7	1	5	1	0	0
5	Λ	1	Total	С	Ν	Ο	S	0	0
5	A	1	14	7	1	5	1	0	0
5	Λ	1	Total	С	Ν	0	S	0	0
0	Л	1	14	7	1	5	1	0	0
5	В	1	Total	С	Ν	0	S	0	0
5	D	1	14	$\overline{7}$	1	5	1	0	0
5	В	1	Total	С	Ν	0	S	0	0
0	D	1	14	7	1	5	1	0	0
5	Р	1	Total	С	Ν	0	S	0	0
0	D	1	14	7	1	5	1	0	0
5	В	1	Total	С	Ν	0	S	0	0
0	D	1	14	7	1	5	1	0	0
5	В	1	Total	С	Ν	0	S	0	0
0	D	1	14	7	1	5	1	U	0
5	B	1	Total	С	Ν	Ο	S	0	0
0		1	14	7	1	5	1	U	0
5	R	1	Total	С	Ν	0	S	0	0
0		L	14	7	1	5	1		U



Continued from previous page...

Mol	Chain	Residues		Ato	\mathbf{pms}			ZeroOcc	AltConf
5	С	1	Total	С	Ν	0	\mathbf{S}	0	0
0	U	1	14	7	1	5	1	0	0
5	С	1	Total	С	Ν	Ο	\mathbf{S}	0	0
0	U	1	14	7	1	5	1	0	0
5	Л	1	Total	С	Ν	0	\mathbf{S}	0	0
0	D	1	14	7	1	5	1	0	0
5	Л	1	Total	С	Ν	0	\mathbf{S}	0	0
0	D	1	14	7	1	5	1	0	0
5	Л	1	Total	С	Ν	0	\mathbf{S}	0	0
0	D	1	14	7	1	5	1	0	0
5	Л	1	Total	С	Ν	0	S	0	0
5		1	14	7	1	5	1		0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	160	Total O 160 160	0	0
6	В	180	Total O 180 180	0	0
6	С	146	Total O 146 146	0	0
6	D	110	Total O 110 110	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-hydroxyacyl-CoA dehydrogenase



MET





• Molecule 2: Putative acyltransferase Rv0859





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	250.94Å 132.80Å 119.29Å	Depositor
a, b, c, α , β , γ	90.00° 110.46° 90.00°	Depositor
Bosolution (Å)	27.08 - 2.18	Depositor
Resolution (A)	117.55 - 2.18	EDS
% Data completeness	76.4 (27.08-2.18)	Depositor
(in resolution range)	76.4(117.55-2.18)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.84 (at 2.18 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R R.	0.191 , 0.219	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.192 , 0.220	DCC
R_{free} test set	7114 reflections (4.90%)	wwPDB-VP
Wilson B-factor $(Å^2)$	46.5	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 39.2	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	0.95	EDS
Total number of atoms	17691	wwPDB-VP
Average B, all atoms $(Å^2)$	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.87% 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: GOL, VXZ, 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).

Mal	Chain	Bond	lengths	Bond	angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.25	0/5471	0.48	0/7406
1	В	0.25	0/5484	0.48	0/7426
2	С	0.25	0/3011	0.51	0/4078
2	D	0.25	0/3013	0.52	0/4080
All	All	0.25	0/16979	0.49	0/22990

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	В	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	598	ARG	Sidechain

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	5371	0	5403	30	0
1	В	5383	0	5405	26	0
2	С	2963	0	2980	26	0
2	D	2965	0	2985	29	0
3	А	25	0	0	0	0
3	В	25	0	0	0	0
3	С	20	0	0	0	0
3	D	15	0	0	0	0
4	А	18	0	24	2	0
4	В	12	0	16	0	0
4	С	6	0	8	1	0
4	D	12	0	16	0	0
5	А	98	0	0	1	0
5	В	98	0	0	1	0
5	С	28	0	0	1	0
5	D	56	0	0	1	0
6	А	160	0	0	2	0
6	В	180	0	0	1	0
6	С	146	0	0	3	0
6	D	110	0	0	0	0
All	All	17691	0	16837	106	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 3.

All (106) 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 (Å)	overlap (Å)
2:C:173:ARG:NH2	2:C:348:LEU:O	2.08	0.85
2:D:382:ARG:HH21	2:D:383:ARG:NH2	1.90	0.69
1:A:412:VAL:HG23	1:A:413:PHE:H	1.60	0.66
2:C:62:VAL:HG12	2:D:62:VAL:HG12	1.78	0.66
1:A:103:LYS:NZ	6:A:902:HOH:O	2.31	0.64
2:C:96:LEU:HD23	2:C:396:VAL:HG13	1.82	0.61
2:C:110:TRP:CD1	2:D:313:ARG:HD3	2.36	0.60
1:A:711:ARG:HB3	4:A:804:GOL:H2	1.82	0.60
2:C:296:PRO:HD3	2:D:81:VAL:HG21	1.84	0.60
1:A:462:HIS:HB3	1:A:474:GLU:HB3	1.85	0.59
1:B:374:LYS:NZ	6:B:901:HOH:O	2.28	0.59
2:C:313:ARG:HD3	2:D:110:TRP:CD1	2.38	0.58
2:D:382:ARG:HG2	2:D:383:ARG:HG3	1.85	0.58
1:A:376:LEU:HD11	1:A:386:SER:HB2	1.86	0.57



	page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:336:LYS:NZ	2:C:340:ASP:OD2	2.34	0.57
1:A:345:ALA:O	1:A:392:ARG:NH1	2.38	0.57
2:D:46:LEU:HD12	2:D:280:LEU:HD21	1.87	0.57
1:B:369:GLU:HG2	1:B:390:LEU:HD13	1.86	0.56
1:B:532:PRO:HB2	1:B:615:LEU:HD13	1.87	0.56
1:B:5:THR:HG22	1:B:37:SER:HB2	1.86	0.56
2:C:81:VAL:HG11	2:D:296:PRO:HD3	1.87	0.56
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.87	0.55
2:D:252:HIS:HE1	2:D:332:SER:H	1.54	0.55
1:B:250:ARG:NH1	2:C:142:TYR:O	2.39	0.55
2:D:390:ILE:HB	2:D:394:MET:HB2	1.89	0.55
1:B:116:GLY:O	1:B:120:ILE:HG12	2.06	0.54
1:B:331:LEU:HD11	1:B:426:ILE:HD13	1.89	0.54
1:A:416:GLN:HG3	1:A:448:LEU:HD23	1.90	0.53
2:C:299:MET:HB3	2:C:300:LEU:HD22	1.90	0.52
1:B:520:ASN:HB3	1:B:581:HIS:CE1	2.44	0.52
2:D:241:LYS:HE2	2:D:295:ASP:OD1	2.09	0.52
1:B:378:ARG:HD2	1:B:380:ARG:HH12	1.75	0.52
1:A:62:LYS:HG3	1:A:63:THR:HG23	1.92	0.52
1:A:182:LYS:NZ	6:A:904:HOH:O	2.35	0.51
2:C:239:LEU:HD21	2:C:248:ILE:HG13	1.92	0.51
1:A:423:PHE:HA	1:A:426:ILE:HG22	1.93	0.51
1:A:532:PRO:HB2	1:A:615:LEU:HD13	1.93	0.51
2:C:45:ASP:N	2:C:45:ASP:OD1	2.44	0.51
2:D:62:VAL:HG11	2:D:130:ASP:HA	1.93	0.51
2:D:326:LEU:HD13	2:D:387:THR:HG23	1.93	0.50
2:D:382:ARG:HE	2:D:383:ARG:CZ	2.24	0.50
2:D:99:VAL:HG13	2:D:269:ILE:HD11	1.93	0.50
2:C:91:PHE:HB2	2:C:390:ILE:HG23	1.93	0.49
2:C:276:LYS:NZ	6:C:603:HOH:O	2.46	0.49
1:A:445:ILE:HD13	1:A:448:LEU:HD12	1.96	0.48
2:D:242:TYR:OH	2:D:298:ILE:HB	2.14	0.48
1:B:698:VAL:HG13	1:B:714:PRO:HG3	1.95	0.48
2:C:173:ARG:HE	2:C:177:LYS:CE	2.27	0.48
1:B:5:THR:HG22	1:B:37:SER:CB	2.43	0.47
1:A:331:LEU:HB2	1:A:410:GLU:HA	1.97	0.47
1:A:65:PHE:O	1:A:117:GLY:HA3	2.15	0.47
1:B:5:THR:HG23	1:B:6:ILE:HG13	1.97	0.47
2:C:62:VAL:HG11	2:C:130:ASP:HA	1.96	0.47
2:C:205:HIS:HB2	6:C:735:HOH:O	2.15	0.47
1:B:415:ASN:OD1	1:B:417:GLU:HG2	2.15	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:382:ARG:HE	2:D:383:ARG:NH1	2.13	0.46
1:A:510:PHE:CD1	1:A:656:LEU:HD11	2.51	0.45
1:A:36:GLU:HG3	1:A:40:LYS:HE3	1.98	0.45
2:D:252:HIS:CE1	2:D:332:SER:H	2.32	0.45
2:C:110:TRP:CZ2	2:D:288:ALA:HA	2.51	0.45
1:A:711:ARG:HH11	4:A:804:GOL:H12	1.82	0.45
1:B:55:VAL:HB	1:B:105:VAL:HG22	1.99	0.45
2:C:134:MET:SD	2:D:75:LEU:HD12	2.57	0.45
1:A:130:ALA:O	1:A:132:VAL:N	2.47	0.45
1:B:140:PRO:HA	1:B:173:GLY:HA3	1.99	0.45
2:D:173:ARG:NH2	2:D:177:LYS:HE3	2.32	0.45
1:A:126:HIS:NE2	1:A:189:GLU:OE2	2.34	0.44
1:B:459:ILE:HD11	1:B:486:LEU:HD12	2.00	0.44
1:B:564:ALA:HB1	1:B:584:GLU:OE2	2.17	0.44
1:A:402:PHE:CB	1:A:426:ILE:HD11	2.48	0.44
1:B:687:SER:HA	1:B:691:GLY:O	2.16	0.44
2:D:2:SER:HB3	2:D:107:ARG:O	2.18	0.44
2:D:170:TYR:O	2:D:173:ARG:HG2	2.18	0.43
1:A:318:GLU:HG3	1:A:319:GLY:N	2.31	0.43
1:B:5:THR:HG21	1:B:34:TYR:HA	2.00	0.43
1:A:363:LYS:HE2	1:A:363:LYS:HB3	1.83	0.43
1:A:253:LEU:HD13	1:A:258:MET:HB2	2.01	0.43
5:B:812:VXZ:O3	5:B:812:VXZ:N	2.52	0.43
2:D:3:GLU:O	2:D:107:ARG:HG2	2.18	0.43
1:B:515:ILE:HD12	1:B:670:ILE:HB	2.01	0.43
1:B:632:LEU:HD12	1:B:635:MET:HE3	2.01	0.43
2:C:59:VAL:HG21	2:C:361:LEU:HB3	2.01	0.43
1:A:471:PRO:HG2	1:A:668:MET:HB3	2.00	0.43
5:D:507:VXZ:O4	5:D:507:VXZ:N	2.51	0.43
1:A:714:PRO:HA	1:A:715:PRO:HD3	1.96	0.42
1:A:126:HIS:HE2	1:A:189:GLU:CD	2.20	0.42
2:C:210:ARG:NH1	6:C:606:HOH:O	2.51	0.42
1:A:355:ASP:OD1	1:A:356:VAL:HG22	2.20	0.42
2:C:203:LEU:HD11	2:C:207:GLU:HG3	2.01	0.42
5:A:807:VXZ:O4	5:A:807:VXZ:N	2.53	0.42
2:C:266:LEU:HD23	2:C:266:LEU:HA	1.88	0.42
2:D:91:PHE:HB2	2:D:390:ILE:CG2	2.50	0.41
2:D:170:TYR:CD1	2:D:173:ARG:HD3	2.55	0.41
1:B:578:TYR:OH	1:B:584:GLU:OE2	2.37	0.41
2:C:390:ILE:HD12	2:C:394:MET:HB2	2.01	0.41
1:A:376:LEU:HD11	1:A:386:SER:CB	2.50	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:390:ILE:HD12	2:D:394:MET:HB2	2.03	0.41
1:B:416:GLN:HE21	1:B:416:GLN:HB2	1.62	0.41
1:B:405:VAL:HB	1:B:430:VAL:HG12	2.01	0.41
1:A:52:ILE:O	1:A:103:LYS:HD3	2.21	0.41
1:A:542:ALA:HB2	1:A:636:ILE:HG23	2.03	0.41
2:C:318:VAL:H	4:C:505:GOL:H12	1.86	0.40
5:C:507:VXZ:O4	5:C:507:VXZ:N	2.53	0.40
2:C:394:MET:HG2	2:D:71:ARG:CZ	2.51	0.40
2:D:354:ALA:HB1	2:D:359:HIS:HB2	2.03	0.40
1:B:476:ILE:HG21	1:B:509:PHE:CE1	2.57	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	Perce	entiles
1	А	719/736~(98%)	693 (96%)	25~(4%)	1 (0%)	51	58
1	В	722/736~(98%)	699~(97%)	22 (3%)	1 (0%)	51	58
2	С	401/403~(100%)	390 (97%)	10 (2%)	1 (0%)	47	52
2	D	401/403~(100%)	386 (96%)	14 (4%)	1 (0%)	47	52
All	All	2243/2278~(98%)	2168 (97%)	71 (3%)	4 (0%)	47	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	С	361	LEU
2	D	361	LEU
1	А	131	ASP
1	В	556	ASN



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	552/566~(98%)	547~(99%)	5 (1%)	78	87	
1	В	552/566~(98%)	547 (99%)	5 (1%)	78	87	
2	С	308/310~(99%)	306~(99%)	2(1%)	86	92	
2	D	309/310~(100%)	309 (100%)	0	100	100	
All	All	1721/1752 (98%)	1709 (99%)	12 (1%)	84	91	

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

Mol	Chain	\mathbf{Res}	Type
1	А	-9	HIS
1	А	258	MET
1	А	307	LEU
1	А	318	GLU
1	А	378	ARG
1	В	5	THR
1	В	101	LEU
1	В	258	MET
1	В	378	ARG
1	В	416	GLN
2	С	173	ARG
2	С	245	VAL

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains identified.

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)

45 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	Tuno	Chain	Dog	Tink	Bond lengths		Bond angles			
	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	С	501	-	4,4,4	0.14	0	6,6,6	0.04	0
4	GOL	D	504	-	$5,\!5,\!5$	0.93	0	$5,\!5,\!5$	1.09	0
5	VXZ	А	810	-	14,14,14	1.02	2 (14%)	21,21,21	0.86	2 (9%)
5	VXZ	А	812	-	14,14,14	0.22	0	21,21,21	0.25	0
5	VXZ	А	811	-	14,14,14	1.03	2 (14%)	21,21,21	0.86	2 (9%)
5	VXZ	А	808	-	14,14,14	1.02	2 (14%)	21,21,21	0.86	2 (9%)
3	SO4	А	802	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	D	502	-	4,4,4	0.14	0	6,6,6	0.07	0
5	VXZ	В	808	-	14,14,14	1.02	2 (14%)	21,21,21	0.87	2 (9%)
5	VXZ	В	811	-	14,14,14	1.02	2 (14%)	21,21,21	0.87	2 (9%)
5	VXZ	А	807	-	14,14,14	1.03	2 (14%)	21,21,21	0.86	2 (9%)
4	GOL	А	804	-	$5,\!5,\!5$	0.86	0	$5,\!5,\!5$	1.02	0
4	GOL	А	805	-	$5,\!5,\!5$	0.81	0	$5,\!5,\!5$	1.06	0
4	GOL	А	806	-	$5,\!5,\!5$	0.82	0	$5,\!5,\!5$	1.04	0
5	VXZ	А	813	-	14,14,14	0.65	1 (7%)	21,21,21	0.23	0
3	SO4	В	801	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	В	813	-	4,4,4	0.17	0	6,6,6	0.20	0
3	SO4	А	803	-	4,4,4	0.14	0	6,6,6	0.05	0
5	VXZ	В	807	-	14,14,14	0.19	0	21,21,21	0.22	0
3	SO4	С	504	-	4,4,4	0.14	0	6,6,6	0.08	0
4	GOL	В	805	-	$5,\!5,\!5$	0.88	0	$5,\!5,\!5$	1.03	0
4	GOL	С	505	-	$5,\!5,\!5$	0.78	0	$5,\!5,\!5$	1.05	0
3	SO4	С	502	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	В	814	-	4,4,4	0.14	0	6,6,6	0.06	0
5	VXZ	В	812	-	14,14,14	0.55	0	21,21,21	0.21	0
3	SO4	C	503	-	4,4,4	0.14	0	6,6,6	0.05	0



Mol	Type	Chain	Dog	Tink	Bond lengths			Bond angles		
	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	VXZ	В	809	-	14,14,14	0.19	0	21,21,21	0.25	0
4	GOL	В	804	-	$5,\!5,\!5$	0.91	0	$5,\!5,\!5$	0.93	0
5	VXZ	D	508	-	14,14,14	0.17	0	21,21,21	0.22	0
5	VXZ	D	506	-	14,14,14	1.03	2 (14%)	21,21,21	0.86	2 (9%)
3	SO4	А	814	-	4,4,4	0.17	0	6,6,6	0.20	0
5	VXZ	С	507	-	14,14,14	1.03	2 (14%)	21,21,21	0.87	2(9%)
5	VXZ	А	809	-	14,14,14	1.02	2 (14%)	21,21,21	0.85	2 (9%)
3	SO4	D	501	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	В	802	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	D	503	-	4,4,4	0.14	0	6,6,6	0.06	0
5	VXZ	D	509	2	14,14,14	0.71	1 (7%)	21,21,21	0.30	0
4	GOL	D	505	-	5,5,5	0.82	0	$5,\!5,\!5$	1.02	0
5	VXZ	D	507	-	14,14,14	1.01	2 (14%)	21,21,21	0.86	2 (9%)
5	VXZ	В	810	-	14,14,14	1.03	2 (14%)	21,21,21	0.87	2 (9%)
5	VXZ	С	506	-	14,14,14	0.20	0	21,21,21	0.25	0
3	SO4	В	803	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	815	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	А	801	-	4,4,4	0.14	0	6,6,6	0.06	0
5	VXZ	В	806	-	14,14,14	1.03	2 (14%)	21,21,21	0.87	2 (9%)

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
4	GOL	D	504	-	-	0/4/4/4	-
5	VXZ	А	810	-	-	0/10/10/10	0/1/1/1
5	VXZ	А	812	-	-	0/10/10/10	0/1/1/1
5	VXZ	А	811	-	-	0/10/10/10	0/1/1/1
5	VXZ	А	808	-	-	0/10/10/10	0/1/1/1
5	VXZ	В	808	-	-	0/10/10/10	0/1/1/1
5	VXZ	В	811	-	-	0/10/10/10	0/1/1/1
5	VXZ	А	807	-	-	0/10/10/10	0/1/1/1
4	GOL	А	804	-	-	4/4/4/4	-
4	GOL	А	806	-	-	2/4/4/4	-
4	GOL	А	805	-	-	2/4/4/4	-
5	VXZ	А	813	-	-	0/10/10/10	0/1/1/1
5	VXZ	В	807	-	-	0/10/10/10	0/1/1/1
4	GOL	В	805	-	-	0/4/4/4	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	С	505	-	-	2/4/4/4	-
5	VXZ	В	812	-	-	0/10/10/10	0/1/1/1
5	VXZ	В	809	-	-	0/10/10/10	0/1/1/1
4	GOL	В	804	-	-	2/4/4/4	-
5	VXZ	D	508	-	-	0/10/10/10	0/1/1/1
5	VXZ	D	506	-	-	2/10/10/10	0/1/1/1
5	VXZ	С	507	-	-	0/10/10/10	0/1/1/1
5	VXZ	А	809	-	-	0/10/10/10	0/1/1/1
5	VXZ	D	509	2	-	0/10/10/10	0/1/1/1
4	GOL	D	505	-	-	4/4/4/4	-
5	VXZ	D	507	-	-	0/10/10/10	0/1/1/1
5	VXZ	В	810	-	-	4/10/10/10	0/1/1/1
5	VXZ	С	506	-	-	0/10/10/10	0/1/1/1
5	VXZ	В	806	-	-	0/10/10/10	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	В	811	VXZ	O4-C6	2.82	1.31	1.22
5	А	810	VXZ	O4-C6	2.81	1.31	1.22
5	А	807	VXZ	O4-C6	2.81	1.31	1.22
5	D	506	VXZ	O4-C6	2.81	1.31	1.22
5	В	808	VXZ	O4-C6	2.80	1.31	1.22
5	А	811	VXZ	O4-C6	2.79	1.31	1.22
5	В	806	VXZ	O4-C6	2.79	1.31	1.22
5	С	507	VXZ	O4-C6	2.78	1.31	1.22
5	А	808	VXZ	O4-C6	2.78	1.31	1.22
5	А	809	VXZ	O4-C6	2.78	1.31	1.22
5	D	507	VXZ	O4-C6	2.78	1.31	1.22
5	В	810	VXZ	O4-C6	2.77	1.31	1.22
5	D	506	VXZ	O3-C6	-2.52	1.22	1.30
5	А	811	VXZ	O3-C6	-2.52	1.22	1.30
5	В	806	VXZ	O3-C6	-2.51	1.22	1.30
5	В	810	VXZ	O3-C6	-2.51	1.22	1.30
5	А	809	VXZ	O3-C6	-2.51	1.22	1.30
5	В	811	VXZ	O3-C6	-2.51	1.22	1.30
5	D	509	VXZ	O2-S	2.50	1.56	1.43
5	С	507	VXZ	O3-C6	-2.50	1.22	1.30
5	D	507	VXZ	O3-C6	-2.50	1.22	1.30
5	А	807	VXZ	O3-C6	-2.49	1.22	1.30
5	А	808	VXZ	O3-C6	-2.49	1.22	1.30



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)			
5	А	810	VXZ	O3-C6	-2.49	1.22	1.30			
5	В	808	VXZ	O3-C6	-2.46	1.23	1.30			
5	А	813	VXZ	O2-S	2.38	1.55	1.43			

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	С	507	VXZ	O4-C6-C5	-3.02	114.60	121.94
5	А	810	VXZ	O4-C6-C5	-3.02	114.61	121.94
5	В	811	VXZ	O4-C6-C5	-3.02	114.62	121.94
5	В	806	VXZ	O4-C6-C5	-3.01	114.62	121.94
5	В	808	VXZ	O4-C6-C5	-3.01	114.63	121.94
5	В	810	VXZ	O4-C6-C5	-3.01	114.64	121.94
5	D	507	VXZ	O4-C6-C5	-3.01	114.64	121.94
5	D	506	VXZ	O4-C6-C5	-3.00	114.66	121.94
5	А	808	VXZ	O4-C6-C5	-2.99	114.67	121.94
5	А	807	VXZ	O4-C6-C5	-2.99	114.68	121.94
5	А	811	VXZ	O4-C6-C5	-2.98	114.71	121.94
5	А	809	VXZ	O4-C6-C5	-2.98	114.71	121.94
5	В	808	VXZ	O3-C6-C5	2.34	122.04	115.31
5	D	507	VXZ	O3-C6-C5	2.34	122.03	115.31
5	А	809	VXZ	O3-C6-C5	2.34	122.03	115.31
5	В	806	VXZ	O3-C6-C5	2.34	122.03	115.31
5	В	811	VXZ	O3-C6-C5	2.33	122.02	115.31
5	С	507	VXZ	O3-C6-C5	2.33	122.02	115.31
5	А	810	VXZ	O3-C6-C5	2.33	122.02	115.31
5	В	810	VXZ	O3-C6-C5	2.33	122.02	115.31
5	D	506	VXZ	O3-C6-C5	2.33	122.01	115.31
5	А	808	VXZ	O3-C6-C5	2.32	122.00	115.31
5	А	807	VXZ	O3-C6-C5	2.32	121.97	115.31
5	А	811	VXZ	O3-C6-C5	2.30	121.94	115.31

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	804	GOL	C1-C2-C3-O3
4	А	806	GOL	O1-C1-C2-C3
4	С	505	GOL	C1-C2-C3-O3
4	D	505	GOL	O1-C1-C2-C3
4	D	505	GOL	C1-C2-C3-O3
4	А	804	GOL	O2-C2-C3-O3



Mol	Chain	Res	Type	Atoms
4	D	505	GOL	O2-C2-C3-O3
4	А	804	GOL	O1-C1-C2-C3
4	В	804	GOL	O1-C1-C2-C3
4	А	806	GOL	O1-C1-C2-O2
4	С	505	GOL	O2-C2-C3-O3
4	D	505	GOL	O1-C1-C2-O2
4	В	804	GOL	O1-C1-C2-O2
4	А	805	GOL	O2-C2-C3-O3
4	А	804	GOL	O1-C1-C2-O2
5	В	810	VXZ	C-C5-C6-O4
5	В	810	VXZ	C-C5-C6-O3
5	В	810	VXZ	C4-C5-C6-O4
5	В	810	VXZ	C4-C5-C6-O3
5	D	506	VXZ	C-C5-C6-O3
5	D	506	VXZ	C-C5-C6-O4
4	А	805	GOL	C1-C2-C3-O3

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There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	А	807	VXZ	1	0
4	А	804	GOL	2	0
4	С	505	GOL	1	0
5	В	812	VXZ	1	0
5	С	507	VXZ	1	0
5	D	507	VXZ	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 sufficient must be 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	723/736~(98%)	0.58	18 (2%) 57 58	35, 54, 90, 152	0
1	В	726/736~(98%)	0.53	13 (1%) 68 69	35, 51, 83, 137	0
2	С	402/403~(99%)	0.60	15 (3%) 41 42	35, 47, 80, 116	0
2	D	402/403~(99%)	0.68	21 (5%) 27 28	33, 48, 86, 150	0
All	All	2253/2278~(98%)	0.58	67 (2%) 50 51	33, 51, 87, 152	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	294	ALA	8.3
1	А	575	GLY	7.0
1	А	576	GLY	6.8
2	D	297	VAL	6.8
1	В	577	THR	6.7
2	D	296	PRO	6.6
2	D	301	THR	6.4
2	С	225	PHE	6.3
2	С	300	LEU	5.2
2	D	300	LEU	5.2
2	С	297	VAL	5.1
1	В	575	GLY	5.0
2	D	298	ILE	4.7
1	А	2	PRO	4.5
2	D	390	ILE	4.4
2	С	390	ILE	4.4
1	А	571	VAL	4.0
1	А	577	THR	3.9
1	А	720	SER	3.8
2	С	294	ALA	3.8
1	В	1	MET	3.8



80	QP
00	ωı

Mal	Chain	Rog	Type	BSB7
0		122		37
	B D	576	CIV	3.6
1	D	202	CIV	3.0
2 0		290 200		0.0 2.6
2	C	298	ILE CIV	3.0 2.5
		293		3.0
2	D	130	LEU	3.4
2	D	391	GLY	3.4
1	A	579	GLN	3.3
1	A	574	ALA	3.1
1	B	578	TYR	3.1
2	D	225	PHE	3.1
2	D	228	LEU	3.0
1	В	568	ARG	2.9
2	С	226	GLU	2.9
2	D	231	LEU	2.8
1	В	689	PRO	2.7
2	С	227	GLY	2.7
1	В	720	SER	2.6
2	D	227	GLY	2.6
2	С	228	LEU	2.6
2	С	134	MET	2.6
2	С	299	MET	2.5
2	D	295	ASP	2.5
2	D	299	MET	2.5
1	А	426	ILE	2.5
1	В	571	VAL	2.5
1	В	692	THR	2.5
1	А	578	TYR	2.4
1	В	377	GLU	2.4
2	D	229	ALA	2.4
1	А	450	THR	2.4
1	В	569	LYS	2.3
2	D	276	LYS	2.3
2	С	295	ASP	2.3
1	A	325	ILE	2.3
1	В	2	PRO	2.3
1	A	442	THR	2.3
2	С	296	PRO	2.2
1	Ā	-9	HIS	2.2
1	A	436	LEU	2.1
1	A	423	PHE	2.1
2	D	393	GLY	2.1
$ \begin{array}{r} 1 \\ 1 \\ 2 \\ 1 \\ 2 \\ 2 \\ 1 \\ 1 \\ 2 \\ 1 \\ 1 \\ 1 \\ 2 \\ 1 \\ 1 \\ 2 \\ 1 \\ 1 \\ 2 \\ 1 \\ 2 \\ 1 \\ 1 \\ 1 \\ 2 \\ 1 \\ 1 \\ 2 \\ 1 \\ $	A B D A B C A B A C A A A A D	$578 \\ 377 \\ 229 \\ 450 \\ 569 \\ 276 \\ 295 \\ 325 \\ 2 \\ 442 \\ 296 \\ -9 \\ 436 \\ 423 \\ 393 $	TYR GLU ALA THR LYS LYS ASP ILE PRO THR PRO HIS LEU PHE GLY	$\begin{array}{r} 2.4 \\ \hline 2.4 \\ \hline 2.4 \\ \hline 2.3 \\ \hline 2.2 \\ \hline 2.2 \\ \hline 2.1 \\ \hline 2.1 \\ \hline 2.1 \end{array}$



Continued from previous page...

Mol	Chain	\mathbf{Res}	Type	RSRZ
2	D	2	SER	2.1
1	А	412	VAL	2.1
2	С	301	THR	2.1
1	А	367	TYR	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, 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
3	SO4	А	802	5/5	0.73	0.18	60,82,100,101	5
5	VXZ	А	811	14/14	0.78	0.24	78,92,130,146	0
4	GOL	В	804	6/6	0.79	0.25	84,86,97,101	0
5	VXZ	А	810	14/14	0.80	0.26	100,112,131,140	0
4	GOL	D	505	6/6	0.81	0.13	$58,\!64,\!74,\!77$	0
5	VXZ	А	812	14/14	0.81	0.23	85,102,125,142	0
4	GOL	С	505	6/6	0.82	0.16	50,65,74,78	0
3	SO4	В	803	5/5	0.83	0.18	55,59,85,87	5
5	VXZ	В	808	14/14	0.83	0.21	67,90,124,145	0
5	VXZ	В	809	14/14	0.83	0.27	97,109,147,148	0
3	SO4	С	501	5/5	0.84	0.16	103,107,123,132	0
4	GOL	D	504	6/6	0.85	0.13	69,73,78,78	0
5	VXZ	В	810	14/14	0.86	0.27	97,103,127,136	0
3	SO4	В	814	5/5	0.88	0.17	$68,\!87,\!102,\!120$	0
3	SO4	С	503	5/5	0.88	0.14	91,92,101,135	0
5	VXZ	В	811	14/14	0.88	0.20	75,88,104,107	0
5	VXZ	D	508	14/14	0.88	0.17	67,79,96,103	0
5	VXZ	С	507	14/14	0.90	0.18	$60,\!70,\!110,\!117$	0
4	GOL	A	806	6/6	0.90	0.22	$7\overline{4,77,83,92}$	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	А	805	6/6	0.91	0.12	46,49,54,59	0
3	SO4	В	801	5/5	0.91	0.20	57,66,83,85	0
3	SO4	С	504	5/5	0.91	0.13	86,95,103,107	0
5	VXZ	D	509	14/14	0.91	0.26	82,94,99,105	14
3	SO4	А	815	5/5	0.92	0.16	74,77,110,137	0
4	GOL	В	805	6/6	0.92	0.16	42,50,59,64	0
4	GOL	А	804	6/6	0.92	0.18	53,60,71,80	0
5	VXZ	В	812	14/14	0.93	0.21	57,76,88,90	0
3	SO4	D	502	5/5	0.93	0.15	77,88,110,117	0
5	VXZ	D	507	14/14	0.94	0.20	68,80,112,117	0
3	SO4	А	814	5/5	0.94	0.18	78,86,102,104	0
3	SO4	В	813	5/5	0.94	0.15	82,83,94,104	0
5	VXZ	А	807	14/14	0.95	0.18	57,74,86,86	0
5	VXZ	А	813	14/14	0.95	0.20	65,81,87,94	0
5	VXZ	С	506	14/14	0.95	0.21	72,82,92,93	0
5	VXZ	В	807	14/14	0.95	0.17	58,76,86,87	0
5	VXZ	D	506	14/14	0.95	0.22	72,84,92,95	0
5	VXZ	А	809	14/14	0.95	0.14	48,64,74,84	0
3	SO4	А	801	5/5	0.95	0.15	57,69,80,88	0
3	SO4	А	803	5/5	0.95	0.14	77,93,100,104	0
3	SO4	D	501	5/5	0.97	0.13	74,80,89,93	0
3	SO4	В	802	5/5	0.97	0.18	78,84,90,98	0
5	VXZ	В	806	14/14	0.97	0.14	58,66,75,78	0
3	SO4	D	503	5/5	0.98	0.14	67,71,79,82	0
3	SO4	С	502	5/5	0.98	0.11	67,70,78,79	0
5	VXZ	A	808	14/14	0.98	0.14	50,55,64,66	0

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.

