



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:25 AM GMT

PDB ID : 3IEL  
Title : Crystal Structure of TTHA0252 from *Thermus thermophilus* HB8 complexed with UMP  
Authors : Ishikawa, H.; Nakagawa, N.; Kuramitsu, S.; Yokoyama, S.; Masui, R.  
Deposited on : 2009-07-23  
Resolution : 2.35 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

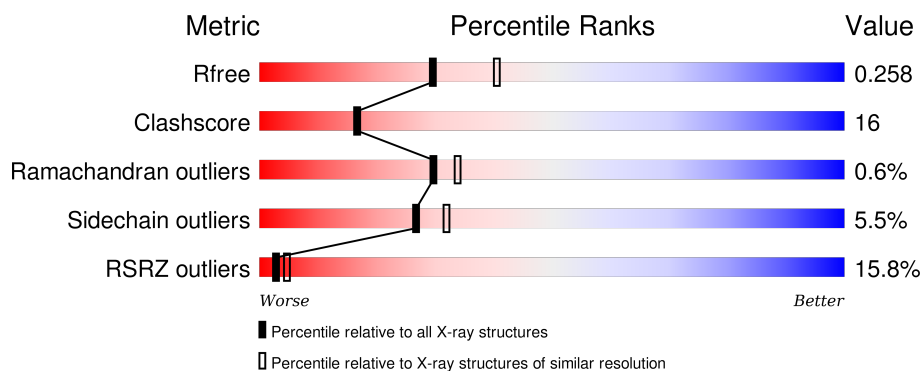
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	431	<div> <div>3%</div> <div>73%</div> <div>24%</div> <div>.</div> </div>
1	B	431	<div> <div>2%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>
1	C	431	<div> <div>27%</div> <div>62%</div> <div>36%</div> <div>.</div> </div>
1	D	431	<div> <div>31%</div> <div>57%</div> <div>41%</div> <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	433	-	-	X	-
2	SO4	A	438	-	-	-	X
2	SO4	A	443	-	-	X	-
2	SO4	A	451	-	-	-	X
2	SO4	A	457	-	-	-	X
2	SO4	A	463	-	-	-	X
2	SO4	B	436	-	-	-	X
2	SO4	B	445	-	-	-	X
2	SO4	C	440	-	-	-	X
2	SO4	C	453	-	-	X	-
2	SO4	D	442	-	-	-	X
3	FLC	A	464	-	-	-	X
3	FLC	B	455	-	-	-	X
4	U5P	A	466	-	-	-	X
4	U5P	A	467	-	-	-	X
4	U5P	B	457	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14251 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 Ribonuclease TTHA0252.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3326	2127	597	594	8			
1	B	431	Total	C	N	O	S	0	0	0
			3326	2127	597	594	8			
1	C	431	Total	C	N	O	S	0	0	0
			3326	2127	597	594	8			
1	D	431	Total	C	N	O	S	0	0	0
			3326	2127	597	594	8			

- 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	A	1	Total	O	S	0	0
			5	4	1		

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

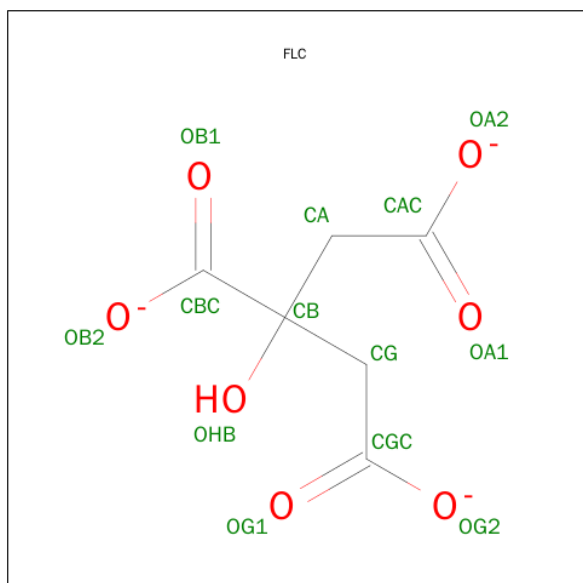
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0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

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula:  $\text{C}_6\text{H}_5\text{O}_7$ ).



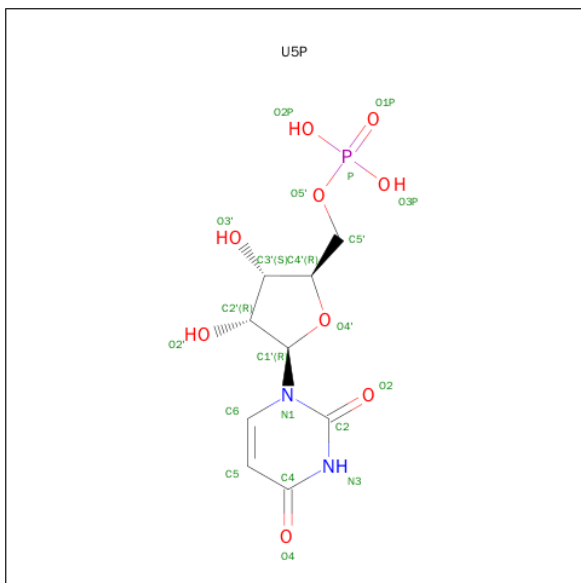
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U5P) (formula:  $C_9H_{13}N_2O_9P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
4	A	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
4	A	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
4	B	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
4	B	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
4	C	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
4	D	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Zn 2	0	0
5	D	2	Total 2	Zn 2	0	0
5	C	2	Total 2	Zn 2	0	0

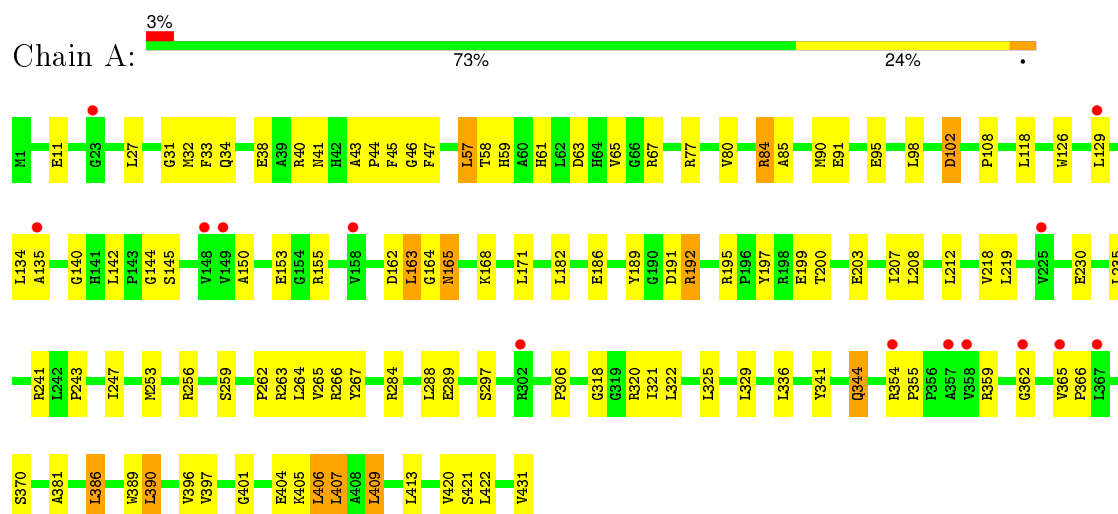
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	118	Total 118	O 118	0	0
6	B	95	Total 95	O 95	0	0
6	C	47	Total 47	O 47	0	0
6	D	26	Total 26	O 26	0	0

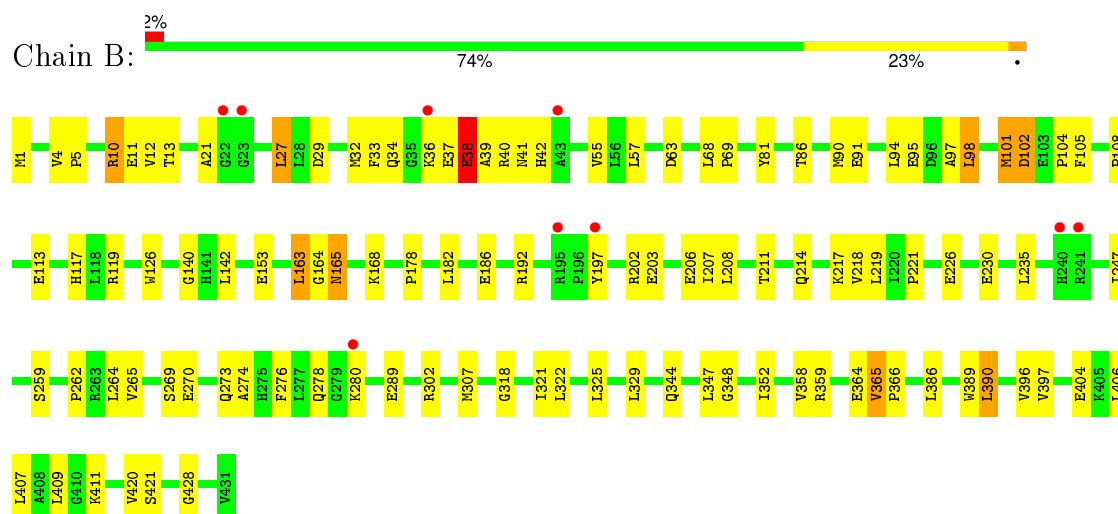
### 3 Residue-property plots

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: Ribonuclease TTHA0252



#### • Molecule 1: Ribonuclease TTHA0252

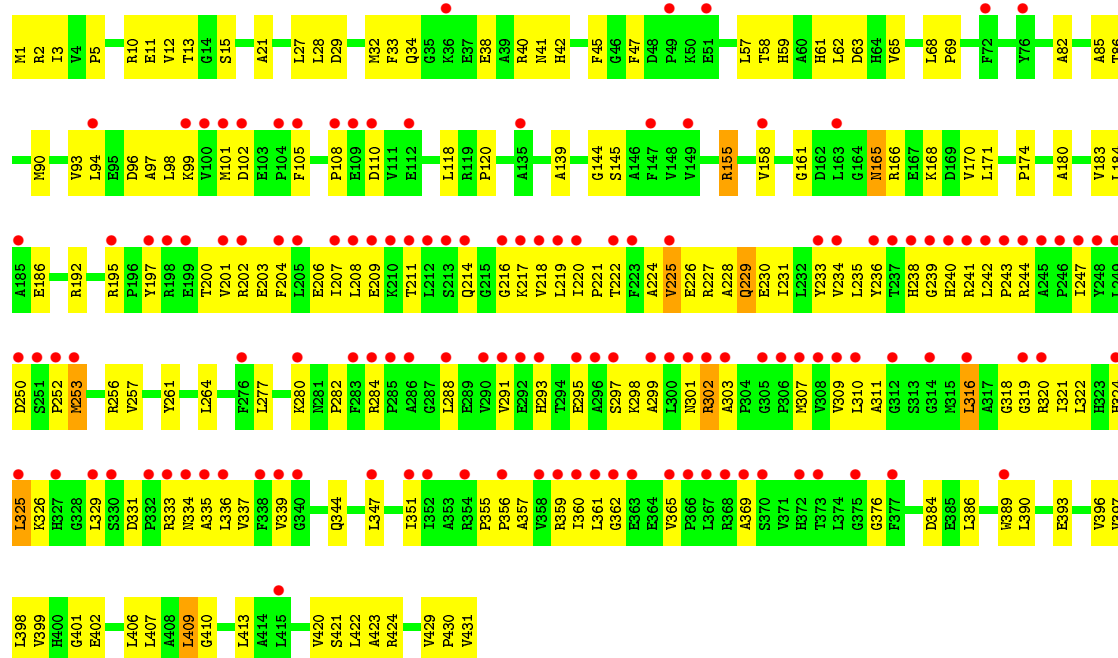


#### • Molecule 1: Ribonuclease TTHA0252





• Molecule 1: Ribonuclease TTHA0252



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.24Å 146.68Å 120.35Å 90.00° 110.11° 90.00°	Depositor
Resolution (Å)	50.00 – 2.35 44.60 – 2.35	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.00-2.35) 95.4 (44.60-2.35)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.28 (at 2.34Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.222 , 0.259 0.222 , 0.258	Depositor DCC
$R_{free}$ test set	9357 reflections (9.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.9	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 97950 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14251	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FLC, ZN, U5P

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	0.37	0/3407	0.65	0/4621
1	B	0.37	0/3407	0.66	1/4621 (0.0%)
1	C	0.32	0/3407	0.59	1/4621 (0.0%)
1	D	0.29	0/3407	0.57	1/4621 (0.0%)
All	All	0.34	0/13628	0.62	3/18484 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	390	LEU	CA-CB-CG	5.37	127.66	115.30
1	C	161	GLY	N-CA-C	-5.22	100.06	113.10
1	D	161	GLY	N-CA-C	-5.03	100.53	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3326	0	3351	90	0
1	B	3326	0	3351	80	0
1	C	3326	0	3351	135	0
1	D	3326	0	3351	154	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	160	0	0	9	0
2	B	115	0	0	0	0
2	C	125	0	0	5	0
2	D	80	0	0	1	0
3	A	13	0	5	1	0
3	B	13	0	5	2	0
4	A	63	0	33	2	0
4	B	42	0	22	2	0
4	C	21	0	11	0	0
4	D	21	0	11	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	118	0	0	5	0
6	B	95	0	0	6	0
6	C	47	0	0	3	0
6	D	26	0	0	1	0
All	All	14251	0	13491	452	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 16.

All (452) 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:98:LEU:HD11	1:C:108:PRO:HA	1.40	1.03
1:D:235:LEU:HD23	1:D:247:ILE:HD13	1.37	1.03
1:B:33:PHE:H	1:B:41:ASN:HD21	1.05	1.01
1:D:33:PHE:H	1:D:41:ASN:HD21	1.10	0.99
1:B:153:GLU:HG2	6:B:519:HOH:O	1.65	0.97
1:A:153:GLU:HG2	2:A:433:SO4:O1	1.63	0.97
1:A:33:PHE:H	1:A:41:ASN:HD21	1.05	0.94
1:A:306:PRO:HD2	1:B:302:ARG:HH22	1.33	0.91
1:C:33:PHE:H	1:C:41:ASN:HD21	1.15	0.89
1:B:265:VAL:HG12	6:B:532:HOH:O	1.76	0.85
1:D:222:THR:HG22	1:D:339:VAL:HG21	1.58	0.83
1:D:284:ARG:HD3	1:D:288:LEU:HD23	1.59	0.83
1:D:1:MET:HG3	1:D:21:ALA:HB2	1.59	0.82
1:A:208:LEU:HD23	1:A:218:VAL:HG21	1.63	0.81
1:C:360:ILE:HG22	1:C:361:LEU:HD13	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:GLU:HA	2:A:433:SO4:O3	1.82	0.80
1:D:98:LEU:HD21	1:D:108:PRO:HB3	1.64	0.80
1:A:168:LYS:HE3	1:A:230:GLU:OE1	1.81	0.79
1:D:168:LYS:HE2	1:D:230:GLU:OE1	1.83	0.79
1:D:322:LEU:HB3	1:D:361:LEU:HD11	1.64	0.78
1:B:97:ALA:O	1:B:101:MET:HB2	1.81	0.78
1:D:211:THR:HG21	1:D:335:ALA:HB2	1.64	0.78
1:B:101:MET:HG2	1:B:104:PRO:HB3	1.68	0.75
1:C:168:LYS:HE3	1:C:230:GLU:OE1	1.87	0.75
1:B:33:PHE:N	1:B:41:ASN:HD21	1.83	0.75
1:A:404:GLU:CD	1:A:404:GLU:H	1.89	0.75
1:C:97:ALA:O	1:C:101:MET:HB2	1.87	0.74
1:C:10:ARG:HH12	1:C:424:ARG:HG2	1.52	0.73
1:A:155:ARG:HD3	1:A:431:VAL:O	1.88	0.73
1:A:34:GLN:HE21	1:A:63:ASP:HB3	1.54	0.73
1:C:10:ARG:HH22	1:C:424:ARG:NH1	1.86	0.73
1:D:407:LEU:HD22	1:D:422:LEU:HD21	1.70	0.73
1:D:360:ILE:HG22	1:D:361:LEU:HD13	1.70	0.72
1:B:208:LEU:HD23	1:B:218:VAL:HG21	1.71	0.72
1:D:309:VAL:HG11	1:D:324:HIS:CD2	2.25	0.71
1:C:43:ALA:HB1	1:C:44:PRO:HD2	1.72	0.71
1:C:229:GLN:CD	1:C:229:GLN:H	1.94	0.71
1:A:34:GLN:NE2	1:A:63:ASP:HB3	2.06	0.71
1:C:34:GLN:HE21	1:C:63:ASP:HB3	1.55	0.70
1:C:218:VAL:HB	1:C:308:VAL:HG12	1.74	0.70
1:D:318:GLY:HA2	1:D:322:LEU:HD11	1.74	0.69
1:B:33:PHE:H	1:B:41:ASN:ND2	1.86	0.69
1:B:278:GLN:HB2	1:B:280:LYS:HD3	1.74	0.69
1:C:33:PHE:N	1:C:41:ASN:HD21	1.91	0.68
1:C:404:GLU:CD	1:C:404:GLU:H	1.96	0.68
1:C:163:LEU:HD21	1:C:389:TRP:CD2	2.29	0.68
1:C:33:PHE:H	1:C:41:ASN:ND2	1.89	0.68
1:C:220:ILE:HG12	1:C:337:VAL:CG2	2.25	0.67
1:C:209:GLU:HG2	1:C:243:PRO:HD3	1.77	0.67
1:C:221:PRO:HB3	1:C:321:ILE:HG12	1.76	0.67
1:D:302:ARG:HG2	1:D:303:ALA:N	2.08	0.67
1:C:362:GLY:O	1:C:363:GLU:HG3	1.95	0.67
1:A:33:PHE:N	1:A:41:ASN:HD21	1.86	0.66
1:D:325:LEU:HD13	1:D:360:ILE:HD13	1.77	0.66
1:D:250:ASP:HA	1:D:291:VAL:HB	1.75	0.66
1:B:42:HIS:ND1	1:B:105:PHE:HB3	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:GLY:HA2	1:D:420:VAL:HG21	1.78	0.66
1:B:289:GLU:HG3	6:B:518:HOH:O	1.94	0.66
1:A:33:PHE:H	1:A:41:ASN:ND2	1.87	0.66
1:D:222:THR:HG22	1:D:339:VAL:CG2	2.26	0.66
1:C:247:ILE:HA	1:C:308:VAL:HG23	1.78	0.65
1:D:99:LYS:HE3	2:D:443:SO4:O2	1.97	0.65
1:C:322:LEU:HB3	1:C:361:LEU:HD11	1.78	0.64
1:C:229:GLN:NE2	1:C:229:GLN:H	1.95	0.64
1:C:235:LEU:HD13	1:C:247:ILE:HD13	1.78	0.64
1:D:401:GLY:HA3	1:D:406:LEU:HD11	1.79	0.64
1:C:83:THR:O	1:C:87:VAL:HG23	1.98	0.64
1:D:298:LYS:HA	1:D:301:ASN:HD22	1.62	0.64
1:D:200:THR:HG21	1:D:376:GLY:HA3	1.78	0.63
1:D:325:LEU:O	1:D:329:LEU:HD13	1.97	0.63
1:D:224:ALA:HB1	1:D:253:MET:HG2	1.80	0.63
1:D:239:GLY:HA2	1:D:242:LEU:HD12	1.80	0.63
1:D:422:LEU:N	1:D:422:LEU:HD12	2.14	0.63
1:A:362:GLY:HA2	2:A:443:SO4:O3	1.98	0.63
1:D:331:ASP:HB3	1:D:334:ASN:ND2	2.13	0.62
1:D:211:THR:HG21	1:D:335:ALA:CB	2.27	0.62
1:D:321:ILE:O	1:D:325:LEU:HG	2.00	0.62
1:A:381:ALA:HB3	1:A:386:LEU:HD13	1.82	0.62
1:C:358:VAL:O	1:C:365:VAL:HG22	2.00	0.62
1:D:253:MET:HA	1:D:256:ARG:HH21	1.65	0.62
1:A:321:ILE:O	1:A:325:LEU:HD13	2.00	0.62
1:D:209:GLU:HG3	1:D:243:PRO:HD3	1.81	0.61
1:D:97:ALA:O	1:D:101:MET:HB2	2.01	0.61
1:D:309:VAL:C	1:D:310:LEU:HD12	2.22	0.60
1:D:12:VAL:HG23	1:D:13:THR:HG23	1.83	0.60
1:C:1:MET:HG2	1:C:431:VAL:HG21	1.83	0.60
1:A:253:MET:HA	1:A:256:ARG:NH2	2.17	0.60
1:D:139:ALA:O	1:D:174:PRO:HG3	2.01	0.60
1:D:208:LEU:HD23	1:D:218:VAL:HG11	1.83	0.60
1:D:10:ARG:NH1	1:D:424:ARG:HG3	2.17	0.60
1:D:253:MET:HA	1:D:256:ARG:NH2	2.16	0.60
1:A:306:PRO:HD2	1:B:302:ARG:NH2	2.12	0.60
1:C:34:GLN:NE2	1:C:63:ASP:HB3	2.17	0.59
1:D:85:ALA:HB3	1:D:144:GLY:HA3	1.83	0.59
1:A:182:LEU:HD11	1:A:397:VAL:HG23	1.84	0.59
1:B:269:SER:O	1:B:273:GLN:HG3	2.01	0.59
1:A:259:SER:O	1:A:262:PRO:HD2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:VAL:HG13	1:C:118:LEU:HD13	1.84	0.59
1:D:33:PHE:H	1:D:41:ASN:ND2	1.90	0.59
1:C:209:GLU:HG2	1:C:243:PRO:CD	2.33	0.58
1:C:424:ARG:HD3	1:C:427:GLU:OE2	2.02	0.58
1:B:289:GLU:CG	6:B:518:HOH:O	2.50	0.58
1:C:85:ALA:HB2	1:C:267:TYR:CD2	2.38	0.58
1:C:222:THR:HG22	1:C:339:VAL:HG21	1.86	0.58
1:C:170:VAL:HG13	1:C:171:LEU:HD13	1.86	0.58
1:D:45:PHE:HB3	1:D:47:PHE:CE1	2.39	0.58
1:B:359:ARG:HD2	1:B:364:GLU:OE2	2.04	0.57
1:B:235:LEU:HD13	1:B:247:ILE:HD13	1.86	0.57
1:D:229:GLN:H	1:D:229:GLN:NE2	2.02	0.57
1:D:59:HIS:CD2	1:D:61:HIS:HB2	2.39	0.57
1:D:98:LEU:HD21	1:D:108:PRO:CB	2.34	0.57
1:A:57:LEU:HG	1:A:65:VAL:HG12	1.85	0.57
1:B:1:MET:HG3	1:B:21:ALA:HB2	1.85	0.57
1:C:86:THR:HG22	1:C:90:MET:CE	2.34	0.57
1:D:34:GLN:HE21	1:D:63:ASP:HB3	1.70	0.57
1:B:12:VAL:HG21	4:B:456:U5P:O2	2.04	0.57
1:B:165:ASN:C	1:B:165:ASN:HD22	2.07	0.57
1:C:217:LYS:HB2	1:C:334:ASN:OD1	2.04	0.57
1:C:98:LEU:HD11	1:C:108:PRO:CA	2.26	0.57
1:C:355:PRO:HB2	1:C:356:PRO:HD2	1.87	0.57
1:A:163:LEU:HD21	1:A:389:TRP:CD2	2.40	0.57
1:C:10:ARG:NH2	1:C:424:ARG:NH1	2.53	0.56
1:C:220:ILE:HG23	1:C:337:VAL:HG23	1.87	0.56
1:C:40:ARG:HD2	6:C:467:HOH:O	2.05	0.56
1:D:355:PRO:HB2	1:D:356:PRO:HD2	1.86	0.56
1:A:129:LEU:HD21	6:A:575:HOH:O	2.05	0.56
1:C:163:LEU:HD21	1:C:389:TRP:CE3	2.40	0.56
1:A:189:TYR:CZ	4:A:465:U5P:H5	2.40	0.56
1:C:225:VAL:O	1:C:257:VAL:HG11	2.06	0.56
1:A:284:ARG:HD3	1:A:288:LEU:HD23	1.88	0.56
1:A:195:ARG:HD2	1:A:199:GLU:OE2	2.05	0.56
1:D:240:HIS:ND1	1:D:241:ARG:N	2.54	0.56
1:C:88:LEU:HB3	1:C:260:LEU:HD21	1.88	0.56
1:C:321:ILE:O	1:C:325:LEU:HD13	2.05	0.55
1:C:59:HIS:CD2	1:C:61:HIS:HB2	2.41	0.55
1:C:402:GLU:HB3	1:C:404:GLU:OE2	2.07	0.55
1:B:86:THR:HG22	1:B:90:MET:HE2	1.89	0.55
1:C:298:LYS:HD2	2:C:453:SO4:O3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:VAL:HG12	1:D:171:LEU:HD12	1.87	0.55
1:D:396:VAL:HG12	1:D:398:LEU:HD12	1.89	0.55
1:D:229:GLN:H	1:D:229:GLN:CD	2.10	0.55
1:C:331:ASP:HB3	1:C:334:ASN:ND2	2.21	0.55
1:C:360:ILE:CG2	1:C:361:LEU:HD13	2.34	0.54
1:D:360:ILE:O	1:D:361:LEU:HB2	2.07	0.54
1:B:27:LEU:HD13	1:B:29:ASP:O	2.07	0.54
1:A:370:SER:HA	2:A:451:SO4:O2	2.07	0.54
1:B:202:ARG:O	1:B:206:GLU:HG3	2.07	0.54
1:C:401:GLY:HA3	1:C:406:LEU:HD11	1.89	0.54
1:D:284:ARG:HD3	1:D:288:LEU:CD2	2.33	0.54
1:C:236:TYR:HD1	1:C:285:PRO:HA	1.73	0.54
1:B:208:LEU:HD21	1:B:218:VAL:HG11	1.90	0.54
1:D:229:GLN:HG3	1:D:261:TYR:CZ	2.42	0.54
1:D:224:ALA:CB	1:D:253:MET:HG2	2.38	0.53
1:C:182:LEU:HD11	1:C:397:VAL:HG23	1.89	0.53
1:D:236:TYR:OH	1:D:280:LYS:HE2	2.08	0.53
1:A:359:ARG:NH1	2:A:443:SO4:O3	2.41	0.53
1:D:86:THR:HG22	1:D:90:MET:CE	2.39	0.53
1:D:225:VAL:O	1:D:257:VAL:HG11	2.08	0.53
1:D:69:PRO:O	1:D:110:ASP:HB3	2.09	0.53
1:C:214:GLN:NE2	1:C:333:ARG:HA	2.24	0.53
1:D:2:ARG:HG3	1:D:430:PRO:HA	1.90	0.53
1:D:1:MET:HG3	1:D:21:ALA:CB	2.35	0.53
1:D:360:ILE:CG2	1:D:361:LEU:HD13	2.38	0.53
1:C:270:GLU:HA	1:C:270:GLU:OE1	2.09	0.52
1:B:226:GLU:HG2	6:B:538:HOH:O	2.08	0.52
1:C:236:TYR:CD1	1:C:285:PRO:HA	2.45	0.52
1:A:344:GLN:HA	1:A:344:GLN:NE2	2.24	0.52
1:C:86:THR:HG22	1:C:90:MET:HE2	1.92	0.52
1:A:98:LEU:HD11	1:A:108:PRO:HA	1.91	0.52
1:C:57:LEU:HG	1:C:65:VAL:HG12	1.92	0.52
1:A:263:ARG:HG2	1:D:277:LEU:HD21	1.91	0.52
1:D:86:THR:HG22	1:D:90:MET:HE2	1.91	0.52
1:B:274:ALA:O	1:B:278:GLN:HG2	2.10	0.52
1:C:5:PRO:HG2	1:C:423:ALA:HB1	1.91	0.52
1:B:411:LYS:HB2	3:B:455:FLC:OHB	2.10	0.52
1:B:42:HIS:CE1	1:B:105:PHE:HB3	2.45	0.52
1:D:214:GLN:HE21	1:D:333:ARG:HA	1.75	0.52
1:C:28:LEU:O	1:C:29:ASP:HB2	2.09	0.52
1:D:68:LEU:N	1:D:69:PRO:HD2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:VAL:HG21	1:D:393:GLU:HG3	1.92	0.51
1:C:294:THR:O	1:C:298:LYS:HG2	2.11	0.51
1:B:102:ASP:HA	6:B:524:HOH:O	2.09	0.51
1:D:155:ARG:HD3	1:D:431:VAL:O	2.11	0.51
1:D:11:GLU:CD	1:D:40:ARG:HH12	2.14	0.51
1:C:309:VAL:C	1:C:310:LEU:HD12	2.30	0.51
1:C:155:ARG:HD3	1:C:431:VAL:O	2.11	0.51
1:A:11:GLU:OE2	1:A:40:ARG:NH1	2.42	0.51
1:C:292:GLU:HB2	2:C:433:SO4:O2	2.11	0.51
1:A:297:SER:OG	1:A:320:ARG:HG2	2.11	0.51
1:C:84:ARG:NH1	2:C:451:SO4:O3	2.36	0.51
1:A:32:MET:HA	1:A:67:ARG:HG3	1.93	0.50
1:D:218:VAL:O	1:D:220:ILE:HG13	2.11	0.50
1:C:59:HIS:HD2	1:C:61:HIS:H	1.58	0.50
1:D:214:GLN:NE2	1:D:333:ARG:HA	2.27	0.50
1:C:409:LEU:HD22	1:C:413:LEU:HG	1.92	0.50
1:B:208:LEU:CD2	1:B:218:VAL:HG11	2.41	0.50
1:C:247:ILE:HG12	1:C:308:VAL:CG2	2.41	0.50
1:A:134:LEU:HD23	1:A:150:ALA:HA	1.92	0.50
1:C:170:VAL:HG13	1:C:171:LEU:CD1	2.41	0.50
1:C:170:VAL:HG22	1:C:171:LEU:HD12	1.93	0.50
1:C:9:ALA:O	1:C:11:GLU:HG2	2.11	0.50
1:B:211:THR:HA	1:B:214:GLN:HG2	1.93	0.50
1:D:208:LEU:CD2	1:D:218:VAL:HG11	2.41	0.50
1:C:10:ARG:HH22	1:C:424:ARG:HH11	1.59	0.50
1:B:12:VAL:HG23	1:B:13:THR:HG23	1.93	0.50
1:A:344:GLN:CA	1:A:344:GLN:HE21	2.25	0.50
1:D:228:ALA:HB3	1:D:229:GLN:NE2	2.27	0.50
1:D:42:HIS:CE1	1:D:105:PHE:HB3	2.47	0.50
1:C:365:VAL:O	1:C:365:VAL:HG23	2.12	0.49
1:D:298:LYS:HA	1:D:301:ASN:ND2	2.25	0.49
1:A:359:ARG:NH2	2:A:444:SO4:O2	2.45	0.49
1:C:381:ALA:HB3	1:C:386:LEU:HD13	1.94	0.49
1:D:299:ALA:HA	1:D:302:ARG:HD2	1.94	0.49
1:D:226:GLU:N	6:D:476:HOH:O	2.44	0.49
1:B:208:LEU:CD2	1:B:218:VAL:HG21	2.41	0.49
1:D:219:LEU:HD21	1:D:324:HIS:O	2.12	0.49
1:B:34:GLN:HA	1:B:38:GLU:HG3	1.94	0.49
1:A:59:HIS:CD2	1:A:61:HIS:HB2	2.47	0.49
1:A:165:ASN:C	1:A:165:ASN:HD22	2.15	0.49
1:D:33:PHE:N	1:D:41:ASN:HD21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:VAL:O	1:A:420:VAL:HA	2.11	0.49
1:D:326:LYS:HD2	1:D:361:LEU:HD22	1.93	0.49
1:A:90:MET:HE1	1:A:118:LEU:HD22	1.94	0.49
1:A:306:PRO:CD	1:B:302:ARG:HH22	2.15	0.49
1:D:322:LEU:HA	1:D:325:LEU:HD11	1.94	0.49
1:C:250:ASP:HA	1:C:291:VAL:HB	1.94	0.49
1:A:168:LYS:HE3	1:A:230:GLU:CD	2.33	0.49
1:C:128:ARG:NH2	6:C:471:HOH:O	2.45	0.49
1:D:240:HIS:CE1	1:D:241:ARG:HB3	2.48	0.49
1:B:34:GLN:HE21	1:B:63:ASP:HB3	1.78	0.49
1:D:65:VAL:CG1	1:D:94:LEU:HD11	2.43	0.49
1:B:163:LEU:HD21	1:B:389:TRP:CE3	2.48	0.49
1:B:11:GLU:OE1	1:B:40:ARG:NH1	2.45	0.48
1:A:389:TRP:HE3	1:A:390:LEU:HD13	1.78	0.48
1:D:239:GLY:HA2	1:D:242:LEU:CD1	2.43	0.48
1:D:329:LEU:HA	1:D:369:ALA:CB	2.43	0.48
1:D:12:VAL:HG12	1:D:401:GLY:HA2	1.95	0.48
1:D:203:GLU:O	1:D:207:ILE:HG13	2.13	0.48
1:D:402:GLU:O	1:D:406:LEU:HD13	2.14	0.48
1:C:366:PRO:HG2	2:C:454:SO4:O2	2.14	0.48
1:D:197:TYR:O	1:D:201:VAL:HG23	2.14	0.48
1:D:221:PRO:HD2	1:D:337:VAL:O	2.13	0.48
1:C:84:ARG:HB3	1:C:267:TYR:OH	2.13	0.48
1:C:323:HIS:ND1	2:C:453:SO4:O2	2.47	0.48
1:D:384:ASP:OD2	1:D:384:ASP:N	2.46	0.48
1:D:62:LEU:HD13	1:D:93:VAL:HG12	1.95	0.48
1:C:325:LEU:HG	1:C:329:LEU:HD11	1.96	0.48
1:C:57:LEU:HD23	1:C:90:MET:CE	2.44	0.48
1:D:280:LYS:O	1:D:282:PRO:HD3	2.14	0.48
1:C:113:GLU:OE2	1:C:117:HIS:HE1	1.96	0.48
1:D:34:GLN:NE2	1:D:63:ASP:HB3	2.29	0.48
1:D:3:ILE:HG12	1:D:184:LEU:HD22	1.95	0.48
1:C:142:LEU:HG	1:C:143:PRO:HD2	1.96	0.48
1:B:168:LYS:HG2	1:B:197:TYR:CE2	2.48	0.48
1:A:43:ALA:HB1	1:A:44:PRO:HD2	1.95	0.48
1:B:11:GLU:OE2	1:B:37:GLU:HG3	2.13	0.47
1:D:227:ARG:HG2	1:D:227:ARG:HH11	1.79	0.47
1:D:165:ASN:C	1:D:165:ASN:HD22	2.16	0.47
1:D:211:THR:OG1	1:D:218:VAL:HG22	2.15	0.47
1:C:247:ILE:HG12	1:C:308:VAL:HG21	1.96	0.47
1:B:168:LYS:HE2	1:B:230:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:LEU:HD22	1:B:226:GLU:HB2	1.96	0.47
1:C:226:GLU:HG2	1:C:261:TYR:OH	2.13	0.47
1:A:163:LEU:HD21	1:A:389:TRP:CE3	2.48	0.47
1:D:329:LEU:HA	1:D:369:ALA:HB2	1.97	0.47
1:D:360:ILE:HD12	1:D:365:VAL:HG11	1.97	0.47
1:B:165:ASN:C	1:B:165:ASN:ND2	2.66	0.47
1:A:389:TRP:CE3	1:A:390:LEU:HD13	2.50	0.47
1:B:221:PRO:HB3	1:B:321:ILE:HG12	1.96	0.47
1:D:399:VAL:HG12	1:D:423:ALA:HB3	1.97	0.47
1:C:211:THR:HG21	1:C:335:ALA:CB	2.45	0.47
1:D:359:ARG:HD3	1:D:362:GLY:HA2	1.97	0.47
1:C:262:PRO:HG3	1:C:281:ASN:ND2	2.30	0.47
1:D:231:ILE:O	1:D:235:LEU:HD13	2.14	0.46
1:C:253:MET:O	1:C:257:VAL:HG23	2.15	0.46
1:D:202:ARG:O	1:D:206:GLU:HG3	2.15	0.46
1:B:420:VAL:HG22	1:B:421:SER:N	2.30	0.46
1:D:65:VAL:HG11	1:D:94:LEU:HD11	1.97	0.46
1:B:404:GLU:HA	1:B:404:GLU:OE2	2.16	0.46
1:D:347:LEU:HD12	1:D:347:LEU:H	1.81	0.46
1:B:68:LEU:N	1:B:69:PRO:HD2	2.30	0.46
1:D:336:LEU:C	1:D:336:LEU:HD23	2.35	0.46
1:D:204:PHE:O	1:D:208:LEU:HG	2.15	0.46
1:D:318:GLY:HA2	1:D:322:LEU:CD1	2.43	0.46
1:A:45:PHE:HB3	1:A:47:PHE:CE1	2.51	0.46
1:A:85:ALA:HB3	1:A:144:GLY:HA3	1.97	0.46
1:A:401:GLY:HA3	1:A:406:LEU:HD13	1.97	0.46
1:B:36:LYS:C	1:B:37:GLU:HG2	2.37	0.46
1:A:153:GLU:CG	2:A:433:SO4:O1	2.50	0.46
1:D:319:GLY:C	1:D:321:ILE:H	2.20	0.46
1:C:57:LEU:HD21	1:C:68:LEU:HD22	1.98	0.46
1:C:214:GLN:HE21	1:C:333:ARG:HA	1.81	0.46
1:D:347:LEU:N	1:D:347:LEU:HD12	2.30	0.46
1:C:192:ARG:HA	1:C:383:GLN:NE2	2.31	0.46
1:B:98:LEU:HD11	1:B:108:PRO:HA	1.97	0.46
1:D:28:LEU:O	1:D:29:ASP:HB2	2.14	0.46
1:C:85:ALA:HB2	1:C:267:TYR:CE2	2.51	0.45
1:C:420:VAL:HG22	1:C:421:SER:N	2.31	0.45
1:B:411:LYS:HD2	3:B:455:FLC:OHB	2.15	0.45
1:B:217:LYS:HG2	1:B:307:MET:HG2	1.97	0.45
1:C:177:PRO:HD3	1:C:389:TRP:CE2	2.51	0.45
1:B:348:GLY:O	1:B:352:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:VAL:O	1:D:238:HIS:HB2	2.17	0.45
1:D:347:LEU:O	1:D:351:ILE:HG13	2.16	0.45
1:D:217:LYS:HG2	1:D:307:MET:HG2	1.99	0.45
1:A:289:GLU:HG3	6:A:502:HOH:O	2.17	0.45
1:B:163:LEU:HD21	1:B:389:TRP:CD2	2.51	0.45
1:C:214:GLN:O	1:C:333:ARG:HD2	2.17	0.45
1:B:140:GLY:O	1:B:164:GLY:HA3	2.17	0.45
1:B:276:PHE:HA	1:B:280:LYS:O	2.17	0.45
1:A:31:GLY:HA3	1:A:63:ASP:O	2.16	0.45
1:C:399:VAL:HG12	1:C:423:ALA:HB3	1.98	0.45
1:C:140:GLY:O	1:C:164:GLY:HA3	2.17	0.45
1:B:178:PRO:HB3	1:C:126:TRP:CE3	2.52	0.45
1:D:326:LYS:O	1:D:326:LYS:HG2	2.17	0.45
1:C:143:PRO:HD3	1:C:226:GLU:HG3	1.99	0.45
1:C:229:GLN:HG3	1:C:261:TYR:CZ	2.53	0.45
1:C:267:TYR:HA	6:C:500:HOH:O	2.16	0.45
1:D:90:MET:HE1	1:D:118:LEU:HD22	1.99	0.45
1:A:192:ARG:NH2	2:A:463:SO4:O2	2.47	0.45
1:B:182:LEU:HD11	1:B:397:VAL:HG23	1.99	0.45
1:D:397:VAL:HG21	1:D:429:VAL:HG11	1.98	0.45
1:A:407:LEU:HD13	1:A:422:LEU:CD2	2.47	0.45
1:B:428:GLY:H	4:B:457:U5P:C5	2.30	0.44
1:D:386:LEU:O	1:D:390:LEU:HD22	2.17	0.44
1:A:235:LEU:HD13	1:A:247:ILE:HD13	1.99	0.44
1:A:318:GLY:HA2	1:A:322:LEU:CD1	2.47	0.44
1:A:262:PRO:O	1:A:265:VAL:HG23	2.18	0.44
1:A:341:TYR:HB3	4:A:465:U5P:H5'2	2.00	0.44
1:C:211:THR:HG21	1:C:335:ALA:HB3	1.98	0.44
1:C:331:ASP:HB3	1:C:334:ASN:HD22	1.83	0.44
1:B:318:GLY:HA2	1:B:322:LEU:CD1	2.48	0.44
1:B:37:GLU:O	1:B:39:ALA:N	2.50	0.44
1:C:312:GLY:HA2	1:C:313:SER:C	2.38	0.44
1:C:1:MET:HG2	1:C:431:VAL:CG2	2.47	0.44
1:C:302:ARG:HG2	1:C:302:ARG:HH21	1.83	0.44
1:B:32:MET:HE2	1:B:105:PHE:HZ	1.82	0.44
1:C:294:THR:O	1:C:297:SER:HB3	2.17	0.44
1:B:259:SER:O	1:B:262:PRO:HD2	2.17	0.44
1:D:235:LEU:O	1:D:239:GLY:HA3	2.17	0.44
1:C:251:SER:HB3	1:C:254:ALA:HB3	2.00	0.44
1:B:91:GLU:O	1:B:95:GLU:HG2	2.18	0.44
1:D:359:ARG:HD2	1:D:359:ARG:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:ILE:HG22	1:D:222:THR:HG23	2.00	0.44
1:D:359:ARG:HD3	1:D:362:GLY:CA	2.48	0.44
1:C:239:GLY:C	1:C:241:ARG:H	2.20	0.44
1:D:422:LEU:CD1	1:D:422:LEU:N	2.80	0.43
1:A:102:ASP:HB2	6:A:580:HOH:O	2.17	0.43
1:A:57:LEU:HD23	1:A:90:MET:HE2	1.98	0.43
1:D:233:TYR:CE1	1:D:282:PRO:HB2	2.53	0.43
1:D:3:ILE:HG23	1:D:3:ILE:O	2.18	0.43
1:A:85:ALA:HB2	1:A:267:TYR:CD2	2.53	0.43
1:B:344:GLN:H	1:B:344:GLN:NE2	2.17	0.43
1:C:10:ARG:NH2	1:C:424:ARG:HH12	2.15	0.43
1:D:252:PRO:O	1:D:256:ARG:HG3	2.18	0.43
1:A:344:GLN:HE21	1:A:344:GLN:HA	1.79	0.43
1:A:266:ARG:HG2	6:A:501:HOH:O	2.17	0.43
1:D:158:VAL:HG23	1:D:180:ALA:HB2	2.01	0.43
1:A:289:GLU:CG	6:A:502:HOH:O	2.67	0.43
1:A:84:ARG:HB2	1:A:84:ARG:HE	1.40	0.43
1:D:235:LEU:HD23	1:D:247:ILE:HG21	2.00	0.43
1:D:325:LEU:HD12	1:D:326:LYS:N	2.34	0.43
1:B:101:MET:HG2	1:B:104:PRO:CB	2.41	0.43
1:D:65:VAL:HG12	1:D:65:VAL:O	2.19	0.43
1:B:113:GLU:OE2	1:B:117:HIS:HE1	2.01	0.43
1:C:229:GLN:HA	1:C:232:LEU:HD12	2.01	0.43
1:D:250:ASP:HB3	1:D:311:ALA:HB2	1.99	0.43
1:A:58:THR:O	1:A:145:SER:HA	2.18	0.43
1:A:212:LEU:CB	1:A:243:PRO:HG2	2.49	0.43
1:D:356:PRO:HG2	1:D:357:ALA:H	1.84	0.43
1:D:389:TRP:HE3	1:D:390:LEU:HD13	1.84	0.43
1:B:270:GLU:OE1	1:C:266:ARG:NH2	2.51	0.43
1:D:316:LEU:HD22	1:D:325:LEU:HD21	2.01	0.43
1:D:216:GLY:HA3	1:D:333:ARG:O	2.19	0.43
1:A:61:HIS:CD2	1:A:142:LEU:HD11	2.53	0.43
1:B:396:VAL:O	1:B:420:VAL:HA	2.19	0.43
1:A:98:LEU:HD11	1:A:108:PRO:CA	2.49	0.43
1:C:386:LEU:O	1:C:390:LEU:HD23	2.18	0.43
1:A:197:TYR:O	1:A:200:THR:HB	2.19	0.43
1:A:203:GLU:O	1:A:207:ILE:HG13	2.19	0.43
1:C:272:VAL:O	1:C:276:PHE:HD2	2.00	0.42
1:B:81:TYR:HA	1:B:119:ARG:O	2.19	0.42
1:B:33:PHE:HB3	1:B:37:GLU:HB2	2.00	0.42
1:D:396:VAL:HG12	1:D:398:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:VAL:HG12	1:D:310:LEU:N	2.32	0.42
1:D:401:GLY:CA	1:D:406:LEU:HD11	2.45	0.42
1:A:80:VAL:HB	1:A:118:LEU:HD23	2.01	0.42
1:D:5:PRO:HG2	1:D:423:ALA:HB1	2.00	0.42
1:B:344:GLN:H	1:B:344:GLN:CD	2.21	0.42
1:A:409:LEU:HD22	1:A:413:LEU:HG	2.01	0.42
1:D:32:MET:HB2	1:D:41:ASN:OD1	2.20	0.42
1:C:12:VAL:HG12	1:C:401:GLY:HA2	2.02	0.42
1:A:59:HIS:CE1	1:A:162:ASP:OD1	2.73	0.42
1:D:220:ILE:HG22	1:D:222:THR:CG2	2.49	0.42
1:B:318:GLY:HA2	1:B:322:LEU:HD11	2.02	0.42
1:B:347:LEU:HD11	1:B:358:VAL:HG11	2.01	0.42
1:B:126:TRP:CE3	1:C:178:PRO:HB3	2.54	0.42
1:A:77:ARG:HD2	2:A:459:SO4:O4	2.20	0.42
1:D:238:HIS:C	1:D:240:HIS:H	2.23	0.42
1:A:46:GLY:HA2	3:A:464:FLC:HG2	2.00	0.42
1:C:59:HIS:NE2	1:C:61:HIS:HB2	2.35	0.42
1:C:386:LEU:O	1:C:390:LEU:CD2	2.68	0.42
1:A:212:LEU:HB2	1:A:243:PRO:HG2	2.01	0.42
1:D:82:ALA:O	1:D:120:PRO:HA	2.20	0.42
1:A:365:VAL:HA	1:A:366:PRO:HD3	1.87	0.42
1:C:326:LYS:HD2	1:C:361:LEU:HD22	2.02	0.42
1:A:321:ILE:HG23	1:A:322:LEU:N	2.34	0.42
1:A:11:GLU:CD	1:A:40:ARG:HH12	2.23	0.42
1:A:191:ASP:CG	1:A:405:LYS:HD2	2.40	0.42
1:B:4:VAL:HA	1:B:5:PRO:HD3	1.85	0.41
1:A:140:GLY:O	1:A:164:GLY:HA3	2.19	0.41
1:D:302:ARG:HG2	1:D:303:ALA:H	1.81	0.41
1:D:297:SER:CB	1:D:320:ARG:HD2	2.50	0.41
1:B:203:GLU:O	1:B:207:ILE:HG13	2.20	0.41
1:D:58:THR:O	1:D:145:SER:HA	2.19	0.41
1:C:10:ARG:CD	1:C:422:LEU:HD23	2.51	0.41
1:A:407:LEU:HD13	1:A:422:LEU:HD21	2.02	0.41
1:A:354:ARG:N	1:A:355:PRO:CD	2.83	0.41
1:C:203:GLU:O	1:C:207:ILE:HG13	2.21	0.41
1:A:57:LEU:HD23	1:A:90:MET:CE	2.51	0.41
1:D:170:VAL:HG12	1:D:171:LEU:CD1	2.51	0.41
1:C:350:GLU:O	1:C:353:ALA:HB3	2.21	0.41
1:C:31:GLY:HA3	1:C:63:ASP:C	2.41	0.41
1:D:347:LEU:CD1	1:D:347:LEU:H	2.34	0.41
1:C:98:LEU:HD12	1:C:111:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:LEU:CD2	1:D:108:PRO:HA	2.51	0.41
1:A:318:GLY:HA2	1:A:322:LEU:HD11	2.02	0.41
1:A:90:MET:HE1	1:A:118:LEU:CD2	2.50	0.41
1:D:397:VAL:HA	1:D:421:SER:O	2.20	0.41
1:C:49:PRO:HB3	1:C:71:LEU:HD12	2.02	0.41
1:B:55:VAL:HG12	1:B:57:LEU:HD13	2.02	0.41
1:D:295:GLU:H	1:D:295:GLU:CD	2.22	0.41
1:B:10:ARG:HH11	1:B:10:ARG:HG2	1.86	0.41
1:A:91:GLU:O	1:A:95:GLU:HG2	2.21	0.41
1:D:409:LEU:HD22	1:D:413:LEU:HD11	2.02	0.41
1:B:365:VAL:HA	1:B:366:PRO:HD3	1.80	0.41
1:D:33:PHE:HD2	1:D:41:ASN:ND2	2.19	0.41
1:C:318:GLY:HA2	1:C:322:LEU:HD11	2.01	0.41
1:C:326:LYS:HE3	1:C:363:GLU:OE1	2.21	0.41
1:C:247:ILE:HG23	1:C:308:VAL:HG23	2.04	0.41
1:C:277:LEU:C	1:C:279:GLY:H	2.24	0.41
1:C:209:GLU:O	1:C:210:LYS:C	2.59	0.40
1:C:32:MET:HE3	1:C:62:LEU:HD22	2.03	0.40
1:A:420:VAL:HG22	1:A:421:SER:N	2.36	0.40
1:D:409:LEU:O	1:D:413:LEU:HG	2.21	0.40
1:C:91:GLU:O	1:C:95:GLU:HG2	2.21	0.40
1:C:227:ARG:HG2	1:C:227:ARG:HH21	1.86	0.40
1:B:32:MET:CE	1:B:105:PHE:HZ	2.34	0.40
1:A:126:TRP:CE3	1:A:135:ALA:HB2	2.56	0.40
1:C:360:ILE:HD12	1:C:365:VAL:HG21	2.03	0.40
1:C:170:VAL:C	1:C:171:LEU:HD12	2.42	0.40
1:C:95:GLU:HA	1:C:95:GLU:OE2	2.21	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	429/431 (100%)	411 (96%)	17 (4%)	1 (0%)	52	63
1	B	429/431 (100%)	413 (96%)	15 (4%)	1 (0%)	52	63
1	C	429/431 (100%)	395 (92%)	32 (8%)	2 (0%)	34	39
1	D	429/431 (100%)	378 (88%)	44 (10%)	7 (2%)	12	10
All	All	1716/1724 (100%)	1597 (93%)	108 (6%)	11 (1%)	30	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	38	GLU
1	D	102	ASP
1	A	102	ASP
1	C	102	ASP
1	C	198	ARG
1	D	166	ARG
1	D	244	ARG
1	D	38	GLU
1	D	316	LEU
1	D	15	SER
1	D	225	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	342/342 (100%)	322 (94%)	20 (6%)	25	29
1	B	342/342 (100%)	321 (94%)	21 (6%)	23	27
1	C	342/342 (100%)	324 (95%)	18 (5%)	28	34
1	D	342/342 (100%)	326 (95%)	16 (5%)	32	41
All	All	1368/1368 (100%)	1293 (94%)	75 (6%)	27	32

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	38	GLU
1	A	57	LEU
1	A	84	ARG
1	A	163	LEU
1	A	165	ASN
1	A	171	LEU
1	A	186	GLU
1	A	192	ARG
1	A	219	LEU
1	A	241	ARG
1	A	264	LEU
1	A	329	LEU
1	A	336	LEU
1	A	344	GLN
1	A	386	LEU
1	A	390	LEU
1	A	406	LEU
1	A	407	LEU
1	A	409	LEU
1	B	10	ARG
1	B	27	LEU
1	B	38	GLU
1	B	94	LEU
1	B	98	LEU
1	B	101	MET
1	B	102	ASP
1	B	163	LEU
1	B	165	ASN
1	B	186	GLU
1	B	192	ARG
1	B	219	LEU
1	B	264	LEU
1	B	325	LEU
1	B	329	LEU
1	B	365	VAL
1	B	386	LEU
1	B	390	LEU
1	B	406	LEU
1	B	407	LEU
1	B	409	LEU
1	C	27	LEU
1	C	28	LEU

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Mol	Chain	Res	Type
1	C	98	LEU
1	C	112	GLU
1	C	155	ARG
1	C	163	LEU
1	C	165	ASN
1	C	173	ASP
1	C	186	GLU
1	C	229	GLN
1	C	253	MET
1	C	336	LEU
1	C	344	GLN
1	C	386	LEU
1	C	398	LEU
1	C	407	LEU
1	C	409	LEU
1	C	415	LEU
1	D	27	LEU
1	D	57	LEU
1	D	96	ASP
1	D	155	ARG
1	D	165	ASN
1	D	186	GLU
1	D	192	ARG
1	D	195	ARG
1	D	229	GLN
1	D	253	MET
1	D	264	LEU
1	D	293	HIS
1	D	302	ARG
1	D	325	LEU
1	D	344	GLN
1	D	409	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	41	ASN
1	A	59	HIS
1	A	165	ASN
1	A	344	GLN
1	A	383	GLN

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Mol	Chain	Res	Type
1	B	34	GLN
1	B	41	ASN
1	B	59	HIS
1	B	61	HIS
1	B	165	ASN
1	B	275	HIS
1	B	383	GLN
1	C	34	GLN
1	C	41	ASN
1	C	59	HIS
1	C	165	ASN
1	C	214	GLN
1	C	229	GLN
1	C	275	HIS
1	C	383	GLN
1	D	34	GLN
1	D	41	ASN
1	D	165	ASN
1	D	194	HIS
1	D	214	GLN
1	D	229	GLN
1	D	301	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 113 ligands modelled in this entry, 8 are monoatomic - leaving 105 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	432	-	4,4,4	1.53	0	6,6,6	0.94	0
2	SO4	A	433	-	4,4,4	1.50	0	6,6,6	0.94	0
2	SO4	A	434	-	4,4,4	1.52	0	6,6,6	0.95	0
2	SO4	A	435	-	4,4,4	1.55	0	6,6,6	0.94	0
2	SO4	A	436	-	4,4,4	1.53	0	6,6,6	0.93	0
2	SO4	A	437	-	4,4,4	1.53	0	6,6,6	0.94	0
2	SO4	A	438	-	4,4,4	1.52	0	6,6,6	0.92	0
2	SO4	A	439	-	4,4,4	1.47	0	6,6,6	0.96	0
2	SO4	A	440	-	4,4,4	1.56	0	6,6,6	0.93	0
2	SO4	A	441	-	4,4,4	1.52	0	6,6,6	0.92	0
2	SO4	A	442	-	4,4,4	1.50	0	6,6,6	0.94	0
2	SO4	A	443	-	4,4,4	1.52	0	6,6,6	0.94	0
2	SO4	A	444	-	4,4,4	1.45	0	6,6,6	0.98	0
2	SO4	A	445	-	4,4,4	1.51	0	6,6,6	0.95	0
2	SO4	A	446	-	4,4,4	1.51	0	6,6,6	0.93	0
2	SO4	A	447	-	4,4,4	1.53	0	6,6,6	0.92	0
2	SO4	A	448	-	4,4,4	1.54	0	6,6,6	0.93	0
2	SO4	A	449	-	4,4,4	1.51	0	6,6,6	0.94	0
2	SO4	A	450	-	4,4,4	1.50	0	6,6,6	0.94	0
2	SO4	A	451	-	4,4,4	1.46	0	6,6,6	0.96	0
2	SO4	A	452	-	4,4,4	1.55	0	6,6,6	0.93	0
2	SO4	A	453	-	4,4,4	1.51	0	6,6,6	0.96	0
2	SO4	A	454	-	4,4,4	1.49	0	6,6,6	0.83	0
2	SO4	A	455	-	4,4,4	1.51	0	6,6,6	0.94	0
2	SO4	A	456	-	4,4,4	1.54	0	6,6,6	0.96	0
2	SO4	A	457	-	4,4,4	1.48	0	6,6,6	0.95	0
2	SO4	A	458	-	4,4,4	1.50	0	6,6,6	0.96	0
2	SO4	A	459	-	4,4,4	1.47	0	6,6,6	0.98	0
2	SO4	A	460	-	4,4,4	1.55	0	6,6,6	0.91	0
2	SO4	A	461	-	4,4,4	1.51	0	6,6,6	0.94	0
2	SO4	A	462	-	4,4,4	1.50	0	6,6,6	0.94	0
2	SO4	A	463	-	4,4,4	1.48	0	6,6,6	0.95	0
3	FLC	A	464	-	3,12,12	0.98	0	3,17,17	0.79	0
4	U5P	A	465	-	16,22,22	1.85	6 (37%)	21,33,33	1.80	1 (4%)
4	U5P	A	466	-	16,22,22	2.03	6 (37%)	21,33,33	2.03	1 (4%)
4	U5P	A	467	-	16,22,22	1.93	6 (37%)	21,33,33	1.91	1 (4%)
2	SO4	B	432	-	4,4,4	1.50	0	6,6,6	0.92	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	B	433	-	4,4,4	1.53	0	6,6,6	0.95	0
2	SO4	B	434	-	4,4,4	1.55	0	6,6,6	0.95	0
2	SO4	B	435	-	4,4,4	1.49	0	6,6,6	0.95	0
2	SO4	B	436	-	4,4,4	1.42	0	6,6,6	1.04	1 (16%)
2	SO4	B	437	-	4,4,4	1.49	0	6,6,6	0.95	0
2	SO4	B	438	-	4,4,4	1.49	0	6,6,6	0.93	0
2	SO4	B	439	-	4,4,4	1.54	0	6,6,6	0.93	0
2	SO4	B	440	-	4,4,4	1.50	0	6,6,6	0.93	0
2	SO4	B	441	-	4,4,4	1.50	0	6,6,6	0.95	0
2	SO4	B	442	-	4,4,4	1.50	0	6,6,6	0.94	0
2	SO4	B	443	-	4,4,4	1.50	0	6,6,6	0.95	0
2	SO4	B	444	-	4,4,4	1.51	0	6,6,6	0.94	0
2	SO4	B	445	-	4,4,4	1.61	0	6,6,6	0.86	0
2	SO4	B	446	-	4,4,4	1.48	0	6,6,6	0.99	0
2	SO4	B	447	-	4,4,4	1.51	0	6,6,6	0.95	0
2	SO4	B	448	-	4,4,4	1.54	0	6,6,6	0.94	0
2	SO4	B	449	-	4,4,4	1.50	0	6,6,6	0.95	0
2	SO4	B	450	-	4,4,4	1.52	0	6,6,6	0.94	0
2	SO4	B	451	-	4,4,4	1.53	0	6,6,6	0.94	0
2	SO4	B	452	-	4,4,4	1.46	0	6,6,6	0.96	0
2	SO4	B	453	-	4,4,4	1.53	0	6,6,6	0.94	0
2	SO4	B	454	-	4,4,4	1.53	0	6,6,6	0.93	0
3	FLC	B	455	-	3,12,12	1.27	0	3,17,17	0.60	0
4	U5P	B	456	-	16,22,22	1.83	5 (31%)	21,33,33	1.82	1 (4%)
4	U5P	B	457	-	16,22,22	1.94	6 (37%)	21,33,33	2.01	1 (4%)
2	SO4	C	432	-	4,4,4	1.51	0	6,6,6	0.94	0
2	SO4	C	433	-	4,4,4	1.52	0	6,6,6	0.96	0
2	SO4	C	434	-	4,4,4	1.48	0	6,6,6	0.95	0
2	SO4	C	435	-	4,4,4	1.50	0	6,6,6	0.94	0
2	SO4	C	436	-	4,4,4	1.49	0	6,6,6	0.95	0
2	SO4	C	437	-	4,4,4	1.52	0	6,6,6	0.93	0
2	SO4	C	438	-	4,4,4	1.48	0	6,6,6	0.96	0
2	SO4	C	439	-	4,4,4	1.51	0	6,6,6	0.95	0
2	SO4	C	440	-	4,4,4	1.50	0	6,6,6	0.94	0
2	SO4	C	441	-	4,4,4	1.49	0	6,6,6	0.96	0
2	SO4	C	442	-	4,4,4	1.50	0	6,6,6	0.95	0
2	SO4	C	443	-	4,4,4	1.53	0	6,6,6	0.92	0
2	SO4	C	444	-	4,4,4	1.51	0	6,6,6	0.96	0
2	SO4	C	445	-	4,4,4	1.52	0	6,6,6	0.96	0
2	SO4	C	446	-	4,4,4	1.51	0	6,6,6	0.94	0
2	SO4	C	447	-	4,4,4	1.52	0	6,6,6	0.94	0
2	SO4	C	448	-	4,4,4	1.51	0	6,6,6	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	C	449	-	4,4,4	1.50	0	6,6,6	0.94	0
2	SO4	C	450	-	4,4,4	1.53	0	6,6,6	0.93	0
2	SO4	C	451	-	4,4,4	1.53	0	6,6,6	0.92	0
2	SO4	C	452	-	4,4,4	1.49	0	6,6,6	0.94	0
2	SO4	C	453	-	4,4,4	1.52	0	6,6,6	0.96	0
2	SO4	C	454	-	4,4,4	1.51	0	6,6,6	0.96	0
2	SO4	C	455	-	4,4,4	1.49	0	6,6,6	0.95	0
2	SO4	C	456	-	4,4,4	1.52	0	6,6,6	0.93	0
4	U5P	C	457	-	16,22,22	1.91	6 (37%)	21,33,33	1.88	1 (4%)
2	SO4	D	432	-	4,4,4	1.48	0	6,6,6	0.95	0
2	SO4	D	433	-	4,4,4	1.50	0	6,6,6	0.92	0
2	SO4	D	434	-	4,4,4	1.54	0	6,6,6	0.94	0
2	SO4	D	435	-	4,4,4	1.51	0	6,6,6	0.95	0
2	SO4	D	436	-	4,4,4	1.51	0	6,6,6	0.94	0
2	SO4	D	437	-	4,4,4	1.50	0	6,6,6	0.94	0
2	SO4	D	438	-	4,4,4	1.48	0	6,6,6	0.95	0
2	SO4	D	439	-	4,4,4	1.49	0	6,6,6	0.95	0
2	SO4	D	440	-	4,4,4	1.50	0	6,6,6	0.95	0
2	SO4	D	441	-	4,4,4	1.51	0	6,6,6	0.94	0
2	SO4	D	442	-	4,4,4	1.51	0	6,6,6	0.95	0
2	SO4	D	443	-	4,4,4	1.48	0	6,6,6	0.95	0
2	SO4	D	444	-	4,4,4	1.50	0	6,6,6	0.94	0
2	SO4	D	445	-	4,4,4	1.51	0	6,6,6	0.93	0
2	SO4	D	446	-	4,4,4	1.51	0	6,6,6	0.94	0
2	SO4	D	447	-	4,4,4	1.51	0	6,6,6	0.95	0
4	U5P	D	448	-	16,22,22	1.96	6 (37%)	21,33,33	1.88	1 (4%)

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	432	-	-	0/0/0/0	0/0/0/0
2	SO4	A	433	-	-	0/0/0/0	0/0/0/0
2	SO4	A	434	-	-	0/0/0/0	0/0/0/0
2	SO4	A	435	-	-	0/0/0/0	0/0/0/0
2	SO4	A	436	-	-	0/0/0/0	0/0/0/0
2	SO4	A	437	-	-	0/0/0/0	0/0/0/0
2	SO4	A	438	-	-	0/0/0/0	0/0/0/0
2	SO4	A	439	-	-	0/0/0/0	0/0/0/0
2	SO4	A	440	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	441	-	-	0/0/0/0	0/0/0/0
2	SO4	A	442	-	-	0/0/0/0	0/0/0/0
2	SO4	A	443	-	-	0/0/0/0	0/0/0/0
2	SO4	A	444	-	-	0/0/0/0	0/0/0/0
2	SO4	A	445	-	-	0/0/0/0	0/0/0/0
2	SO4	A	446	-	-	0/0/0/0	0/0/0/0
2	SO4	A	447	-	-	0/0/0/0	0/0/0/0
2	SO4	A	448	-	-	0/0/0/0	0/0/0/0
2	SO4	A	449	-	-	0/0/0/0	0/0/0/0
2	SO4	A	450	-	-	0/0/0/0	0/0/0/0
2	SO4	A	451	-	-	0/0/0/0	0/0/0/0
2	SO4	A	452	-	-	0/0/0/0	0/0/0/0
2	SO4	A	453	-	-	0/0/0/0	0/0/0/0
2	SO4	A	454	-	-	0/0/0/0	0/0/0/0
2	SO4	A	455	-	-	0/0/0/0	0/0/0/0
2	SO4	A	456	-	-	0/0/0/0	0/0/0/0
2	SO4	A	457	-	-	0/0/0/0	0/0/0/0
2	SO4	A	458	-	-	0/0/0/0	0/0/0/0
2	SO4	A	459	-	-	0/0/0/0	0/0/0/0
2	SO4	A	460	-	-	0/0/0/0	0/0/0/0
2	SO4	A	461	-	-	0/0/0/0	0/0/0/0
2	SO4	A	462	-	-	0/0/0/0	0/0/0/0
2	SO4	A	463	-	-	0/0/0/0	0/0/0/0
3	FLC	A	464	-	-	0/6/16/16	0/0/0/0
4	U5P	A	465	-	-	0/6/26/26	0/2/2/2
4	U5P	A	466	-	-	0/6/26/26	0/2/2/2
4	U5P	A	467	-	-	0/6/26/26	0/2/2/2
2	SO4	B	432	-	-	0/0/0/0	0/0/0/0
2	SO4	B	433	-	-	0/0/0/0	0/0/0/0
2	SO4	B	434	-	-	0/0/0/0	0/0/0/0
2	SO4	B	435	-	-	0/0/0/0	0/0/0/0
2	SO4	B	436	-	-	0/0/0/0	0/0/0/0
2	SO4	B	437	-	-	0/0/0/0	0/0/0/0
2	SO4	B	438	-	-	0/0/0/0	0/0/0/0
2	SO4	B	439	-	-	0/0/0/0	0/0/0/0
2	SO4	B	440	-	-	0/0/0/0	0/0/0/0
2	SO4	B	441	-	-	0/0/0/0	0/0/0/0
2	SO4	B	442	-	-	0/0/0/0	0/0/0/0
2	SO4	B	443	-	-	0/0/0/0	0/0/0/0
2	SO4	B	444	-	-	0/0/0/0	0/0/0/0
2	SO4	B	445	-	-	0/0/0/0	0/0/0/0
2	SO4	B	446	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	B	447	-	-	0/0/0/0	0/0/0/0
2	SO4	B	448	-	-	0/0/0/0	0/0/0/0
2	SO4	B	449	-	-	0/0/0/0	0/0/0/0
2	SO4	B	450	-	-	0/0/0/0	0/0/0/0
2	SO4	B	451	-	-	0/0/0/0	0/0/0/0
2	SO4	B	452	-	-	0/0/0/0	0/0/0/0
2	SO4	B	453	-	-	0/0/0/0	0/0/0/0
2	SO4	B	454	-	-	0/0/0/0	0/0/0/0
3	FLC	B	455	-	-	0/6/16/16	0/0/0/0
4	U5P	B	456	-	-	0/6/26/26	0/2/2/2
4	U5P	B	457	-	-	0/6/26/26	0/2/2/2
2	SO4	C	432	-	-	0/0/0/0	0/0/0/0
2	SO4	C	433	-	-	0/0/0/0	0/0/0/0
2	SO4	C	434	-	-	0/0/0/0	0/0/0/0
2	SO4	C	435	-	-	0/0/0/0	0/0/0/0
2	SO4	C	436	-	-	0/0/0/0	0/0/0/0
2	SO4	C	437	-	-	0/0/0/0	0/0/0/0
2	SO4	C	438	-	-	0/0/0/0	0/0/0/0
2	SO4	C	439	-	-	0/0/0/0	0/0/0/0
2	SO4	C	440	-	-	0/0/0/0	0/0/0/0
2	SO4	C	441	-	-	0/0/0/0	0/0/0/0
2	SO4	C	442	-	-	0/0/0/0	0/0/0/0
2	SO4	C	443	-	-	0/0/0/0	0/0/0/0
2	SO4	C	444	-	-	0/0/0/0	0/0/0/0
2	SO4	C	445	-	-	0/0/0/0	0/0/0/0
2	SO4	C	446	-	-	0/0/0/0	0/0/0/0
2	SO4	C	447	-	-	0/0/0/0	0/0/0/0
2	SO4	C	448	-	-	0/0/0/0	0/0/0/0
2	SO4	C	449	-	-	0/0/0/0	0/0/0/0
2	SO4	C	450	-	-	0/0/0/0	0/0/0/0
2	SO4	C	451	-	-	0/0/0/0	0/0/0/0
2	SO4	C	452	-	-	0/0/0/0	0/0/0/0
2	SO4	C	453	-	-	0/0/0/0	0/0/0/0
2	SO4	C	454	-	-	0/0/0/0	0/0/0/0
2	SO4	C	455	-	-	0/0/0/0	0/0/0/0
2	SO4	C	456	-	-	0/0/0/0	0/0/0/0
4	U5P	C	457	-	-	0/6/26/26	0/2/2/2
2	SO4	D	432	-	-	0/0/0/0	0/0/0/0
2	SO4	D	433	-	-	0/0/0/0	0/0/0/0
2	SO4	D	434	-	-	0/0/0/0	0/0/0/0
2	SO4	D	435	-	-	0/0/0/0	0/0/0/0
2	SO4	D	436	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	D	437	-	-	0/0/0/0	0/0/0/0
2	SO4	D	438	-	-	0/0/0/0	0/0/0/0
2	SO4	D	439	-	-	0/0/0/0	0/0/0/0
2	SO4	D	440	-	-	0/0/0/0	0/0/0/0
2	SO4	D	441	-	-	0/0/0/0	0/0/0/0
2	SO4	D	442	-	-	0/0/0/0	0/0/0/0
2	SO4	D	443	-	-	0/0/0/0	0/0/0/0
2	SO4	D	444	-	-	0/0/0/0	0/0/0/0
2	SO4	D	445	-	-	0/0/0/0	0/0/0/0
2	SO4	D	446	-	-	0/0/0/0	0/0/0/0
2	SO4	D	447	-	-	0/0/0/0	0/0/0/0
4	U5P	D	448	-	-	0/6/26/26	0/2/2/2

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	457	U5P	P-O5'	-2.97	1.50	1.60
4	A	465	U5P	P-O5'	-2.86	1.50	1.60
4	D	448	U5P	P-O5'	-2.85	1.50	1.60
4	B	456	U5P	P-O5'	-2.78	1.50	1.60
4	A	467	U5P	P-O5'	-2.70	1.51	1.60
4	B	457	U5P	P-O5'	-2.55	1.51	1.60
4	A	466	U5P	P-O5'	-2.43	1.52	1.60
4	A	465	U5P	P-O2P	2.12	1.62	1.54
4	A	467	U5P	P-O2P	2.30	1.63	1.54
4	D	448	U5P	P-O2P	2.34	1.63	1.54
4	B	457	U5P	P-O2P	2.44	1.63	1.54
4	C	457	U5P	P-O2P	2.47	1.63	1.54
4	A	465	U5P	C6-C5	2.49	1.43	1.38
4	B	456	U5P	O4'-C1'	2.51	1.44	1.41
4	A	466	U5P	P-O2P	2.55	1.63	1.54
4	B	456	U5P	C6-C5	2.57	1.43	1.38
4	C	457	U5P	O4'-C1'	2.63	1.44	1.41
4	D	448	U5P	C6-C5	2.72	1.44	1.38
4	A	465	U5P	C6-N1	2.76	1.39	1.35
4	C	457	U5P	C6-C5	2.79	1.44	1.38
4	A	467	U5P	C6-C5	2.80	1.44	1.38
4	B	457	U5P	C6-C5	2.83	1.44	1.38
4	A	466	U5P	C6-C5	2.91	1.44	1.38
4	B	457	U5P	C4-N3	3.03	1.38	1.33
4	A	467	U5P	O4'-C1'	3.03	1.45	1.41
4	B	457	U5P	C6-N1	3.15	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	456	U5P	C6-N1	3.19	1.40	1.35
4	A	465	U5P	O4'-C1'	3.20	1.45	1.41
4	D	448	U5P	O4'-C1'	3.22	1.45	1.41
4	A	466	U5P	O4'-C1'	3.27	1.45	1.41
4	C	457	U5P	C4-N3	3.37	1.39	1.33
4	C	457	U5P	C6-N1	3.39	1.40	1.35
4	D	448	U5P	C4-N3	3.45	1.39	1.33
4	A	467	U5P	C4-N3	3.47	1.39	1.33
4	A	465	U5P	C4-N3	3.48	1.39	1.33
4	A	467	U5P	C6-N1	3.52	1.40	1.35
4	D	448	U5P	C6-N1	3.54	1.40	1.35
4	B	456	U5P	C4-N3	3.59	1.39	1.33
4	B	457	U5P	O4'-C1'	3.75	1.45	1.41
4	A	466	U5P	C6-N1	3.76	1.41	1.35
4	A	466	U5P	C4-N3	3.79	1.40	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	436	SO4	O2-S-O1	-2.03	103.06	109.50
4	A	465	U5P	C4-N3-C2	7.42	121.49	114.14
4	B	456	U5P	C4-N3-C2	7.56	121.63	114.14
4	C	457	U5P	C4-N3-C2	7.84	121.90	114.14
4	D	448	U5P	C4-N3-C2	7.89	121.96	114.14
4	A	467	U5P	C4-N3-C2	7.95	122.02	114.14
4	B	457	U5P	C4-N3-C2	8.14	122.21	114.14
4	A	466	U5P	C4-N3-C2	8.16	122.23	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	433	SO4	3	0
2	A	443	SO4	2	0
2	A	444	SO4	1	0
2	A	451	SO4	1	0
2	A	459	SO4	1	0
2	A	463	SO4	1	0
3	A	464	FLC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	465	U5P	2	0
3	B	455	FLC	2	0
4	B	456	U5P	1	0
4	B	457	U5P	1	0
2	C	433	SO4	1	0
2	C	451	SO4	1	0
2	C	453	SO4	2	0
2	C	454	SO4	1	0
2	D	443	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	431/431 (100%)	0.34	14 (3%) 51 64	26, 39, 62, 83	0
1	B	431/431 (100%)	0.27	9 (2%) 67 79	23, 40, 64, 83	0
1	C	431/431 (100%)	1.36	117 (27%) 1 1	26, 61, 109, 121	0
1	D	431/431 (100%)	1.62	132 (30%) 1 0	36, 69, 124, 144	0
All	All	1724/1724 (100%)	0.90	272 (15%) 3 5	23, 48, 111, 144	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	212	LEU	9.2
1	D	363	GLU	8.5
1	D	306	PRO	8.1
1	D	325	LEU	7.9
1	D	208	LEU	7.4
1	D	334	ASN	7.1
1	D	332	PRO	7.0
1	C	301	ASN	7.0
1	C	333	ARG	7.0
1	D	244	ARG	7.0
1	C	329	LEU	6.8
1	D	286	ALA	6.6
1	D	205	LEU	6.4
1	D	240	HIS	6.3
1	D	242	LEU	6.3
1	D	241	ARG	6.2
1	C	242	LEU	6.2
1	D	213	SER	6.0
1	D	335	ALA	5.9
1	D	214	GLN	5.9
1	D	365	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	D	329	LEU	5.8
1	C	241	ARG	5.7
1	D	299	ALA	5.7
1	D	285	PRO	5.7
1	D	250	ASP	5.5
1	D	333	ARG	5.5
1	C	216	GLY	5.5
1	C	210	LYS	5.5
1	C	307	MET	5.5
1	D	300	LEU	5.4
1	D	249	LEU	5.4
1	D	367	LEU	5.3
1	C	367	LEU	5.3
1	D	201	VAL	5.3
1	C	297	SER	5.3
1	D	358	VAL	5.2
1	C	326	LYS	5.2
1	C	240	HIS	5.2
1	C	415	LEU	5.2
1	D	239	GLY	5.1
1	C	286	ALA	5.0
1	D	351	ILE	5.0
1	D	100	VAL	4.9
1	C	244	ARG	4.9
1	C	300	LEU	4.9
1	C	214	GLN	4.9
1	D	327	HIS	4.9
1	D	360	ILE	4.8
1	D	308	VAL	4.7
1	D	102	ASP	4.7
1	C	354	ARG	4.7
1	C	213	SER	4.6
1	C	334	ASN	4.6
1	D	210	LYS	4.6
1	C	212	LEU	4.6
1	C	292	GLU	4.6
1	D	218	VAL	4.5
1	C	335	ALA	4.5
1	C	215	GLY	4.5
1	D	324	HIS	4.5
1	D	209	GLU	4.4
1	D	291	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	302	ARG	4.3
1	C	280	LYS	4.3
1	D	415	LEU	4.3
1	C	199	GLU	4.3
1	D	246	PRO	4.3
1	D	368	ARG	4.3
1	D	377	PHE	4.2
1	D	301	ASN	4.2
1	C	332	PRO	4.2
1	D	339	VAL	4.2
1	C	248	TYR	4.2
1	C	296	ALA	4.2
1	D	243	PRO	4.2
1	D	245	ALA	4.2
1	D	293	HIS	4.1
1	D	207	ILE	4.1
1	D	297	SER	4.1
1	D	338	PHE	4.1
1	C	323	HIS	4.1
1	A	362	GLY	4.1
1	D	307	MET	4.0
1	C	295	GLU	4.0
1	C	356	PRO	3.9
1	C	196	PRO	3.9
1	D	354	ARG	3.9
1	D	369	ALA	3.9
1	D	292	GLU	3.9
1	C	245	ALA	3.9
1	D	108	PRO	3.8
1	C	358	VAL	3.8
1	C	219	LEU	3.7
1	D	216	GLY	3.7
1	D	280	LYS	3.7
1	C	303	ALA	3.6
1	D	219	LEU	3.6
1	D	361	LEU	3.6
1	D	314	GLY	3.6
1	D	290	VAL	3.6
1	D	330	SER	3.6
1	C	293	HIS	3.6
1	D	359	ARG	3.5
1	D	248	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	149	VAL	3.5
1	D	234	VAL	3.5
1	D	252	PRO	3.5
1	C	288	LEU	3.5
1	C	359	ARG	3.5
1	D	238	HIS	3.5
1	C	357	ALA	3.5
1	C	148	VAL	3.4
1	C	361	LEU	3.4
1	C	238	HIS	3.4
1	D	253	MET	3.4
1	D	336	LEU	3.4
1	C	208	LEU	3.4
1	D	199	GLU	3.4
1	D	310	LEU	3.4
1	C	209	GLU	3.4
1	A	365	VAL	3.3
1	C	243	PRO	3.3
1	C	412	LEU	3.3
1	C	362	GLY	3.3
1	D	101	MET	3.3
1	C	365	VAL	3.3
1	C	246	PRO	3.3
1	C	202	ARG	3.3
1	C	320	ARG	3.3
1	D	296	ALA	3.3
1	C	306	PRO	3.3
1	C	353	ALA	3.2
1	D	104	PRO	3.2
1	D	149	VAL	3.2
1	C	289	GLU	3.2
1	C	363	GLU	3.2
1	C	294	THR	3.2
1	C	360	ILE	3.2
1	D	316	LEU	3.2
1	C	58	THR	3.2
1	C	211	THR	3.1
1	C	276	PHE	3.1
1	C	287	GLY	3.1
1	C	366	PRO	3.1
1	C	207	ILE	3.1
1	D	340	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	217	LYS	3.1
1	B	241	ARG	3.0
1	C	325	LEU	3.0
1	D	362	GLY	3.0
1	C	247	ILE	3.0
1	D	366	PRO	3.0
1	C	373	THR	3.0
1	B	36	LYS	2.9
1	B	240	HIS	2.9
1	C	305	GLY	2.9
1	C	355	PRO	2.9
1	C	198	ARG	2.9
1	C	239	GLY	2.9
1	D	288	LEU	2.9
1	B	22	GLY	2.9
1	C	302	ARG	2.8
1	C	364	GLU	2.8
1	D	223	PHE	2.8
1	C	235	LEU	2.8
1	D	112	GLU	2.8
1	D	211	THR	2.8
1	D	370	SER	2.8
1	D	295	GLU	2.8
1	C	299	ALA	2.8
1	C	319	GLY	2.8
1	C	236	TYR	2.8
1	D	158	VAL	2.7
1	C	147	PHE	2.7
1	C	350	GLU	2.7
1	D	204	PHE	2.7
1	A	354	ARG	2.7
1	C	368	ARG	2.7
1	D	372	HIS	2.7
1	A	23	GLY	2.7
1	D	94	LEU	2.7
1	D	185	ALA	2.7
1	C	250	ASP	2.7
1	A	302	ARG	2.7
1	C	304	PRO	2.7
1	D	236	TYR	2.6
1	C	290	VAL	2.6
1	C	324	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	370	SER	2.6
1	A	158	VAL	2.6
1	D	303	ALA	2.6
1	C	327	HIS	2.6
1	A	358	VAL	2.6
1	C	414	ALA	2.6
1	D	352	ILE	2.6
1	C	160	SER	2.5
1	D	389	TRP	2.5
1	A	135	ALA	2.5
1	C	283	PHE	2.5
1	D	320	ARG	2.5
1	C	274	ALA	2.5
1	B	43	ALA	2.5
1	D	202	ARG	2.5
1	D	319	GLY	2.4
1	C	205	LEU	2.4
1	C	322	LEU	2.4
1	C	371	VAL	2.4
1	D	305	GLY	2.4
1	D	76	TYR	2.4
1	D	195	ARG	2.4
1	D	99	LYS	2.4
1	D	237	THR	2.4
1	D	233	TYR	2.3
1	C	135	ALA	2.3
1	C	369	ALA	2.3
1	D	222	THR	2.3
1	C	217	LYS	2.3
1	C	225	VAL	2.3
1	D	356	PRO	2.3
1	B	280	LYS	2.3
1	C	298	LYS	2.3
1	C	279	GLY	2.3
1	D	51	GLU	2.3
1	D	284	ARG	2.3
1	D	347	LEU	2.3
1	D	135	ALA	2.3
1	D	109	GLU	2.3
1	D	247	ILE	2.2
1	A	129	LEU	2.2
1	C	57	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	49	PRO	2.2
1	D	110	ASP	2.2
1	B	197	TYR	2.2
1	D	163	LEU	2.2
1	A	357	ALA	2.2
1	D	251	SER	2.2
1	C	266	ARG	2.2
1	C	158	VAL	2.2
1	D	309	VAL	2.2
1	C	159	TYR	2.2
1	D	225	VAL	2.2
1	C	146	ALA	2.2
1	D	105	PHE	2.2
1	D	147	PHE	2.2
1	C	233	TYR	2.1
1	D	276	PHE	2.1
1	D	283	PHE	2.1
1	C	112	GLU	2.1
1	C	175	SER	2.1
1	D	72	PHE	2.1
1	C	56	LEU	2.1
1	C	163	LEU	2.1
1	D	312	GLY	2.1
1	D	197	TYR	2.1
1	C	161	GLY	2.1
1	D	36	LYS	2.1
1	D	375	GLY	2.1
1	D	198	ARG	2.1
1	C	275	HIS	2.1
1	D	220	ILE	2.1
1	C	200	THR	2.0
1	A	367	LEU	2.0
1	C	195	ARG	2.0
1	A	148	VAL	2.0
1	B	23	GLY	2.0
1	C	285	PRO	2.0
1	A	225	VAL	2.0
1	C	291	VAL	2.0
1	D	373	THR	2.0
1	C	28	LEU	2.0
1	B	195	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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	FLC	B	455	13/13	0.52	0.47	24.46	84,97,99,100	0
3	FLC	A	464	13/13	0.43	0.53	13.98	125,127,128,128	0
4	U5P	A	467	21/21	0.69	0.39	12.81	140,144,145,146	0
2	SO4	B	436	5/5	0.88	0.38	9.89	94,95,95,97	0
4	U5P	B	457	21/21	0.63	0.37	9.27	106,108,110,111	0
2	SO4	C	440	5/5	0.76	0.34	6.21	174,174,174,174	0
2	SO4	A	463	5/5	0.81	0.29	4.86	142,142,143,143	0
2	SO4	A	457	5/5	0.88	0.17	4.35	129,129,129,130	0
2	SO4	B	445	5/5	0.95	0.18	3.70	58,60,62,63	0
2	SO4	A	451	5/5	0.76	0.43	2.62	130,130,130,130	0
4	U5P	A	466	21/21	0.83	0.23	2.12	60,71,74,76	0
2	SO4	A	438	5/5	0.79	0.37	2.09	143,144,144,144	0
2	SO4	C	445	5/5	0.90	0.20	1.68	99,99,100,100	0
2	SO4	D	442	5/5	0.65	0.67	1.56	167,167,167,167	0
2	SO4	A	434	5/5	0.72	0.21	1.55	140,140,140,140	0
4	U5P	A	465	21/21	0.97	0.16	1.54	33,51,52,57	0
4	U5P	B	456	21/21	0.96	0.19	1.54	34,53,56,59	0
2	SO4	B	434	5/5	0.93	0.20	0.76	84,84,85,85	0
2	SO4	C	435	5/5	0.93	0.20	0.68	113,114,114,114	0
4	U5P	C	457	21/21	0.94	0.19	0.61	61,73,75,76	0
2	SO4	A	437	5/5	0.93	0.16	0.19	87,87,88,89	0
2	SO4	D	433	5/5	0.76	0.39	0.14	141,141,142,142	0
2	SO4	A	454	5/5	0.96	0.16	0.06	54,54,55,57	0
2	SO4	C	443	5/5	0.85	0.16	0.03	117,117,118,118	0
2	SO4	B	433	5/5	0.98	0.14	0.01	65,65,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	U5P	D	448	21/21	0.91	0.21	-0.05	88,94,95,96	0
2	SO4	A	435	5/5	0.79	0.21	-0.39	126,126,127,127	0
2	SO4	C	453	5/5	0.68	0.35	-0.59	152,152,152,152	0
2	SO4	B	432	5/5	0.94	0.15	-0.66	83,84,85,86	0
2	SO4	A	456	5/5	0.88	0.12	-0.88	90,90,91,91	0
2	SO4	D	435	5/5	0.95	0.15	-0.90	87,87,88,88	0
2	SO4	D	432	5/5	0.87	0.14	-1.64	132,132,132,132	0
2	SO4	D	445	5/5	0.82	0.19	-1.69	131,131,132,132	0
2	SO4	A	440	5/5	0.98	0.10	-1.89	58,58,60,60	0
5	ZN	A	469	1/1	0.93	0.11	-1.99	95,95,95,95	0
5	ZN	A	468	1/1	0.96	0.09	-3.37	74,74,74,74	0
5	ZN	C	458	1/1	0.83	0.09	-3.43	96,96,96,96	0
5	ZN	B	459	1/1	0.97	0.08	-3.77	84,84,84,84	0
5	ZN	C	459	1/1	0.94	0.08	-4.76	97,97,97,97	0
2	SO4	A	453	5/5	0.97	0.09	-4.80	84,85,85,86	0
5	ZN	D	450	1/1	0.90	0.05	-5.28	102,102,102,102	0
5	ZN	B	458	1/1	0.95	0.07	-6.19	70,70,70,70	0
5	ZN	D	449	1/1	0.88	0.07	-6.47	106,106,106,106	0
2	SO4	A	442	5/5	0.72	0.69	-	159,159,159,159	0
2	SO4	B	446	5/5	0.87	0.26	-	135,135,135,136	0
2	SO4	C	456	5/5	0.75	0.15	-	136,137,137,137	0
2	SO4	A	446	5/5	0.60	0.42	-	167,167,167,167	0
2	SO4	C	452	5/5	0.63	0.33	-	149,149,149,149	0
2	SO4	D	437	5/5	0.78	0.41	-	141,141,142,142	0
2	SO4	B	438	5/5	0.70	0.25	-	133,133,133,133	0
2	SO4	B	440	5/5	0.62	0.41	-	140,140,140,141	0
2	SO4	C	434	5/5	0.95	0.12	-	70,71,71,72	0
2	SO4	B	449	5/5	0.85	0.26	-	141,141,141,141	0
2	SO4	D	434	5/5	0.85	0.24	-	123,123,123,123	0
2	SO4	C	436	5/5	0.91	0.21	-	129,130,130,130	0
2	SO4	C	448	5/5	0.81	0.28	-	141,141,141,141	0
2	SO4	A	432	5/5	0.88	0.11	-	123,123,124,124	0
2	SO4	B	454	5/5	0.78	0.24	-	147,147,148,148	0
2	SO4	A	452	5/5	0.85	0.28	-	120,120,120,120	0
2	SO4	A	436	5/5	0.52	0.26	-	159,159,159,159	0
2	SO4	A	459	5/5	0.83	0.38	-	118,119,119,119	0
2	SO4	C	455	5/5	0.86	0.28	-	138,138,139,139	0
2	SO4	D	436	5/5	0.93	0.17	-	108,108,108,108	0
2	SO4	D	440	5/5	0.71	0.20	-	139,139,139,139	0
2	SO4	D	444	5/5	0.98	0.12	-	72,72,73,73	0
2	SO4	A	462	5/5	0.92	0.15	-	127,128,128,128	0
2	SO4	C	454	5/5	0.73	0.21	-	143,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	D	441	5/5	0.69	0.31	-	173,173,173,174	0
2	SO4	C	450	5/5	0.71	0.35	-	142,142,143,143	0
2	SO4	B	443	5/5	0.95	0.11	-	80,81,82,82	0
2	SO4	C	451	5/5	0.92	0.14	-	111,111,111,111	0
2	SO4	C	446	5/5	0.88	0.33	-	155,155,155,156	0
2	SO4	B	447	5/5	0.90	0.18	-	142,142,142,142	0
2	SO4	A	441	5/5	0.94	0.15	-	101,101,101,101	0
2	SO4	A	460	5/5	0.87	0.19	-	101,101,101,102	0
2	SO4	B	437	5/5	0.87	0.20	-	119,119,119,119	0
2	SO4	C	437	5/5	0.86	0.38	-	142,142,142,142	0
2	SO4	A	449	5/5	0.89	0.25	-	156,156,156,156	0
2	SO4	A	433	5/5	0.79	0.64	-	157,158,158,158	0
2	SO4	C	449	5/5	0.87	0.30	-	148,148,148,148	0
2	SO4	C	438	5/5	0.81	0.26	-	123,123,124,124	0
2	SO4	B	435	5/5	0.80	0.22	-	132,132,133,133	0
2	SO4	C	447	5/5	0.41	0.43	-	186,186,186,186	0
2	SO4	B	452	5/5	0.88	0.22	-	103,103,103,104	0
2	SO4	C	441	5/5	0.84	0.17	-	130,130,130,130	0
2	SO4	C	444	5/5	0.86	0.15	-	124,124,124,124	0
2	SO4	A	445	5/5	0.89	0.17	-	125,125,125,126	0
2	SO4	D	446	5/5	0.59	0.29	-	165,165,166,166	0
2	SO4	C	442	5/5	0.77	0.27	-	150,151,151,151	0
2	SO4	C	432	5/5	0.92	0.11	-	108,108,108,108	0
2	SO4	A	455	5/5	0.89	0.24	-	114,114,114,114	0
2	SO4	B	453	5/5	0.93	0.19	-	124,124,124,125	0
2	SO4	D	443	5/5	0.45	0.42	-	185,185,185,185	0
2	SO4	A	447	5/5	0.75	0.24	-	145,145,145,146	0
2	SO4	A	439	5/5	0.84	0.27	-	131,131,131,131	0
2	SO4	A	450	5/5	0.76	0.34	-	166,166,166,166	0
2	SO4	D	447	5/5	0.79	0.25	-	161,161,161,161	0
2	SO4	B	439	5/5	0.87	0.22	-	135,135,135,135	0
2	SO4	C	433	5/5	0.71	0.39	-	138,138,138,138	0
2	SO4	B	451	5/5	0.76	0.20	-	143,143,143,143	0
2	SO4	A	458	5/5	0.83	0.30	-	124,124,125,125	0
2	SO4	D	439	5/5	0.86	0.43	-	131,131,132,132	0
2	SO4	A	448	5/5	0.84	0.24	-	125,125,125,125	0
2	SO4	C	439	5/5	0.92	0.10	-	111,111,112,112	0
2	SO4	B	450	5/5	0.91	0.16	-	122,122,123,123	0
2	SO4	B	444	5/5	0.90	0.17	-	109,110,110,110	0
2	SO4	A	444	5/5	0.73	0.48	-	138,138,138,138	0
2	SO4	A	443	5/5	0.72	0.29	-	141,141,142,142	0
2	SO4	B	441	5/5	0.87	0.15	-	107,107,108,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	442	5/5	0.88	0.12	-	106,106,107,107	0
2	SO4	D	438	5/5	0.88	0.12	-	159,159,159,159	0
2	SO4	B	448	5/5	0.90	0.12	-	105,105,106,106	0
2	SO4	A	461	5/5	0.79	0.26	-	125,125,126,126	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.