



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:43 AM GMT

PDB ID : 2Y4A  
Title : UNEXPECTED TRICOVALENT BINDING MODE OF BORONIC ACIDS  
WITHIN THE ACTIVE SITE OF A PENICILLIN BINDING PROTEIN  
Authors : Sauvage, E.; Zervosen, A.; Herman, R.; Kerff, F.; Rocaboy, M.; Charlier, P.  
Deposited on : 2011-01-05  
Resolution : 2.70 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

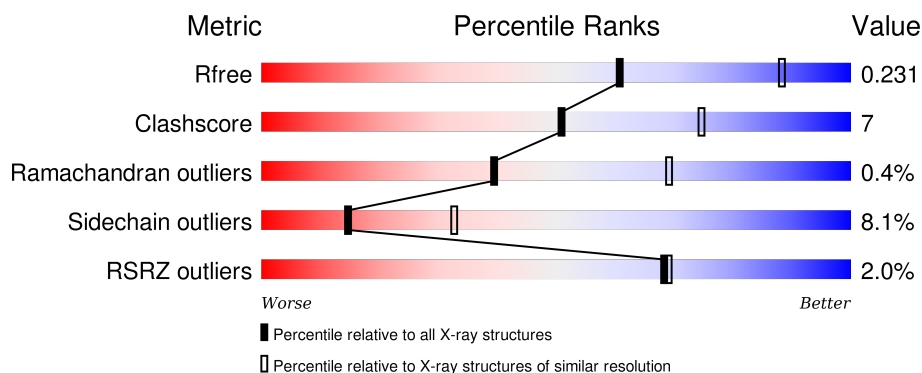
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	466	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>%</span> <span>78%</span> <span>20%</span> </div> </div>
1	B	466	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>%</span> <span>81%</span> <span>18%</span> </div> </div>
1	C	466	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>2%</span> <span>87%</span> <span>11%</span> </div> </div>
1	D	466	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>5%</span> <span>80%</span> <span>18%</span> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BH6	D	500	-	-	-	X
3	SO4	B	604	-	-	-	X
3	SO4	D	600	-	-	-	X
4	MG	A	611	-	-	-	X

## 2 Entry composition [i](#)

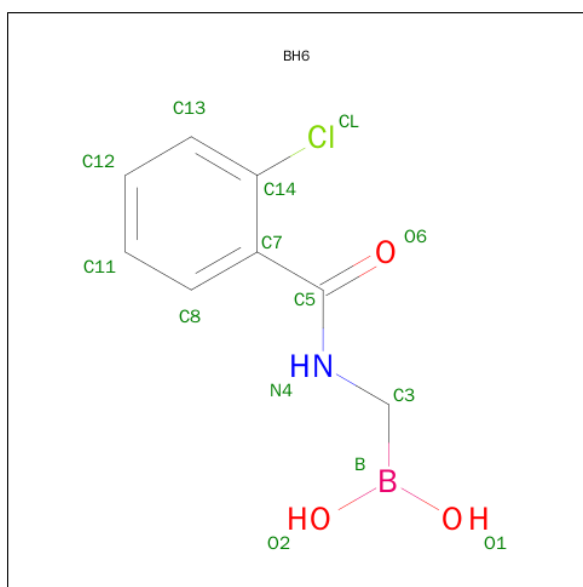
There are 5 unique types of molecules in this entry. The entry contains 13712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	466	Total	C	N	O	S	0	0	0
			3353	2076	564	707	6			

- Molecule 2 is {[ (2-CHLOROBENZOYL)AMINO]METHYL}BORONIC ACID (three-letter code: BH6) (formula: C<sub>8</sub>H<sub>9</sub>BClNO<sub>3</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	B	C	Cl	N	O	0	0
			14	1	8	1	1	3		
2	B	1	Total	B	C	Cl	N	O	0	0
			12	1	8	1	1	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	B	C	Cl	N	O	0	0
			12	1	8	1	1	1		
2	D	1	Total	B	C	Cl	N	O	0	0
			14	1	8	1	1	3		

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

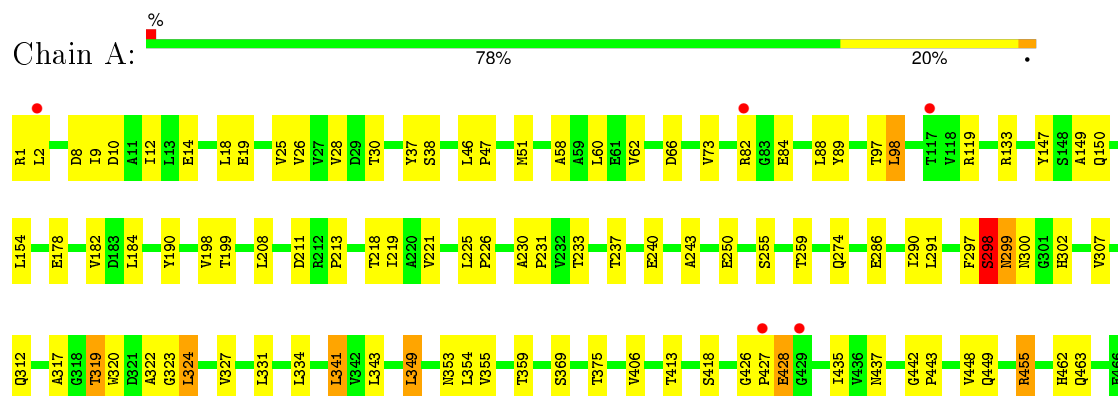
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	39	Total O 39 39	0	0
5	B	48	Total O 48 48	0	0
5	C	47	Total O 47 47	0	0
5	D	28	Total O 28 28	0	0

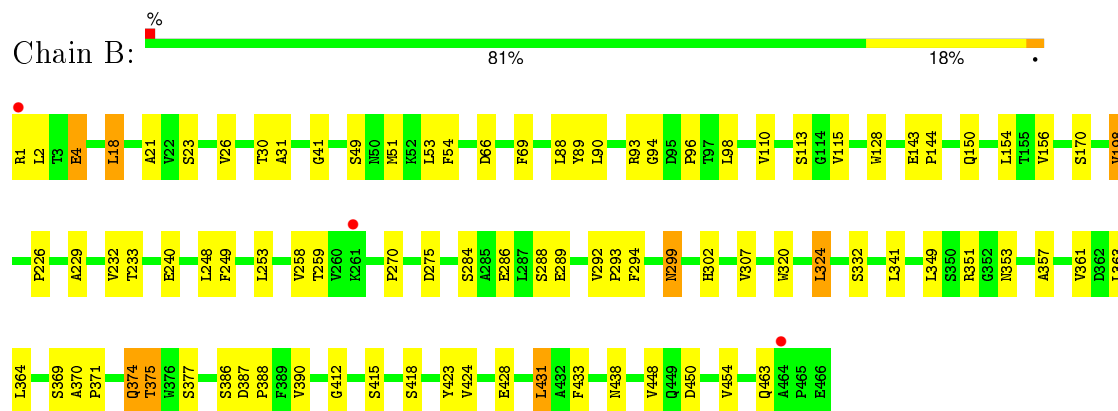
### 3 Residue-property plots

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.

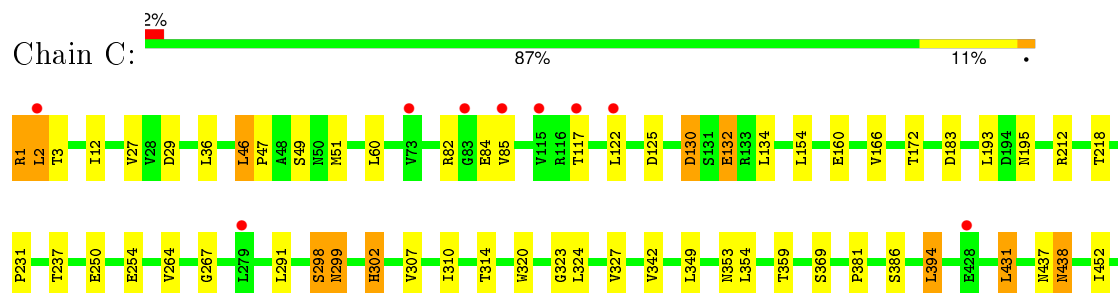
#### • Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE



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

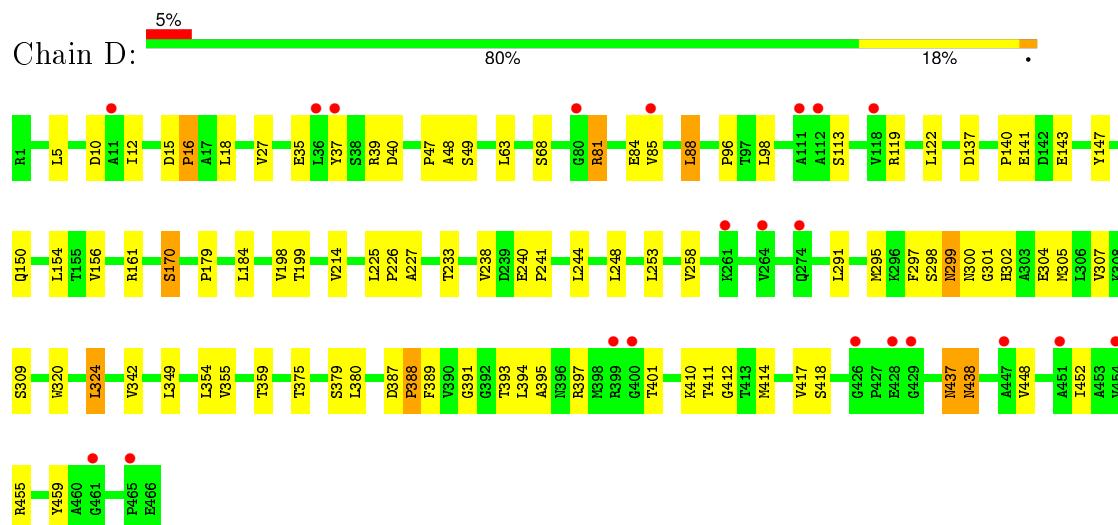


#### • Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE





● 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, $\alpha$ , $\beta$ , $\gamma$	103.31Å 91.57Å 106.87Å 90.00° 94.37° 90.00°	Depositor
Resolution (Å)	46.10 – 2.70 46.05 – 2.69	Depositor EDS
% Data completeness (in resolution range)	97.3 (46.10-2.70) 97.0 (46.05-2.69)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, $R_{free}$	0.187 , 0.225 0.198 , 0.231	Depositor DCC
$R_{free}$ test set	2784 reflections (5.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.6	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 30.0	EDS
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 53629 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13712	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, BH6

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	0.60	0/3412	0.74	1/4666 (0.0%)
1	B	0.61	0/3403	0.74	2/4656 (0.0%)
1	C	0.61	0/3403	0.74	1/4656 (0.0%)
1	D	0.55	0/3412	0.70	0/4666
All	All	0.59	0/13630	0.73	4/18644 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	VAL	CB-CA-C	-6.19	99.63	111.40
1	C	46	LEU	CA-CB-CG	5.94	128.96	115.30
1	A	98	LEU	CA-CB-CG	5.42	127.76	115.30
1	B	53	LEU	CB-CG-CD1	-5.01	102.48	111.00

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	3200	53	0
1	B	3344	0	3193	48	0
1	C	3344	0	3193	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3353	0	3200	49	0
2	A	14	0	9	1	0
2	B	12	0	7	1	0
2	C	12	0	7	3	0
2	D	14	0	9	3	0
3	A	25	0	0	0	0
3	B	25	0	0	0	0
3	C	25	0	0	1	0
3	D	25	0	0	0	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	A	39	0	0	1	0
5	B	48	0	0	0	0
5	C	47	0	0	0	0
5	D	28	0	0	0	0
All	All	13712	0	12818	181	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 7.

All (181) 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:374:GLN:HA	1:B:374:GLN:HE21	1.37	0.90
1:A:150:GLN:HE22	1:A:240:GLU:H	1.17	0.90
1:A:82:ARG:HB2	1:A:84:GLU:HG3	1.54	0.90
1:B:299:ASN:ND2	1:B:302:HIS:H	1.74	0.86
1:C:1:ARG:HG2	1:C:2:LEU:H	1.44	0.81
1:A:60:LEU:HD11	1:A:291:LEU:HD11	1.66	0.78
1:D:342:VAL:HB	1:D:354:LEU:HB2	1.67	0.75
1:A:150:GLN:NE2	1:A:240:GLU:H	1.85	0.73
1:A:51:MET:HE2	1:A:353:ASN:HB3	1.69	0.73
1:A:133:ARG:HB3	1:A:150:GLN:HG2	1.69	0.73
1:B:288:SER:HB2	1:B:375:THR:HG21	1.70	0.73
1:C:1:ARG:HG2	1:C:2:LEU:N	2.06	0.70
1:A:299:ASN:HD22	1:A:302:HIS:H	1.37	0.69
1:A:1:ARG:HH12	1:A:455:ARG:HH22	1.40	0.69
1:A:319:THR:HG22	1:A:322:ALA:H	1.58	0.68
1:A:1:ARG:HH22	1:A:455:ARG:NH2	1.93	0.67
1:B:66:ASP:HA	1:B:286:GLU:OE1	1.96	0.66
1:D:238:VAL:HG21	1:D:244:LEU:HD22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:VAL:HG21	1:A:462:HIS:CE1	2.31	0.65
1:C:47:PRO:HG3	1:C:51:MET:HE2	1.76	0.65
1:D:414:MET:HG2	2:D:500:BH6:H11	1.79	0.63
1:A:51:MET:CE	1:A:353:ASN:HB3	2.30	0.62
1:A:38:SER:OG	5:A:2002:HOH:O	2.16	0.62
1:C:298:SER:CB	2:C:500:BH6:C3	2.78	0.62
1:A:299:ASN:ND2	1:A:302:HIS:H	1.98	0.61
1:C:29:ASP:HA	1:C:431:LEU:HD12	1.82	0.61
1:C:381:PRO:HB2	1:C:394:LEU:HD22	1.83	0.61
1:B:307:VAL:HG11	1:B:324:LEU:HD13	1.82	0.61
1:B:51:MET:HE2	1:B:353:ASN:HB3	1.82	0.61
1:A:8:ASP:OD2	1:A:455:ARG:NH1	2.34	0.60
1:B:299:ASN:HD22	1:B:302:HIS:H	1.47	0.58
1:B:292:VAL:HB	1:B:293:PRO:CD	2.33	0.58
1:D:147:TYR:HB2	1:D:300:ASN:ND2	2.18	0.58
1:D:253:LEU:HB3	1:D:258:VAL:HB	1.85	0.58
1:B:69:PHE:N	1:B:284:SER:OG	2.31	0.57
1:C:310:ILE:O	1:C:314:THR:HB	2.05	0.57
1:B:424:VAL:HB	1:B:431:LEU:HB2	1.85	0.57
1:C:166:VAL:HG12	1:C:237:THR:HA	1.86	0.57
1:D:5:LEU:HD22	1:D:459:TYR:CD1	2.39	0.57
1:C:47:PRO:HG3	1:C:51:MET:CE	2.35	0.57
1:B:351:ARG:NH2	1:B:415:SER:O	2.30	0.57
1:A:1:ARG:NH1	1:A:455:ARG:HH22	2.03	0.57
1:B:361:VAL:HA	1:B:364:LEU:HD12	1.86	0.57
1:D:414:MET:HB2	1:D:417:VAL:HB	1.88	0.56
1:A:225:LEU:HD12	1:A:226:PRO:HD2	1.87	0.56
1:B:450:ASP:O	1:B:454:VAL:HG23	2.04	0.56
1:C:1:ARG:CG	1:C:2:LEU:H	2.18	0.56
1:A:47:PRO:HG3	1:A:355:VAL:HG13	1.86	0.56
1:A:97:THR:HG21	1:A:290:ILE:HG12	1.87	0.56
1:B:374:GLN:HA	1:B:374:GLN:NE2	2.16	0.56
1:D:414:MET:HG2	2:D:500:BH6:C11	2.36	0.55
1:B:18:LEU:HD22	1:B:448:VAL:HG11	1.88	0.55
1:B:387:ASP:HB3	1:B:390:VAL:HB	1.87	0.55
1:B:294:PHE:HB2	1:B:302:HIS:HD2	1.71	0.55
1:D:455:ARG:O	1:D:455:ARG:NH1	2.40	0.55
1:B:156:VAL:HG21	1:B:248:LEU:HD12	1.88	0.55
1:D:225:LEU:HD12	1:D:226:PRO:HD2	1.87	0.55
1:C:172:THR:HG22	1:C:231:PRO:HB3	1.89	0.54
1:B:49:SER:CB	2:B:500:BH6:C3	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:GLN:HE21	1:B:374:GLN:CA	2.17	0.53
1:D:170:SER:HB3	1:D:233:THR:HG22	1.88	0.53
1:D:18:LEU:HD11	1:D:448:VAL:HG11	1.89	0.53
1:A:413:THR:H	2:A:500:BH6:HO1	1.56	0.53
1:D:307:VAL:HG11	1:D:324:LEU:HD13	1.91	0.53
1:B:150:GLN:HE22	1:B:240:GLU:H	1.56	0.52
1:A:349:LEU:HD23	1:A:349:LEU:O	2.09	0.52
1:B:170:SER:HA	1:B:232:VAL:O	2.10	0.52
1:D:299:ASN:ND2	1:D:302:HIS:H	2.09	0.51
1:B:51:MET:CE	1:B:353:ASN:HB3	2.41	0.51
1:D:156:VAL:HG21	1:D:248:LEU:HD12	1.93	0.51
1:B:299:ASN:HD22	1:B:299:ASN:C	2.15	0.50
1:A:426:GLY:C	1:A:428:GLU:H	2.15	0.50
1:B:18:LEU:CD2	1:B:448:VAL:HG11	2.42	0.50
1:D:437:ASN:C	1:D:438:ASN:HD22	2.15	0.49
1:D:47:PRO:HB3	1:D:355:VAL:HG22	1.93	0.49
1:D:394:LEU:HD23	1:D:397:ARG:HD3	1.94	0.49
1:C:437:ASN:C	1:C:438:ASN:HD22	2.16	0.49
1:C:130:ASP:HB3	1:C:132:GLU:H	1.78	0.48
1:D:150:GLN:NE2	1:D:240:GLU:H	2.12	0.48
1:A:297:PHE:O	1:A:298:SER:CB	2.60	0.48
1:B:150:GLN:NE2	1:B:240:GLU:H	2.12	0.48
1:A:184:LEU:HD22	1:A:219:ILE:HG13	1.96	0.48
1:A:1:ARG:HH22	1:A:455:ARG:HH22	1.61	0.48
1:C:82:ARG:HB3	1:C:84:GLU:HG3	1.96	0.48
1:D:438:ASN:N	1:D:438:ASN:HD22	2.12	0.48
1:C:299:ASN:HD22	1:C:302:HIS:H	1.62	0.48
1:D:12:ILE:HG21	1:D:452:ILE:HG13	1.96	0.48
1:A:198:VAL:HG22	1:A:199:THR:N	2.29	0.47
1:B:294:PHE:HB2	1:B:302:HIS:CD2	2.49	0.47
1:A:10:ASP:O	1:A:14:GLU:HG2	2.14	0.47
1:A:182:VAL:HG11	1:A:221:VAL:HG21	1.95	0.47
1:C:36:LEU:HD13	1:C:459:TYR:CE2	2.50	0.47
1:D:304:GLU:OE1	1:D:304:GLU:HA	2.14	0.47
1:B:54:PHE:CD1	1:B:363:LEU:HD22	2.50	0.47
1:A:66:ASP:O	1:A:286:GLU:HG2	2.15	0.47
1:B:26:VAL:O	1:B:433:PHE:HA	2.15	0.47
1:D:47:PRO:HB3	1:D:355:VAL:CG2	2.45	0.47
1:A:323:GLY:O	1:A:327:VAL:HG23	2.15	0.46
1:A:18:LEU:HD11	1:A:448:VAL:HG11	1.97	0.46
1:D:179:PRO:HA	1:D:198:VAL:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:TYR:HA	1:B:431:LEU:O	2.15	0.46
1:B:143:GLU:N	1:B:144:PRO:CD	2.79	0.46
1:A:307:VAL:HG11	1:A:324:LEU:HD13	1.98	0.46
1:D:141:GLU:OE1	1:D:141:GLU:N	2.46	0.46
1:C:60:LEU:HD11	1:C:291:LEU:HD11	1.97	0.46
1:A:25:VAL:HG22	1:A:435:ILE:HG23	1.98	0.46
1:D:49:SER:HB3	1:D:410:LYS:NZ	2.31	0.46
1:D:301:GLY:O	1:D:305:MET:HG3	2.15	0.46
1:B:94:GLY:O	1:B:96:PRO:HD3	2.16	0.46
1:B:226:PRO:HB2	1:B:229:ALA:HB2	1.98	0.46
1:C:298:SER:CB	2:C:500:BH6:H3	2.45	0.45
1:B:1:ARG:CG	1:B:4:GLU:HB2	2.46	0.45
1:C:51:MET:CE	1:C:353:ASN:HB3	2.47	0.45
1:A:149:ALA:HA	1:A:237:THR:HG21	1.96	0.45
1:A:58:ALA:O	1:A:62:VAL:HG23	2.17	0.45
1:B:412:GLY:O	1:B:418:SER:HA	2.16	0.45
1:D:49:SER:OG	1:D:298:SER:OG	2.35	0.45
1:D:39:ARG:O	1:D:40:ASP:C	2.56	0.44
1:C:342:VAL:HB	1:C:354:LEU:HB2	1.99	0.44
1:A:312:GLN:HA	1:A:317:ALA:H	1.82	0.44
1:D:391:GLY:HA3	1:D:395:ALA:HA	1.99	0.44
1:A:426:GLY:C	1:A:428:GLU:N	2.70	0.44
1:D:15:ASP:HA	1:D:16:PRO:HD2	1.65	0.44
1:A:334:LEU:HD12	1:A:334:LEU:HA	1.86	0.44
1:D:27:VAL:HG23	1:D:37:TYR:HB3	1.99	0.44
1:A:26:VAL:HA	1:A:37:TYR:O	2.17	0.44
1:B:93:ARG:HG2	1:B:128:TRP:CG	2.53	0.44
1:D:140:PRO:HA	1:D:143:GLU:OE2	2.17	0.44
1:D:199:THR:CG2	1:D:227:ALA:HA	2.48	0.44
1:C:49:SER:HB2	2:C:500:BH6:CL	2.55	0.43
1:D:225:LEU:HA	1:D:225:LEU:HD12	1.79	0.43
1:C:125:ASP:HB2	1:C:267:GLY:O	2.17	0.43
1:C:323:GLY:O	1:C:327:VAL:HG23	2.18	0.43
1:C:160:GLU:HG2	3:C:604:SO4:O2	2.18	0.43
1:B:110:VAL:HG12	1:B:115:VAL:HB	1.99	0.43
1:A:418:SER:OG	1:A:449:GLN:NE2	2.51	0.43
1:D:299:ASN:HD22	1:D:302:HIS:H	1.63	0.43
1:D:295:MET:HB2	1:D:379:SER:HB2	2.01	0.43
1:D:387:ASP:O	1:D:389:PHE:N	2.52	0.43
1:D:85:VAL:HG21	1:D:88:LEU:HD23	2.01	0.43
1:C:27:VAL:HG21	1:C:456:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LEU:HD13	1:A:343:LEU:HD11	2.01	0.43
1:C:12:ILE:HG21	1:C:452:ILE:HG13	2.01	0.43
1:B:41:GLY:HA2	1:B:357:ALA:HB3	2.01	0.42
1:D:240:GLU:O	1:D:241:PRO:C	2.58	0.42
1:A:230:ALA:HA	1:A:231:PRO:HD2	1.82	0.42
1:A:1:ARG:NH2	1:A:455:ARG:HH22	2.18	0.42
1:A:147:TYR:HB2	1:A:300:ASN:ND2	2.34	0.42
1:D:412:GLY:O	1:D:418:SER:HA	2.20	0.42
1:A:353:ASN:O	1:A:354:LEU:HD23	2.20	0.42
1:A:9:ILE:HA	1:A:12:ILE:HD12	2.02	0.42
1:B:21:ALA:HB1	1:B:438:ASN:O	2.19	0.42
1:C:212:ARG:HA	1:C:218:THR:O	2.19	0.42
1:B:89:TYR:CZ	1:B:270:PRO:HD3	2.55	0.42
1:D:161:ARG:HG2	1:D:297:PHE:CE2	2.55	0.41
1:B:341:LEU:HA	1:B:341:LEU:HD23	1.87	0.41
1:B:387:ASP:O	1:B:388:PRO:C	2.58	0.41
1:D:96:PRO:O	1:D:302:HIS:CE1	2.73	0.41
2:D:500:BH6:O6	2:D:500:BH6:CL	2.75	0.41
1:B:1:ARG:HG2	1:B:4:GLU:HB2	2.03	0.41
1:B:51:MET:HE2	1:B:353:ASN:CB	2.50	0.41
1:A:198:VAL:HG22	1:A:199:THR:H	1.86	0.41
1:C:307:VAL:O	1:C:323:GLY:HA3	2.20	0.41
1:A:66:ASP:C	1:A:286:GLU:HG2	2.41	0.41
1:B:90:LEU:HD22	1:B:249:PHE:HB2	2.03	0.41
1:A:442:GLY:HA3	1:A:443:PRO:HD2	1.89	0.41
1:B:463:GLN:HB2	1:B:463:GLN:HE21	1.63	0.41
1:D:12:ILE:HG22	1:D:448:VAL:HG13	2.03	0.41
1:D:47:PRO:O	1:D:48:ALA:C	2.59	0.40
1:A:327:VAL:O	1:A:331:LEU:HG	2.20	0.40
1:D:387:ASP:HA	1:D:388:PRO:HD2	1.89	0.40
1:C:122:LEU:HD23	1:C:264:VAL:HG22	2.03	0.40
1:A:213:PRO:HD2	1:A:218:THR:O	2.21	0.40
1:D:199:THR:HA	1:D:225:LEU:O	2.20	0.40
1:A:73:VAL:HA	1:A:89:TYR:O	2.21	0.40
1:C:193:LEU:HD11	1:C:195:ASN:HB2	2.04	0.40
1:B:370:ALA:HB1	1:B:371:PRO:HD2	2.02	0.40
1:D:88:LEU:HB3	1:D:122:LEU:HD13	2.03	0.40
1:A:190:TYR:OH	1:A:243:ALA:HB3	2.22	0.40
1:D:297:PHE:O	1:D:298:SER:HB3	2.21	0.40
1:B:253:LEU:HB3	1:B:258:VAL:HB	2.02	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	464/466 (100%)	438 (94%)	24 (5%)	2 (0%)	39	69
1	B	464/466 (100%)	437 (94%)	26 (6%)	1 (0%)	52	80
1	C	464/466 (100%)	437 (94%)	26 (6%)	1 (0%)	52	80
1	D	464/466 (100%)	426 (92%)	34 (7%)	4 (1%)	21	49
All	All	1856/1864 (100%)	1738 (94%)	110 (6%)	8 (0%)	39	69

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	130	ASP
1	A	427	PRO
1	D	81	ARG
1	A	298	SER
1	D	16	PRO
1	B	31	ALA
1	D	35	GLU
1	D	388	PRO

### 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	339/339 (100%)	308 (91%)	31 (9%)	12	26
1	B	338/339 (100%)	312 (92%)	26 (8%)	16	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	338/339 (100%)	314 (93%)	24 (7%)	18	41
1	D	339/339 (100%)	311 (92%)	28 (8%)	14	31
All	All	1354/1356 (100%)	1245 (92%)	109 (8%)	15	33

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	19	GLU
1	A	28	VAL
1	A	30	THR
1	A	46	LEU
1	A	88	LEU
1	A	98	LEU
1	A	119	ARG
1	A	154	LEU
1	A	178	GLU
1	A	208	LEU
1	A	211	ASP
1	A	233	THR
1	A	250	GLU
1	A	255	SER
1	A	259	THR
1	A	274	GLN
1	A	298	SER
1	A	299	ASN
1	A	319	THR
1	A	320	TRP
1	A	324	LEU
1	A	341	LEU
1	A	349	LEU
1	A	359	THR
1	A	369	SER
1	A	375	THR
1	A	428	GLU
1	A	437	ASN
1	A	455	ARG
1	A	463	GLN
1	B	2	LEU
1	B	4	GLU
1	B	18	LEU

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Mol	Chain	Res	Type
1	B	23	SER
1	B	30	THR
1	B	88	LEU
1	B	98	LEU
1	B	113	SER
1	B	154	LEU
1	B	198	VAL
1	B	233	THR
1	B	259	THR
1	B	275	ASP
1	B	289	GLU
1	B	299	ASN
1	B	320	TRP
1	B	324	LEU
1	B	332	SER
1	B	349	LEU
1	B	369	SER
1	B	374	GLN
1	B	375	THR
1	B	377	SER
1	B	386	SER
1	B	428	GLU
1	B	431	LEU
1	C	1	ARG
1	C	2	LEU
1	C	3	THR
1	C	46	LEU
1	C	85	VAL
1	C	117	THR
1	C	132	GLU
1	C	134	LEU
1	C	154	LEU
1	C	183	ASP
1	C	250	GLU
1	C	254	GLU
1	C	298	SER
1	C	299	ASN
1	C	302	HIS
1	C	320	TRP
1	C	324	LEU
1	C	349	LEU
1	C	359	THR

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Mol	Chain	Res	Type
1	C	369	SER
1	C	386	SER
1	C	394	LEU
1	C	431	LEU
1	C	438	ASN
1	D	10	ASP
1	D	63	LEU
1	D	68	SER
1	D	81	ARG
1	D	84	GLU
1	D	88	LEU
1	D	98	LEU
1	D	113	SER
1	D	119	ARG
1	D	137	ASP
1	D	154	LEU
1	D	170	SER
1	D	184	LEU
1	D	214	VAL
1	D	291	LEU
1	D	299	ASN
1	D	309	SER
1	D	320	TRP
1	D	324	LEU
1	D	349	LEU
1	D	359	THR
1	D	375	THR
1	D	380	LEU
1	D	393	THR
1	D	401	THR
1	D	411	THR
1	D	437	ASN
1	D	438	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	150	GLN
1	A	158	HIS
1	A	299	ASN
1	A	312	GLN

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Mol	Chain	Res	Type
1	A	462	HIS
1	A	463	GLN
1	B	50	ASN
1	B	150	GLN
1	B	158	HIS
1	B	299	ASN
1	B	302	HIS
1	B	374	GLN
1	B	396	ASN
1	B	463	GLN
1	C	44	GLN
1	C	50	ASN
1	C	282	HIS
1	C	299	ASN
1	C	302	HIS
1	C	366	GLN
1	D	150	GLN
1	D	299	ASN
1	D	302	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	BH6	A	500	1	11,14,14	1.43	2 (18%)	14,18,18	1.05	1 (7%)
3	SO4	A	600	-	4,4,4	0.15	0	6,6,6	0.23	0
3	SO4	A	601	-	4,4,4	0.30	0	6,6,6	0.24	0
3	SO4	A	602	-	4,4,4	0.20	0	6,6,6	0.32	0
3	SO4	A	603	-	4,4,4	0.06	0	6,6,6	0.42	0
3	SO4	A	604	-	4,4,4	0.11	0	6,6,6	0.36	0
2	BH6	B	500	1	10,12,14	1.40	1 (10%)	14,15,18	1.56	2 (14%)
3	SO4	B	601	-	4,4,4	0.33	0	6,6,6	0.44	0
3	SO4	B	602	-	4,4,4	0.19	0	6,6,6	0.20	0
3	SO4	B	603	-	4,4,4	0.35	0	6,6,6	0.62	0
3	SO4	B	604	-	4,4,4	0.13	0	6,6,6	0.12	0
3	SO4	B	605	-	4,4,4	0.11	0	6,6,6	0.32	0
2	BH6	C	500	1	10,12,14	1.47	1 (10%)	14,15,18	1.39	4 (28%)
3	SO4	C	601	-	4,4,4	0.29	0	6,6,6	0.24	0
3	SO4	C	602	-	4,4,4	0.20	0	6,6,6	0.25	0
3	SO4	C	603	-	4,4,4	0.14	0	6,6,6	0.25	0
3	SO4	C	604	-	4,4,4	0.03	0	6,6,6	0.17	0
3	SO4	C	605	-	4,4,4	0.10	0	6,6,6	0.15	0
2	BH6	D	500	1	11,14,14	1.27	2 (18%)	14,18,18	1.10	1 (7%)
3	SO4	D	600	-	4,4,4	0.19	0	6,6,6	0.15	0
3	SO4	D	601	-	4,4,4	0.24	0	6,6,6	0.15	0
3	SO4	D	602	-	4,4,4	0.09	0	6,6,6	0.32	0
3	SO4	D	603	-	4,4,4	0.16	0	6,6,6	0.20	0
3	SO4	D	604	-	4,4,4	0.02	0	6,6,6	0.24	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	BH6	A	500	1	-	0/6/9/9	0/1/1/1
3	SO4	A	600	-	-	0/0/0/0	0/0/0/0
3	SO4	A	601	-	-	0/0/0/0	0/0/0/0
3	SO4	A	602	-	-	0/0/0/0	0/0/0/0
3	SO4	A	603	-	-	0/0/0/0	0/0/0/0
3	SO4	A	604	-	-	0/0/0/0	0/0/0/0
2	BH6	B	500	1	-	0/6/7/9	0/1/1/1
3	SO4	B	601	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	602	-	-	0/0/0/0	0/0/0/0
3	SO4	B	603	-	-	0/0/0/0	0/0/0/0
3	SO4	B	604	-	-	0/0/0/0	0/0/0/0
3	SO4	B	605	-	-	0/0/0/0	0/0/0/0
2	BH6	C	500	1	-	0/6/7/9	0/1/1/1
3	SO4	C	601	-	-	0/0/0/0	0/0/0/0
3	SO4	C	602	-	-	0/0/0/0	0/0/0/0
3	SO4	C	603	-	-	0/0/0/0	0/0/0/0
3	SO4	C	604	-	-	0/0/0/0	0/0/0/0
3	SO4	C	605	-	-	0/0/0/0	0/0/0/0
2	BH6	D	500	1	-	0/6/9/9	0/1/1/1
3	SO4	D	600	-	-	0/0/0/0	0/0/0/0
3	SO4	D	601	-	-	0/0/0/0	0/0/0/0
3	SO4	D	602	-	-	0/0/0/0	0/0/0/0
3	SO4	D	603	-	-	0/0/0/0	0/0/0/0
3	SO4	D	604	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	BH6	B-C3	2.73	1.60	1.56
2	A	500	BH6	B-C3	2.92	1.60	1.56
2	D	500	BH6	C14-CL	2.94	1.80	1.73
2	A	500	BH6	C14-CL	3.44	1.82	1.73
2	B	500	BH6	C14-CL	3.60	1.82	1.73
2	C	500	BH6	C14-CL	3.73	1.82	1.73

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	BH6	O6-C5-C7	-2.38	116.40	120.95
2	C	500	BH6	C13-C14-C7	-2.01	119.01	121.35
2	B	500	BH6	C8-C7-C14	2.01	120.19	117.77
2	C	500	BH6	C8-C7-C14	2.22	120.44	117.77
2	D	500	BH6	C8-C7-C14	2.45	120.71	117.77
2	A	500	BH6	C8-C7-C14	2.61	120.92	117.77
2	C	500	BH6	C3-N4-C5	2.97	127.29	121.89
2	B	500	BH6	C3-N4-C5	4.80	130.62	121.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	BH6	1	0
2	B	500	BH6	1	0
2	C	500	BH6	3	0
3	C	604	SO4	1	0
2	D	500	BH6	3	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%)	-0.12	5 (1%) 82 83	27, 42, 70, 116	0
1	B	466/466 (100%)	0.01	3 (0%) 90 91	27, 41, 66, 114	0
1	C	466/466 (100%)	-0.12	9 (1%) 70 70	25, 39, 61, 99	0
1	D	466/466 (100%)	0.17	21 (4%) 37 36	27, 55, 98, 121	0
All	All	1864/1864 (100%)	-0.02	38 (2%) 68 69	25, 43, 81, 121	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	80	GLY	7.2
1	D	429	GLY	4.1
1	A	429	GLY	3.8
1	A	427	PRO	3.6
1	D	400	GLY	3.3
1	C	117	THR	3.2
1	D	111	ALA	3.2
1	D	461	GLY	2.9
1	D	264	VAL	2.8
1	D	261	LYS	2.7
1	C	279	LEU	2.7
1	D	399	ARG	2.7
1	B	261	LYS	2.6
1	D	37	TYR	2.6
1	D	447	ALA	2.6
1	D	451	ALA	2.6
1	C	122	LEU	2.6
1	C	2	LEU	2.5
1	C	428	GLU	2.5
1	D	118	VAL	2.4
1	C	115	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	2	LEU	2.3
1	D	11	ALA	2.3
1	D	465	PRO	2.3
1	D	274	GLN	2.3
1	B	1	ARG	2.3
1	A	82	ARG	2.1
1	B	464	ALA	2.1
1	C	85	VAL	2.1
1	D	428	GLU	2.0
1	D	36	LEU	2.0
1	A	117	THR	2.0
1	D	85	VAL	2.0
1	C	83	GLY	2.0
1	D	426	GLY	2.0
1	D	112	ALA	2.0
1	C	73	VAL	2.0
1	D	454	VAL	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	SO4	B	604	5/5	0.76	0.26	6.75	129,130,130,130	0
3	SO4	D	600	5/5	0.88	0.30	6.60	118,118,118,118	0
4	MG	A	611	1/1	0.76	0.25	2.66	66,66,66,66	0
2	BH6	D	500	14/14	0.93	0.20	2.04	43,52,55,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BH6	A	500	14/14	0.94	0.17	0.86	35,48,53,57	0
3	SO4	C	604	5/5	0.94	0.15	0.54	81,82,83,83	0
2	BH6	C	500	12/14	0.92	0.15	0.16	22,58,61,66	0
3	SO4	A	604	5/5	0.90	0.15	-0.07	100,100,101,101	0
3	SO4	A	600	5/5	0.99	0.13	-0.29	59,59,60,62	0
3	SO4	D	602	5/5	0.89	0.14	-0.81	86,86,86,86	0
2	BH6	B	500	12/14	0.94	0.12	-0.97	23,57,61,67	0
4	MG	D	610	1/1	0.99	0.07	-1.92	26,26,26,26	0
3	SO4	D	604	5/5	0.95	0.13	-2.18	76,77,78,78	0
4	MG	A	610	1/1	0.96	0.05	-2.19	28,28,28,28	0
3	SO4	C	605	5/5	0.96	0.12	-3.92	74,75,76,76	0
3	SO4	C	602	5/5	0.96	0.13	-	68,68,69,69	0
3	SO4	A	602	5/5	0.92	0.15	-	81,81,82,82	0
3	SO4	A	603	5/5	0.95	0.22	-	61,64,65,65	0
3	SO4	B	602	5/5	0.94	0.14	-	59,59,60,60	0
3	SO4	D	601	5/5	0.94	0.15	-	68,69,69,69	0
3	SO4	B	605	5/5	0.95	0.13	-	63,63,64,65	0
3	SO4	C	603	5/5	0.98	0.12	-	45,45,46,48	0
3	SO4	C	601	5/5	0.98	0.09	-	46,47,49,50	0
3	SO4	D	603	5/5	0.97	0.14	-	44,45,46,46	0
3	SO4	B	601	5/5	0.97	0.11	-	43,44,46,47	0
3	SO4	A	601	5/5	0.97	0.11	-	39,40,41,41	0
3	SO4	B	603	5/5	0.97	0.12	-	44,44,45,46	0
4	MG	D	611	1/1	0.85	0.11	-	51,51,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.