



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 03:33 PM BST

PDB ID : 4B4Z  
Title : Crystal structure of a complex between Actinomadura R39 DD-peptidase and a sulfonamide boronate inhibitor  
Authors : Cannella, S.E.; Sauvage, E.; Herman, R.; Kerff, F.; Rocaboy, M.; Charlier, P.  
Deposited on : 2012-08-02  
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

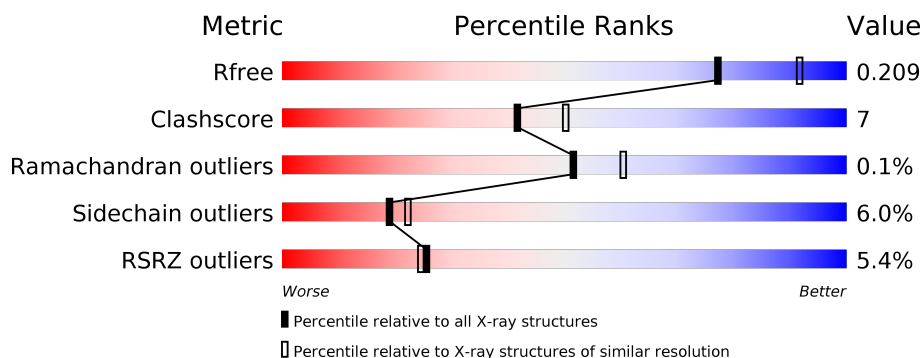
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	466	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>
1	B	466	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>
1	C	466	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>.</div> </div> </div>
1	D	466	<div> <div>12%</div> <div> <div></div> <div>81%</div> <div>16%</div> <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
4	SO4	A	1473	-	-	X	-
4	SO4	B	1472	-	-	X	-
4	SO4	C	1472	-	-	X	-
4	SO4	D	1471	-	-	X	-

## 2 Entry composition [i](#)

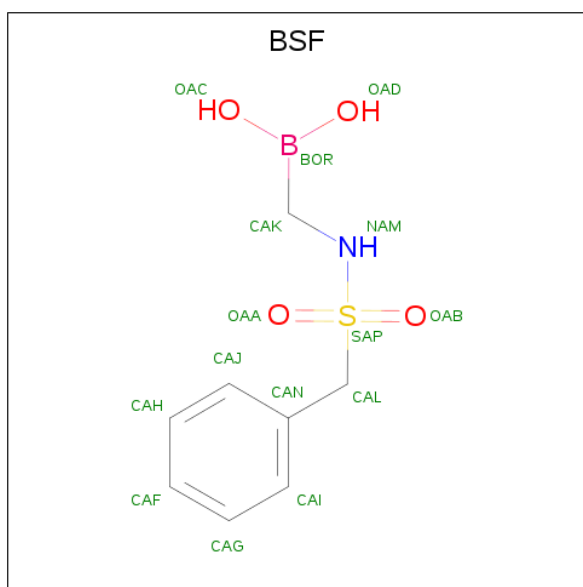
There are 5 unique types of molecules in this entry. The entry contains 14610 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-ALANYL-D-ALANINE CARBOXYPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3353	2076	564	707	6			
1	B	466	Total	C	N	O	S	0	0	1
			3344	2071	564	703	6			
1	C	466	Total	C	N	O	S	0	0	1
			3344	2071	564	703	6			
1	D	461	Total	C	N	O	S	0	0	0
			3310	2049	556	699	6			

- Molecule 2 is {[ (benzylsulfonyl)amino]methyl}boronic acid (three-letter code: BSF) (formula: C<sub>8</sub>H<sub>12</sub>BNO<sub>4</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	S	0	0
			13	1	8	1	2	1		
2	B	1	Total	B	C	N	O	S	0	0
			13	1	8	1	2	1		

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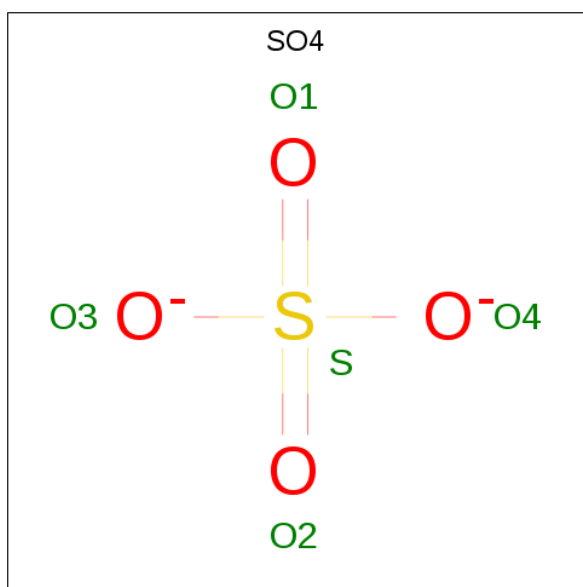
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	B	C	N	O	S	0	0
			13	1	8	1	2	1		
2	D	1	Total	B	C	N	O	S	0	0
			13	1	8	1	2	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		

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



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

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

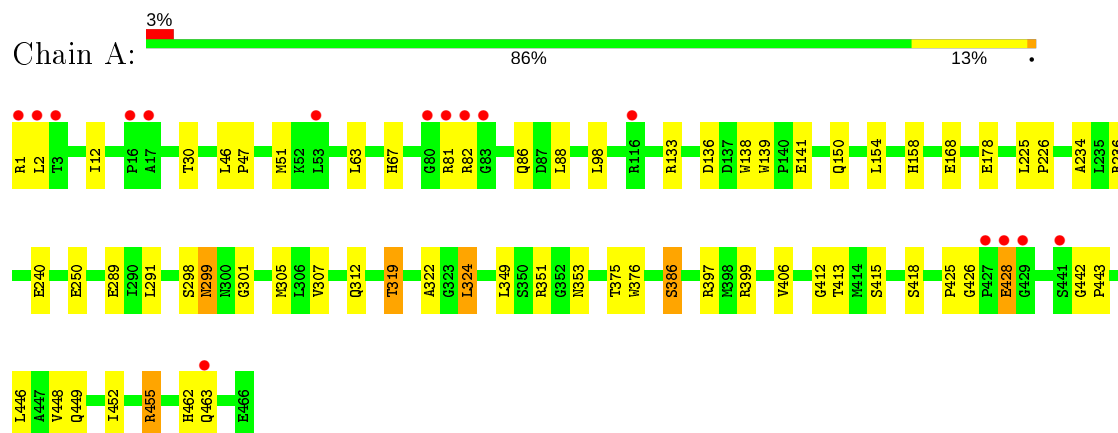
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	288	Total 288	O 288	0	0
5	B	279	Total 279	O 279	0	0
5	C	298	Total 298	O 298	0	0
5	D	208	Total 208	O 208	0	0

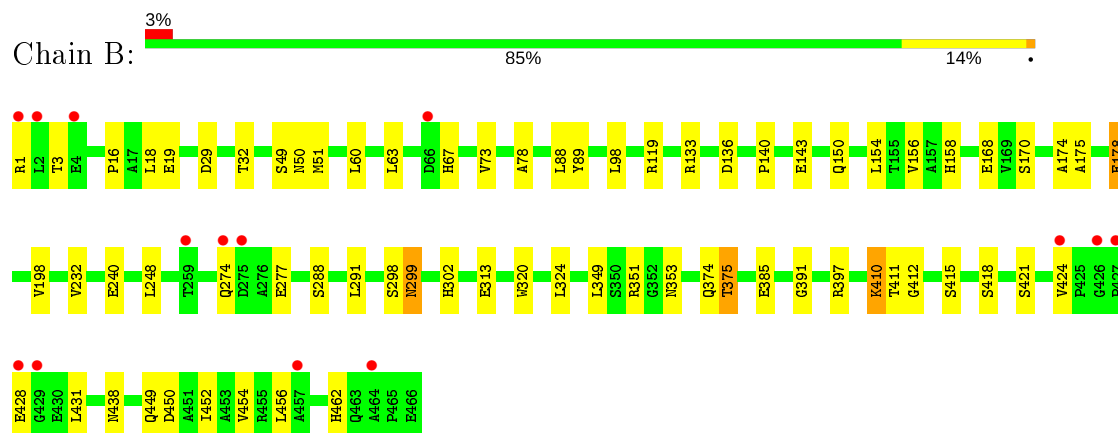
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

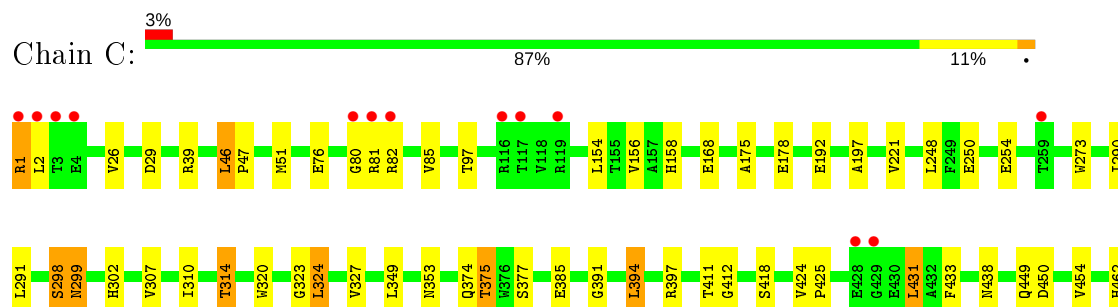
#### • Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE



#### • Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE



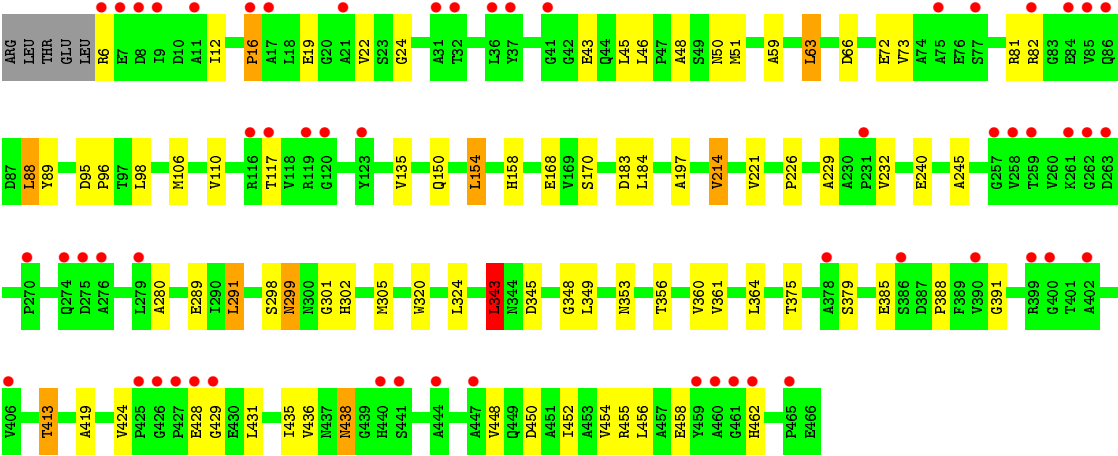
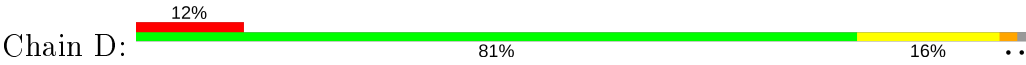
#### • Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE





Q463  
A464  
P465  
E466

● Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.12Å 90.69Å 105.73Å 90.00° 94.52° 90.00°	Depositor
Resolution (Å)	35.25 – 2.20 35.25 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (35.25-2.20) 99.3 (35.25-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.206 , 0.260 0.206 , 0.209	Depositor DCC
$R_{free}$ test set	4852 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 35.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14610	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.46	0/3412	0.63	0/4666
1	B	0.45	0/3403	0.61	0/4656
1	C	0.47	0/3403	0.61	1/4656 (0.0%)
1	D	0.44	0/3369	0.60	2/4608 (0.0%)
All	All	0.46	0/13587	0.61	3/18586 (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	D	343	LEU	CA-CB-CG	5.73	128.49	115.30
1	C	46	LEU	CA-CB-CG	5.56	128.10	115.30
1	D	214	VAL	CB-CA-C	-5.17	101.57	111.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3353	0	3199	41	0
1	B	3344	0	3193	48	0
1	C	3344	0	3193	40	0
1	D	3310	0	3148	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	13	0	10	2	0
2	B	13	0	10	3	0
2	C	13	0	10	1	0
2	D	13	0	10	3	0
3	A	2	0	0	0	0
3	D	2	0	0	0	0
4	A	35	0	0	3	0
4	B	35	0	0	6	0
4	C	35	0	0	8	0
4	D	25	0	0	5	0
5	A	288	0	0	4	0
5	B	279	0	0	4	0
5	C	298	0	0	2	0
5	D	208	0	0	9	1
All	All	14610	0	12773	184	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 (184) 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:B:168:GLU:OE2	4:B:1472:SO4:S	2.02	1.17
1:C:168:GLU:OE2	4:C:1472:SO4:S	2.04	1.14
1:D:24:GLY:O	5:D:2004:HOH:O	1.66	1.10
1:C:158:HIS:NE2	4:C:1472:SO4:S	2.38	0.95
1:C:47:PRO:HG3	1:C:51:MET:HE2	1.52	0.92
1:B:288:SER:HB2	1:B:375:THR:HG21	1.52	0.91
1:B:168:GLU:OE2	4:B:1472:SO4:O2	1.87	0.91
1:C:47:PRO:HG3	1:C:51:MET:CE	2.05	0.86
1:B:168:GLU:OE2	4:B:1472:SO4:O3	1.93	0.85
1:A:150:GLN:HE22	1:A:240:GLU:H	1.26	0.84
1:C:158:HIS:NE2	4:C:1472:SO4:O3	2.14	0.80
1:A:319:THR:HG22	1:A:322:ALA:H	1.45	0.80
1:B:158:HIS:NE2	4:B:1472:SO4:S	2.52	0.80
1:C:168:GLU:OE2	4:C:1472:SO4:O3	2.00	0.78
1:C:168:GLU:OE2	4:C:1472:SO4:O2	2.01	0.78
1:B:462:HIS:ND1	5:B:2268:HOH:O	2.15	0.78
1:D:50:ASN:ND2	1:D:419:ALA:HB1	2.02	0.75
1:B:150:GLN:HE22	1:B:240:GLU:H	1.35	0.73
1:C:397:ARG:HH22	1:C:449:GLN:HE21	1.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:THR:HG23	5:D:2174:HOH:O	1.89	0.72
1:A:150:GLN:NE2	1:A:240:GLU:H	1.87	0.71
1:A:158:HIS:NE2	4:A:1473:SO4:O1	2.23	0.70
1:B:158:HIS:NE2	4:B:1472:SO4:O3	2.23	0.69
1:B:49:SER:CB	2:B:500:BSF:CAK	2.70	0.68
1:D:298:SER:CB	2:D:500:BSF:CAK	2.73	0.67
1:D:435:ILE:HA	5:D:2004:HOH:O	1.94	0.66
1:D:73:VAL:O	5:D:2033:HOH:O	2.14	0.66
1:C:307:VAL:HG11	1:C:324:LEU:HD13	1.78	0.65
1:B:175:ALA:O	1:B:178:GLU:HG2	1.97	0.65
1:A:406:VAL:HG21	1:A:462:HIS:CE1	2.31	0.65
1:D:72:GLU:OE2	5:D:2032:HOH:O	2.15	0.64
1:D:291:LEU:HD12	1:D:379:SER:CB	2.28	0.64
1:B:150:GLN:NE2	1:B:240:GLU:H	1.94	0.64
1:A:298:SER:CB	2:A:500:BSF:CAK	2.75	0.63
1:B:51:MET:CE	1:B:353:ASN:HB3	2.27	0.63
1:C:197:ALA:HB2	1:C:221:VAL:HG12	1.80	0.63
1:C:310:ILE:O	1:C:314:THR:HB	1.99	0.62
1:B:51:MET:HE2	1:B:353:ASN:HB3	1.81	0.62
1:D:16:PRO:O	1:D:19:GLU:HG2	2.00	0.62
1:A:136:ASP:HB3	5:A:2106:HOH:O	1.99	0.61
1:A:158:HIS:CE1	4:A:1473:SO4:O1	2.53	0.61
1:D:388:PRO:HA	5:D:2180:HOH:O	2.01	0.61
1:D:150:GLN:HE22	1:D:240:GLU:H	1.47	0.60
1:D:150:GLN:NE2	1:D:240:GLU:H	1.98	0.60
1:B:299:ASN:HD22	1:B:302:HIS:H	1.50	0.60
1:B:397:ARG:HH22	1:B:449:GLN:HE21	1.50	0.59
1:B:351:ARG:NH2	1:B:415:SER:O	2.32	0.59
1:A:351:ARG:NH2	1:A:415:SER:O	2.31	0.59
1:B:49:SER:CB	2:B:500:BSF:HAK	2.33	0.59
1:C:158:HIS:NE2	4:C:1472:SO4:O2	2.34	0.59
1:A:397:ARG:HH22	1:A:449:GLN:HE21	1.51	0.58
1:C:51:MET:CE	1:C:353:ASN:HB3	2.34	0.58
1:A:51:MET:CE	1:A:353:ASN:HB3	2.34	0.58
1:D:226:PRO:HG2	1:D:229:ALA:HB2	1.87	0.57
1:D:197:ALA:HB2	1:D:221:VAL:HG12	1.86	0.56
1:B:49:SER:HB3	2:B:500:BSF:HAK	1.88	0.55
1:D:298:SER:CB	2:D:500:BSF:HAKA	2.36	0.55
1:B:136:ASP:OD2	5:B:2097:HOH:O	2.18	0.54
1:A:307:VAL:HG11	1:A:324:LEU:HD13	1.90	0.54
1:B:299:ASN:ND2	1:B:302:HIS:H	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:HIS:HE1	4:D:1471:SO4:O4	1.90	0.54
1:C:158:HIS:CE1	4:C:1472:SO4:O3	2.60	0.54
1:D:158:HIS:CE1	4:D:1471:SO4:O4	2.60	0.54
1:C:397:ARG:NH2	1:C:449:GLN:HE21	2.05	0.53
1:D:45:LEU:HD22	1:D:438:ASN:HB2	1.90	0.53
1:B:410:LYS:HE3	5:B:2200:HOH:O	2.08	0.53
1:C:298:SER:CB	2:C:500:BSF:CAK	2.87	0.53
1:B:410:LYS:HE2	1:B:411:THR:O	2.09	0.52
1:C:397:ARG:HH22	1:C:449:GLN:NE2	2.06	0.52
1:C:51:MET:HE3	1:C:353:ASN:HB3	1.91	0.52
1:A:51:MET:HE2	1:A:353:ASN:HB3	1.90	0.52
1:A:168:GLU:OE2	4:A:1473:SO4:O2	2.28	0.52
1:A:386:SER:HA	1:A:399:ARG:NH2	2.25	0.52
1:B:424:VAL:HB	1:B:431:LEU:HB2	1.91	0.51
1:D:291:LEU:HD12	1:D:379:SER:HB2	1.91	0.51
1:D:48:ALA:O	1:D:348:GLY:HA3	2.11	0.51
1:D:106:MET:O	1:D:110:VAL:HG23	2.11	0.51
1:D:73:VAL:CG1	1:D:88:LEU:HD11	2.40	0.51
1:D:436:VAL:N	5:D:2004:HOH:O	2.28	0.51
1:B:397:ARG:NH2	1:B:449:GLN:HE21	2.09	0.50
1:A:63:LEU:O	1:A:67:HIS:HB2	2.12	0.50
1:C:323:GLY:O	1:C:327:VAL:HG23	2.12	0.50
1:C:394:LEU:HD13	1:C:411:THR:CG2	2.41	0.50
1:C:424:VAL:HB	1:C:431:LEU:HB2	1.93	0.49
1:A:141:GLU:H	1:A:141:GLU:CD	2.15	0.49
1:D:301:GLY:O	1:D:305:MET:HG3	2.13	0.49
1:D:12:ILE:HG22	1:D:448:VAL:HG13	1.94	0.49
1:C:168:GLU:OE2	4:C:1472:SO4:O1	2.30	0.48
1:A:289:GLU:HG2	5:A:2215:HOH:O	2.13	0.48
1:D:158:HIS:HD2	5:D:2103:HOH:O	1.95	0.48
1:D:6:ARG:HA	1:D:6:ARG:HH11	1.79	0.48
1:D:168:GLU:OE2	4:D:1471:SO4:O3	2.31	0.48
1:D:455:ARG:HH12	1:D:458:GLU:HB2	1.79	0.48
1:A:406:VAL:HG13	1:A:425:PRO:HD2	1.96	0.48
1:B:1:ARG:NH1	1:D:429:GLY:O	2.46	0.48
1:D:22:VAL:HG11	1:D:43:GLU:HG2	1.96	0.48
1:B:158:HIS:NE2	4:B:1472:SO4:O2	2.46	0.47
1:B:78:ALA:HA	1:B:277:GLU:HG2	1.95	0.47
1:D:413:THR:HG23	2:D:500:BSF:OAA	2.13	0.47
1:A:133:ARG:HB3	1:A:150:GLN:HG2	1.96	0.47
1:B:133:ARG:HB3	1:B:150:GLN:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ARG:HH22	1:D:455:ARG:HH21	1.60	0.47
1:A:12:ILE:HG22	1:A:448:VAL:HG13	1.97	0.47
1:B:63:LEU:O	1:B:67:HIS:HB2	2.15	0.47
1:B:119:ARG:HG2	1:B:119:ARG:HH11	1.80	0.47
1:B:29:ASP:HB3	1:B:32:THR:OG1	2.14	0.47
1:D:158:HIS:CE1	4:D:1471:SO4:S	3.08	0.47
1:A:386:SER:HA	1:A:399:ARG:HH21	1.79	0.47
1:A:1:ARG:HH22	1:A:455:ARG:NH2	2.14	0.46
1:A:298:SER:CB	2:A:500:BSF:HAKA	2.45	0.46
1:D:424:VAL:HB	1:D:431:LEU:HB2	1.98	0.46
1:A:86:GLN:HB3	5:A:2058:HOH:O	2.15	0.46
1:C:80:GLY:O	1:C:82:ARG:N	2.47	0.46
1:A:301:GLY:O	1:A:305:MET:HG3	2.16	0.46
1:D:343:LEU:N	1:D:343:LEU:HD23	2.30	0.46
1:D:385:GLU:O	1:D:391:GLY:HA3	2.15	0.46
1:B:19:GLU:OE2	5:B:2004:HOH:O	2.21	0.46
1:C:156:VAL:HG21	1:C:248:LEU:HD12	1.98	0.46
1:D:452:ILE:O	1:D:456:LEU:HG	2.15	0.46
1:A:225:LEU:HD12	1:A:226:PRO:HD2	1.98	0.46
1:C:450:ASP:O	1:C:454:VAL:HG23	2.17	0.45
1:C:425:PRO:O	1:C:462:HIS:NE2	2.46	0.45
1:A:299:ASN:HD22	1:A:299:ASN:C	2.18	0.45
1:A:426:GLY:C	1:A:428:GLU:N	2.70	0.45
1:A:12:ILE:HG21	1:A:452:ILE:HG13	1.99	0.45
1:A:47:PRO:HG3	1:A:51:MET:CE	2.47	0.45
1:B:385:GLU:O	1:B:391:GLY:HA3	2.16	0.45
1:B:450:ASP:O	1:B:454:VAL:HG23	2.16	0.45
1:C:462:HIS:HE1	5:C:2281:HOH:O	2.00	0.45
1:C:51:MET:HE1	1:C:353:ASN:HB3	1.98	0.45
1:D:356:THR:O	1:D:360:VAL:HG23	2.16	0.45
1:D:458:GLU:HA	1:D:462:HIS:O	2.17	0.45
1:D:59:ALA:O	1:D:63:LEU:HB2	2.17	0.45
1:C:175:ALA:O	1:C:178:GLU:HB2	2.17	0.45
1:B:140:PRO:HA	1:B:143:GLU:OE2	2.17	0.44
1:D:135:VAL:HG21	1:D:345:ASP:HB3	2.00	0.44
1:D:280:ALA:O	5:D:2033:HOH:O	2.21	0.44
1:C:39:ARG:NH1	5:C:2003:HOH:O	2.42	0.44
1:D:158:HIS:NE2	4:D:1471:SO4:O3	2.44	0.44
1:B:170:SER:HA	1:B:232:VAL:O	2.17	0.44
1:A:81:ARG:HD3	1:B:313:GLU:OE2	2.17	0.44
1:B:298:SER:HB2	1:B:410:LYS:NZ	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:GLY:O	1:B:418:SER:HA	2.17	0.44
1:C:299:ASN:HD22	1:C:302:HIS:H	1.66	0.44
1:B:288:SER:CB	1:B:375:THR:HG21	2.35	0.43
1:C:374:GLN:NE2	1:C:375:THR:HG22	2.33	0.43
1:C:97:THR:HG21	1:C:290:ILE:HG12	1.99	0.43
1:D:450:ASP:O	1:D:454:VAL:HG23	2.18	0.43
1:A:234:ALA:HB1	1:A:236:ARG:NH1	2.33	0.43
1:B:60:LEU:HD11	1:B:291:LEU:HD11	1.99	0.43
1:D:51:MET:HE2	1:D:353:ASN:HB3	2.00	0.43
1:A:1:ARG:HH22	1:A:455:ARG:HH22	1.67	0.43
1:A:1:ARG:HH12	1:A:455:ARG:HH22	1.67	0.43
1:C:26:VAL:O	1:C:433:PHE:HA	2.19	0.43
1:C:76:GLU:HG3	1:C:273:TRP:CD1	2.53	0.43
1:D:343:LEU:H	1:D:343:LEU:HD23	1.83	0.43
1:C:29:ASP:HA	1:C:431:LEU:HD12	2.01	0.43
1:D:50:ASN:HD21	1:D:419:ALA:HB1	1.83	0.43
1:D:455:ARG:NH1	1:D:458:GLU:HB2	2.34	0.43
1:A:138:TRP:HB3	5:A:2111:HOH:O	2.19	0.42
1:B:175:ALA:H	1:B:178:GLU:HG3	1.84	0.42
1:D:299:ASN:C	1:D:299:ASN:HD22	2.23	0.42
1:C:47:PRO:HG3	1:C:51:MET:HE3	1.96	0.42
1:A:397:ARG:NH1	1:A:446:LEU:HD22	2.34	0.42
1:D:170:SER:HB2	1:D:183:ASP:HB3	2.02	0.42
1:A:412:GLY:O	1:A:418:SER:HA	2.20	0.42
1:B:298:SER:CB	1:B:410:LYS:HZ2	2.30	0.42
1:B:50:ASN:ND2	1:B:421:SER:OG	2.53	0.41
1:B:73:VAL:HA	1:B:89:TYR:O	2.19	0.41
1:D:73:VAL:CG1	1:D:88:LEU:CD1	2.98	0.41
1:A:397:ARG:HH22	1:A:449:GLN:NE2	2.15	0.41
1:B:156:VAL:HG21	1:B:248:LEU:HD12	2.02	0.41
1:B:452:ILE:O	1:B:456:LEU:HG	2.20	0.41
1:B:16:PRO:HA	1:B:19:GLU:HG2	2.03	0.41
1:C:385:GLU:O	1:C:391:GLY:HA3	2.21	0.41
1:A:139:TRP:HB3	1:A:141:GLU:OE2	2.21	0.41
1:C:412:GLY:O	1:C:418:SER:HA	2.20	0.41
1:D:361:VAL:HA	1:D:364:LEU:HD12	2.02	0.41
1:C:1:ARG:HD3	1:C:2:LEU:H	1.86	0.40
1:D:154:LEU:HD13	1:D:245:ALA:HB3	2.04	0.40
1:D:73:VAL:HA	1:D:89:TYR:O	2.22	0.40
1:D:95:ASP:HA	1:D:96:PRO:HD3	1.95	0.40
1:A:442:GLY:HA3	1:A:443:PRO:HD2	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:SER:HA	1:D:232:VAL:O	2.21	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)
5:D:2197:HOH:O	5:D:2321:HOH:O[2_645]	2.06	0.14

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	464/466 (100%)	450 (97%)	14 (3%)	0	100	100
1	B	464/466 (100%)	449 (97%)	14 (3%)	1 (0%)	47	55
1	C	464/466 (100%)	450 (97%)	13 (3%)	1 (0%)	47	55
1	D	459/466 (98%)	440 (96%)	19 (4%)	0	100	100
All	All	1851/1864 (99%)	1789 (97%)	60 (3%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	81	ARG
1	B	174	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/339 (100%)	317 (94%)	22 (6%)	17	19
1	B	338/339 (100%)	321 (95%)	17 (5%)	24	30
1	C	338/339 (100%)	319 (94%)	19 (6%)	21	25
1	D	334/339 (98%)	311 (93%)	23 (7%)	15	16
All	All	1349/1356 (100%)	1268 (94%)	81 (6%)	19	22

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	30	THR
1	A	46	LEU
1	A	82	ARG
1	A	88	LEU
1	A	98	LEU
1	A	154	LEU
1	A	178	GLU
1	A	250	GLU
1	A	291	LEU
1	A	299	ASN
1	A	312	GLN
1	A	319	THR
1	A	324	LEU
1	A	349	LEU
1	A	375	THR
1	A	376	TRP
1	A	386	SER
1	A	413	THR
1	A	428	GLU
1	A	455	ARG
1	A	463	GLN
1	B	3	THR
1	B	18	LEU
1	B	88	LEU
1	B	98	LEU
1	B	154	LEU
1	B	178	GLU
1	B	198	VAL
1	B	274	GLN

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Mol	Chain	Res	Type
1	B	299	ASN
1	B	320	TRP
1	B	324	LEU
1	B	349	LEU
1	B	374	GLN
1	B	375	THR
1	B	410	LYS
1	B	428	GLU
1	B	438	ASN
1	C	1	ARG
1	C	46	LEU
1	C	85	VAL
1	C	154	LEU
1	C	192	GLU
1	C	250	GLU
1	C	254	GLU
1	C	291	LEU
1	C	298	SER
1	C	299	ASN
1	C	314	THR
1	C	320	TRP
1	C	324	LEU
1	C	349	LEU
1	C	375	THR
1	C	377	SER
1	C	394	LEU
1	C	431	LEU
1	C	438	ASN
1	D	16	PRO
1	D	46	LEU
1	D	63	LEU
1	D	66	ASP
1	D	81	ARG
1	D	82	ARG
1	D	88	LEU
1	D	98	LEU
1	D	117	THR
1	D	154	LEU
1	D	184	LEU
1	D	214	VAL
1	D	289	GLU
1	D	291	LEU

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Mol	Chain	Res	Type
1	D	299	ASN
1	D	302	HIS
1	D	320	TRP
1	D	324	LEU
1	D	343	LEU
1	D	349	LEU
1	D	413	THR
1	D	428	GLU
1	D	438	ASN

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

Mol	Chain	Res	Type
1	A	44	GLN
1	A	50	ASN
1	A	150	GLN
1	A	299	ASN
1	A	312	GLN
1	A	366	GLN
1	A	437	ASN
1	A	449	GLN
1	A	462	HIS
1	A	463	GLN
1	B	44	GLN
1	B	50	ASN
1	B	67	HIS
1	B	150	GLN
1	B	299	ASN
1	B	302	HIS
1	B	396	ASN
1	B	437	ASN
1	B	449	GLN
1	C	50	ASN
1	C	299	ASN
1	C	302	HIS
1	C	366	GLN
1	C	437	ASN
1	C	449	GLN
1	D	44	GLN
1	D	50	ASN
1	D	67	HIS
1	D	150	GLN

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Mol	Chain	Res	Type
1	D	299	ASN
1	D	302	HIS
1	D	366	GLN
1	D	437	ASN
1	D	449	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 4 are monoatomic - leaving 30 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	$\# Z  > 2$
4	SO4	A	1472	-	4,4,4	0.12	0	6,6,6	0.08	0
4	SO4	C	1471	-	4,4,4	0.15	0	6,6,6	0.16	0
4	SO4	B	1470	-	4,4,4	0.15	0	6,6,6	0.12	0
4	SO4	D	1470	-	4,4,4	0.15	0	6,6,6	0.08	0
4	SO4	A	1473	-	4,4,4	0.60	0	6,6,6	0.35	0
4	SO4	B	1471	-	4,4,4	0.16	0	6,6,6	0.09	0
4	SO4	A	1470	-	4,4,4	0.15	0	6,6,6	0.11	0
4	SO4	C	1468	-	4,4,4	0.20	0	6,6,6	0.14	0
4	SO4	C	1466	-	4,4,4	0.16	0	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	B	1472	-	4,4,4	0.28	0	6,6,6	0.64	0
4	SO4	B	1466	-	4,4,4	0.15	0	6,6,6	0.22	0
4	SO4	B	1469	-	4,4,4	0.12	0	6,6,6	0.19	0
4	SO4	A	1471	-	4,4,4	0.14	0	6,6,6	0.11	0
2	BSF	B	500	1	11,13,15	0.97	0	15,17,20	2.05	1 (6%)
2	BSF	D	500	1	11,13,15	0.74	0	15,17,20	2.49	3 (20%)
4	SO4	C	1470	-	4,4,4	0.15	0	6,6,6	0.17	0
4	SO4	B	1467	-	4,4,4	0.13	0	6,6,6	0.19	0
4	SO4	D	1467	-	4,4,4	0.12	0	6,6,6	0.18	0
4	SO4	D	1469	-	4,4,4	0.20	0	6,6,6	0.23	0
2	BSF	C	500	1	11,13,15	0.89	0	15,17,20	2.12	2 (13%)
4	SO4	B	1468	-	4,4,4	0.15	0	6,6,6	0.11	0
4	SO4	D	1468	-	4,4,4	0.11	0	6,6,6	0.18	0
4	SO4	C	1472	-	4,4,4	0.23	0	6,6,6	0.58	0
4	SO4	A	1467	-	4,4,4	0.11	0	6,6,6	0.28	0
4	SO4	A	1468	-	4,4,4	0.14	0	6,6,6	0.14	0
2	BSF	A	500	1	11,13,15	0.75	0	15,17,20	1.66	2 (13%)
4	SO4	A	1469	-	4,4,4	0.16	0	6,6,6	0.29	0
4	SO4	C	1467	-	4,4,4	0.11	0	6,6,6	0.14	0
4	SO4	C	1469	-	4,4,4	0.14	0	6,6,6	0.10	0
4	SO4	D	1471	-	4,4,4	0.20	0	6,6,6	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BSF	B	500	1	-	0/8/9/11	0/1/1/1
2	BSF	D	500	1	-	0/8/9/11	0/1/1/1
2	BSF	A	500	1	-	0/8/9/11	0/1/1/1
2	BSF	C	500	1	-	1/8/9/11	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	BSF	OAB-SAP-OAA	-8.31	107.31	119.35
2	C	500	BSF	OAB-SAP-OAA	-7.54	108.43	119.35
2	B	500	BSF	OAB-SAP-OAA	-7.53	108.44	119.35
2	A	500	BSF	OAB-SAP-OAA	-5.29	111.69	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	BSF	CAN-CAL-SAP	-3.01	105.91	112.34
2	C	500	BSF	OAA-SAP-CAL	2.28	111.77	108.30
2	A	500	BSF	OAB-SAP-CAL	2.19	111.64	108.30
2	D	500	BSF	CAJ-CAN-CAI	2.05	121.39	118.17

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	500	BSF	CAN-CAL-SAP-OAA

There are no ring outliers.

8 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1473	SO4	3	0
4	B	1472	SO4	6	0
2	B	500	BSF	3	0
2	D	500	BSF	3	0
2	C	500	BSF	1	0
4	C	1472	SO4	8	0
2	A	500	BSF	2	0
4	D	1471	SO4	5	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	466/466 (100%)	0.05	16 (3%)	45	43	19, 30, 55, 75	0
1	B	466/466 (100%)	0.05	14 (3%)	50	48	20, 32, 54, 74	0
1	C	466/466 (100%)	-0.08	14 (3%)	50	48	18, 28, 47, 66	0
1	D	461/466 (98%)	0.55	57 (12%)	4	3	20, 40, 69, 81	0
All	All	1859/1864 (99%)	0.14	101 (5%)	25	24	18, 32, 60, 81	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	427	PRO	5.7
1	C	2	LEU	5.5
1	A	429	GLY	5.2
1	B	464	ALA	4.8
1	D	400	GLY	4.8
1	D	276	ALA	4.4
1	C	81	ARG	4.4
1	C	82	ARG	4.2
1	D	429	GLY	4.1
1	D	274	GLN	4.1
1	B	429	GLY	4.1
1	A	427	PRO	3.9
1	A	3	THR	3.8
1	D	426	GLY	3.8
1	D	465	PRO	3.8
1	A	81	ARG	3.7
1	B	426	GLY	3.7
1	C	259	THR	3.7
1	B	428	GLU	3.7
1	D	21	ALA	3.7
1	A	80	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	120	GLY	3.6
1	D	428	GLU	3.5
1	C	119	ARG	3.5
1	D	41	GLY	3.5
1	D	85	VAL	3.5
1	D	117	THR	3.5
1	D	257	GLY	3.5
1	D	82	ARG	3.4
1	D	17	ALA	3.3
1	D	460	ALA	3.2
1	D	119	ARG	3.2
1	D	86	GLN	3.2
1	D	9	ILE	3.1
1	D	261	LYS	3.1
1	B	427	PRO	3.1
1	C	116	ARG	3.0
1	D	116	ARG	3.0
1	D	390	VAL	3.0
1	C	4	GLU	3.0
1	D	399	ARG	3.0
1	A	116	ARG	2.9
1	D	75	ALA	2.9
1	C	3	THR	2.8
1	D	77	SER	2.8
1	D	36	LEU	2.8
1	C	1	ARG	2.8
1	D	259	THR	2.8
1	D	386	SER	2.8
1	A	17	ALA	2.7
1	D	6	ARG	2.8
1	C	117	THR	2.7
1	A	82	ARG	2.7
1	D	84	GLU	2.7
1	D	32	THR	2.7
1	D	8	ASP	2.6
1	D	402	ALA	2.5
1	A	1	ARG	2.5
1	D	263	ASP	2.5
1	D	262	GLY	2.4
1	A	441	SER	2.4
1	B	275	ASP	2.4
1	D	31	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	425	PRO	2.4
1	D	459	TYR	2.3
1	A	428	GLU	2.3
1	B	1	ARG	2.3
1	D	444	ALA	2.3
1	B	274	GLN	2.3
1	D	37	TYR	2.3
1	C	464	ALA	2.3
1	B	4	GLU	2.2
1	B	259	THR	2.2
1	D	258	VAL	2.2
1	B	457	ALA	2.2
1	C	429	GLY	2.2
1	D	275	ASP	2.2
1	D	279	LEU	2.2
1	D	461	GLY	2.2
1	D	231	PRO	2.2
1	D	441	SER	2.2
1	C	80	GLY	2.2
1	D	378	ALA	2.2
1	D	11	ALA	2.1
1	D	123	TYR	2.1
1	B	66	ASP	2.1
1	D	462	HIS	2.1
1	A	53	LEU	2.1
1	B	2	LEU	2.1
1	D	16	PRO	2.1
1	D	7	GLU	2.1
1	D	270	PRO	2.1
1	A	2	LEU	2.1
1	A	16	PRO	2.0
1	A	463	GLN	2.0
1	B	424	VAL	2.0
1	C	428	GLU	2.0
1	D	447	ALA	2.0
1	D	406	VAL	2.0
1	D	440	HIS	2.0
1	A	83	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	D	1471	5/5	0.56	0.28	74,76,76,76	0
4	SO4	A	1473	5/5	0.60	0.21	84,85,86,86	0
4	SO4	A	1470	5/5	0.66	0.27	110,111,111,111	0
4	SO4	D	1470	5/5	0.72	0.26	119,119,119,119	0
4	SO4	D	1467	5/5	0.73	0.22	78,79,79,79	0
3	MG	A	611	1/1	0.76	0.18	54,54,54,54	0
4	SO4	C	1471	5/5	0.82	0.25	88,88,88,88	0
4	SO4	A	1471	5/5	0.83	0.28	94,94,94,94	0
4	SO4	C	1469	5/5	0.86	0.23	99,100,100,100	0
4	SO4	B	1469	5/5	0.88	0.16	84,84,85,85	0
4	SO4	A	1472	5/5	0.88	0.44	98,98,98,98	0
4	SO4	B	1471	5/5	0.89	0.22	80,81,81,81	0
3	MG	A	610	1/1	0.90	0.09	37,37,37,37	0
2	BSF	D	500	13/15	0.91	0.16	36,41,43,44	0
2	BSF	A	500	13/15	0.91	0.15	30,44,46,47	0
4	SO4	A	1468	5/5	0.93	0.13	76,76,76,76	0
3	MG	D	610	1/1	0.93	0.11	40,40,40,40	0
4	SO4	B	1470	5/5	0.95	0.31	82,82,83,83	0
4	SO4	B	1467	5/5	0.95	0.10	64,64,64,64	0
3	MG	D	611	1/1	0.95	0.11	42,42,42,42	0
4	SO4	D	1468	5/5	0.95	0.09	67,68,68,68	0
4	SO4	B	1472	5/5	0.95	0.13	31,34,36,37	0
2	BSF	B	500	13/15	0.96	0.18	25,29,40,40	0
4	SO4	C	1470	5/5	0.96	0.15	55,56,57,57	0
4	SO4	C	1472	5/5	0.97	0.10	33,35,37,38	0
4	SO4	A	1469	5/5	0.97	0.12	48,49,51,51	0
4	SO4	A	1467	5/5	0.97	0.12	37,38,38,39	0
4	SO4	B	1466	5/5	0.97	0.13	53,53,53,54	0
4	SO4	D	1469	5/5	0.97	0.09	35,35,37,38	0
4	SO4	C	1466	5/5	0.98	0.08	40,40,42,42	0
4	SO4	B	1468	5/5	0.98	0.15	38,39,39,40	0
4	SO4	C	1468	5/5	0.98	0.11	36,38,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	C	1467	5/5	0.98	0.08	59,59,60,60	0
2	BSF	C	500	13/15	0.98	0.15	21,25,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.