



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:18 am GMT

PDB ID : 4E3R  
Title : PLP-bound aminotransferase mutant crystal structure from *Vibrio fluvialis*  
Authors : Midelfort, K.S.; Kumar, R.; Han, S.; Karmilowicz, M.J.; McConnell, K.; Gehlhaar, D.K.; Mistry, A.; Chang, J.S.; Anderson, M.; Vilalobos, A.; Minshull, J.; Govindarajan, S.; Wong, J.W.  
Deposited on : 2012-03-10  
Resolution : 1.90 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	:	trunk28620
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)	:	recalc28949

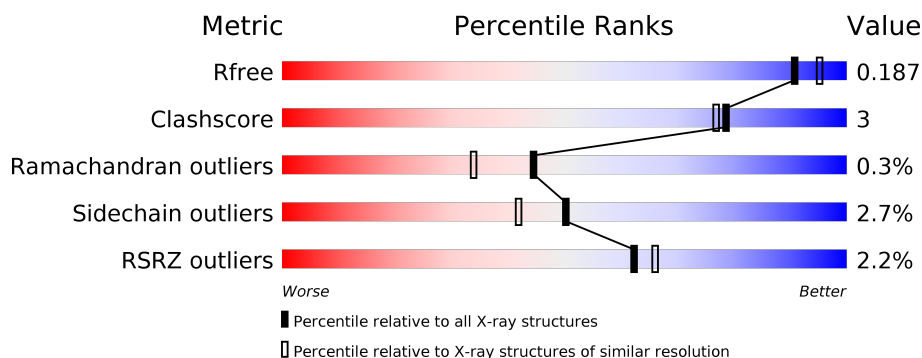
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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 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	473	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>•</div> </div> </div>
1	B	473	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>• •</div> </div> </div>
1	C	473	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>5%</div> </div> </div>
1	D	473	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>5%</div> </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
2	SO4	A	501	-	-	X	X
2	SO4	B	501	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15618 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 Pyruvate transaminase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	P	S	0	0	0
			3528	2257	594	656	1	20			
1	B	452	Total	C	N	O	P	S	0	0	0
			3528	2257	594	656	1	20			
1	C	451	Total	C	N	O	P	S	0	0	0
			3523	2254	593	655	1	20			
1	D	451	Total	C	N	O	P	S	0	0	0
			3523	2254	593	655	1	20			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP F2XBU9
A	-18	GLY	-	EXPRESSION TAG	UNP F2XBU9
A	-17	SER	-	EXPRESSION TAG	UNP F2XBU9
A	-16	SER	-	EXPRESSION TAG	UNP F2XBU9
A	-15	HIS	-	EXPRESSION TAG	UNP F2XBU9
A	-14	HIS	-	EXPRESSION TAG	UNP F2XBU9
A	-13	HIS	-	EXPRESSION TAG	UNP F2XBU9
A	-12	HIS	-	EXPRESSION TAG	UNP F2XBU9
A	-11	HIS	-	EXPRESSION TAG	UNP F2XBU9
A	-10	HIS	-	EXPRESSION TAG	UNP F2XBU9
A	-9	SER	-	EXPRESSION TAG	UNP F2XBU9
A	-8	SER	-	EXPRESSION TAG	UNP F2XBU9
A	-7	GLY	-	EXPRESSION TAG	UNP F2XBU9
A	-6	LEU	-	EXPRESSION TAG	UNP F2XBU9
A	-5	VAL	-	EXPRESSION TAG	UNP F2XBU9
A	-4	PRO	-	EXPRESSION TAG	UNP F2XBU9
A	-3	ARG	-	EXPRESSION TAG	UNP F2XBU9
A	-2	GLY	-	EXPRESSION TAG	UNP F2XBU9
A	-1	SER	-	EXPRESSION TAG	UNP F2XBU9
A	0	HIS	-	EXPRESSION TAG	UNP F2XBU9
A	19	TRP	PHE	ENGINEERED MUTATION	UNP F2XBU9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	57	PHE	TRP	ENGINEERED MUTATION	UNP F2XBU9
A	85	ALA	PHE	ENGINEERED MUTATION	UNP F2XBU9
A	88	LYS	ARG	ENGINEERED MUTATION	UNP F2XBU9
A	153	ALA	VAL	ENGINEERED MUTATION	UNP F2XBU9
A	163	PHE	LYS	ENGINEERED MUTATION	UNP F2XBU9
A	259	VAL	ILE	ENGINEERED MUTATION	UNP F2XBU9
A	415	PHE	ARG	ENGINEERED MUTATION	UNP F2XBU9
B	-19	MET	-	EXPRESSION TAG	UNP F2XBU9
B	-18	GLY	-	EXPRESSION TAG	UNP F2XBU9
B	-17	SER	-	EXPRESSION TAG	UNP F2XBU9
B	-16	SER	-	EXPRESSION TAG	UNP F2XBU9
B	-15	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	-14	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	-13	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	-12	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	-11	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	-10	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	-9	SER	-	EXPRESSION TAG	UNP F2XBU9
B	-8	SER	-	EXPRESSION TAG	UNP F2XBU9
B	-7	GLY	-	EXPRESSION TAG	UNP F2XBU9
B	-6	LEU	-	EXPRESSION TAG	UNP F2XBU9
B	-5	VAL	-	EXPRESSION TAG	UNP F2XBU9
B	-4	PRO	-	EXPRESSION TAG	UNP F2XBU9
B	-3	ARG	-	EXPRESSION TAG	UNP F2XBU9
B	-2	GLY	-	EXPRESSION TAG	UNP F2XBU9
B	-1	SER	-	EXPRESSION TAG	UNP F2XBU9
B	0	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	19	TRP	PHE	ENGINEERED MUTATION	UNP F2XBU9
B	57	PHE	TRP	ENGINEERED MUTATION	UNP F2XBU9
B	85	ALA	PHE	ENGINEERED MUTATION	UNP F2XBU9
B	88	LYS	ARG	ENGINEERED MUTATION	UNP F2XBU9
B	153	ALA	VAL	ENGINEERED MUTATION	UNP F2XBU9
B	163	PHE	LYS	ENGINEERED MUTATION	UNP F2XBU9
B	259	VAL	ILE	ENGINEERED MUTATION	UNP F2XBU9
B	415	PHE	ARG	ENGINEERED MUTATION	UNP F2XBU9
C	-19	MET	-	EXPRESSION TAG	UNP F2XBU9
C	-18	GLY	-	EXPRESSION TAG	UNP F2XBU9
C	-17	SER	-	EXPRESSION TAG	UNP F2XBU9
C	-16	SER	-	EXPRESSION TAG	UNP F2XBU9
C	-15	HIS	-	EXPRESSION TAG	UNP F2XBU9
C	-14	HIS	-	EXPRESSION TAG	UNP F2XBU9
C	-13	HIS	-	EXPRESSION TAG	UNP F2XBU9

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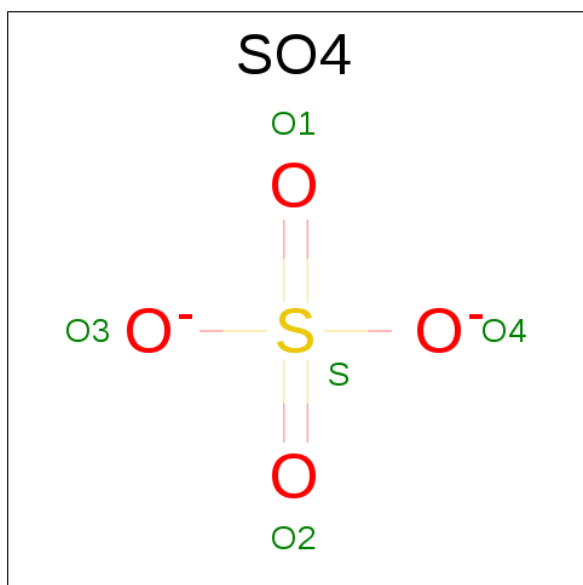
Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	EXPRESSION TAG	UNP F2XBU9
C	-11	HIS	-	EXPRESSION TAG	UNP F2XBU9
C	-10	HIS	-	EXPRESSION TAG	UNP F2XBU9
C	-9	SER	-	EXPRESSION TAG	UNP F2XBU9
C	-8	SER	-	EXPRESSION TAG	UNP F2XBU9
C	-7	GLY	-	EXPRESSION TAG	UNP F2XBU9
C	-6	LEU	-	EXPRESSION TAG	UNP F2XBU9
C	-5	VAL	-	EXPRESSION TAG	UNP F2XBU9
C	-4	PRO	-	EXPRESSION TAG	UNP F2XBU9
C	-3	ARG	-	EXPRESSION TAG	UNP F2XBU9
C	-2	GLY	-	EXPRESSION TAG	UNP F2XBU9
C	-1	SER	-	EXPRESSION TAG	UNP F2XBU9
C	0	HIS	-	EXPRESSION TAG	UNP F2XBU9
C	19	TRP	PHE	ENGINEERED MUTATION	UNP F2XBU9
C	57	PHE	TRP	ENGINEERED MUTATION	UNP F2XBU9
C	85	ALA	PHE	ENGINEERED MUTATION	UNP F2XBU9
C	88	LYS	ARG	ENGINEERED MUTATION	UNP F2XBU9
C	153	ALA	VAL	ENGINEERED MUTATION	UNP F2XBU9
C	163	PHE	LYS	ENGINEERED MUTATION	UNP F2XBU9
C	259	VAL	ILE	ENGINEERED MUTATION	UNP F2XBU9
C	415	PHE	ARG	ENGINEERED MUTATION	UNP F2XBU9
D	-19	MET	-	EXPRESSION TAG	UNP F2XBU9
D	-18	GLY	-	EXPRESSION TAG	UNP F2XBU9
D	-17	SER	-	EXPRESSION TAG	UNP F2XBU9
D	-16	SER	-	EXPRESSION TAG	UNP F2XBU9
D	-15	HIS	-	EXPRESSION TAG	UNP F2XBU9
D	-14	HIS	-	EXPRESSION TAG	UNP F2XBU9
D	-13	HIS	-	EXPRESSION TAG	UNP F2XBU9
D	-12	HIS	-	EXPRESSION TAG	UNP F2XBU9
D	-11	HIS	-	EXPRESSION TAG	UNP F2XBU9
D	-10	HIS	-	EXPRESSION TAG	UNP F2XBU9
D	-9	SER	-	EXPRESSION TAG	UNP F2XBU9
D	-8	SER	-	EXPRESSION TAG	UNP F2XBU9
D	-7	GLY	-	EXPRESSION TAG	UNP F2XBU9
D	-6	LEU	-	EXPRESSION TAG	UNP F2XBU9
D	-5	VAL	-	EXPRESSION TAG	UNP F2XBU9
D	-4	PRO	-	EXPRESSION TAG	UNP F2XBU9
D	-3	ARG	-	EXPRESSION TAG	UNP F2XBU9
D	-2	GLY	-	EXPRESSION TAG	UNP F2XBU9
D	-1	SER	-	EXPRESSION TAG	UNP F2XBU9
D	0	HIS	-	EXPRESSION TAG	UNP F2XBU9
D	19	TRP	PHE	ENGINEERED MUTATION	UNP F2XBU9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	57	PHE	TRP	ENGINEERED MUTATION	UNP F2XBU9
D	85	ALA	PHE	ENGINEERED MUTATION	UNP F2XBU9
D	88	LYS	ARG	ENGINEERED MUTATION	UNP F2XBU9
D	153	ALA	VAL	ENGINEERED MUTATION	UNP F2XBU9
D	163	PHE	LYS	ENGINEERED MUTATION	UNP F2XBU9
D	259	VAL	ILE	ENGINEERED MUTATION	UNP F2XBU9
D	415	PHE	ARG	ENGINEERED MUTATION	UNP F2XBU9

- 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		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total 1	Na 1	0	0
3	C	1	Total 1	Na 1	0	0

- Molecule 4 is water.

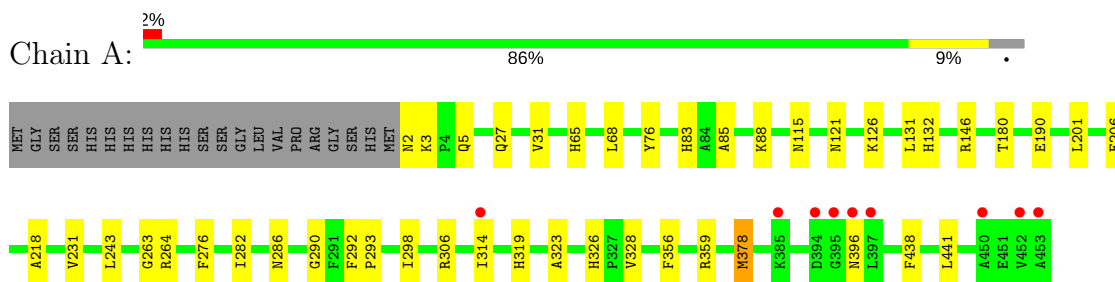
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	379	Total 379	O 379	0	0
4	B	405	Total 405	O 405	0	0
4	C	371	Total 371	O 371	0	0
4	D	342	Total 342	O 342	0	0



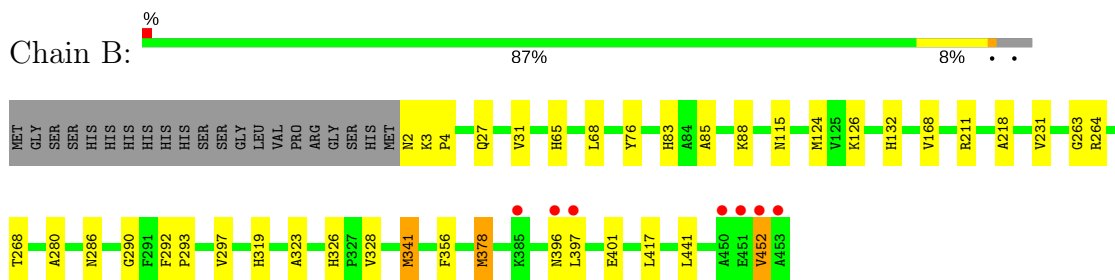
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

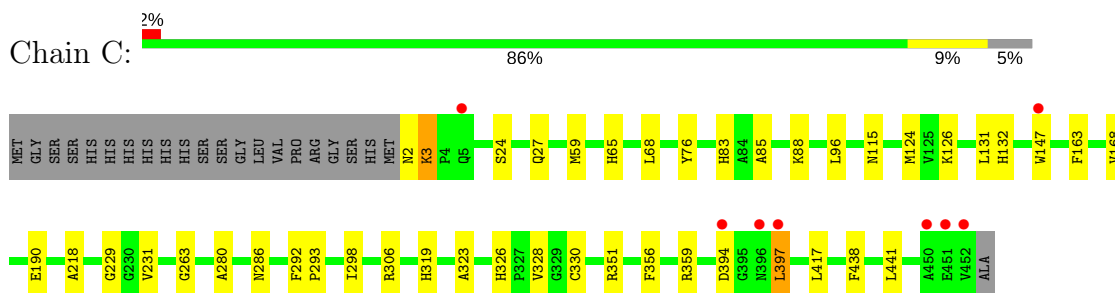
#### • Molecule 1: Pyruvate transaminase



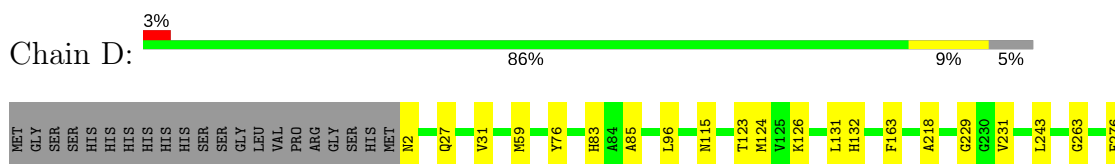
#### • Molecule 1: Pyruvate transaminase



#### • Molecule 1: Pyruvate transaminase



#### • Molecule 1: Pyruvate transaminase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.98Å 161.94Å 179.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 1.90 29.88 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.88-1.90) 98.7 (29.88-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 1.91Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
R, $R_{free}$	0.157 , 0.190 0.156 , 0.187	Depositor DCC
$R_{free}$ test set	7175 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.6	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.3	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	0.97	EDS
Total number of atoms	15618	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.74 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.7728e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: NA, LLP, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.51	1/3595 (0.0%)	0.64	2/4876 (0.0%)
1	B	0.52	2/3595 (0.1%)	0.62	1/4876 (0.0%)
1	C	0.49	1/3590 (0.0%)	0.63	2/4869 (0.0%)
1	D	0.49	0/3590	0.63	2/4869 (0.0%)
All	All	0.50	4/14370 (0.0%)	0.63	7/19490 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	298	ILE	C-N	-5.61	1.21	1.34
1	A	378	MET	SD-CE	-5.37	1.47	1.77
1	B	378	MET	SD-CE	-5.35	1.47	1.77
1	B	341	MET	SD-CE	-5.05	1.49	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	298	ILE	O-C-N	-6.74	111.91	122.70
1	D	298	ILE	O-C-N	-5.72	113.54	122.70
1	A	298	ILE	O-C-N	-5.63	113.69	122.70
1	D	263	GLY	N-CA-C	5.59	127.07	113.10
1	C	263	GLY	N-CA-C	5.35	126.47	113.10
1	B	263	GLY	N-CA-C	5.31	126.37	113.10
1	A	263	GLY	N-CA-C	5.23	126.17	113.10

There are no chirality outliers.

There are no planarity outliers.

## 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	3528	0	3432	26	0
1	B	3528	0	3432	28	0
1	C	3523	0	3426	27	0
1	D	3523	0	3427	25	0
2	A	5	0	0	2	0
2	B	5	0	0	1	0
2	D	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	379	0	0	1	0
4	B	405	0	0	1	0
4	C	371	0	0	0	0
4	D	342	0	0	2	0
All	All	15618	0	13717	93	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 (93) 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:A:83:HIS:HD2	1:A:85:ALA:H	1.30	0.79
1:D:83:HIS:HD2	1:D:85:ALA:H	1.30	0.77
1:B:4:PRO:HA	2:B:501:SO4:O4	1.83	0.77
1:A:65:HIS:HD2	1:A:68:LEU:H	1.32	0.76
1:B:83:HIS:HD2	1:B:85:ALA:H	1.34	0.75
1:C:65:HIS:HD2	1:C:68:LEU:H	1.34	0.74
1:B:65:HIS:HD2	1:B:68:LEU:H	1.36	0.72
1:C:83:HIS:HD2	1:C:85:ALA:H	1.37	0.72
1:C:115:ASN:HD21	1:C:323:ALA:HB3	1.60	0.66
1:B:124:MET:CE	1:B:297:VAL:HG13	2.26	0.66
1:C:126:LYS:NZ	1:C:319:HIS:HD2	1.95	0.65
1:B:126:LYS:NZ	1:B:319:HIS:HD2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:MET:HE2	1:B:297:VAL:HG13	1.80	0.63
1:A:5:GLN:HB3	2:A:501:SO4:O4	2.00	0.62
1:A:83:HIS:CD2	1:A:85:ALA:H	2.17	0.60
1:A:314:ILE:HD13	1:B:168:VAL:HG11	1.83	0.60
1:D:126:LYS:NZ	1:D:319:HIS:HD2	2.00	0.59
1:A:115:ASN:HD21	1:A:323:ALA:HB3	1.68	0.59
1:A:326:HIS:HD2	1:A:328:VAL:H	1.51	0.58
1:C:124:MET:HE1	1:C:280:ALA:HB1	1.86	0.57
1:D:124:MET:HE1	1:D:280:ALA:HB1	1.87	0.57
1:B:132:HIS:HE1	1:B:218:ALA:O	1.88	0.57
1:B:115:ASN:HD21	1:B:323:ALA:HB3	1.71	0.56
1:A:126:LYS:NZ	1:A:319:HIS:HD2	2.05	0.54
1:B:326:HIS:HD2	1:B:328:VAL:H	1.56	0.54
1:C:131:LEU:HD11	1:C:306:ARG:HB3	1.89	0.54
1:A:132:HIS:HD2	4:A:641:HOH:O	1.92	0.53
1:C:326:HIS:HD2	1:C:328:VAL:H	1.57	0.53
1:C:88:LYS:HG2	1:D:31:VAL:HB	1.89	0.53
1:B:132:HIS:HD2	4:B:704:HOH:O	1.91	0.53
1:C:132:HIS:HE1	1:C:218:ALA:O	1.92	0.52
1:A:180:THR:HB	1:A:201:LEU:HD22	1.93	0.51
1:C:76:TYR:CE2	1:C:328:VAL:HG11	2.46	0.51
1:D:115:ASN:HD21	1:D:323:ALA:HB3	1.75	0.51
1:B:126:LYS:HZ3	1:B:319:HIS:HD2	1.57	0.50
1:D:76:TYR:CE2	1:D:328:VAL:HG11	2.46	0.50
1:B:124:MET:HE1	1:B:280:ALA:HB1	1.94	0.49
1:B:126:LYS:NZ	1:B:319:HIS:CD2	2.78	0.49
1:C:394:ASP:HB2	1:C:397:LEU:HD22	1.95	0.49
1:D:83:HIS:CD2	1:D:85:ALA:H	2.21	0.48
1:C:168:VAL:HG11	1:D:314:ILE:HD13	1.95	0.48
1:A:264:ARG:HB3	1:A:378:MET:HE2	1.96	0.48
1:C:126:LYS:HZ3	1:C:319:HIS:HD2	1.60	0.48
1:A:290:GLY:O	1:B:326:HIS:HE1	1.98	0.47
1:C:163:PHE:HZ	1:C:229:GLY:HA2	1.78	0.47
1:D:132:HIS:HD2	4:D:620:HOH:O	1.96	0.47
1:A:132:HIS:HE1	1:A:218:ALA:O	1.96	0.47
1:A:76:TYR:CE2	1:A:328:VAL:HG11	2.49	0.47
1:C:96:LEU:HD22	1:C:330:CYS:HA	1.96	0.47
1:C:124:MET:HE3	1:C:280:ALA:HB3	1.96	0.47
1:C:126:LYS:NZ	1:C:319:HIS:CD2	2.79	0.47
1:D:123:THR:OG1	1:D:319:HIS:HE1	1.98	0.46
1:C:326:HIS:CD2	1:C:328:VAL:H	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:TYR:CE2	1:B:328:VAL:HG11	2.51	0.46
1:D:163:PHE:HZ	1:D:229:GLY:HA2	1.80	0.46
1:C:126:LYS:HZ2	1:C:319:HIS:HD2	1.62	0.46
1:B:83:HIS:CD2	1:B:85:ALA:H	2.23	0.46
1:A:326:HIS:HE1	1:B:290:GLY:O	1.98	0.45
1:D:126:LYS:HZ3	1:D:319:HIS:HD2	1.64	0.45
1:D:243:LEU:HD22	1:D:276:PHE:HB2	1.99	0.45
1:D:285:LLP:O3	1:D:285:LLP:NZ	2.49	0.45
1:C:326:HIS:HE1	1:D:290:GLY:O	1.99	0.45
1:D:394:ASP:HB2	1:D:397:LEU:HD23	1.98	0.45
1:C:83:HIS:CD2	1:C:85:ALA:H	2.26	0.45
1:D:132:HIS:HE1	1:D:218:ALA:O	2.00	0.45
1:A:88:LYS:HG2	1:B:31:VAL:HB	2.00	0.44
1:D:126:LYS:NZ	1:D:319:HIS:CD2	2.83	0.44
1:A:326:HIS:CD2	1:A:328:VAL:H	2.33	0.44
1:A:131:LEU:HD11	1:A:306:ARG:HB3	2.00	0.44
1:C:293:PRO:HD3	1:D:292:PHE:CZ	2.53	0.44
1:B:124:MET:HE1	1:B:297:VAL:HG13	1.99	0.43
1:A:293:PRO:HD3	1:B:292:PHE:CZ	2.52	0.43
1:B:264:ARG:HB3	1:B:378:MET:HE2	1.99	0.43
1:C:124:MET:CE	1:C:280:ALA:CB	2.97	0.43
1:A:292:PHE:CZ	1:B:293:PRO:HD3	2.54	0.43
1:C:359:ARG:HG2	1:C:438:PHE:CG	2.54	0.43
1:D:124:MET:HE2	1:D:297:VAL:HG13	2.00	0.43
1:B:397:LEU:HD13	1:B:452:VAL:HG22	2.00	0.42
1:C:292:PHE:CZ	1:D:293:PRO:HD3	2.53	0.42
1:B:326:HIS:CD2	1:B:328:VAL:H	2.36	0.42
1:A:31:VAL:HB	1:B:88:LYS:HG2	2.00	0.42
1:B:211:ARG:HD2	1:C:147:TRP:CE2	2.55	0.42
1:A:359:ARG:HG2	1:A:438:PHE:CG	2.55	0.42
1:D:131:LEU:HD11	1:D:306:ARG:HB3	2.02	0.42
1:A:126:LYS:HZ2	1:A:319:HIS:HD2	1.67	0.42
1:D:124:MET:HE1	1:D:280:ALA:CB	2.49	0.41
1:D:355:ARG:HB2	4:D:719:HOH:O	2.20	0.41
1:A:5:GLN:N	2:A:501:SO4:O3	2.40	0.41
1:C:124:MET:CE	1:C:280:ALA:HB1	2.50	0.41
1:D:96:LEU:HD22	1:D:330:CYS:HA	2.01	0.41
1:A:243:LEU:CD2	1:A:276:PHE:HB2	2.51	0.41
1:B:268:THR:CG2	1:B:341:MET:HE1	2.51	0.41
1:A:121:ASN:ND2	1:A:282:ILE:HG13	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/473 (95%)	436 (97%)	12 (3%)	1 (0%)	51	41
1	B	449/473 (95%)	435 (97%)	13 (3%)	1 (0%)	51	41
1	C	448/473 (95%)	432 (96%)	14 (3%)	2 (0%)	38	26
1	D	448/473 (95%)	434 (97%)	13 (3%)	1 (0%)	51	41
All	All	1794/1892 (95%)	1737 (97%)	52 (3%)	5 (0%)	44	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	3	LYS
1	A	231	VAL
1	B	231	VAL
1	C	231	VAL
1	D	231	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	365/383 (95%)	355 (97%)	10 (3%)	50	42
1	B	365/383 (95%)	355 (97%)	10 (3%)	50	42
1	C	365/383 (95%)	353 (97%)	12 (3%)	43	33
1	D	365/383 (95%)	357 (98%)	8 (2%)	57	51
All	All	1460/1532 (95%)	1420 (97%)	40 (3%)	50	42



All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	3	LYS
1	A	27	GLN
1	A	146	ARG
1	A	190	GLU
1	A	206	GLU
1	A	286	ASN
1	A	356	PHE
1	A	396	ASN
1	A	441	LEU
1	B	2	ASN
1	B	3	LYS
1	B	27	GLN
1	B	286	ASN
1	B	356	PHE
1	B	396	ASN
1	B	401	GLU
1	B	417	LEU
1	B	441	LEU
1	B	452	VAL
1	C	2	ASN
1	C	3	LYS
1	C	24	SER
1	C	27	GLN
1	C	59	MET
1	C	190	GLU
1	C	286	ASN
1	C	351	ARG
1	C	356	PHE
1	C	397	LEU
1	C	417	LEU
1	C	441	LEU
1	D	2	ASN
1	D	27	GLN
1	D	59	MET
1	D	286	ASN
1	D	356	PHE
1	D	396	ASN
1	D	417	LEU
1	D	441	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	65	HIS
1	A	83	HIS
1	A	115	ASN
1	A	121	ASN
1	A	132	HIS
1	A	267	ASN
1	A	319	HIS
1	A	326	HIS
1	A	368	ASN
1	B	2	ASN
1	B	65	HIS
1	B	83	HIS
1	B	115	ASN
1	B	121	ASN
1	B	132	HIS
1	B	319	HIS
1	B	326	HIS
1	B	368	ASN
1	C	26	HIS
1	C	65	HIS
1	C	83	HIS
1	C	115	ASN
1	C	121	ASN
1	C	132	HIS
1	C	319	HIS
1	C	326	HIS
1	C	368	ASN
1	D	2	ASN
1	D	83	HIS
1	D	115	ASN
1	D	121	ASN
1	D	132	HIS
1	D	319	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	LLP	A	285	1	24,24,25	3.06	10 (41%)	28,32,34	1.92	8 (28%)
1	LLP	B	285	1	24,24,25	2.99	9 (37%)	28,32,34	2.17	9 (32%)
1	LLP	C	285	1	24,24,25	2.89	8 (33%)	28,32,34	1.93	6 (21%)
1	LLP	D	285	1	24,24,25	2.81	9 (37%)	28,32,34	1.81	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	285	1	-	0/15/17/19	0/1/1/1
1	LLP	B	285	1	-	0/15/17/19	0/1/1/1
1	LLP	C	285	1	-	0/15/17/19	0/1/1/1
1	LLP	D	285	1	-	0/15/17/19	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	285	LLP	O3-C3	-2.48	1.31	1.37
1	B	285	LLP	P-OP2	-2.14	1.46	1.54
1	A	285	LLP	P-OP4	-2.08	1.53	1.60
1	D	285	LLP	O3-C3	-2.06	1.32	1.37
1	D	285	LLP	C2'-C2	2.00	1.54	1.50
1	D	285	LLP	CD-CE	2.06	1.58	1.51
1	A	285	LLP	CD-CE	2.11	1.58	1.51
1	A	285	LLP	C4-C3	2.13	1.44	1.40
1	A	285	LLP	CA-C	2.14	1.53	1.50
1	B	285	LLP	CB-CA	2.29	1.56	1.53
1	A	285	LLP	C6-N1	2.30	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	285	LLP	C4-C3	2.33	1.44	1.40
1	A	285	LLP	CB-CA	2.39	1.56	1.53
1	D	285	LLP	C4-C5	2.42	1.45	1.42
1	C	285	LLP	C6-N1	2.48	1.39	1.34
1	D	285	LLP	C6-N1	2.49	1.39	1.34
1	A	285	LLP	C2'-C2	2.57	1.55	1.50
1	B	285	LLP	C4-C3	2.70	1.45	1.40
1	C	285	LLP	CA-C	2.73	1.53	1.50
1	D	285	LLP	CA-C	2.98	1.54	1.50
1	C	285	LLP	CE-NZ	3.05	1.53	1.46
1	C	285	LLP	C4-C5	3.12	1.46	1.42
1	B	285	LLP	CE-NZ	3.45	1.54	1.46
1	B	285	LLP	CA-C	3.52	1.54	1.50
1	B	285	LLP	C4-C5	3.60	1.46	1.42
1	A	285	LLP	C4-C5	4.09	1.47	1.42
1	D	285	LLP	CB-CA	4.16	1.59	1.53
1	B	285	LLP	C6-N1	4.23	1.43	1.34
1	D	285	LLP	C4-C4'	5.46	1.56	1.46
1	B	285	LLP	C4-C4'	6.39	1.58	1.46
1	C	285	LLP	C4-C4'	6.96	1.59	1.46
1	A	285	LLP	C4-C4'	7.60	1.60	1.46
1	B	285	LLP	C4'-NZ	9.11	1.53	1.27
1	C	285	LLP	C4'-NZ	9.30	1.54	1.27
1	D	285	LLP	C4'-NZ	9.50	1.54	1.27
1	A	285	LLP	C4'-NZ	9.81	1.55	1.27

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	LLP	C3-C4-C5	-5.11	114.35	118.24
1	C	285	LLP	C3-C4-C5	-4.44	114.86	118.24
1	B	285	LLP	C4-C4'-NZ	-4.33	103.65	124.66
1	C	285	LLP	C4-C4'-NZ	-4.23	104.12	124.66
1	D	285	LLP	C3-C4-C5	-4.03	115.17	118.24
1	B	285	LLP	C3-C4-C5	-4.03	115.17	118.24
1	A	285	LLP	C4-C4'-NZ	-3.99	105.26	124.66
1	B	285	LLP	C2'-C2-C3	-3.91	116.30	120.96
1	C	285	LLP	C2'-C2-C3	-3.69	116.56	120.96
1	B	285	LLP	CD-CE-NZ	-3.52	103.10	110.88
1	D	285	LLP	C4-C4'-NZ	-3.31	108.57	124.66
1	B	285	LLP	C5-C6-N1	-2.55	119.55	123.87
1	B	285	LLP	O-C-CA	-2.55	117.98	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	LLP	C2'-C2-C3	-2.40	118.11	120.96
1	C	285	LLP	O-C-CA	-2.33	118.60	125.02
1	A	285	LLP	CD-CE-NZ	-2.25	105.92	110.88
1	A	285	LLP	O-C-CA	-2.15	119.07	125.02
1	D	285	LLP	O-C-CA	-2.14	119.10	125.02
1	D	285	LLP	C5-C4-C4'	2.03	124.40	121.36
1	B	285	LLP	C5-C4-C4'	2.25	124.72	121.36
1	A	285	LLP	CB-CA-C	2.31	115.46	111.65
1	A	285	LLP	C5-C4-C4'	2.50	125.10	121.36
1	C	285	LLP	C2'-C2-N1	2.83	123.54	117.89
1	B	285	LLP	C2'-C2-N1	2.93	123.74	117.89
1	A	285	LLP	C4-C3-C2	3.71	122.43	120.15
1	B	285	LLP	C4-C3-C2	4.27	122.78	120.15
1	C	285	LLP	C4-C3-C2	4.53	122.94	120.15
1	D	285	LLP	C4-C3-C2	4.83	123.13	120.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	285	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	501	-	4,4,4	0.68	0	6,6,6	0.27	0
2	SO4	B	501	-	4,4,4	0.34	0	6,6,6	0.20	0
2	SO4	D	501	-	4,4,4	0.20	0	6,6,6	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	SO4	D	501	-	-	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SO4	2	0
2	B	501	SO4	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	451/473 (95%)	-0.27	9 (1%) 65 69	13, 21, 43, 80	0
1	B	451/473 (95%)	-0.26	7 (1%) 72 75	14, 22, 45, 82	0
1	C	450/473 (95%)	-0.22	8 (1%) 69 72	15, 24, 46, 63	0
1	D	450/473 (95%)	-0.04	15 (3%) 47 50	14, 26, 49, 72	0
All	All	1802/1892 (95%)	-0.20	39 (2%) 62 66	13, 23, 46, 82	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	453	ALA	5.1
1	D	396	ASN	5.0
1	D	452	VAL	4.6
1	A	396	ASN	4.2
1	D	388	ALA	3.9
1	A	452	VAL	3.5
1	D	397	LEU	3.5
1	C	452	VAL	3.5
1	D	451	GLU	3.5
1	B	397	LEU	3.4
1	C	397	LEU	3.0
1	C	396	ASN	3.0
1	B	452	VAL	3.0
1	A	314	ILE	2.9
1	B	396	ASN	2.9
1	C	394	ASP	2.8
1	B	453	ALA	2.7
1	C	450	ALA	2.6
1	A	385	LYS	2.6
1	D	394	ASP	2.5
1	B	450	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	394	ASP	2.5
1	A	397	LEU	2.5
1	D	391	THR	2.4
1	A	450	ALA	2.4
1	D	450	ALA	2.4
1	D	367	PRO	2.3
1	D	393	PHE	2.3
1	C	5	GLN	2.3
1	D	314	ILE	2.3
1	B	385	LYS	2.2
1	A	395	GLY	2.2
1	B	451	GLU	2.2
1	C	451	GLU	2.2
1	D	385	LYS	2.2
1	D	448	VAL	2.2
1	D	449	PHE	2.2
1	D	392	PRO	2.1
1	C	147	TRP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
1	LLP	B	285	24/25	0.95	0.14	-	17,22,27,30	0
1	LLP	D	285	24/25	0.96	0.12	-	19,25,28,32	0
1	LLP	A	285	24/25	0.96	0.13	-	16,23,28,31	0
1	LLP	C	285	24/25	0.95	0.14	-	18,21,25,27	0

## 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
2	SO4	B	501	5/5	0.64	0.92	16.30	180,184,185,185	0
2	SO4	A	501	5/5	0.85	0.27	2.92	76,80,83,83	0
3	NA	D	502	1/1	0.98	0.14	1.54	30,30,30,30	0
3	NA	B	502	1/1	1.00	0.07	-0.52	25,25,25,25	0
2	SO4	D	501	5/5	0.97	0.13	-0.57	40,42,46,46	0
3	NA	C	501	1/1	0.94	0.09	-0.58	29,29,29,29	0
3	NA	A	502	1/1	0.97	0.08	-0.58	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.