



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2017 – 05:35 PM EDT

PDB ID : 4ZXF  
Title : Crystal Structure of a Soluble Variant of Monoglyceride Lipase from *Saccharomyces Cerevisiae* in Complex with a Substrate Analog  
Authors : Aschauer, P.; Lichtenegger, J.; Rengachari, S.; Gruber, K.; Oberer, M.  
Deposited on : unknown  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

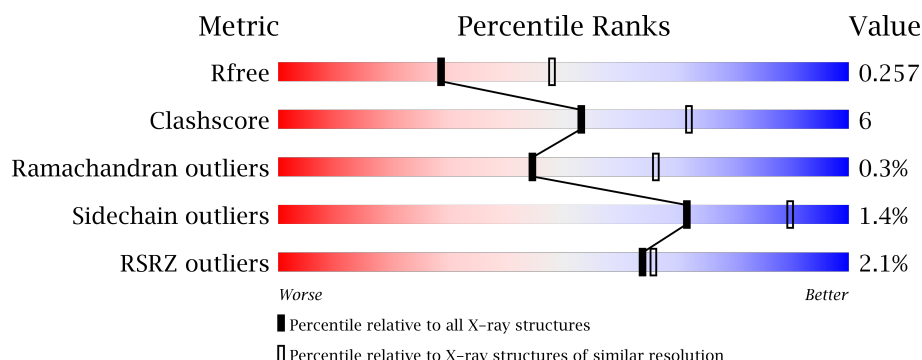
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	340	<div> <div>81%</div> <div>9%</div> <div>9%</div> </div>
1	B	340	<div> <div>7%</div> <div>77%</div> <div>12%</div> <div>10%</div> </div>
1	C	340	<div> <div>79%</div> <div>11%</div> <div>10%</div> </div>
1	D	340	<div> <div>7%</div> <div>66%</div> <div>18%</div> <div>14%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	4S7	C	500	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9958 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 Monoglyceride lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2469	1581	424	451	13			
1	B	307	Total	C	N	O	S	0	0	0
			2462	1578	422	448	14			
1	C	307	Total	C	N	O	S	0	0	0
			2463	1578	423	448	14			
1	D	293	Total	C	N	O	S	0	1	0
			2368	1520	407	429	12			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	initiating methionine	UNP P28321
A	-25	SER	-	expression tag	UNP P28321
A	-24	TYR	-	expression tag	UNP P28321
A	-23	TYR	-	expression tag	UNP P28321
A	-22	HIS	-	expression tag	UNP P28321
A	-21	HIS	-	expression tag	UNP P28321
A	-20	HIS	-	expression tag	UNP P28321
A	-19	HIS	-	expression tag	UNP P28321
A	-18	HIS	-	expression tag	UNP P28321
A	-17	HIS	-	expression tag	UNP P28321
A	-16	ASP	-	expression tag	UNP P28321
A	-15	TYR	-	expression tag	UNP P28321
A	-14	ASP	-	expression tag	UNP P28321
A	-13	ILE	-	expression tag	UNP P28321
A	-12	PRO	-	expression tag	UNP P28321
A	-11	THR	-	expression tag	UNP P28321
A	-10	THR	-	expression tag	UNP P28321
A	-9	GLU	-	expression tag	UNP P28321
A	-8	ASN	-	expression tag	UNP P28321
A	-7	LEU	-	expression tag	UNP P28321
A	-6	TYR	-	expression tag	UNP P28321

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	PHE	-	expression tag	UNP P28321
A	-4	GLN	-	expression tag	UNP P28321
A	-3	GLY	-	expression tag	UNP P28321
A	-2	ALA	-	expression tag	UNP P28321
A	-1	MET	-	expression tag	UNP P28321
A	0	GLY	-	expression tag	UNP P28321
A	175	SER	LEU	engineered mutation	UNP P28321
A	264	ARG	GLN	engineered mutation	UNP P28321
B	-26	MET	-	initiating methionine	UNP P28321
B	-25	SER	-	expression tag	UNP P28321
B	-24	TYR	-	expression tag	UNP P28321
B	-23	TYR	-	expression tag	UNP P28321
B	-22	HIS	-	expression tag	UNP P28321
B	-21	HIS	-	expression tag	UNP P28321
B	-20	HIS	-	expression tag	UNP P28321
B	-19	HIS	-	expression tag	UNP P28321
B	-18	HIS	-	expression tag	UNP P28321
B	-17	HIS	-	expression tag	UNP P28321
B	-16	ASP	-	expression tag	UNP P28321
B	-15	TYR	-	expression tag	UNP P28321
B	-14	ASP	-	expression tag	UNP P28321
B	-13	ILE	-	expression tag	UNP P28321
B	-12	PRO	-	expression tag	UNP P28321
B	-11	THR	-	expression tag	UNP P28321
B	-10	THR	-	expression tag	UNP P28321
B	-9	GLU	-	expression tag	UNP P28321
B	-8	ASN	-	expression tag	UNP P28321
B	-7	LEU	-	expression tag	UNP P28321
B	-6	TYR	-	expression tag	UNP P28321
B	-5	PHE	-	expression tag	UNP P28321
B	-4	GLN	-	expression tag	UNP P28321
B	-3	GLY	-	expression tag	UNP P28321
B	-2	ALA	-	expression tag	UNP P28321
B	-1	MET	-	expression tag	UNP P28321
B	0	GLY	-	expression tag	UNP P28321
B	175	SER	LEU	engineered mutation	UNP P28321
B	264	ARG	GLN	engineered mutation	UNP P28321
C	-26	MET	-	initiating methionine	UNP P28321
C	-25	SER	-	expression tag	UNP P28321
C	-24	TYR	-	expression tag	UNP P28321
C	-23	TYR	-	expression tag	UNP P28321
C	-22	HIS	-	expression tag	UNP P28321

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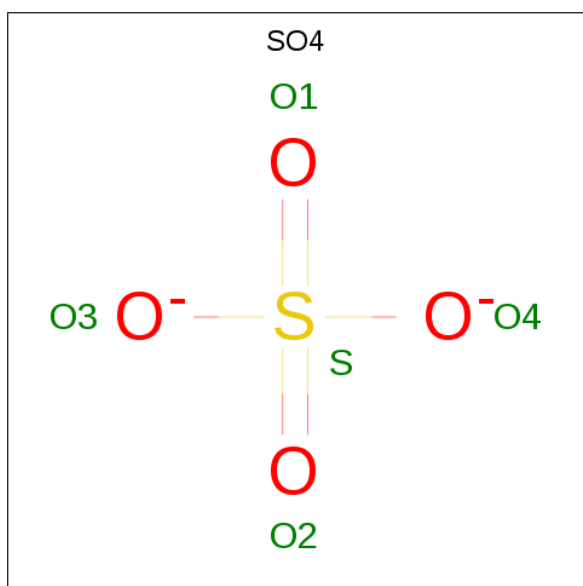
Chain	Residue	Modelled	Actual	Comment	Reference
C	-21	HIS	-	expression tag	UNP P28321
C	-20	HIS	-	expression tag	UNP P28321
C	-19	HIS	-	expression tag	UNP P28321
C	-18	HIS	-	expression tag	UNP P28321
C	-17	HIS	-	expression tag	UNP P28321
C	-16	ASP	-	expression tag	UNP P28321
C	-15	TYR	-	expression tag	UNP P28321
C	-14	ASP	-	expression tag	UNP P28321
C	-13	ILE	-	expression tag	UNP P28321
C	-12	PRO	-	expression tag	UNP P28321
C	-11	THR	-	expression tag	UNP P28321
C	-10	THR	-	expression tag	UNP P28321
C	-9	GLU	-	expression tag	UNP P28321
C	-8	ASN	-	expression tag	UNP P28321
C	-7	LEU	-	expression tag	UNP P28321
C	-6	TYR	-	expression tag	UNP P28321
C	-5	PHE	-	expression tag	UNP P28321
C	-4	GLN	-	expression tag	UNP P28321
C	-3	GLY	-	expression tag	UNP P28321
C	-2	ALA	-	expression tag	UNP P28321
C	-1	MET	-	expression tag	UNP P28321
C	0	GLY	-	expression tag	UNP P28321
C	175	SER	LEU	engineered mutation	UNP P28321
C	264	ARG	GLN	engineered mutation	UNP P28321
D	-26	MET	-	initiating methionine	UNP P28321
D	-25	SER	-	expression tag	UNP P28321
D	-24	TYR	-	expression tag	UNP P28321
D	-23	TYR	-	expression tag	UNP P28321
D	-22	HIS	-	expression tag	UNP P28321
D	-21	HIS	-	expression tag	UNP P28321
D	-20	HIS	-	expression tag	UNP P28321
D	-19	HIS	-	expression tag	UNP P28321
D	-18	HIS	-	expression tag	UNP P28321
D	-17	HIS	-	expression tag	UNP P28321
D	-16	ASP	-	expression tag	UNP P28321
D	-15	TYR	-	expression tag	UNP P28321
D	-14	ASP	-	expression tag	UNP P28321
D	-13	ILE	-	expression tag	UNP P28321
D	-12	PRO	-	expression tag	UNP P28321
D	-11	THR	-	expression tag	UNP P28321
D	-10	THR	-	expression tag	UNP P28321
D	-9	GLU	-	expression tag	UNP P28321

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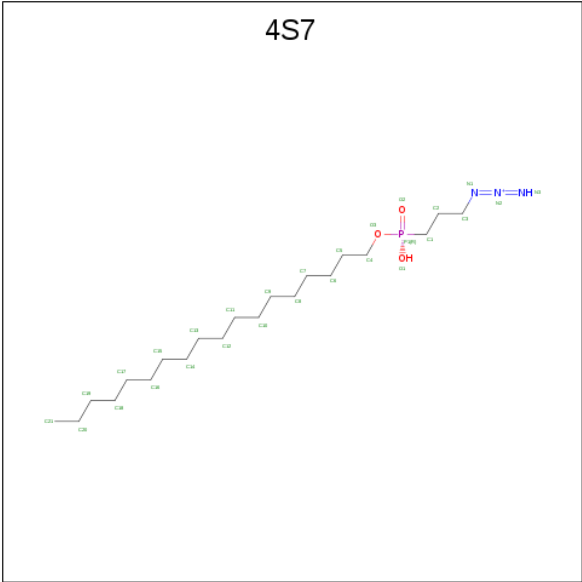
Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	ASN	-	expression tag	UNP P28321
D	-7	LEU	-	expression tag	UNP P28321
D	-6	TYR	-	expression tag	UNP P28321
D	-5	PHE	-	expression tag	UNP P28321
D	-4	GLN	-	expression tag	UNP P28321
D	-3	GLY	-	expression tag	UNP P28321
D	-2	ALA	-	expression tag	UNP P28321
D	-1	MET	-	expression tag	UNP P28321
D	0	GLY	-	expression tag	UNP P28321
D	175	SER	LEU	engineered mutation	UNP P28321
D	264	ARG	GLN	engineered mutation	UNP P28321

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



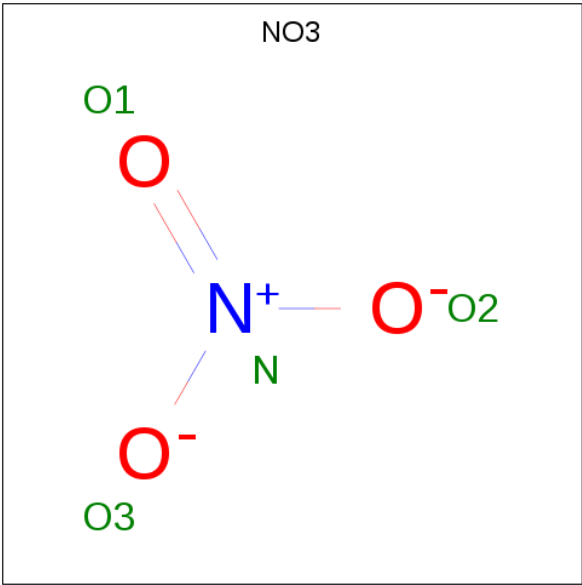
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1-{3-[(R)-hydroxy(octadecyloxy)phosphoryl]propyl} triaza-1,2-dien-2-ium (three-letter code: 4S7) (formula: C<sub>21</sub>H<sub>45</sub>N<sub>3</sub>O<sub>3</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			27	21	3	2	1		

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



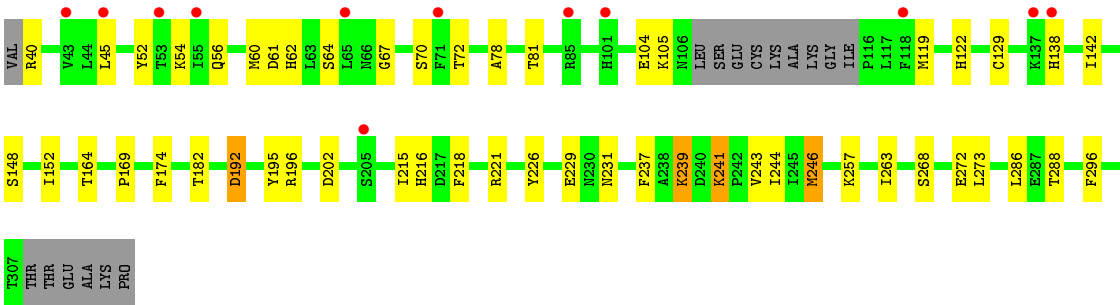
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	N	O	0	0
			4	1	3		
4	D	1	Total	N	O	0	0
			4	1	3		

- Molecule 5 is water.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	54	Total 54	O 54	0	0
5	B	45	Total 45	O 45	0	0
5	C	28	Total 28	O 28	0	0
5	D	24	Total 24	O 24	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.76Å 107.13Å 165.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.48 – 2.50 69.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (65.48-2.50) 99.5 (69.63-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.201 , 0.257 0.201 , 0.257	Depositor DCC
$R_{free}$ test set	2409 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.8	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9958	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4S7, SO4, NO3

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	0.23	0/2537	0.42	0/3425
1	B	0.24	0/2529	0.42	0/3411
1	C	0.25	0/2531	0.43	0/3415
1	D	0.30	0/2437	0.51	2/3285 (0.1%)
All	All	0.26	0/10034	0.45	2/13536 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	12	VAL	C-N-CD	6.61	142.28	128.40
1	D	14	GLU	N-CA-C	-6.49	93.47	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	12	VAL	Peptide

## 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	2469	0	2413	19	0
1	B	2462	0	2411	27	0
1	C	2463	0	2411	31	0
1	D	2368	0	2309	47	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	C	27	0	0	7	0
4	D	8	0	0	1	0
5	A	54	0	0	0	0
5	B	45	0	0	1	0
5	C	28	0	0	0	0
5	D	24	0	0	1	0
All	All	9958	0	9544	119	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:THR:HB	1:D:33:GLN:OE1	1.28	1.31
1:D:10:THR:CB	1:D:33:GLN:OE1	2.19	0.91
1:D:237:PHE:HZ	1:D:243:VAL:HG11	1.44	0.81
1:D:11:THR:OG1	1:D:33:GLN:NE2	2.19	0.76
1:B:92:GLU:OE1	1:B:221:ARG:NH1	2.23	0.71
1:C:184:LEU:HD21	3:C:500:4S7:N3	2.05	0.71
1:C:123:SER:OG	3:C:500:4S7:P1	2.50	0.69
1:D:40:ARG:N	1:D:67:GLY:O	2.28	0.67
1:D:263:ILE:HG13	1:D:273:LEU:HB2	1.76	0.67
1:C:124:MET:HB2	3:C:500:4S7:O2	1.95	0.66
1:C:246:MET:HB2	1:C:276:TYR:HE2	1.60	0.66
1:D:237:PHE:CZ	1:D:243:VAL:HG11	2.30	0.66
1:D:52:TYR:CE2	1:D:54:LYS:HB3	2.32	0.65
1:A:177:ARG:HB2	1:A:177:ARG:HH11	1.62	0.64
1:A:305:LYS:O	1:C:235:LYS:NZ	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:THR:HG22	1:B:310:GLU:H	1.65	0.62
1:D:142:ILE:O	1:D:241:LYS:NZ	2.33	0.61
1:C:124:MET:CB	3:C:500:4S7:O2	2.50	0.60
1:D:6:TYR:OH	1:D:61:ASP:OD2	2.18	0.58
1:D:12:VAL:HB	1:D:13:PRO:HD3	1.85	0.57
1:C:123:SER:CB	3:C:500:4S7:P1	2.92	0.57
1:B:263:ILE:HG13	1:B:273:LEU:HB2	1.86	0.57
1:B:171:LEU:HD13	1:D:164:THR:HG22	1.87	0.56
1:C:32:VAL:HG12	1:C:34:ASN:OD1	2.06	0.55
1:A:167:ILE:HA	1:A:170:LEU:HD12	1.89	0.55
1:C:123:SER:HB3	3:C:500:4S7:P1	2.47	0.55
1:B:270:ASP:OD2	1:B:306:HIS:NE2	2.28	0.55
1:A:196:ARG:NH2	2:A:401:SO4:O4	2.32	0.54
1:A:18:GLU:OE2	1:A:101:HIS:NE2	2.38	0.54
1:D:10:THR:OG1	1:D:61:ASP:OD1	2.19	0.54
1:D:237:PHE:HE2	1:D:268:SER:HB2	1.73	0.54
1:D:27:TYR:CE1	1:D:105:LYS:HE2	2.43	0.54
1:D:52:TYR:HE2	1:D:54:LYS:HB3	1.70	0.54
1:C:138:HIS:ND1	1:C:141:GLU:OE1	2.36	0.53
1:C:208:LEU:HD13	3:C:500:4S7:N3	2.24	0.53
1:B:32:VAL:HG23	1:B:69:GLU:HG3	1.91	0.53
1:B:42:ARG:HH12	1:B:109:GLU:HB2	1.74	0.53
1:B:178:VAL:HG22	1:D:182:THR:HA	1.92	0.52
1:C:34:ASN:OD1	1:C:34:ASN:N	2.42	0.52
1:D:14:GLU:HB2	1:D:29:PHE:H	1.75	0.52
1:C:62:HIS:O	1:C:66:ASN:ND2	2.36	0.51
1:B:32:VAL:HG12	1:B:34:ASN:HB2	1.92	0.51
1:C:257:LYS:HE3	1:D:257:LYS:HZ2	1.75	0.51
1:D:104:GLU:OE1	1:D:138:HIS:NE2	2.43	0.51
1:D:20:PHE:O	1:D:22:GLY:N	2.43	0.51
1:C:162:LYS:NZ	1:C:165:GLN:HG3	2.25	0.51
1:D:237:PHE:HZ	1:D:243:VAL:CG1	2.18	0.51
1:C:1:MET:HB2	1:C:201:SER:HB3	1.93	0.51
1:B:18:GLU:OE1	1:B:105:LYS:HE3	2.10	0.51
1:D:195:TYR:HB3	1:D:286:LEU:HD12	1.93	0.51
1:D:215:ILE:HA	1:D:218:PHE:CE2	2.46	0.50
1:A:169:PRO:HG3	1:A:215:ILE:HG22	1.94	0.50
1:B:62:HIS:HB3	1:B:296:PHE:CZ	2.47	0.49
1:C:66:ASN:HB3	1:C:300:LYS:HE3	1.93	0.49
1:D:237:PHE:CE2	1:D:268:SER:HB2	2.48	0.49
1:A:62:HIS:HB3	1:A:296:PHE:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:ILE:HG13	1:C:273:LEU:HB2	1.94	0.49
1:C:184:LEU:HD22	1:C:189:ILE:HD11	1.94	0.48
1:B:231:ASN:HB2	1:B:235:LYS:HE3	1.95	0.48
1:D:196:ARG:NH2	4:D:402:NO3:O2	2.44	0.47
1:B:166:ILE:O	1:B:170:LEU:HG	2.14	0.47
1:D:13:PRO:HB3	1:D:30:TRP:CE3	2.50	0.47
1:B:257:LYS:NZ	5:B:507:HOH:O	2.47	0.47
1:B:207:PRO:HG2	1:B:209:TYR:CE2	2.49	0.47
1:A:245:ILE:HG21	1:A:259:SER:HB3	1.97	0.46
1:A:202:ASP:HB3	1:A:205:SER:HB2	1.96	0.46
1:A:158:THR:OG1	1:A:253:ILE:HA	2.15	0.46
1:A:302:TRP:O	1:A:306:HIS:ND1	2.47	0.46
1:C:215:ILE:HA	1:C:218:PHE:CE2	2.51	0.46
1:B:242:PRO:HA	1:B:270:ASP:O	2.16	0.46
1:C:91:ASP:HB3	1:C:213:ARG:HG2	1.98	0.45
1:A:215:ILE:HA	1:A:218:PHE:CE2	2.51	0.45
1:A:54:LYS:HA	1:A:57:PHE:CD1	2.52	0.45
1:D:244:ILE:HG23	1:D:246:MET:HE1	1.97	0.45
1:A:177:ARG:HB2	1:A:177:ARG:NH1	2.30	0.45
1:D:56:GLN:O	1:D:60:MET:HG3	2.16	0.45
1:D:62:HIS:HB3	1:D:296:PHE:CE2	2.51	0.45
1:A:179:ARG:HA	1:A:211:SER:HA	1.99	0.45
1:D:192:ASP:HB3	1:D:288:THR:HG22	1.99	0.44
1:D:218:PHE:HA	1:D:221:ARG:HG2	1.99	0.44
1:B:218:PHE:HA	1:B:221:ARG:HG2	1.99	0.44
1:C:162:LYS:HZ1	1:C:165:GLN:HG3	1.82	0.44
1:D:52:TYR:OH	1:D:202:ASP:OD2	2.36	0.44
1:B:18:GLU:OE2	1:B:101:HIS:NE2	2.39	0.44
1:C:2:ALA:HB3	1:C:198:PHE:HA	2.00	0.44
1:D:152:ILE:HG22	1:D:226:TYR:HB2	2.00	0.44
1:A:169:PRO:HB3	1:A:216:HIS:HA	2.00	0.44
1:C:17:TYR:HD2	1:C:24:LYS:HG2	1.83	0.43
1:C:270:ASP:OD2	1:C:306:HIS:NE2	2.33	0.43
1:D:18:GLU:HG2	1:D:19:ASN:H	1.82	0.43
1:A:176:PRO:HD2	1:A:177:ARG:NH2	2.33	0.43
1:D:122:HIS:HA	1:D:148:SER:HB3	2.00	0.43
1:D:239:LYS:HD2	1:D:239:LYS:HA	1.70	0.43
1:D:45:LEU:HB2	1:D:72:THR:HB	1.99	0.43
1:D:12:VAL:CB	1:D:13:PRO:HD3	2.49	0.43
1:A:152:ILE:HG22	1:A:226:TYR:HB2	2.01	0.43
1:C:224:LYS:HB3	1:C:224:LYS:HE2	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:LEU:H	1:C:208:LEU:HD23	1.84	0.42
1:C:257:LYS:HE3	1:D:257:LYS:NZ	2.33	0.42
1:D:30:TRP:CD1	1:D:64:SER:HB2	2.55	0.42
1:B:215:ILE:HA	1:B:218:PHE:CE2	2.54	0.42
1:D:231:ASN:OD1	5:D:501:HOH:O	2.21	0.42
1:B:1:MET:HB2	1:B:201:SER:HB3	2.01	0.42
1:D:169:PRO:HA	1:D:216:HIS:HB2	2.01	0.42
1:C:184:LEU:HG	1:C:208:LEU:HD22	2.02	0.42
1:B:96:PHE:O	1:B:100:GLU:HG2	2.19	0.41
1:D:78:ALA:O	1:D:81:THR:HG22	2.20	0.41
1:B:309:THR:HG22	1:B:310:GLU:N	2.33	0.41
1:B:68:TYR:CZ	1:B:303:LEU:HB3	2.55	0.41
1:D:119:MET:HG2	1:D:129:CYS:SG	2.60	0.41
1:A:109:GLU:O	1:A:113:LYS:HG2	2.20	0.41
1:B:145:TYR:HB2	1:B:243:VAL:HG13	2.03	0.41
1:D:244:ILE:HA	1:D:272:GLU:O	2.21	0.41
1:D:16:GLN:HB2	1:D:27:TYR:CE2	2.56	0.40
1:B:12:VAL:HA	1:B:13:PRO:HD3	1.90	0.40
1:B:122:HIS:CE1	1:B:282:SER:HA	2.56	0.40
1:B:242:PRO:HB2	1:B:302:TRP:CZ2	2.57	0.40
1:C:241:LYS:HA	1:C:242:PRO:HD3	1.90	0.40
1:C:96:PHE:CE2	1:C:221:ARG:HD2	2.56	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	A	306/340 (90%)	300 (98%)	6 (2%)	0	100	100
1	B	303/340 (89%)	293 (97%)	10 (3%)	0	100	100
1	C	305/340 (90%)	295 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	288/340 (85%)	266 (92%)	18 (6%)	4 (1%)	13	23
All	All	1202/1360 (88%)	1154 (96%)	44 (4%)	4 (0%)	44	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	13	PRO
1	D	21	ASP
1	D	239	LYS
1	D	12	VAL

### 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	267/295 (90%)	265 (99%)	2 (1%)	87	96
1	B	266/295 (90%)	263 (99%)	3 (1%)	78	92
1	C	266/295 (90%)	263 (99%)	3 (1%)	78	92
1	D	256/295 (87%)	249 (97%)	7 (3%)	50	77
All	All	1055/1180 (89%)	1040 (99%)	15 (1%)	71	90

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	SER
1	A	177	ARG
1	B	213	ARG
1	B	221	ARG
1	B	243	VAL
1	C	36	THR
1	C	213	ARG
1	C	289	ASP
1	D	12	VAL
1	D	70	SER

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Mol	Chain	Res	Type
1	D	174	PHE
1	D	192	ASP
1	D	229	GLU
1	D	241	LYS
1	D	246	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	33	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	A	401	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	B	401	-	4,4,4	0.16	0	6,6,6	0.05	0
3	4S7	C	500	-	22,26,27	0.44	0	20,26,29	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NO3	D	401	-	1,3,3	0.86	0	0,3,3	0.00	-
4	NO3	D	402	-	1,3,3	0.85	0	0,3,3	0.00	-

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
2	SO4	A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	B	401	-	-	0/0/0/0	0/0/0/0
3	4S7	C	500	-	-	0/21/25/27	0/0/0/0
4	NO3	D	401	-	-	0/0/0/0	0/0/0/0
4	NO3	D	402	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SO4	1	0
3	C	500	4S7	7	0
4	D	402	NO3	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	308/340 (90%)	-0.26	0 100 100	24, 34, 48, 79	0
1	B	307/340 (90%)	-0.16	2 (0%) 87 88	27, 40, 58, 79	0
1	C	307/340 (90%)	-0.15	1 (0%) 93 94	27, 44, 63, 82	0
1	D	293/340 (86%)	0.44	23 (7%) 14 14	26, 58, 81, 90	0
All	All	1215/1360 (89%)	-0.04	26 (2%) 64 66	24, 41, 72, 90	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	26	GLY	9.3
1	D	43	VAL	4.6
1	D	137	LYS	4.5
1	D	28	MET	3.8
1	D	12	VAL	3.6
1	D	101	HIS	3.3
1	D	118	PHE	3.1
1	C	38	GLU	3.0
1	D	138	HIS	2.8
1	D	65	LEU	2.8
1	D	27	TYR	2.7
1	D	5	PRO	2.6
1	B	166	ILE	2.5
1	D	15	LEU	2.5
1	D	9	GLN	2.5
1	D	53	THR	2.5
1	D	11	THR	2.5
1	D	85	ARG	2.4
1	D	55	ILE	2.4
1	B	112	ALA	2.3
1	D	205	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	29	PHE	2.2
1	D	17	TYR	2.2
1	D	18	GLU	2.1
1	D	45	LEU	2.1
1	D	71	PHE	2.1

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	4S7	C	500	27/28	0.76	0.27	4.62	26,40,56,58	27
4	NO3	D	401	4/4	0.90	0.10	-2.67	45,46,60,65	0
4	NO3	D	402	4/4	0.90	0.14	-	68,71,72,73	0
2	SO4	B	401	5/5	0.95	0.11	-	72,75,80,87	0
2	SO4	A	401	5/5	0.96	0.10	-	62,63,70,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.