



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:04 am GMT

PDB ID : 2WB4  
Title : ACTIVATED DIGUANYLATE CYCLASE PLED IN COMPLEX WITH C-DI-GMP  
Authors : Wassmann, P.; Schirmer, T.  
Deposited on : 2009-02-20  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

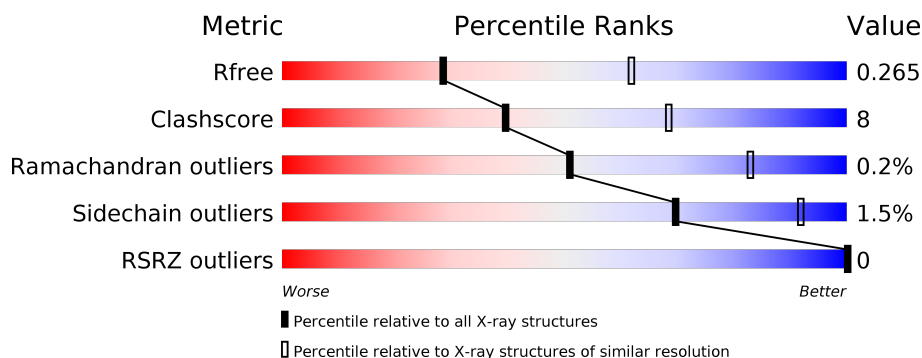
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	459	
1	B	459	

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
5	SO4	A	1461	-	-	X	-

## 2 Entry composition [i](#)

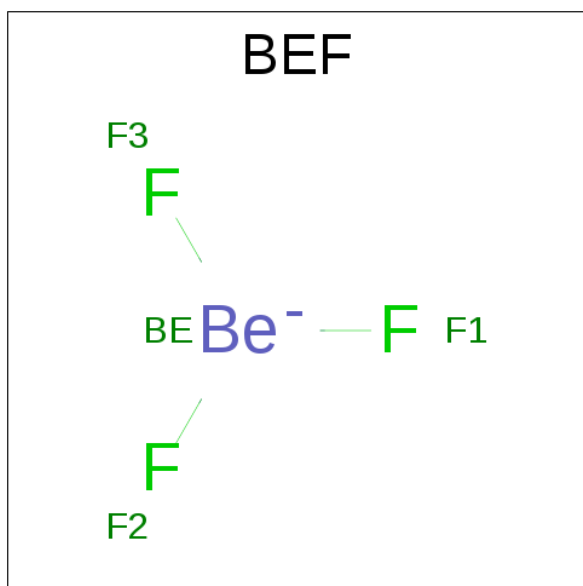
There are 6 unique types of molecules in this entry. The entry contains 7214 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIGUANYLATE CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	124	0	0
			3521	2190	651	665	15			
1	B	441	Total	C	N	O	S	78	0	0
			3387	2110	615	648	14			

- Molecule 2 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF<sub>3</sub>).

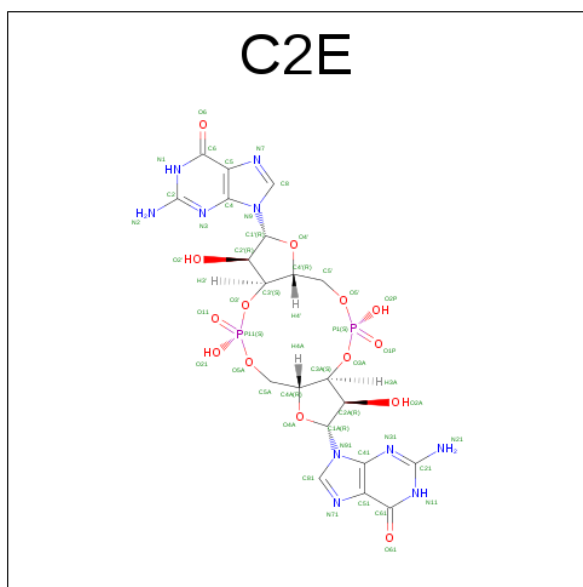


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Be	F	0	0
			4	1	3		
2	B	1	Total	Be	F	0	0
			4	1	3		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mg 2 2	0	0
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is 9,9'-[(2R,3R,3AS,5S,7AR,9R,10R,10AS,12S,14AR)-3,5,10,12-TETRAHYDROXY-5,12-DIOXIDOOCTAHYDRO-2H,7H-DIFURO[3,2-D:3',2'-J][1,3,7,9,2,8]TETRAOXADIPHOSPHACYCLODODECINE-2,9-DIYL]BIS(2-AMINO-1,9-DIHYDRO-6H-PURIN-6-ONE) (three-letter code: C2E) (formula:  $C_{20}H_{24}N_{10}O_{14}P_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 46 20 10 14 2	0	0
4	A	1	Total C N O P 46 20 10 14 2	0	0
4	B	1	Total C N O P 46 20 10 14 2	0	0
4	B	1	Total C N O P 46 20 10 14 2	0	0
4	B	1	Total C N O P 46 20 10 14 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

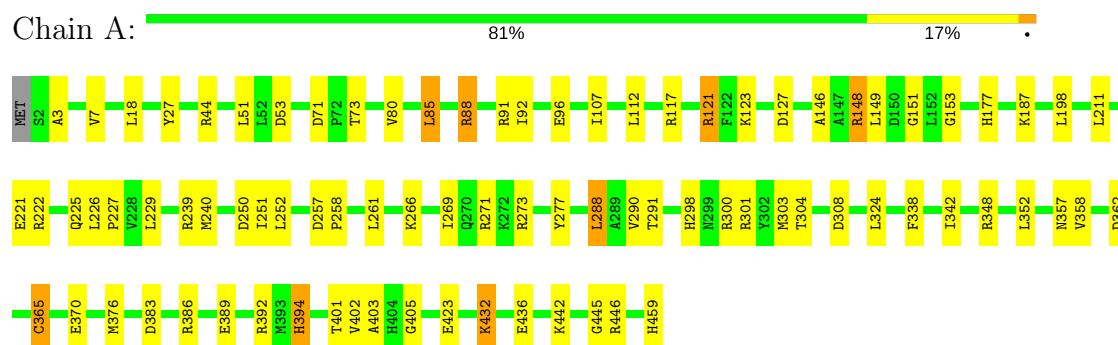
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	25	Total	O	0	0
			25	25		
6	B	25	Total	O	0	0
			25	25		

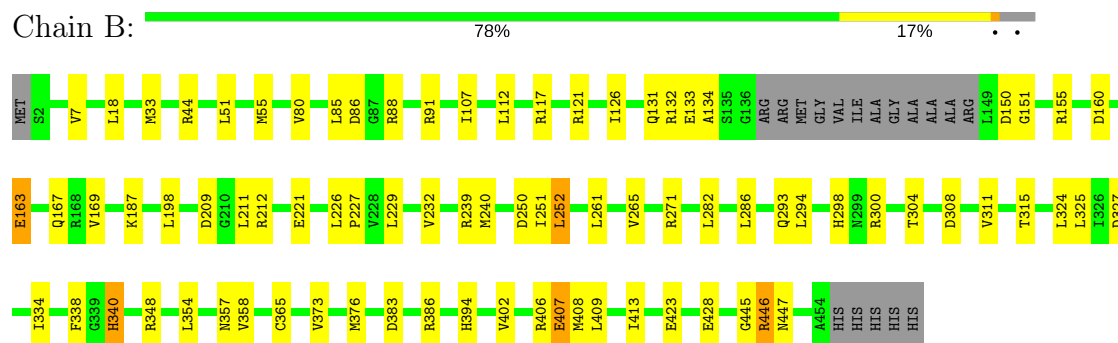
### 3 Residue-property plots

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



#### • Molecule 1: DIGUANYLATE CYCLASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.56Å 127.43Å 88.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 2.80 63.71 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.5 (60.00-2.80) 86.6 (63.71-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.41 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.239 , 0.268 0.239 , 0.265	Depositor DCC
$R_{free}$ test set	1691 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	7214	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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, BEF, SO4, C2E

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	0.78	8/3569 (0.2%)	1.23	25/4825 (0.5%)
1	B	0.79	7/3429 (0.2%)	1.20	26/4636 (0.6%)
All	All	0.79	15/6998 (0.2%)	1.21	51/9461 (0.5%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	ARG	CZ-NH1	-9.47	1.20	1.33
1	B	88	ARG	CZ-NH1	-9.45	1.20	1.33
1	B	88	ARG	CZ-NH2	-8.09	1.22	1.33
1	A	88	ARG	CZ-NH2	-6.81	1.24	1.33
1	B	133	GLU	CG-CD	6.71	1.62	1.51
1	A	365	CYS	CB-SG	-6.38	1.71	1.82
1	A	96	GLU	CG-CD	6.00	1.60	1.51
1	A	85	LEU	CG-CD2	-5.95	1.29	1.51
1	A	432	LYS	CE-NZ	5.86	1.63	1.49
1	B	160	ASP	CG-OD1	-5.81	1.11	1.25
1	A	222	ARG	CB-CG	-5.43	1.37	1.52
1	B	293	GLN	CD-NE2	-5.26	1.19	1.32
1	B	428	GLU	CG-CD	5.22	1.59	1.51
1	B	293	GLN	CD-OE1	-5.17	1.12	1.24
1	A	221	GLU	CB-CG	5.14	1.61	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ARG	NE-CZ-NH1	-23.16	108.72	120.30
1	B	44	ARG	NE-CZ-NH2	-21.63	109.49	120.30
1	B	121	ARG	NE-CZ-NH2	-21.52	109.54	120.30
1	A	44	ARG	NE-CZ-NH1	-20.74	109.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ARG	NE-CZ-NH2	20.18	130.39	120.30
1	A	117	ARG	NE-CZ-NH2	-20.08	110.26	120.30
1	B	44	ARG	NE-CZ-NH1	19.88	130.24	120.30
1	B	121	ARG	NE-CZ-NH1	19.63	130.11	120.30
1	A	121	ARG	NE-CZ-NH1	-19.57	110.52	120.30
1	B	117	ARG	NE-CZ-NH2	18.52	129.56	120.30
1	A	44	ARG	NE-CZ-NH2	18.48	129.54	120.30
1	B	117	ARG	NE-CZ-NH1	-18.31	111.15	120.30
1	A	117	ARG	NE-CZ-NH1	17.88	129.24	120.30
1	A	121	ARG	NE-CZ-NH2	17.20	128.90	120.30
1	B	91	ARG	NE-CZ-NH2	-15.43	112.58	120.30
1	B	91	ARG	NE-CZ-NH1	13.99	127.29	120.30
1	A	308	ASP	CB-CG-OD1	13.76	130.68	118.30
1	A	301	ARG	CG-CD-NE	13.68	140.53	111.80
1	A	88	ARG	NE-CZ-NH1	13.46	127.03	120.30
1	B	327	ASP	CB-CG-OD2	13.10	130.09	118.30
1	B	88	ARG	NE-CZ-NH1	11.41	126.01	120.30
1	B	155	ARG	CG-CD-NE	10.95	134.80	111.80
1	A	88	ARG	NH1-CZ-NH2	-9.78	108.64	119.40
1	A	117	ARG	CD-NE-CZ	9.68	137.15	123.60
1	B	44	ARG	CD-NE-CZ	9.48	136.87	123.60
1	B	88	ARG	NH1-CZ-NH2	-9.31	109.16	119.40
1	B	121	ARG	CD-NE-CZ	9.19	136.46	123.60
1	B	117	ARG	CD-NE-CZ	9.07	136.30	123.60
1	B	88	ARG	NE-CZ-NH2	9.06	124.83	120.30
1	A	121	ARG	CD-NE-CZ	8.97	136.16	123.60
1	A	91	ARG	CD-NE-CZ	8.91	136.08	123.60
1	A	44	ARG	CD-NE-CZ	8.81	135.93	123.60
1	A	88	ARG	NE-CZ-NH2	8.05	124.33	120.30
1	B	327	ASP	CB-CG-OD1	-8.00	111.10	118.30
1	A	394	HIS	CB-CA-C	-7.82	94.77	110.40
1	B	86	ASP	CB-CG-OD2	-7.55	111.51	118.30
1	B	308	ASP	CB-CG-OD1	7.36	124.92	118.30
1	A	308	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	B	163	GLU	CB-CG-CD	6.82	132.63	114.20
1	B	160	ASP	CB-CG-OD1	6.74	124.36	118.30
1	A	445	GLY	N-CA-C	-6.13	97.78	113.10
1	B	91	ARG	CD-NE-CZ	6.05	132.07	123.60
1	B	308	ASP	CB-CG-OD2	-5.92	112.98	118.30
1	A	187	LYS	CD-CE-NZ	-5.86	98.22	111.70
1	A	53	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	B	407	GLU	N-CA-CB	-5.65	100.43	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	LYS	CG-CD-CE	-5.63	95.00	111.90
1	A	423	GLU	CA-CB-CG	5.54	125.59	113.40
1	B	187	LYS	CB-CG-CD	5.54	126.00	111.60
1	B	33	MET	CB-CG-SD	5.41	128.63	112.40
1	A	225	GLN	CA-CB-CG	5.19	124.81	113.40

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	3521	0	3581	64	0
1	B	3387	0	3451	52	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	92	0	44	1	0
4	B	138	0	66	1	0
5	A	10	0	0	3	0
5	B	5	0	0	0	0
6	A	25	0	0	3	0
6	B	25	0	0	1	0
All	All	7214	0	7142	117	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 8.

All (117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:LEU:HD13	1:A:376:MET:CE	1.73	1.17
1:A:324:LEU:HD13	1:A:376:MET:HE1	1.16	1.13
1:B:324:LEU:HD13	1:B:376:MET:HE2	1.27	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LEU:HD11	1:A:291:THR:OG1	1.53	1.06
1:B:324:LEU:HD13	1:B:376:MET:CE	1.89	1.01
1:B:357:ASN:ND2	1:B:394:HIS:CE1	2.30	1.00
1:B:357:ASN:ND2	1:B:394:HIS:HE1	1.60	0.98
1:A:240:MET:HE3	1:A:251:ILE:HG21	1.45	0.97
1:B:357:ASN:HD21	1:B:394:HIS:HE1	1.09	0.95
1:B:357:ASN:HD21	1:B:394:HIS:CE1	1.96	0.80
1:A:240:MET:CE	1:A:251:ILE:HG21	2.12	0.79
1:B:240:MET:HE2	1:B:251:ILE:HG21	1.72	0.72
1:A:107:ILE:HD13	1:A:112:LEU:HD22	1.71	0.71
1:A:324:LEU:HD13	1:A:376:MET:HE3	1.73	0.70
4:B:507:C2E:H8	4:B:507:C2E:O5'	1.90	0.69
1:B:357:ASN:CG	1:B:394:HIS:CE1	2.68	0.67
1:B:107:ILE:HD13	1:B:112:LEU:HD22	1.77	0.67
1:B:402:VAL:O	1:B:406:ARG:NH1	2.28	0.66
1:A:342:ILE:HG23	1:A:402:VAL:CG1	2.26	0.66
1:A:288:LEU:CD1	1:A:291:THR:OG1	2.39	0.65
1:A:401:THR:O	1:A:402:VAL:HG23	1.97	0.65
4:A:505:C2E:O21	6:A:2024:HOH:O	2.13	0.64
1:A:370:GLU:OE1	6:A:2015:HOH:O	2.15	0.64
1:B:240:MET:CE	1:B:251:ILE:HG21	2.28	0.63
1:A:324:LEU:CD1	1:A:376:MET:CE	2.66	0.61
1:B:338:PHE:HZ	1:B:408:MET:HB2	1.65	0.61
1:A:107:ILE:CD1	1:A:112:LEU:HD22	2.30	0.61
1:A:148:ARG:HB3	1:B:340:HIS:CD2	2.36	0.61
1:A:342:ILE:HG23	1:A:402:VAL:HG13	1.83	0.60
1:A:151:GLY:HA2	1:A:269:ILE:HG22	1.83	0.60
1:A:401:THR:HG23	1:A:405:GLY:HA2	1.84	0.60
1:B:445:GLY:O	1:B:446:ARG:HB2	2.01	0.59
1:A:153:GLY:O	1:A:177:HIS:ND1	2.34	0.58
1:B:211:LEU:HD12	1:B:239:ARG:NH1	2.19	0.58
1:A:300:ARG:O	1:A:304:THR:HG23	2.03	0.58
1:A:446:ARG:NH1	5:A:1461:SO4:O2	2.38	0.57
1:A:342:ILE:CG2	1:A:402:VAL:HG11	2.35	0.57
1:A:146:ALA:HB2	1:A:277:TYR:CE2	2.41	0.56
1:B:324:LEU:CD1	1:B:376:MET:CE	2.76	0.56
1:B:413:ILE:O	1:B:447:ASN:HA	2.06	0.56
1:A:229:LEU:CD1	1:A:250:ASP:HB3	2.36	0.55
1:B:324:LEU:HD13	1:B:376:MET:HE1	1.86	0.55
1:A:211:LEU:HD12	1:A:239:ARG:NH1	2.22	0.55
1:A:121:ARG:NH2	5:A:1460:SO4:O2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ILE:CD1	1:B:112:LEU:HD22	2.36	0.54
1:B:126:ILE:HD11	1:B:271:ARG:HE	1.71	0.54
1:B:55:MET:SD	1:B:85:LEU:HD21	2.48	0.54
1:B:229:LEU:CD1	1:B:250:ASP:HB3	2.38	0.53
1:B:315:THR:HB	1:B:423:GLU:HA	1.91	0.53
1:A:88:ARG:HH11	1:A:92:ILE:HD11	1.73	0.53
1:A:389:GLU:OE2	1:A:392:ARG:NH1	2.43	0.52
1:B:338:PHE:CZ	1:B:408:MET:HB2	2.44	0.52
1:B:294:LEU:HD12	1:B:348:ARG:HH21	1.75	0.51
1:A:298:HIS:O	1:A:365:CYS:HB2	2.11	0.50
1:A:291:THR:HG23	6:A:2010:HOH:O	2.11	0.50
1:A:402:VAL:HG12	1:A:403:ALA:N	2.27	0.50
1:A:229:LEU:HD12	1:A:250:ASP:O	2.12	0.49
1:A:402:VAL:CG1	1:A:403:ALA:N	2.75	0.49
1:B:325:LEU:HD13	1:B:373:VAL:HG22	1.95	0.49
1:A:383:ASP:OD1	1:A:386:ARG:NH2	2.39	0.49
1:A:123:LYS:O	1:A:127:ASP:CB	2.61	0.49
1:B:126:ILE:HD11	1:B:271:ARG:NE	2.27	0.49
1:A:226:LEU:HD12	1:A:227:PRO:HD2	1.95	0.49
1:A:342:ILE:HG23	1:A:402:VAL:HG11	1.92	0.48
1:B:338:PHE:HZ	1:B:408:MET:CB	2.25	0.48
1:B:354:LEU:O	1:B:358:VAL:HG22	2.14	0.47
1:A:432:LYS:O	1:A:436:GLU:HG2	2.14	0.47
1:B:232:VAL:CG2	1:B:251:ILE:HG23	2.44	0.47
1:B:298:HIS:O	1:B:365:CYS:HB2	2.15	0.47
1:A:348:ARG:O	1:A:352:LEU:CD1	2.62	0.47
1:A:348:ARG:O	1:A:352:LEU:HD13	2.15	0.47
1:B:163:GLU:O	1:B:167:GLN:HG2	2.14	0.47
1:B:383:ASP:OD1	1:B:386:ARG:NH2	2.41	0.46
1:A:290:VAL:O	1:A:290:VAL:CG1	2.64	0.46
1:A:342:ILE:CG2	1:A:402:VAL:CG1	2.91	0.46
1:B:334:ILE:HG12	1:B:409:LEU:HD21	1.98	0.46
1:A:442:LYS:NZ	5:A:1461:SO4:O1	2.36	0.46
1:B:232:VAL:HG22	1:B:251:ILE:HG23	1.98	0.45
1:A:88:ARG:HD2	1:A:257:ASP:OD2	2.16	0.45
1:B:229:LEU:HD12	1:B:250:ASP:O	2.16	0.45
1:A:258:PRO:O	1:A:261:LEU:HB3	2.17	0.45
1:B:7:VAL:HG13	1:B:18:LEU:HD23	1.99	0.45
1:A:146:ALA:O	1:A:149:LEU:HD23	2.17	0.44
1:A:358:VAL:HG13	1:A:362:ASP:OD2	2.17	0.44
1:A:342:ILE:HG21	1:A:402:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LEU:HG	1:A:252:LEU:HD12	1.99	0.44
1:A:401:THR:O	1:A:402:VAL:CG2	2.63	0.44
1:A:401:THR:C	1:A:402:VAL:HG23	2.37	0.44
1:B:51:LEU:HD23	1:B:80:VAL:HB	2.00	0.44
1:A:123:LYS:O	1:A:127:ASP:HB2	2.18	0.44
1:A:338:PHE:HB3	1:A:342:ILE:HD12	2.00	0.44
1:A:71:ASP:OD2	1:A:73:THR:HB	2.18	0.44
1:B:7:VAL:CG1	1:B:18:LEU:HD23	2.48	0.44
1:A:229:LEU:HD13	1:A:250:ASP:HB3	1.99	0.43
1:A:7:VAL:HG13	1:A:18:LEU:HD23	2.01	0.43
1:B:229:LEU:HG	1:B:252:LEU:CD1	2.49	0.43
1:B:300:ARG:HD3	6:B:2019:HOH:O	2.19	0.43
1:B:324:LEU:CD1	1:B:376:MET:HE1	2.47	0.42
1:B:169:VAL:HG13	1:B:261:LEU:HD21	2.01	0.42
1:B:300:ARG:O	1:B:304:THR:HG23	2.19	0.42
1:B:150:ASP:OD1	1:B:151:GLY:N	2.50	0.42
1:B:229:LEU:HD13	1:B:250:ASP:HB3	2.00	0.42
1:B:209:ASP:HB3	1:B:212:ARG:HB3	2.02	0.41
1:B:226:LEU:HD12	1:B:227:PRO:HD2	2.02	0.41
1:A:7:VAL:CG1	1:A:18:LEU:HD23	2.50	0.41
1:A:149:LEU:HA	1:A:149:LEU:HD13	1.92	0.41
1:A:3:ALA:HB3	1:A:27:TYR:CD1	2.55	0.41
1:A:324:LEU:CD1	1:A:376:MET:HE3	2.43	0.41
1:A:357:ASN:OD1	1:A:394:HIS:CE1	2.74	0.41
1:A:149:LEU:HD12	1:A:273:ARG:HB3	2.03	0.41
1:A:303:MET:HG3	1:A:365:CYS:SG	2.60	0.41
1:B:198:LEU:CD2	1:B:265:VAL:HG22	2.50	0.41
1:A:51:LEU:HD23	1:A:80:VAL:HB	2.02	0.41
1:B:406:ARG:C	1:B:408:MET:H	2.25	0.41
1:B:311:VAL:O	1:B:315:THR:HG23	2.21	0.40
1:B:131:GLN:O	1:B:134:ALA:HB3	2.21	0.40
1:A:198:LEU:HD12	1:A:227:PRO:O	2.22	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	456/459 (99%)	444 (97%)	12 (3%)	0	100	100
1	B	437/459 (95%)	422 (97%)	13 (3%)	2 (0%)	32	67
All	All	893/918 (97%)	866 (97%)	25 (3%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	446	ARG
1	B	407	GLU

### 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	373/374 (100%)	368 (99%)	5 (1%)	73	93
1	B	362/374 (97%)	356 (98%)	6 (2%)	66	90
All	All	735/748 (98%)	724 (98%)	11 (2%)	70	92

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	148	ARG
1	A	271	ARG
1	A	288	LEU
1	A	459	HIS
1	B	132	ARG
1	B	221	GLU
1	B	252	LEU
1	B	282	LEU
1	B	286	LEU

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Mol	Chain	Res	Type
1	B	340	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	93	GLN
1	A	280	ASN
1	A	394	HIS
1	A	459	HIS
1	B	93	GLN
1	B	340	HIS
1	B	357	ASN
1	B	394	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 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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
5	SO4	A	1460	-	4,4,4	0.37	0	6,6,6	0.80	0
5	SO4	A	1461	-	4,4,4	0.19	0	6,6,6	0.45	0
2	BEF	A	501	1,3	0,3,3	0.00	-	0,3,3	0.00	-
4	C2E	A	503	-	44,52,52	0.84	1 (2%)	50,82,82	1.70	13 (26%)
4	C2E	A	505	-	44,52,52	0.81	0	50,82,82	1.84	12 (24%)
5	SO4	B	1455	-	4,4,4	0.35	0	6,6,6	0.24	0
2	BEF	B	501	1,3	0,3,3	0.00	-	0,3,3	0.00	-
4	C2E	B	503	-	44,52,52	0.68	0	50,82,82	1.99	15 (30%)
4	C2E	B	505	-	44,52,52	0.85	2 (4%)	50,82,82	1.68	12 (24%)
4	C2E	B	507	3	44,52,52	0.78	0	50,82,82	1.83	17 (34%)

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
5	SO4	A	1460	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1461	-	-	0/0/0/0	0/0/0/0
2	BEF	A	501	1,3	-	0/0/0/0	0/0/0/0
4	C2E	A	503	-	-	0/22/62/62	0/6/7/7
4	C2E	A	505	-	-	0/22/62/62	0/6/7/7
5	SO4	B	1455	-	-	0/0/0/0	0/0/0/0
2	BEF	B	501	1,3	-	0/0/0/0	0/0/0/0
4	C2E	B	503	-	-	0/22/62/62	0/6/7/7
4	C2E	B	505	-	-	0/22/62/62	0/6/7/7
4	C2E	B	507	3	-	0/22/62/62	0/6/7/7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	505	C2E	C61-C51	-2.52	1.36	1.41
4	B	505	C2E	C21-N11	-2.33	1.31	1.35
4	A	503	C2E	O4A-C1A	2.82	1.45	1.41

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	C2E	N31-C21-N11	-4.58	120.77	127.46
4	B	507	C2E	N31-C21-N11	-4.42	121.00	127.46
4	B	503	C2E	N3-C2-N1	-4.11	121.45	127.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	505	C2E	N3-C2-N1	-4.07	121.52	127.46
4	A	503	C2E	N3-C2-N1	-4.06	121.53	127.46
4	A	505	C2E	N31-C21-N11	-4.04	121.56	127.46
4	B	505	C2E	N3-C2-N1	-3.67	122.09	127.46
4	A	503	C2E	C51-C61-N11	-3.49	118.51	123.48
4	A	503	C2E	N31-C21-N11	-3.43	122.45	127.46
4	A	505	C2E	C5-C6-N1	-3.27	118.83	123.48
4	B	507	C2E	C51-C61-N11	-3.24	118.87	123.48
4	B	507	C2E	N3-C2-N1	-3.07	122.98	127.46
4	B	507	C2E	C5-C6-N1	-3.06	119.12	123.48
4	B	505	C2E	C51-C61-N11	-3.05	119.14	123.48
4	B	505	C2E	N31-C21-N11	-2.92	123.19	127.46
4	B	507	C2E	C1A-N91-C41	-2.92	121.59	126.64
4	A	505	C2E	C61-C51-C41	-2.90	117.96	120.84
4	B	507	C2E	O5A-P11-O11	-2.89	97.61	109.25
4	B	503	C2E	C5-C6-N1	-2.88	119.39	123.48
4	B	503	C2E	C2'-C3'-C4'	-2.86	98.12	103.23
4	A	505	C2E	C2A-C3A-C4A	-2.82	98.18	103.23
4	B	503	C2E	C51-C61-N11	-2.82	119.47	123.48
4	A	503	C2E	C5-C6-N1	-2.57	119.83	123.48
4	B	507	C2E	C61-C51-C41	-2.54	118.32	120.84
4	B	503	C2E	C2A-C3A-C4A	-2.31	99.10	103.23
4	A	503	C2E	C4-C5-N7	-2.15	107.33	109.41
4	A	503	C2E	C6-C5-C4	-2.12	118.73	120.84
4	B	507	C2E	C41-C51-N71	-2.09	107.39	109.41
4	A	503	C2E	C2'-C3'-C4'	-2.08	99.51	103.23
4	B	505	C2E	C6-C5-C4	-2.06	118.79	120.84
4	B	503	C2E	O5A-P11-O11	-2.05	100.96	109.25
4	B	507	C2E	O21-P11-O11	2.04	122.83	112.28
4	B	507	C2E	N21-C21-N11	2.14	120.66	117.24
4	B	505	C2E	N21-C21-N31	2.14	121.70	117.75
4	B	503	C2E	N2-C2-N3	2.18	121.78	117.75
4	B	505	C2E	C6-N1-C2	2.22	119.25	116.06
4	B	507	C2E	C2-N3-C4	2.24	117.77	115.16
4	B	507	C2E	C3'-C2'-C1'	2.38	105.30	99.95
4	A	503	C2E	C3'-C2'-C1'	2.41	105.36	99.95
4	A	503	C2E	C21-N31-C41	2.42	117.99	115.16
4	B	505	C2E	C3A-C2A-C1A	2.50	105.56	99.95
4	B	505	C2E	O5A-C5A-C4A	2.58	118.13	109.00
4	B	507	C2E	C4A-O4A-C1A	2.59	112.53	109.77
4	B	507	C2E	C6-N1-C2	2.69	119.92	116.06
4	A	503	C2E	N2-C2-N3	2.76	122.85	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	505	C2E	C61-N11-C21	2.82	120.12	116.06
4	B	507	C2E	C3A-C2A-C1A	2.85	106.36	99.95
4	A	505	C2E	C3'-C2'-C1'	2.87	106.39	99.95
4	B	505	C2E	C3'-C2'-C1'	2.93	106.52	99.95
4	B	503	C2E	N21-C21-N31	3.05	123.37	117.75
4	A	505	C2E	C3A-C2A-C1A	3.14	107.00	99.95
4	B	505	C2E	C4'-O4'-C1'	3.18	113.15	109.77
4	B	503	C2E	C3A-C2A-C1A	3.20	107.14	99.95
4	A	505	C2E	C2-N3-C4	3.23	118.93	115.16
4	A	505	C2E	C21-N31-C41	3.27	118.98	115.16
4	A	505	C2E	C4'-O4'-C1'	3.31	113.29	109.77
4	B	503	C2E	C2-N3-C4	3.39	119.12	115.16
4	A	505	C2E	C6-N1-C2	3.45	121.02	116.06
4	B	505	C2E	C61-N11-C21	3.48	121.06	116.06
4	B	503	C2E	C6-N1-C2	3.50	121.10	116.06
4	A	503	C2E	C2-N3-C4	3.58	119.34	115.16
4	B	507	C2E	C61-N11-C21	3.61	121.26	116.06
4	A	503	C2E	C61-N11-C21	3.74	121.44	116.06
4	B	507	C2E	C21-N31-C41	3.75	119.53	115.16
4	B	505	C2E	C2-N3-C4	3.79	119.59	115.16
4	A	503	C2E	C6-N1-C2	3.82	121.55	116.06
4	B	503	C2E	C21-N31-C41	3.82	119.62	115.16
4	B	503	C2E	C61-N11-C21	3.88	121.65	116.06
4	B	503	C2E	C3'-C2'-C1'	3.90	108.72	99.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1460	SO4	1	0
5	A	1461	SO4	2	0
4	A	505	C2E	1	0
4	B	507	C2E	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	458/459 (99%)	-0.33	0 100 100	2, 13, 21, 37	40 (8%)
1	B	441/459 (96%)	-0.22	0 100 100	2, 13, 27, 51	29 (6%)
All	All	899/918 (97%)	-0.28	0 100 100	2, 13, 25, 51	69 (7%)

There are no RSRZ outliers to report.

### 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
2	BEF	A	501	4/4	0.89	0.22	0.37	13,14,19,23	0
5	SO4	B	1455	5/5	0.98	0.16	-0.45	32,33,36,41	0
4	C2E	B	507	46/46	0.96	0.12	-1.07	2,17,24,28	0
4	C2E	A	505	46/46	0.97	0.12	-1.40	2,5,14,18	0
2	BEF	B	501	4/4	0.97	0.11	-1.71	3,5,6,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	C2E	B	503	46/46	0.97	0.11	-2.38	6,16,22,25	0
3	MG	A	502	1/1	0.90	0.04	-2.53	15,15,15,15	0
4	C2E	B	505	46/46	0.96	0.12	-2.76	2,10,16,23	0
5	SO4	A	1461	5/5	0.97	0.10	-2.79	21,28,33,34	0
3	MG	B	502	1/1	0.96	0.07	-3.30	12,12,12,12	0
4	C2E	A	503	46/46	0.98	0.09	-3.70	2,2,9,13	0
5	SO4	A	1460	5/5	0.94	0.18	-	31,34,41,44	0
3	MG	B	509	1/1	0.91	0.12	-	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.