



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:52 PM GMT

PDB ID : 1VI9  
Title : Crystal structure of pyridoxamine kinase  
Authors : Structural GenomiX  
Deposited on : 2003-12-01  
Resolution : 1.96 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

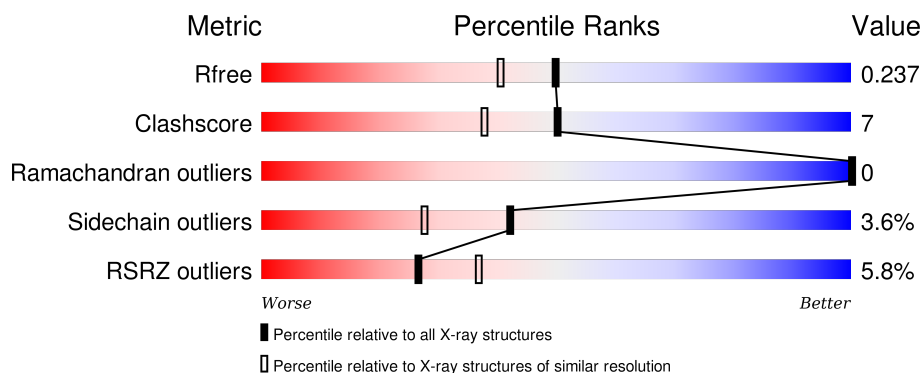
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	299	<div> <div>5%</div> <div>80%15% . .</div> </div>
1	B	299	<div> <div>6%</div> <div>82%13% . .</div> </div>
1	C	299	<div> <div>8%</div> <div>76%17% . .</div> </div>
1	D	299	<div> <div>3%</div> <div>83%12% . .</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	298	-	-	-	X
2	SO4	C	298	-	-	-	X
2	SO4	D	298	-	-	-	X
3	BME	D	300[A]	-	-	-	X
3	BME	D	300[B]	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9760 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 Pyridoxamine kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	Se	0	1	0
			2200	1401	382	403	5	9			
1	B	288	Total	C	N	O	S	Se	0	0	0
			2205	1403	384	405	5	8			
1	C	288	Total	C	N	O	S	Se	0	1	0
			2198	1401	381	402	5	9			
1	D	288	Total	C	N	O	S	Se	0	1	0
			2203	1403	381	405	5	9			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	cloning artifact	UNP P77150
A	0	SER	-	cloning artifact	UNP P77150
A	1	LEU	-	cloning artifact	UNP P77150
A	2	MSE	MET	modified residue	UNP P77150
A	26	MSE	MET	modified residue	UNP P77150
A	53	CSD	CYS	modified residue	UNP P77150
A	55	MSE	MET	modified residue	UNP P77150
A	115	MSE	MET	modified residue	UNP P77150
A	196	MSE	MET	modified residue	UNP P77150
A	216	MSE	MET	modified residue	UNP P77150
A	255	MSE	MET	modified residue	UNP P77150
A	261	MSE	MET	modified residue	UNP P77150
A	288	GLU	-	cloning artifact	UNP P77150
A	289	GLY	-	cloning artifact	UNP P77150
A	290	GLY	-	cloning artifact	UNP P77150
A	291	SER	-	cloning artifact	UNP P77150
A	292	HIS	-	cloning artifact	UNP P77150
A	293	HIS	-	cloning artifact	UNP P77150
A	294	HIS	-	cloning artifact	UNP P77150
A	295	HIS	-	cloning artifact	UNP P77150
A	296	HIS	-	cloning artifact	UNP P77150

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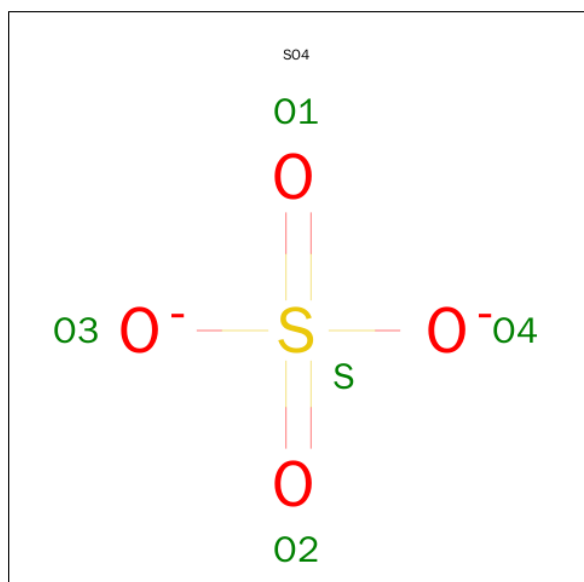
Chain	Residue	Modelled	Actual	Comment	Reference
A	297	HIS	-	cloning artifact	UNP P77150
B	-1	MSE	-	cloning artifact	UNP P77150
B	0	SER	-	cloning artifact	UNP P77150
B	1	LEU	-	cloning artifact	UNP P77150
B	2	MSE	MET	modified residue	UNP P77150
B	26	MSE	MET	modified residue	UNP P77150
B	53	CSD	CYS	modified residue	UNP P77150
B	55	MSE	MET	modified residue	UNP P77150
B	115	MSE	MET	modified residue	UNP P77150
B	196	MSE	MET	modified residue	UNP P77150
B	216	MSE	MET	modified residue	UNP P77150
B	255	MSE	MET	modified residue	UNP P77150
B	261	MSE	MET	modified residue	UNP P77150
B	288	GLU	-	cloning artifact	UNP P77150
B	289	GLY	-	cloning artifact	UNP P77150
B	290	GLY	-	cloning artifact	UNP P77150
B	291	SER	-	cloning artifact	UNP P77150
B	292	HIS	-	cloning artifact	UNP P77150
B	293	HIS	-	cloning artifact	UNP P77150
B	294	HIS	-	cloning artifact	UNP P77150
B	295	HIS	-	cloning artifact	UNP P77150
B	296	HIS	-	cloning artifact	UNP P77150
B	297	HIS	-	cloning artifact	UNP P77150
C	-1	MSE	-	cloning artifact	UNP P77150
C	0	SER	-	cloning artifact	UNP P77150
C	1	LEU	-	cloning artifact	UNP P77150
C	2	MSE	MET	modified residue	UNP P77150
C	26	MSE	MET	modified residue	UNP P77150
C	53	CSD	CYS	modified residue	UNP P77150
C	55	MSE	MET	modified residue	UNP P77150
C	115	MSE	MET	modified residue	UNP P77150
C	196	MSE	MET	modified residue	UNP P77150
C	216	MSE	MET	modified residue	UNP P77150
C	255	MSE	MET	modified residue	UNP P77150
C	261	MSE	MET	modified residue	UNP P77150
C	288	GLU	-	cloning artifact	UNP P77150
C	289	GLY	-	cloning artifact	UNP P77150
C	290	GLY	-	cloning artifact	UNP P77150
C	291	SER	-	cloning artifact	UNP P77150
C	292	HIS	-	cloning artifact	UNP P77150
C	293	HIS	-	cloning artifact	UNP P77150
C	294	HIS	-	cloning artifact	UNP P77150

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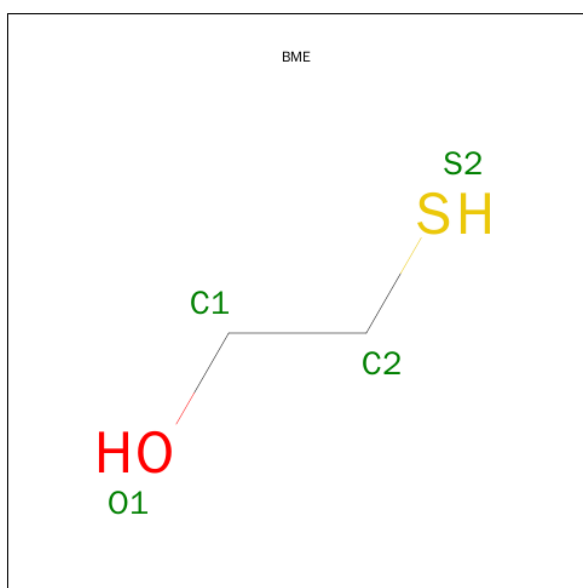
Chain	Residue	Modelled	Actual	Comment	Reference
C	295	HIS	-	cloning artifact	UNP P77150
C	296	HIS	-	cloning artifact	UNP P77150
C	297	HIS	-	cloning artifact	UNP P77150
D	-1	MSE	-	cloning artifact	UNP P77150
D	0	SER	-	cloning artifact	UNP P77150
D	1	LEU	-	cloning artifact	UNP P77150
D	2	MSE	MET	modified residue	UNP P77150
D	26	MSE	MET	modified residue	UNP P77150
D	53	CSD	CYS	modified residue	UNP P77150
D	55	MSE	MET	modified residue	UNP P77150
D	115	MSE	MET	modified residue	UNP P77150
D	196	MSE	MET	modified residue	UNP P77150
D	216	MSE	MET	modified residue	UNP P77150
D	255	MSE	MET	modified residue	UNP P77150
D	261	MSE	MET	modified residue	UNP P77150
D	288	GLU	-	cloning artifact	UNP P77150
D	289	GLY	-	cloning artifact	UNP P77150
D	290	GLY	-	cloning artifact	UNP P77150
D	291	SER	-	cloning artifact	UNP P77150
D	292	HIS	-	cloning artifact	UNP P77150
D	293	HIS	-	cloning artifact	UNP P77150
D	294	HIS	-	cloning artifact	UNP P77150
D	295	HIS	-	cloning artifact	UNP P77150
D	296	HIS	-	cloning artifact	UNP P77150
D	297	HIS	-	cloning artifact	UNP P77150

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

- Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O S 4 2 1 1	0	0
3	D	1	Total C O S 7 4 2 1	0	1

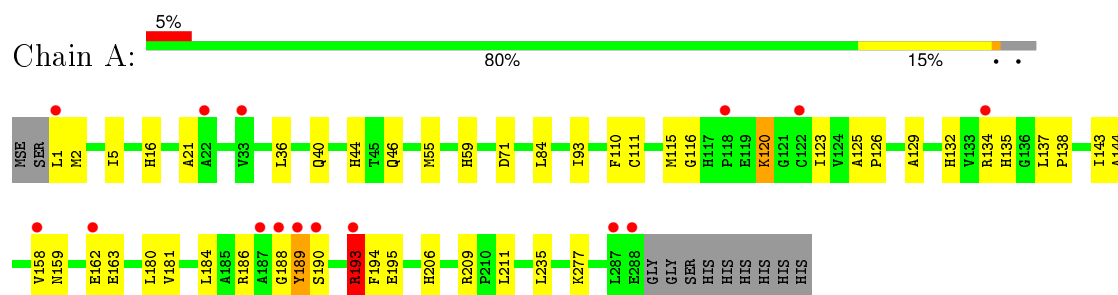
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	235	Total O 235 235	0	0
4	B	241	Total O 241 241	0	0
4	C	216	Total O 216 216	0	0
4	D	231	Total O 231 231	0	0

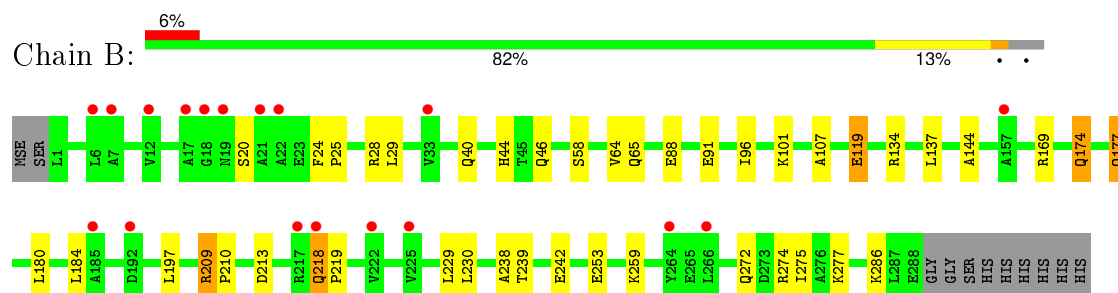
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

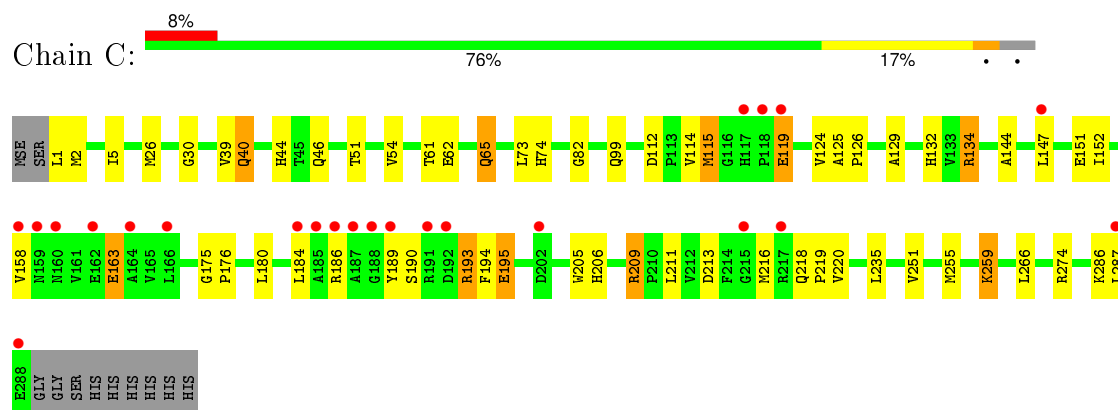
- Molecule 1: Pyridoxamine kinase



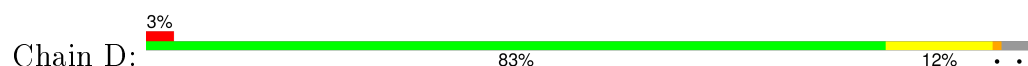
- Molecule 1: Pyridoxamine kinase



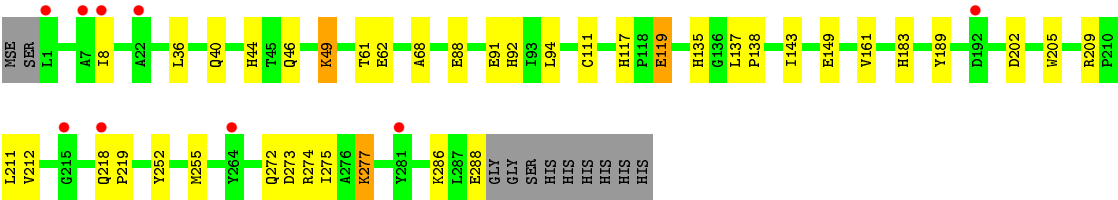
- Molecule 1: Pyridoxamine kinase



- Molecule 1: Pyridoxamine kinase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.38 Å 92.59 Å 122.24 Å 90.00° 99.42° 90.00°	Depositor
Resolution (Å)	43.03 – 1.96 43.22 – 1.96	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.03-1.96) 98.7 (43.22-1.96)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 1.95 Å)	Xtriage
Refinement program	REFMAC 4	Depositor
R, $R_{free}$	0.198 , 0.256 0.189 , 0.237	Depositor DCC
$R_{free}$ test set	4166 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 63.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 83507 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9760	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, SO4, BME

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	0.59	0/2235	1.08	4/3029 (0.1%)
1	B	0.59	0/2237	1.15	7/3032 (0.2%)
1	C	0.57	0/2233	1.09	11/3026 (0.4%)
1	D	0.57	0/2239	1.06	5/3035 (0.2%)
All	All	0.58	0/8944	1.10	27/12122 (0.2%)

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

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

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	ARG	NE-CZ-NH2	16.29	128.45	120.30
1	B	209	ARG	NE-CZ-NH1	-11.32	114.64	120.30
1	B	209	ARG	CD-NE-CZ	10.82	138.75	123.60
1	C	209	ARG	CD-NE-CZ	9.53	136.94	123.60
1	C	163	GLU	CA-CB-CG	8.40	131.88	113.40
1	C	134	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	C	186	ARG	NE-CZ-NH1	-7.81	116.40	120.30
1	D	252	TYR	CB-CG-CD1	-7.53	116.48	121.00
1	C	209	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	B	28	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	209	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	D	252	TYR	CB-CG-CD2	6.71	125.03	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	274	ARG	CD-NE-CZ	6.50	132.71	123.60
1	D	209	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	193	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	B	169	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	B	28	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	C	193	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	115	MSE	CA-CB-CG	5.33	122.36	113.30
1	A	40	GLN	CB-CA-C	5.33	121.06	110.40
1	C	40	GLN	CB-CA-C	5.33	121.06	110.40
1	B	40	GLN	CB-CA-C	5.32	121.05	110.40
1	A	193	ARG	CD-NE-CZ	5.29	131.01	123.60
1	D	274	ARG	CD-NE-CZ	5.23	130.92	123.60
1	C	193	ARG	CD-NE-CZ	5.21	130.89	123.60
1	D	49	LYS	CA-CB-CG	5.13	124.70	113.40
1	C	134	ARG	CD-NE-CZ	5.09	130.73	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	40	GLN	Mainchain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2200	0	2203	32	0
1	B	2205	0	2205	22	0
1	C	2198	0	2201	49	0
1	D	2203	0	2199	21	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	B	4	0	5	0	0
3	D	7	0	10	0	0
4	A	235	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	241	0	0	5	1
4	C	216	0	0	5	0
4	D	231	0	0	5	0
All	All	9760	0	8823	123	1

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 7.

All (123) 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:C:115:MSE:HE3	1:C:132:HIS:HB2	1.29	1.08
1:C:115:MSE:CE	1:C:132:HIS:HB2	1.96	0.96
1:A:115:MSE:HE3	1:A:132:HIS:HB2	1.49	0.94
1:A:115:MSE:CE	1:A:132:HIS:HB2	1.98	0.92
1:A:115:MSE:HE2	1:A:129:ALA:HA	1.53	0.89
1:C:115:MSE:HE2	1:C:129:ALA:HA	1.54	0.89
1:C:51:THR:HB	1:D:62:GLU:HG2	1.60	0.81
1:C:115:MSE:HE3	1:C:132:HIS:CB	2.13	0.78
1:A:115:MSE:HE3	1:A:132:HIS:CB	2.24	0.67
1:C:125:ALA:HB1	1:C:126:PRO:HD2	1.77	0.67
1:B:239:THR:OG1	1:B:242:GLU:HG2	1.96	0.66
1:B:218:GLN:HG2	4:B:485:HOH:O	1.94	0.66
1:A:190:SER:HB3	1:A:193:ARG:NH1	2.13	0.64
1:B:286:LYS:HE2	4:B:540:HOH:O	1.97	0.63
1:C:115:MSE:HE2	1:C:129:ALA:CA	2.29	0.62
1:C:193:ARG:NH1	4:C:433:HOH:O	2.32	0.62
1:C:40:GLN:HB2	4:C:452:HOH:O	2.00	0.61
1:C:2:MSE:HE3	1:C:30:GLY:O	2.01	0.61
1:C:61:THR:HG22	1:C:65:GLN:HE22	1.66	0.59
1:A:159:ASN:HA	1:A:186:ARG:HH11	1.68	0.58
1:C:255[A]:MSE:SE	1:C:266:LEU:HD21	2.53	0.58
1:A:194:PHE:HB2	1:A:211:LEU:HD23	1.87	0.57
1:C:115:MSE:SE	4:C:514:HOH:O	2.72	0.57
1:A:116:GLY:HA2	1:A:123:ILE:HG12	1.85	0.57
1:C:251:VAL:O	1:C:255[B]:MSE:HG3	2.05	0.56
1:D:117:HIS:HE1	1:D:149:GLU:OE1	1.89	0.56
1:A:55:MSE:HE3	1:A:59:HIS:NE2	2.21	0.56
1:C:1:LEU:HA	4:C:497:HOH:O	2.06	0.55
1:D:119:GLU:HB3	4:D:461:HOH:O	2.07	0.55
1:D:119:GLU:CD	1:D:119:GLU:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:MSE:HE2	1:A:129:ALA:CA	2.32	0.54
1:A:159:ASN:HA	1:A:186:ARG:NH1	2.22	0.54
1:B:29:LEU:HD22	1:B:229:LEU:HD22	1.89	0.53
1:C:5:ILE:HD11	1:C:235:LEU:HD12	1.90	0.53
1:A:189:TYR:HB2	1:A:195:GLU:OE1	2.09	0.53
1:C:39:VAL:HG12	1:C:54:VAL:HA	1.91	0.52
1:C:205:TRP:CH2	1:C:286:LYS:HB2	2.44	0.52
1:D:205:TRP:CZ2	1:D:286:LYS:HE2	2.44	0.52
1:A:158:VAL:HA	1:A:163:GLU:HG3	1.92	0.52
1:C:115:MSE:HE2	1:C:129:ALA:O	2.10	0.51
1:C:184:LEU:HD12	1:C:195:GLU:HB3	1.91	0.51
1:B:137:LEU:HD21	1:B:174:GLN:HG3	1.92	0.51
1:A:144:ALA:HA	1:A:180:LEU:O	2.10	0.50
1:C:46:GLN:HG3	1:C:220:VAL:CG2	2.42	0.49
1:D:94:LEU:HD11	1:D:135:HIS:HB3	1.93	0.49
1:C:193:ARG:NH2	1:C:195:GLU:OE2	2.45	0.49
1:C:46:GLN:HG3	1:C:220:VAL:HG21	1.95	0.49
1:C:73:LEU:CD2	1:C:99:GLN:HG2	2.43	0.49
1:C:147:LEU:O	1:C:151:GLU:HG3	2.11	0.49
1:C:194:PHE:HB2	1:C:211:LEU:HD23	1.93	0.49
1:A:120:LYS:HB3	1:A:120:LYS:NZ	2.29	0.48
1:B:210:PRO:HB2	4:B:451:HOH:O	2.12	0.48
1:D:61:THR:OG1	1:D:92:HIS:HD2	1.96	0.48
1:A:193:ARG:CG	1:A:193:ARG:HH11	2.26	0.48
1:D:92:HIS:HE1	4:D:478:HOH:O	1.97	0.48
1:A:193:ARG:HH11	1:A:193:ARG:HG2	1.80	0.47
1:D:88:GLU:O	1:D:91:GLU:HG2	2.15	0.47
1:C:5:ILE:HG21	1:C:26:MSE:HE1	1.97	0.47
1:D:8:ILE:HA	1:D:36:LEU:O	2.15	0.47
1:C:195:GLU:HG2	1:C:206:HIS:NE2	2.30	0.46
1:B:253:GLU:HG3	1:B:274:ARG:HB3	1.96	0.46
1:B:24:PHE:HB3	1:B:25:PRO:HD3	1.98	0.46
1:B:88:GLU:O	1:B:91:GLU:HG2	2.16	0.45
1:C:195:GLU:HG2	1:C:206:HIS:HE2	1.82	0.45
1:B:238:ALA:HB1	1:B:242:GLU:HG3	1.99	0.45
1:B:44:HIS:CE1	1:B:46:GLN:HB3	2.52	0.45
1:C:115:MSE:HE3	1:C:132:HIS:CG	2.51	0.44
1:A:162:GLU:H	1:A:162:GLU:CD	2.20	0.44
1:B:177:GLN:NE2	4:B:384:HOH:O	2.50	0.44
1:B:272:GLN:HA	1:B:275:ILE:HD12	2.00	0.44
1:C:115:MSE:SE	1:C:152:ILE:HG21	2.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASP:HB2	4:A:384:HOH:O	2.17	0.44
1:B:213:ASP:O	1:B:259:LYS:NZ	2.31	0.44
1:D:218:GLN:HA	1:D:219:PRO:HD3	1.85	0.44
1:B:119:GLU:H	1:B:119:GLU:CD	2.20	0.44
1:D:272:GLN:HA	1:D:275:ILE:HD12	2.00	0.44
1:B:180:LEU:HD22	1:B:230:LEU:HD22	1.99	0.44
1:D:273:ASP:O	1:D:277:LYS:HE2	2.17	0.44
1:D:68:ALA:HA	4:D:450:HOH:O	2.18	0.43
1:B:218:GLN:HA	1:B:219:PRO:HD3	1.93	0.43
1:B:101:LYS:HE2	1:B:107:ALA:O	2.19	0.43
1:C:193:ARG:HE	1:C:193:ARG:HB2	1.58	0.43
1:C:218:GLN:HA	1:C:219:PRO:HD3	1.93	0.43
1:A:5:ILE:HD11	1:A:235:LEU:HD12	2.01	0.43
1:C:119:GLU:H	1:C:119:GLU:HG3	1.56	0.42
1:C:115:MSE:HE3	1:C:132:HIS:ND1	2.34	0.42
1:C:114:VAL:O	1:C:124:VAL:HG11	2.19	0.42
1:D:137:LEU:HB3	1:D:138:PRO:HD3	2.00	0.42
1:D:111:CYS:O	1:D:143:ILE:HA	2.19	0.42
1:B:184:LEU:HD11	1:B:197:LEU:HG	2.00	0.42
1:C:44:HIS:CD2	1:C:46:GLN:HB2	2.55	0.42
1:C:144:ALA:HA	1:C:180:LEU:O	2.20	0.42
1:A:125:ALA:HB1	1:A:126:PRO:HD2	2.02	0.42
1:C:189:TYR:HB2	1:C:193:ARG:NH2	2.34	0.42
1:C:44:HIS:HD2	1:C:46:GLN:H	1.66	0.42
1:B:144:ALA:HA	1:B:180:LEU:O	2.20	0.42
1:A:195:GLU:OE1	1:A:206:HIS:NE2	2.51	0.42
1:A:135:HIS:HD2	4:A:482:HOH:O	2.02	0.42
1:C:74:HIS:HD2	4:C:341:HOH:O	2.02	0.42
1:A:44:HIS:CE1	1:A:46:GLN:HB2	2.55	0.42
1:A:16:HIS:HB3	1:A:21:ALA:HA	2.01	0.41
1:A:111:CYS:O	1:A:143:ILE:HA	2.20	0.41
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.96	0.41
1:A:184:LEU:HD13	1:A:188:GLY:HA2	2.03	0.41
1:B:20:SER:HB3	4:B:337:HOH:O	2.20	0.41
1:C:195:GLU:OE2	1:C:206:HIS:NE2	2.53	0.41
1:D:212:VAL:HG21	1:D:255[B]:MSE:HB3	2.02	0.41
1:B:64:VAL:HG21	1:B:96:ILE:HG12	2.03	0.41
1:C:61:THR:HG22	1:C:65:GLN:NE2	2.34	0.41
1:C:175:GLY:N	1:C:176:PRO:HD2	2.36	0.41
1:C:206:HIS:HB2	1:C:287:LEU:HD11	2.03	0.41
1:D:91:GLU:HG3	4:D:483:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:HG11	1:A:184:LEU:HD23	2.03	0.41
1:A:84:LEU:HD21	1:A:93:ILE:HD12	2.03	0.40
1:C:158:VAL:HA	1:C:163:GLU:HG3	2.02	0.40
1:C:213:ASP:O	1:C:259:LYS:HE2	2.20	0.40
1:A:137:LEU:N	1:A:138:PRO:HD2	2.36	0.40
1:D:161:VAL:HG21	1:D:189:TYR:CZ	2.57	0.40
1:C:82:GLY:HA2	1:C:112:ASP:HB3	2.04	0.40
1:C:189:TYR:CD1	1:C:195:GLU:OE2	2.74	0.40
1:A:159:ASN:OD1	1:A:186:ARG:NH1	2.54	0.40
1:D:183:HIS:HE1	4:D:377:HOH:O	2.03	0.40
1:D:44:HIS:CE1	1:D:46:GLN:HB3	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:436:HOH:O	4:B:540:HOH:O[2_655]	2.19	0.01

## 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	286/299 (96%)	274 (96%)	12 (4%)	0	100	100
1	B	285/299 (95%)	281 (99%)	4 (1%)	0	100	100
1	C	286/299 (96%)	276 (96%)	10 (4%)	0	100	100
1	D	286/299 (96%)	281 (98%)	5 (2%)	0	100	100
All	All	1143/1196 (96%)	1112 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.



### 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	230/232 (99%)	221 (96%)	9 (4%)	39	24
1	B	231/232 (100%)	222 (96%)	9 (4%)	39	24
1	C	229/232 (99%)	220 (96%)	9 (4%)	39	24
1	D	231/232 (100%)	225 (97%)	6 (3%)	54	43
All	All	921/928 (99%)	888 (96%)	33 (4%)	42	28

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	2	MSE
1	A	36	LEU
1	A	110	PHE
1	A	120	LYS
1	A	134	ARG
1	A	189	TYR
1	A	193	ARG
1	A	277	LYS
1	B	58	SER
1	B	65	GLN
1	B	119	GLU
1	B	134	ARG
1	B	174	GLN
1	B	177	GLN
1	B	209	ARG
1	B	218	GLN
1	B	277	LYS
1	C	62	GLU
1	C	65	GLN
1	C	119	GLU
1	C	134	ARG
1	C	190	SER
1	C	195	GLU

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Mol	Chain	Res	Type
1	C	209	ARG
1	C	216	MSE
1	C	259	LYS
1	D	49	LYS
1	D	119	GLU
1	D	202	ASP
1	D	211	LEU
1	D	277	LYS
1	D	288	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
1	A	183	HIS
1	B	65	GLN
1	B	99	GLN
1	B	174	GLN
1	B	177	GLN
1	B	218	GLN
1	C	44	HIS
1	C	65	GLN
1	C	99	GLN
1	D	92	HIS
1	D	117	HIS
1	D	183	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	CSD	A	53	1	3,7,8	0.65	0	3,8,10	0.85	0
1	CSD	B	53	1	3,7,8	0.57	0	3,8,10	1.14	0
1	CSD	C	53	1	3,7,8	0.48	0	3,8,10	1.52	0
1	CSD	D	53	1	3,7,8	0.62	0	3,8,10	1.28	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
1	CSD	A	53	1	-	0/2/6/8	0/0/0/0
1	CSD	B	53	1	-	0/2/6/8	0/0/0/0
1	CSD	C	53	1	-	0/2/6/8	0/0/0/0
1	CSD	D	53	1	-	0/2/6/8	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.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 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	298	-	4,4,4	0.95	0	6,6,6	0.22	0
2	SO4	B	298	-	4,4,4	0.98	0	6,6,6	0.26	0
3	BME	B	300	1	3,3,3	0.46	0	2,2,2	0.64	0
2	SO4	C	298	-	4,4,4	0.97	0	6,6,6	0.23	0
2	SO4	D	298	-	4,4,4	0.96	0	6,6,6	0.15	0
3	BME	D	300[A]	-	3,3,3	0.45	0	2,2,2	0.50	0
3	BME	D	300[B]	-	3,3,3	0.50	0	2,2,2	0.52	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	298	-	-	0/0/0/0	0/0/0/0
2	SO4	B	298	-	-	0/0/0/0	0/0/0/0
3	BME	B	300	1	-	0/1/1/1	0/0/0/0
2	SO4	C	298	-	-	0/0/0/0	0/0/0/0
2	SO4	D	298	-	-	0/0/0/0	0/0/0/0
3	BME	D	300[A]	-	-	0/1/1/1	0/0/0/0
3	BME	D	300[B]	-	-	0/1/1/1	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.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	279/299 (93%)	0.29	15 (5%) 29 41	13, 24, 45, 58	0
1	B	279/299 (93%)	0.33	18 (6%) 22 32	13, 21, 34, 51	0
1	C	279/299 (93%)	0.49	23 (8%) 14 23	16, 25, 49, 65	0
1	D	279/299 (93%)	0.23	9 (3%) 51 61	15, 23, 38, 58	0
All	All	1116/1196 (93%)	0.33	65 (5%) 26 37	13, 23, 42, 65	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	215	GLY	5.4
1	A	288	GLU	5.0
1	D	1	LEU	5.0
1	C	118	PRO	4.7
1	C	191	ARG	4.4
1	C	158	VAL	4.0
1	C	119	GLU	4.0
1	C	189	TYR	3.9
1	D	218	GLN	3.8
1	A	189	TYR	3.8
1	C	288	GLU	3.7
1	C	187	ALA	3.7
1	C	192	ASP	3.6
1	A	118	PRO	3.6
1	D	264	TYR	3.6
1	B	21	ALA	3.5
1	C	188	GLY	3.4
1	D	192	ASP	3.2
1	D	281	TYR	3.2
1	B	33	VAL	3.2
1	A	190	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	188	GLY	3.1
1	A	33	VAL	3.0
1	C	217	ARG	2.9
1	A	1	LEU	2.9
1	B	22	ALA	2.9
1	C	215	GLY	2.9
1	A	187	ALA	2.8
1	C	287	LEU	2.7
1	A	134	ARG	2.7
1	B	192	ASP	2.6
1	A	122	CYS	2.6
1	A	287	LEU	2.6
1	C	160	ASN	2.5
1	D	22	ALA	2.4
1	A	158	VAL	2.4
1	B	222	VAL	2.4
1	B	225	VAL	2.4
1	C	185	ALA	2.4
1	C	186	ARG	2.4
1	C	147	LEU	2.4
1	D	8	ILE	2.3
1	A	22	ALA	2.3
1	B	7	ALA	2.3
1	C	184	LEU	2.3
1	A	193	ARG	2.3
1	C	162	GLU	2.3
1	A	162	GLU	2.2
1	B	157	ALA	2.2
1	C	164	ALA	2.2
1	C	202	ASP	2.2
1	B	264	TYR	2.2
1	B	266	LEU	2.2
1	B	18	GLY	2.1
1	B	17	ALA	2.1
1	B	19	ASN	2.1
1	B	218	GLN	2.1
1	B	6	LEU	2.1
1	C	159	ASN	2.1
1	C	166	LEU	2.1
1	C	117	HIS	2.1
1	B	12	VAL	2.0
1	B	185	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	7	ALA	2.0
1	B	217	ARG	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	CSD	D	53	8/9	0.93	0.11	-	25,28,37,39	0
1	CSD	A	53	8/9	0.92	0.12	-	19,24,32,37	0
1	CSD	C	53	8/9	0.91	0.11	-	28,30,36,39	0
1	CSD	B	53	8/9	0.90	0.11	-	20,24,33,37	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
3	BME	D	300[B]	4/4	0.83	0.36	8.25	30,31,31,31	3
3	BME	D	300[A]	4/4	0.83	0.36	7.98	30,30,31,31	3
2	SO4	A	298	5/5	0.83	0.21	7.16	65,66,67,67	0
2	SO4	C	298	5/5	0.72	0.23	3.42	74,74,74,74	0
2	SO4	D	298	5/5	0.84	0.21	2.18	67,67,67,67	0
2	SO4	B	298	5/5	0.92	0.18	0.97	49,49,49,50	0
3	BME	B	300	4/4	0.94	0.12	-0.42	29,32,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.