



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:51 AM GMT

PDB ID : 2V0N  
Title : ACTIVATED RESPONSE REGULATOR PLED IN COMPLEX WITH C-DIGMP AND GTP-ALPHA-S  
Authors : Wassmann, P.; Schirmer, T.  
Deposited on : 2007-05-15  
Resolution : 2.71 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

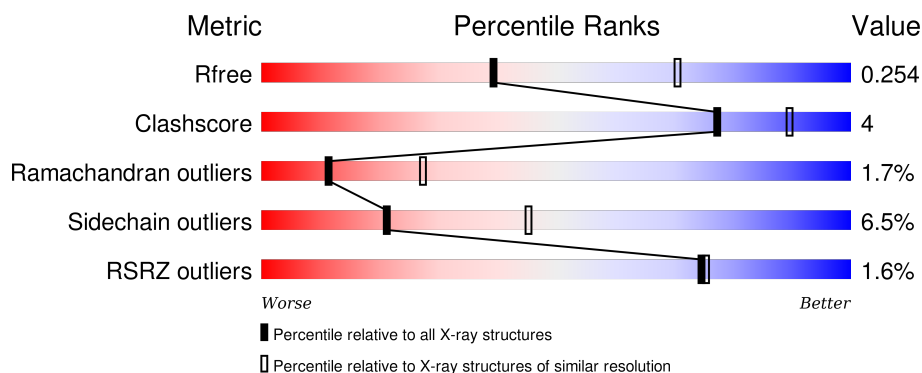
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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	459	<div> <div></div> <div>85%13% ..</div> </div>
1	B	459	<div> <div>2%</div> <div>83%13% ..</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
4	C2E	A	503	X	-	-	-
4	C2E	A	505	X	-	-	-
4	C2E	B	503	X	-	-	-
4	C2E	B	505	X	-	-	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7298 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.

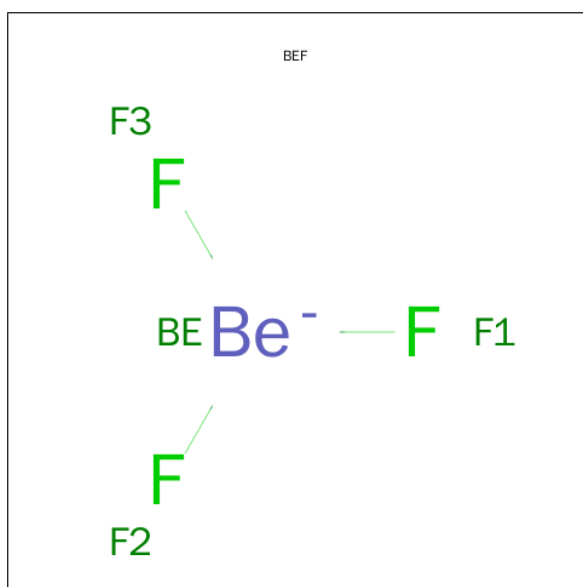
- Molecule 1 is a protein called RESPONSE REGULATOR PLED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	96	0	0
			3531	2196	654	666	15			
1	B	454	Total	C	N	O	S	97	0	0
			3481	2166	639	661	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	455	HIS	-	EXPRESSION TAG	UNP Q9A5I5
A	456	HIS	-	EXPRESSION TAG	UNP Q9A5I5
A	457	HIS	-	EXPRESSION TAG	UNP Q9A5I5
A	458	HIS	-	EXPRESSION TAG	UNP Q9A5I5
A	459	HIS	-	EXPRESSION TAG	UNP Q9A5I5
A	460	HIS	-	EXPRESSION TAG	UNP Q9A5I5
B	455	HIS	-	EXPRESSION TAG	UNP Q9A5I5
B	456	HIS	-	EXPRESSION TAG	UNP Q9A5I5
B	457	HIS	-	EXPRESSION TAG	UNP Q9A5I5
B	458	HIS	-	EXPRESSION TAG	UNP Q9A5I5
B	459	HIS	-	EXPRESSION TAG	UNP Q9A5I5
B	460	HIS	-	EXPRESSION TAG	UNP Q9A5I5

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

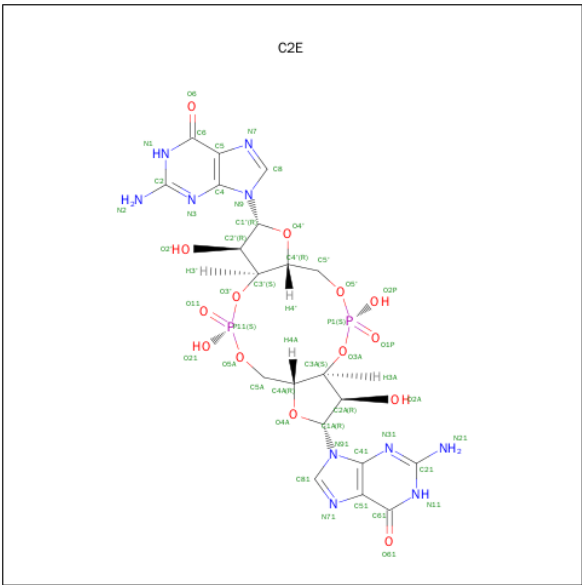


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Be	F	0	0
			4	1	3		
2	B	1	Total	Be	F	0	0
			4	1	3		

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

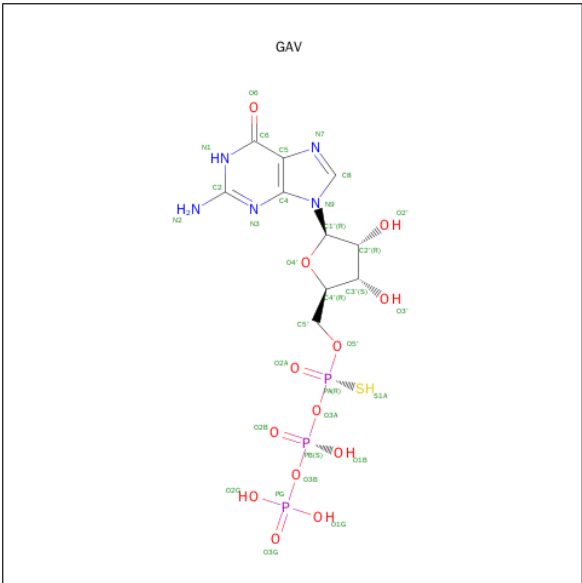
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	3	Total	Mg	0	0
			3	3		

- 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<sub>20</sub>H<sub>24</sub>N<sub>10</sub>O<sub>14</sub>P<sub>2</sub>).



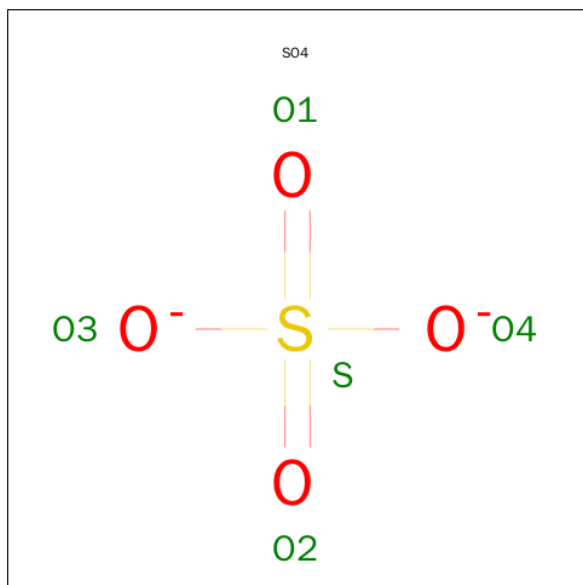
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 46	C 20	N 10	O 14	P 2	0	0
4	A	1	Total 46	C 20	N 10	O 14	P 2	0	0
4	B	1	Total 46	C 20	N 10	O 14	P 2	0	0
4	B	1	Total 46	C 20	N 10	O 14	P 2	0	0

- Molecule 5 is GUANOSINE-5'-RP-ALPHA-THIO-TRIPHOSPHATE (three-letter code: GAV) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	
			32	10	5	13	3	1	
5	B	1	Total	C	N	O	P	S	
			32	10	5	13	3	1	

- Molecule 6 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl		
			1	1	0	0

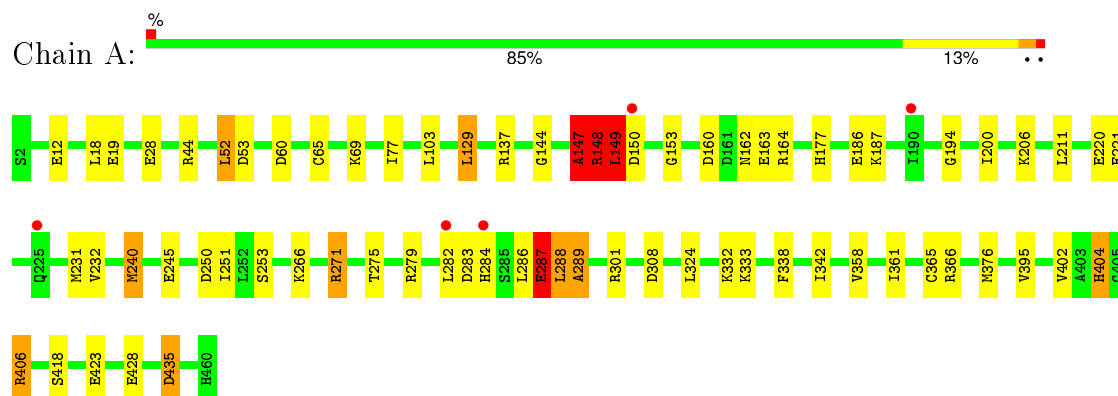
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	8	Total	O		
			8	8	0	0
8	B	6	Total	O		
			6	6	0	0

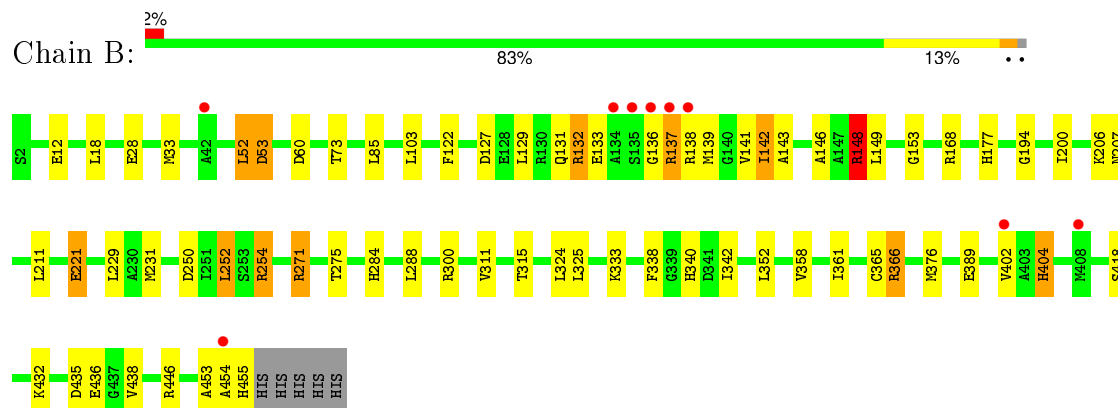
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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: RESPONSE REGULATOR PLED



#### • Molecule 1: RESPONSE REGULATOR PLED





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.97Å 132.56Å 88.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.71 73.56 – 2.71	Depositor EDS
% Data completeness (in resolution range)	94.0 (30.00-2.71) 94.0 (73.56-2.71)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.215 , 0.252 0.219 , 0.254	Depositor DCC
$R_{free}$ test set	1969 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.1	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.5	EDS
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 39295 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7298	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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, CL, GAV, 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	2.47	24/3580 (0.7%)	3.00	48/4840 (1.0%)
1	B	1.04	12/3524 (0.3%)	0.97	18/4762 (0.4%)
All	All	1.90	36/7104 (0.5%)	2.24	66/9602 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	1
All	All	0	10

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	GLU	CD-OE2	111.38	2.48	1.25
1	A	44	ARG	NE-CZ	-50.31	0.67	1.33
1	A	12	GLU	CG-CD	-33.96	1.01	1.51
1	A	406	ARG	NE-CZ	30.01	1.72	1.33
1	A	206	LYS	CG-CD	-28.49	0.55	1.52
1	B	254	ARG	CD-NE	-25.32	1.03	1.46
1	A	435	ASP	CG-OD1	-22.63	0.73	1.25
1	B	12	GLU	CG-CD	-21.67	1.19	1.51
1	B	148	ARG	C-N	20.55	1.81	1.34
1	A	19	GLU	CD-OE1	-19.56	1.04	1.25
1	B	333	LYS	CG-CD	-17.96	0.91	1.52
1	A	423	GLU	CG-CD	-15.55	1.28	1.51
1	A	271	ARG	CG-CD	-14.83	1.14	1.51
1	B	138	ARG	C-O	-14.01	0.96	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	435	ASP	CG-OD2	14.00	1.57	1.25
1	A	287	GLU	C-N	-13.74	1.02	1.34
1	B	206	LYS	CD-CE	13.56	1.85	1.51
1	A	332	LYS	CG-CD	-12.24	1.10	1.52
1	B	168	ARG	NE-CZ	12.16	1.48	1.33
1	A	147	ALA	C-N	-11.83	1.06	1.34
1	B	389	GLU	CB-CG	-11.36	1.30	1.52
1	A	160	ASP	CG-OD1	-11.15	0.99	1.25
1	A	288	LEU	C-N	10.83	1.58	1.34
1	A	186	GLU	CD-OE1	-10.04	1.14	1.25
1	A	187	LYS	CD-CE	9.44	1.74	1.51
1	A	308	ASP	CG-OD1	-8.58	1.05	1.25
1	A	149	LEU	C-N	8.54	1.53	1.34
1	A	220	GLU	CB-CG	-7.89	1.37	1.52
1	B	127	ASP	CB-CG	-6.82	1.37	1.51
1	A	333	LYS	CD-CE	-6.42	1.35	1.51
1	A	19	GLU	CD-OE2	-6.15	1.18	1.25
1	B	142	ILE	N-CA	-5.96	1.34	1.46
1	B	221	GLU	CD-OE2	5.70	1.31	1.25
1	B	28	GLU	CG-CD	-5.67	1.43	1.51
1	A	65	CYS	CB-SG	-5.62	1.72	1.81
1	A	245	GLU	CG-CD	-5.21	1.44	1.51

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ARG	NE-CZ-NH2	-110.75	64.93	120.30
1	A	44	ARG	NE-CZ-NH1	94.48	167.54	120.30
1	A	186	GLU	OE1-CD-OE2	-50.93	62.18	123.30
1	A	406	ARG	NE-CZ-NH1	-46.14	97.23	120.30
1	A	287	GLU	O-C-N	-45.42	50.03	122.70
1	A	435	ASP	CB-CG-OD2	-38.78	83.40	118.30
1	A	406	ARG	NE-CZ-NH2	36.62	138.61	120.30
1	A	147	ALA	O-C-N	-34.19	68.00	122.70
1	A	150	ASP	N-CA-CB	-33.06	51.10	110.60
1	A	149	LEU	O-C-N	-32.33	70.97	122.70
1	A	186	GLU	CG-CD-OE2	-30.97	56.35	118.30
1	A	435	ASP	CB-CG-OD1	-27.75	93.32	118.30
1	A	19	GLU	OE1-CD-OE2	27.04	155.74	123.30
1	A	147	ALA	CA-C-N	23.52	168.94	117.20
1	A	160	ASP	CB-CG-OD2	-20.15	100.17	118.30
1	A	308	ASP	CB-CG-OD2	-19.51	100.74	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	LEU	CA-C-N	18.97	158.93	117.20
1	B	254	ARG	CD-NE-CZ	17.98	148.77	123.60
1	A	287	GLU	C-N-CA	17.55	165.59	121.70
1	A	287	GLU	CA-C-N	17.42	155.53	117.20
1	B	366	ARG	NE-CZ-NH2	-16.86	111.87	120.30
1	B	366	ARG	NE-CZ-NH1	16.29	128.45	120.30
1	A	206	LYS	CB-CG-CD	16.22	153.76	111.60
1	A	206	LYS	CG-CD-CE	14.47	155.31	111.90
1	B	138	ARG	N-CA-CB	-14.00	85.41	110.60
1	B	138	ARG	CA-C-O	13.25	147.93	120.10
1	A	366	ARG	NE-CZ-NH1	-12.54	114.03	120.30
1	B	206	LYS	CD-CE-NZ	12.44	140.32	111.70
1	B	141	VAL	C-N-CA	-12.16	91.30	121.70
1	A	366	ARG	NE-CZ-NH2	11.96	126.28	120.30
1	A	147	ALA	C-N-CA	11.79	151.18	121.70
1	A	160	ASP	OD1-CG-OD2	11.59	145.31	123.30
1	A	12	GLU	CB-CG-CD	10.31	142.03	114.20
1	A	423	GLU	CB-CG-CD	9.45	139.72	114.20
1	B	142	ILE	CA-C-N	-9.08	97.23	117.20
1	A	19	GLU	CG-CD-OE1	-9.07	100.15	118.30
1	A	44	ARG	CD-NE-CZ	9.06	136.28	123.60
1	B	148	ARG	C-N-CA	-8.96	99.29	121.70
1	B	333	LYS	CB-CG-CD	8.87	134.67	111.60
1	B	389	GLU	CA-CB-CG	8.85	132.87	113.40
1	A	423	GLU	CG-CD-OE1	-8.65	101.00	118.30
1	A	423	GLU	CG-CD-OE2	8.63	135.57	118.30
1	A	12	GLU	CG-CD-OE1	8.41	135.12	118.30
1	A	12	GLU	CG-CD-OE2	-8.38	101.55	118.30
1	A	435	ASP	OD1-CG-OD2	8.33	139.13	123.30
1	A	19	GLU	CG-CD-OE2	-7.78	102.74	118.30
1	A	308	ASP	CB-CG-OD1	7.39	124.95	118.30
1	B	366	ARG	CD-NE-CZ	7.02	133.43	123.60
1	A	245	GLU	CB-CG-CD	6.91	132.86	114.20
1	A	288	LEU	O-C-N	-6.80	111.82	122.70
1	A	187	LYS	CG-CD-CE	-6.78	91.55	111.90
1	A	266	LYS	CG-CD-CE	-6.57	92.19	111.90
1	B	142	ILE	O-C-N	6.50	133.10	122.70
1	A	28	GLU	CA-CB-CG	-6.04	100.11	113.40
1	B	127	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	150	ASP	CA-CB-CG	-5.95	100.31	113.40
1	A	271	ARG	CG-CD-NE	-5.72	99.78	111.80
1	B	254	ARG	CG-CD-NE	5.55	123.46	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	ARG	CD-NE-CZ	5.47	131.26	123.60
1	A	308	ASP	OD1-CG-OD2	5.46	133.68	123.30
1	A	160	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	A	406	ARG	CD-NE-CZ	5.22	130.91	123.60
1	B	12	GLU	CB-CG-CD	5.19	128.20	114.20
1	B	53	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	A	245	GLU	CG-CD-OE2	5.03	128.35	118.30
1	B	127	ASP	CA-CB-CG	5.02	124.44	113.40

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	ALA	Mainchain
1	A	148	ARG	Peptide
1	A	149	LEU	Mainchain,Peptide
1	A	287	GLU	Mainchain,Peptide
1	A	288	LEU	Mainchain
1	A	406	ARG	Sidechain
1	A	435	ASP	Sidechain
1	B	146	ALA	Peptide

## 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	3531	0	3586	19	0
1	B	3481	0	3551	30	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
4	A	92	0	44	3	0
4	B	92	0	43	2	0
5	A	32	0	13	0	0
5	B	32	0	13	0	0
6	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
8	A	8	0	0	0	0
8	B	6	0	0	1	0
All	All	7298	0	7250	52	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 4.

All (52) 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:HE1	1.36	1.02
1:B:324:LEU:HD13	1:B:376:MET:HE1	1.50	0.92
1:B:324:LEU:HD13	1:B:376:MET:CE	2.00	0.92
1:A:324:LEU:HD13	1:A:376:MET:CE	1.99	0.91
1:B:229:LEU:HD13	1:B:250:ASP:HB3	1.68	0.73
1:B:338:PHE:HB3	1:B:342:ILE:HD12	1.72	0.70
1:A:153:GLY:O	1:A:177:HIS:ND1	2.25	0.69
1:B:52:LEU:HD22	1:B:53:ASP:O	1.93	0.68
1:B:432:LYS:O	1:B:436:GLU:HG2	1.95	0.67
1:B:229:LEU:CD1	1:B:250:ASP:HB3	2.31	0.61
1:A:338:PHE:HB3	1:A:342:ILE:HD12	1.84	0.60
1:B:324:LEU:HD13	1:B:376:MET:HE3	1.79	0.60
1:B:311:VAL:O	1:B:315:THR:HG23	2.03	0.59
1:A:240:MET:HG3	1:A:251:ILE:HD13	1.88	0.56
1:B:200:ILE:HG22	1:B:231:MET:HE3	1.88	0.55
1:B:453:ALA:HB2	8:B:2005:HOH:O	2.08	0.54
1:B:229:LEU:HD21	1:B:252:LEU:HD11	1.91	0.52
1:B:153:GLY:O	1:B:177:HIS:ND1	2.40	0.51
4:A:505:C2E:C81	4:A:505:C2E:H4A	2.41	0.50
1:A:283:ASP:OD2	1:B:132:ARG:NH1	2.45	0.49
1:B:435:ASP:O	1:B:438:VAL:HG22	2.12	0.49
1:B:132:ARG:NE	1:B:132:ARG:HA	2.28	0.49
4:B:505:C2E:H4A	4:B:505:C2E:C81	2.43	0.48
1:A:250:ASP:OD1	1:A:251:ILE:N	2.46	0.48
1:A:162:ASN:O	1:A:163:GLU:C	2.52	0.48
1:A:52:LEU:HD22	1:A:53:ASP:O	2.14	0.48
1:A:289:ALA:HB3	1:A:301:ARG:HH22	1.79	0.47
1:B:200:ILE:HG22	1:B:231:MET:CE	2.43	0.47
1:A:200:ILE:HG22	1:A:231:MET:HE3	1.97	0.47
1:B:133:GLU:O	1:B:136:GLY:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:NH2	1:A:144:GLY:O	2.49	0.46
1:A:361:ILE:HD11	1:B:361:ILE:HD11	1.99	0.45
1:A:271:ARG:O	1:A:275:THR:HG23	2.16	0.45
1:B:284:HIS:CE1	1:B:288:LEU:HD21	2.52	0.45
1:B:271:ARG:O	1:B:275:THR:HG23	2.17	0.44
1:B:229:LEU:HG	1:B:252:LEU:HD12	1.99	0.44
4:B:503:C2E:H4'	4:B:503:C2E:C8	2.48	0.44
1:B:122:PHE:HB3	1:B:271:ARG:HH22	1.83	0.43
1:A:60:ASP:C	1:A:60:ASP:OD1	2.56	0.43
1:B:229:LEU:HD12	1:B:250:ASP:O	2.19	0.43
1:A:232:VAL:HG22	1:A:251:ILE:HG23	2.02	0.42
1:B:137:ARG:HG3	1:B:137:ARG:O	2.19	0.42
1:A:240:MET:CG	1:A:251:ILE:HD13	2.49	0.42
1:A:129:LEU:HD21	1:A:279:ARG:NH1	2.34	0.42
4:A:505:C2E:H4A	4:A:505:C2E:H81	2.01	0.41
1:B:325:LEU:CD2	1:B:435:ASP:HB3	2.50	0.41
1:B:432:LYS:HA	1:B:435:ASP:OD1	2.21	0.41
1:B:207:ASN:N	1:B:207:ASN:HD22	2.19	0.41
1:B:60:ASP:OD1	1:B:60:ASP:C	2.59	0.41
1:A:69:LYS:NZ	1:A:77:ILE:O	2.55	0.40
1:B:284:HIS:O	1:B:288:LEU:HD23	2.21	0.40
4:A:503:C2E:C8	4:A:503:C2E:H4'	2.51	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	457/459 (100%)	437 (96%)	13 (3%)	7 (2%)	13	31
1	B	450/459 (98%)	427 (95%)	15 (3%)	8 (2%)	11	25
All	All	907/918 (99%)	864 (95%)	28 (3%)	15 (2%)	11	27

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	ALA
1	A	149	LEU
1	A	289	ALA
1	B	143	ALA
1	B	149	LEU
1	A	404	HIS
1	B	137	ARG
1	B	194	GLY
1	B	404	HIS
1	B	454	ALA
1	A	287	GLU
1	B	148	ARG
1	A	148	ARG
1	A	194	GLY
1	B	142	ILE

### 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	374/374 (100%)	353 (94%)	21 (6%)	26	53
1	B	369/374 (99%)	342 (93%)	27 (7%)	17	39
All	All	743/748 (99%)	695 (94%)	48 (6%)	21	45

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	52	LEU
1	A	103	LEU
1	A	129	LEU
1	A	148	ARG
1	A	149	LEU
1	A	164	ARG
1	A	211	LEU

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Mol	Chain	Res	Type
1	A	221	GLU
1	A	240	MET
1	A	253	SER
1	A	282	LEU
1	A	284	HIS
1	A	286	LEU
1	A	358	VAL
1	A	365	CYS
1	A	395	VAL
1	A	402	VAL
1	A	404	HIS
1	A	418	SER
1	A	428	GLU
1	B	18	LEU
1	B	33	MET
1	B	52	LEU
1	B	73	THR
1	B	85	LEU
1	B	103	LEU
1	B	129	LEU
1	B	131	GLN
1	B	132	ARG
1	B	139	MET
1	B	148	ARG
1	B	211	LEU
1	B	221	GLU
1	B	252	LEU
1	B	254	ARG
1	B	271	ARG
1	B	300	ARG
1	B	340	HIS
1	B	352	LEU
1	B	358	VAL
1	B	365	CYS
1	B	366	ARG
1	B	402	VAL
1	B	404	HIS
1	B	418	SER
1	B	446	ARG
1	B	455	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	280	ASN
1	B	93	GLN
1	B	207	ASN
1	B	280	ASN
1	B	293	GLN
1	B	335	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 6 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	$\# Z  > 2$
6	SO4	A	1470	-	4,4,4	0.07	0	6,6,6	0.27	0
6	SO4	A	1471	-	4,4,4	0.07	0	6,6,6	0.12	0
2	BEF	A	501	1,3	0,3,3	0.00	-	0,3,3	0.00	-
4	C2E	A	503	-	42,52,52	0.73	1 (2%)	50,82,82	2.04	18 (36%)
4	C2E	A	505	-	42,52,52	0.58	0	50,82,82	2.30	20 (40%)
5	GAV	A	600	3	23,34,34	1.15	2 (8%)	32,54,54	1.94	8 (25%)
2	BEF	B	501	1,3	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	C2E	B	503	-	42,52,52	0.61	0	50,82,82	2.41	20 (40%)
4	C2E	B	505	-	42,52,52	0.63	0	50,82,82	2.25	16 (32%)
5	GAV	B	600	3	23,34,34	1.06	2 (8%)	32,54,54	1.75	5 (15%)

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
6	SO4	A	1470	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1471	-	-	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	-	1/1/10/10	0/22/62/62	0/6/7/7
4	C2E	A	505	-	2/2/10/10	0/22/62/62	0/6/7/7
5	GAV	A	600	3	-	0/13/38/38	0/3/3/3
2	BEF	B	501	1,3	-	0/0/0/0	0/0/0/0
4	C2E	B	503	-	2/2/10/10	0/22/62/62	0/6/7/7
4	C2E	B	505	-	2/2/10/10	0/22/62/62	0/6/7/7
5	GAV	B	600	3	-	0/13/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	C2E	C21-N11	-2.19	1.31	1.35
5	B	600	GAV	C6-N1	2.10	1.37	1.33
5	B	600	GAV	PA-O5'	2.47	1.61	1.58
5	A	600	GAV	C6-N1	3.02	1.38	1.33
5	A	600	GAV	PA-O5'	3.10	1.62	1.58

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	505	C2E	C4A-O4A-C1A	-7.29	101.71	109.72
4	B	505	C2E	C4A-O4A-C1A	-7.23	101.77	109.72
4	B	503	C2E	C4A-O4A-C1A	-6.98	102.05	109.72
4	A	503	C2E	C4'-O4'-C1'	-5.47	103.71	109.72
4	B	505	C2E	C4'-O4'-C1'	-5.39	103.80	109.72
5	B	600	GAV	C4'-O4'-C1'	-5.33	103.87	109.72
5	A	600	GAV	N3-C2-N1	-5.15	119.60	127.44
4	A	505	C2E	C4'-O4'-C1'	-4.78	104.46	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	600	GAV	N3-C2-N1	-4.31	120.88	127.44
4	B	505	C2E	N3-C2-N1	-4.12	121.17	127.44
4	B	503	C2E	C4'-O4'-C1'	-4.09	105.22	109.72
4	B	503	C2E	C51-C61-N11	-4.07	118.03	123.59
4	B	503	C2E	N3-C2-N1	-4.02	121.33	127.44
4	A	505	C2E	N3-C2-N1	-3.87	121.56	127.44
4	A	503	C2E	C5-C6-N1	-3.78	118.42	123.59
4	A	505	C2E	O5A-C5A-C4A	-3.78	95.17	109.12
5	A	600	GAV	C4'-O4'-C1'	-3.75	105.60	109.72
4	A	505	C2E	C51-C61-N11	-3.74	118.47	123.59
4	A	503	C2E	C51-C61-N11	-3.62	118.64	123.59
4	B	503	C2E	N31-C21-N11	-3.60	121.96	127.44
4	B	505	C2E	N31-C21-N11	-3.57	122.00	127.44
4	B	505	C2E	O5A-C5A-C4A	-3.54	96.07	109.12
4	B	503	C2E	C5-C6-N1	-3.51	118.78	123.59
4	B	505	C2E	C51-C61-N11	-3.49	118.82	123.59
4	A	505	C2E	C41-C51-N71	-3.32	106.42	109.48
4	B	503	C2E	O5'-C5'-C4'	-3.19	97.35	109.12
5	A	600	GAV	C1'-N9-C4	-3.18	122.15	126.94
4	A	503	C2E	N3-C2-N1	-3.15	122.65	127.44
4	B	503	C2E	O5A-C5A-C4A	-3.14	97.55	109.12
4	A	503	C2E	N31-C21-N11	-3.13	122.68	127.44
4	B	503	C2E	C2A-C3A-C4A	-3.11	97.45	103.29
4	A	505	C2E	O5'-P1-O1P	-3.05	97.76	109.62
4	A	505	C2E	N31-C21-N11	-3.05	122.80	127.44
4	B	505	C2E	C5-C6-N1	-3.04	119.44	123.59
4	A	505	C2E	O5'-C5'-C4'	-2.98	98.12	109.12
4	A	503	C2E	C41-C51-N71	-2.93	106.78	109.48
4	A	503	C2E	O5'-C5'-C4'	-2.88	98.51	109.12
4	B	505	C2E	C41-C51-N71	-2.82	106.88	109.48
4	A	505	C2E	C4-C5-N7	-2.81	106.89	109.48
5	B	600	GAV	C2'-C1'-N9	-2.81	110.00	114.29
4	A	505	C2E	C5-C6-N1	-2.80	119.76	123.59
4	A	505	C2E	O5A-P11-O11	-2.80	98.76	109.62
4	B	503	C2E	C2'-C1'-N9	-2.69	110.18	114.29
4	A	503	C2E	C2A-C3A-C4A	-2.65	98.31	103.29
4	B	503	C2E	C41-C51-N71	-2.64	107.05	109.48
5	A	600	GAV	C6-C5-C4	-2.46	117.95	120.90
5	A	600	GAV	C4-C5-N7	-2.38	107.29	109.48
5	B	600	GAV	PB-O3A-PA	-2.30	125.36	133.44
4	B	503	C2E	C2A-C1A-N91	-2.18	110.97	114.29
5	B	600	GAV	PB-O3B-PG	-2.18	125.37	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	C2E	O5'-P1-O1P	-2.16	101.25	109.62
4	A	503	C2E	O5A-P11-O11	-2.13	101.35	109.62
4	B	505	C2E	C2A-C3A-C4A	-2.13	99.30	103.29
4	A	503	C2E	C2'-C1'-N9	-2.10	111.08	114.29
4	B	505	C2E	C2'-C3'-C4'	-2.10	99.35	103.29
4	A	505	C2E	C2'-C3'-C4'	-2.09	99.36	103.29
4	A	505	C2E	C2A-C1A-N91	-2.06	111.14	114.29
5	A	600	GAV	N2-C2-N1	2.04	120.58	117.20
4	B	503	C2E	O4A-C4A-C5A	2.11	116.86	109.32
4	A	505	C2E	C3A-C2A-C1A	2.12	105.07	99.98
4	A	505	C2E	C5'-C4'-C3'	2.13	121.98	114.31
4	A	505	C2E	O4A-C1A-N91	2.21	112.71	108.10
4	B	505	C2E	C5'-C4'-C3'	2.23	122.36	114.31
4	B	503	C2E	C3'-C2'-C1'	2.26	105.41	99.98
4	A	503	C2E	O4A-C4A-C3A	2.27	110.10	104.86
4	A	503	C2E	C3'-C2'-C1'	2.28	105.45	99.98
5	A	600	GAV	C6-N1-C2	2.32	119.16	115.94
4	B	505	C2E	O4A-C1A-N91	2.33	112.97	108.10
4	A	503	C2E	O4'-C1'-N9	2.40	113.12	108.10
4	A	503	C2E	C5'-C4'-C3'	2.50	123.32	114.31
4	B	505	C2E	C3A-C2A-C1A	2.72	106.50	99.98
4	B	503	C2E	O4A-C1A-N91	2.79	113.94	108.10
4	A	505	C2E	C6-N1-C2	2.93	120.00	115.94
4	A	503	C2E	C3A-C2A-C1A	3.03	107.25	99.98
4	A	505	C2E	C3'-C2'-C1'	3.11	107.45	99.98
4	B	503	C2E	C5A-C4A-C3A	3.18	125.78	114.31
4	B	505	C2E	C3'-C2'-C1'	3.20	107.65	99.98
4	B	503	C2E	O4A-C4A-C3A	3.35	112.59	104.86
4	A	505	C2E	C61-N11-C21	3.36	120.60	115.94
4	B	505	C2E	C6-N1-C2	3.41	120.67	115.94
4	B	503	C2E	C3A-C2A-C1A	3.44	108.23	99.98
4	B	505	C2E	C61-N11-C21	3.60	120.94	115.94
4	A	503	C2E	C6-N1-C2	3.78	121.18	115.94
4	A	503	C2E	C61-N11-C21	3.87	121.32	115.94
4	B	503	C2E	C61-N11-C21	3.93	121.40	115.94
4	B	503	C2E	C6-N1-C2	4.17	121.73	115.94
5	A	600	GAV	O4'-C1'-N9	4.60	117.74	108.10

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	505	C2E	C4'

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Mol	Chain	Res	Type	Atom
4	B	505	C2E	C4A
4	A	505	C2E	C4'
4	A	505	C2E	C4A
4	A	503	C2E	C4'
4	B	503	C2E	C4'
4	B	503	C2E	C4A

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
4	A	503	C2E	1	0
4	A	505	C2E	2	0
4	B	503	C2E	1	0
4	B	505	C2E	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	456/459 (99%)	0.36	5 (1%) 82 83	23, 42, 51, 83	23 (5%)
1	B	444/459 (96%)	0.39	9 (2%) 68 69	25, 42, 53, 80	10 (2%)
All	All	900/918 (98%)	0.38	14 (1%) 74 75	23, 42, 52, 83	33 (3%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	137	ARG	3.9
1	A	284	HIS	3.5
1	B	138	ARG	3.3
1	B	134	ALA	2.8
1	B	136	GLY	2.6
1	B	408	MET	2.5
1	A	190	ILE	2.4
1	B	402	VAL	2.4
1	A	150	ASP	2.4
1	A	282	LEU	2.3
1	B	454	ALA	2.2
1	B	135	SER	2.2
1	A	225	GLN	2.1
1	B	42	ALA	2.1

### 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 carbohydrates 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. 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	MG	B	502	1/1	0.97	0.20	1.10	36,36,36,36	0
4	C2E	A	505	46/46	0.97	0.20	-0.05	37,41,43,45	0
4	C2E	A	503	46/46	0.97	0.19	-0.56	37,42,44,45	0
4	C2E	B	505	46/46	0.97	0.18	-0.65	37,41,43,44	0
5	GAV	B	600	32/32	0.94	0.16	-0.77	33,41,64,70	0
5	GAV	A	600	32/32	0.93	0.16	-1.16	48,60,70,76	0
3	MG	A	502	1/1	0.82	0.14	-1.40	37,37,37,37	0
2	BEF	A	501	4/4	0.97	0.12	-1.85	35,35,39,39	0
4	C2E	B	503	46/46	0.96	0.16	-2.03	37,41,43,44	0
2	BEF	B	501	4/4	0.95	0.11	-3.32	35,35,39,39	0
7	CL	A	1472	1/1	0.96	0.13	-4.14	38,38,38,38	0
3	MG	B	601	1/1	0.87	0.06	-4.59	46,46,46,46	0
3	MG	A	601	1/1	0.84	0.12	-5.38	45,45,45,45	0
3	MG	A	602	1/1	0.78	0.16	-	52,52,52,52	0
6	SO4	A	1470	5/5	0.94	0.22	-	71,76,79,80	0
6	SO4	A	1471	5/5	0.88	0.28	-	85,86,88,89	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.