



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:37 AM GMT

PDB ID : 1K8T  
Title : Crystal structure of the adenylyl cyclase domain of anthrax edema factor (EF)  
Authors : Drum, C.L.; Yan, S.-Z.; Bard, J.; Shen, Y.-Q.; Lu, D.; Soelaiman, S.;  
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Deposited on : 2001-10-25  
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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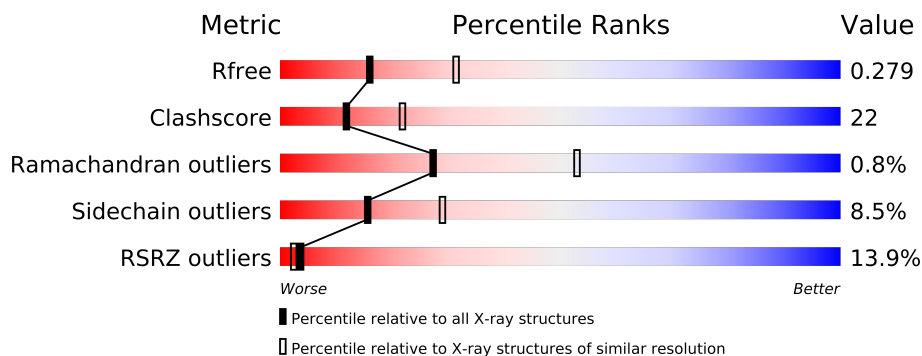
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	510	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4142 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CALMODULIN-SENSITIVE ADENYLATE CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			4025	2574	685	763	3			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ni 1	0	0

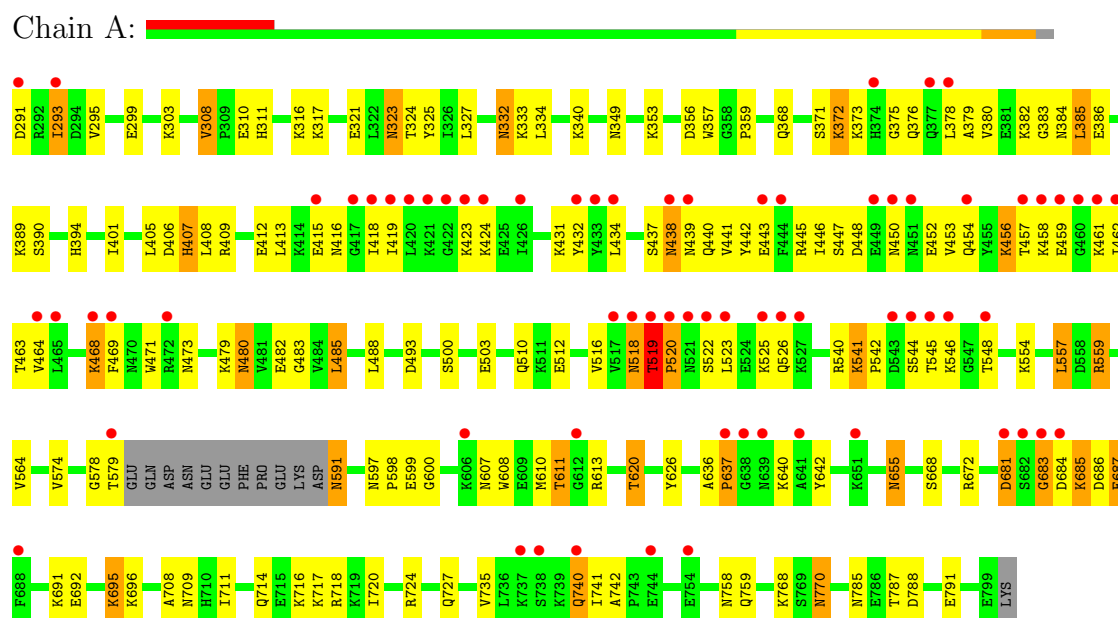
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	96	Total 96	O 96	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: CALMODULIN-SENSITIVE ADENYLATE CYCLASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.48Å 203.60Å 74.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 37.02 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.60) 98.2 (37.02-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.94 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.229 , 0.276 0.231 , 0.279	Depositor DCC
$R_{free}$ test set	2364 reflections (9.89%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.2	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 23920 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4142	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.55	1/4101 (0.0%)	0.72	3/5519 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	637	PRO	N-CA	6.26	1.57	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	683	GLY	N-CA-C	-7.99	93.13	113.10
1	A	519	THR	C-N-CD	-5.74	107.97	120.60
1	A	685	LYS	N-CA-C	-5.06	97.34	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4025	0	4060	176	0
2	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	96	0	0	3	0
All	All	4142	0	4060	176	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (176) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:519:THR:CB	1:A:520:PRO:HD2	1.65	1.17
1:A:439:ASN:ND2	1:A:442:TYR:HB2	1.61	1.12
1:A:519:THR:HB	1:A:520:PRO:CD	1.82	1.08
1:A:540:ARG:HD2	1:A:548:THR:HG23	1.38	1.01
1:A:785:ASN:OD1	1:A:787:THR:HG22	1.60	1.01
1:A:454:GLN:HG3	1:A:473:ASN:HD22	1.37	0.90
1:A:684:ASP:HB3	1:A:687:GLU:HB3	1.55	0.89
1:A:540:ARG:CD	1:A:548:THR:HG23	2.02	0.89
1:A:716:LYS:HE2	1:A:720:ILE:HD11	1.56	0.88
1:A:332:ASN:HD22	1:A:332:ASN:C	1.80	0.85
1:A:519:THR:HB	1:A:520:PRO:HD2	0.85	0.84
1:A:711:ILE:CD1	1:A:720:ILE:HD12	2.08	0.84
1:A:317:LYS:HE2	1:A:321:GLU:OE1	1.78	0.83
1:A:578:GLY:O	1:A:579:THR:HB	1.77	0.82
1:A:407:HIS:CD2	1:A:407:HIS:H	1.96	0.80
1:A:519:THR:CB	1:A:520:PRO:CD	2.52	0.80
1:A:525:LYS:HE2	1:A:724:ARG:HH12	1.47	0.80
1:A:724:ARG:HH21	1:A:727:GLN:HE22	1.28	0.80
1:A:439:ASN:HD21	1:A:442:TYR:HB2	1.46	0.79
1:A:439:ASN:HD22	1:A:442:TYR:HB2	1.45	0.78
1:A:332:ASN:ND2	1:A:334:LEU:H	1.83	0.77
1:A:353:LYS:H	1:A:368:GLN:HE22	1.30	0.77
1:A:711:ILE:HD13	1:A:720:ILE:HD12	1.65	0.76
1:A:758:ASN:ND2	1:A:759:GLN:HE21	1.84	0.76
1:A:450:ASN:ND2	1:A:452:GLU:HB2	2.01	0.75
1:A:540:ARG:HD2	1:A:548:THR:CG2	2.17	0.74
1:A:308:VAL:HG22	1:A:311:HIS:CG	2.25	0.72
1:A:637:PRO:HG3	1:A:642:TYR:CE2	2.25	0.71
1:A:456:LYS:HG2	1:A:471:TRP:CE2	2.26	0.70
1:A:626:TYR:H	1:A:709:ASN:HD21	1.40	0.70
1:A:758:ASN:HD22	1:A:759:GLN:HE21	1.41	0.68
1:A:685:LYS:HD3	1:A:686:ASP:N	2.08	0.68
1:A:770:ASN:H	1:A:770:ASN:HD22	1.40	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:454:GLN:HG3	1:A:473:ASN:ND2	2.09	0.67
1:A:708:ALA:HB1	1:A:717:LYS:HG2	1.77	0.66
1:A:446:ILE:HG12	1:A:447:SER:H	1.59	0.66
1:A:711:ILE:HD11	1:A:720:ILE:HD12	1.78	0.66
1:A:607:ASN:O	1:A:611:THR:HG22	1.96	0.66
1:A:620:THR:HG21	4:A:57:HOH:O	1.95	0.66
1:A:564:VAL:HG21	1:A:574:VAL:HG21	1.79	0.65
1:A:597:ASN:HB2	1:A:598:PRO:CD	2.27	0.64
1:A:353:LYS:N	1:A:368:GLN:HE22	1.94	0.64
1:A:440:GLN:O	1:A:458:LYS:HD2	1.97	0.64
1:A:446:ILE:HG12	1:A:447:SER:N	2.13	0.63
1:A:413:LEU:HD12	1:A:418:ILE:HG21	1.80	0.63
1:A:681:ASP:OD2	1:A:740:GLN:NE2	2.28	0.63
1:A:480:ASN:HD21	1:A:483:GLY:H	1.47	0.62
1:A:480:ASN:ND2	1:A:483:GLY:H	1.98	0.62
1:A:439:ASN:ND2	1:A:442:TYR:CB	2.51	0.61
1:A:368:GLN:HG3	1:A:383:GLY:HA3	1.82	0.61
1:A:373:LYS:HD2	1:A:376:GLN:NE2	2.16	0.61
1:A:353:LYS:H	1:A:368:GLN:NE2	1.99	0.60
1:A:695:LYS:HA	1:A:695:LYS:HE3	1.81	0.60
1:A:332:ASN:HD22	1:A:334:LEU:H	1.50	0.60
1:A:416:ASN:N	1:A:416:ASN:HD22	1.98	0.59
1:A:332:ASN:C	1:A:332:ASN:ND2	2.53	0.59
1:A:375:GLY:CA	1:A:464:VAL:HG11	2.33	0.59
1:A:456:LYS:HG2	1:A:471:TRP:CZ2	2.37	0.58
1:A:522:SER:C	1:A:523:LEU:HD12	2.23	0.58
1:A:578:GLY:O	1:A:579:THR:CB	2.52	0.57
1:A:431:LYS:HD2	1:A:448:ASP:OD1	2.04	0.57
1:A:724:ARG:HD3	1:A:727:GLN:NE2	2.20	0.57
1:A:608:TRP:HA	1:A:611:THR:HG23	1.87	0.57
1:A:500:SER:HB3	1:A:503:GLU:HB2	1.85	0.57
1:A:655:ASN:C	1:A:655:ASN:HD22	2.08	0.57
1:A:559:ARG:NH2	4:A:55:HOH:O	2.37	0.57
1:A:380:VAL:HG12	1:A:384:ASN:HD21	1.70	0.57
1:A:525:LYS:CE	1:A:724:ARG:HH12	2.15	0.56
1:A:685:LYS:O	1:A:686:ASP:HB2	2.03	0.56
1:A:405:LEU:HG	1:A:453:VAL:HG21	1.87	0.56
1:A:597:ASN:HB2	1:A:598:PRO:HD2	1.87	0.56
1:A:741:ILE:HG22	1:A:742:ALA:O	2.06	0.56
1:A:323:ASN:HD22	1:A:598:PRO:HB3	1.71	0.56
1:A:522:SER:O	1:A:523:LEU:HD12	2.06	0.55
1:A:332:ASN:HD22	1:A:333:LYS:N	2.05	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:480:ASN:HD21	1:A:483:GLY:N	2.06	0.53
1:A:413:LEU:HD12	1:A:418:ILE:CG2	2.38	0.53
1:A:720:ILE:O	1:A:724:ARG:HG2	2.09	0.53
1:A:295:VAL:HG12	1:A:610:MET:SD	2.48	0.53
1:A:457:THR:HG21	1:A:468:LYS:CB	2.39	0.53
1:A:681:ASP:OD1	1:A:681:ASP:N	2.24	0.53
1:A:457:THR:CG2	1:A:469:PHE:H	2.21	0.53
1:A:390:SER:O	1:A:394:HIS:HD2	1.92	0.53
1:A:409:ARG:O	1:A:413:LEU:HD23	2.09	0.52
1:A:457:THR:HG22	1:A:469:PHE:H	1.73	0.52
1:A:458:LYS:HB2	1:A:461:LYS:HB2	1.91	0.52
1:A:457:THR:HG21	1:A:468:LYS:HB2	1.91	0.52
1:A:316:LYS:HG3	1:A:600:GLY:CA	2.40	0.52
1:A:443:GLU:HB2	1:A:456:LYS:HE2	1.93	0.51
1:A:523:LEU:HD23	1:A:716:LYS:HE3	1.93	0.51
1:A:459:GLU:CD	1:A:459:GLU:H	2.14	0.51
1:A:526:GLN:HE22	1:A:711:ILE:HA	1.76	0.50
1:A:607:ASN:O	1:A:611:THR:CG2	2.58	0.50
1:A:480:ASN:C	1:A:480:ASN:HD22	2.15	0.50
1:A:375:GLY:HA2	1:A:464:VAL:HG11	1.92	0.50
1:A:687:GLU:O	1:A:691:LYS:HG3	2.11	0.50
1:A:293:ILE:O	1:A:610:MET:CE	2.60	0.50
1:A:692:GLU:HG3	1:A:696:LYS:HE3	1.93	0.49
1:A:316:LYS:HG3	1:A:600:GLY:HA2	1.95	0.49
1:A:637:PRO:HG3	1:A:642:TYR:CD2	2.48	0.49
1:A:418:ILE:O	1:A:419:ILE:HG23	2.12	0.49
1:A:724:ARG:HD3	1:A:727:GLN:HE21	1.76	0.48
1:A:735:VAL:HG13	1:A:741:ILE:HD11	1.94	0.48
1:A:293:ILE:O	1:A:610:MET:SD	2.71	0.48
1:A:714:GLN:HA	1:A:717:LYS:HD2	1.95	0.48
1:A:334:LEU:CD1	1:A:356:ASP:O	2.62	0.48
1:A:787:THR:O	1:A:791:GLU:HG2	2.13	0.48
1:A:716:LYS:O	1:A:720:ILE:HG13	2.14	0.47
1:A:432:TYR:CE1	1:A:445:ARG:CZ	2.97	0.47
1:A:545:THR:OG1	1:A:548:THR:HB	2.13	0.47
1:A:456:LYS:HG2	1:A:471:TRP:CD2	2.50	0.47
1:A:409:ARG:NE	1:A:413:LEU:HD21	2.29	0.47
1:A:416:ASN:ND2	1:A:416:ASN:N	2.61	0.47
1:A:461:LYS:HD2	1:A:461:LYS:HA	1.50	0.47
1:A:724:ARG:NH2	1:A:727:GLN:HE22	2.04	0.46
1:A:376:GLN:HB2	1:A:379:ALA:HB3	1.98	0.46
1:A:291:ASP:C	1:A:293:ILE:H	2.19	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:545:THR:O	1:A:546:LYS:C	2.53	0.46
1:A:462:ILE:HG22	1:A:463:THR:O	2.16	0.46
1:A:787:THR:HG23	1:A:788:ASP:N	2.30	0.46
1:A:454:GLN:HG3	1:A:473:ASN:HA	1.97	0.46
1:A:685:LYS:HD3	1:A:685:LYS:C	2.36	0.46
1:A:371:SER:C	1:A:373:LYS:H	2.18	0.45
1:A:415:GLU:C	1:A:416:ASN:HD22	2.19	0.45
1:A:446:ILE:CG1	1:A:447:SER:H	2.28	0.45
1:A:431:LYS:HB2	1:A:448:ASP:OD1	2.16	0.45
1:A:683:GLY:O	1:A:684:ASP:C	2.55	0.45
1:A:353:LYS:HB3	1:A:372:LYS:HD3	1.98	0.45
1:A:371:SER:C	1:A:373:LYS:N	2.69	0.45
1:A:655:ASN:C	1:A:655:ASN:ND2	2.69	0.45
1:A:770:ASN:N	1:A:770:ASN:HD22	2.05	0.44
1:A:735:VAL:CG1	1:A:741:ILE:HD11	2.47	0.44
1:A:518:ASN:O	1:A:519:THR:HG23	2.17	0.44
1:A:310:GLU:CD	1:A:310:GLU:H	2.20	0.44
1:A:770:ASN:ND2	1:A:770:ASN:H	2.12	0.43
1:A:357:TRP:HH2	1:A:439:ASN:ND2	2.16	0.43
1:A:541:LYS:H	1:A:541:LYS:HG2	1.48	0.43
1:A:408:LEU:O	1:A:412:GLU:HG3	2.18	0.43
1:A:446:ILE:CG1	1:A:447:SER:N	2.81	0.43
1:A:523:LEU:HB3	1:A:716:LYS:CE	2.49	0.42
1:A:457:THR:HG22	1:A:469:PHE:O	2.19	0.42
1:A:413:LEU:HB3	1:A:419:ILE:HG12	2.01	0.42
1:A:349:ASN:HB3	1:A:394:HIS:CE1	2.54	0.42
1:A:687:GLU:OE1	1:A:687:GLU:N	2.52	0.42
1:A:385:LEU:HD22	1:A:389:LYS:HE2	2.01	0.42
1:A:479:LYS:HB2	1:A:488:LEU:HD21	2.01	0.42
1:A:445:ARG:HD3	1:A:471:TRP:CZ3	2.54	0.42
1:A:308:VAL:CG2	1:A:311:HIS:CG	3.01	0.42
1:A:636:ALA:HA	1:A:637:PRO:HD3	1.80	0.42
1:A:557:LEU:HD12	1:A:557:LEU:HA	1.85	0.42
1:A:327:LEU:HD12	1:A:327:LEU:N	2.35	0.42
1:A:523:LEU:HB3	1:A:716:LYS:HE3	2.01	0.42
1:A:768:LYS:HG2	1:A:770:ASN:ND2	2.35	0.41
1:A:564:VAL:HG11	1:A:574:VAL:HG11	2.01	0.41
1:A:293:ILE:CB	4:A:90:HOH:O	2.68	0.41
1:A:440:GLN:HG2	1:A:441:VAL:HG23	2.03	0.41
1:A:418:ILE:O	1:A:419:ILE:CG2	2.68	0.41
1:A:324:THR:HG22	1:A:325:TYR:O	2.21	0.41
1:A:406:ASP:HB2	1:A:407:HIS:HD2	1.86	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:640:LYS:HG2	1:A:640:LYS:H	1.57	0.41
1:A:540:ARG:CZ	1:A:544:SER:HB2	2.50	0.41
1:A:443:GLU:HB2	1:A:456:LYS:CE	2.50	0.41
1:A:382:LYS:O	1:A:386:GLU:HG3	2.21	0.41
1:A:591:ASN:HD22	1:A:591:ASN:C	2.24	0.41
1:A:447:SER:HB3	1:A:450:ASN:O	2.21	0.40
1:A:359:PRO:CB	1:A:405:LEU:HD11	2.50	0.40
1:A:299:GLU:HG3	1:A:303:LYS:HD3	2.03	0.40
1:A:526:GLN:NE2	1:A:711:ILE:HG13	2.35	0.40
1:A:512:GLU:O	1:A:516:VAL:HG23	2.20	0.40
1:A:787:THR:CG2	1:A:788:ASP:N	2.84	0.40
1:A:613:ARG:CZ	1:A:636:ALA:HB2	2.51	0.40
1:A:359:PRO:HB3	1:A:405:LEU:HD11	2.02	0.40
1:A:437:SER:C	1:A:439:ASN:H	2.25	0.40
1:A:711:ILE:O	1:A:717:LYS:HE2	2.21	0.40
1:A:482:GLU:HG3	1:A:482:GLU:O	2.22	0.40
1:A:401:ILE:HG21	1:A:485:LEU:HB3	2.03	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	494/510 (97%)	452 (92%)	38 (8%)	4 (1%)	27 53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	520	PRO
1	A	438	ASN
1	A	518	ASN
1	A	293	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	437/455 (96%)	400 (92%)	37 (8%)	15	29

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	308	VAL
1	A	323	ASN
1	A	332	ASN
1	A	340	LYS
1	A	372	LYS
1	A	378	LEU
1	A	385	LEU
1	A	407	HIS
1	A	423	LYS
1	A	424	LYS
1	A	434	LEU
1	A	438	ASN
1	A	456	LYS
1	A	468	LYS
1	A	480	ASN
1	A	485	LEU
1	A	493	ASP
1	A	510	GLN
1	A	519	THR
1	A	541	LYS
1	A	542	PRO
1	A	554	LYS
1	A	557	LEU
1	A	559	ARG
1	A	591	ASN
1	A	599	GLU
1	A	611	THR
1	A	620	THR
1	A	655	ASN
1	A	668	SER
1	A	672	ARG

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Mol	Chain	Res	Type
1	A	681	ASP
1	A	687	GLU
1	A	695	LYS
1	A	718	ARG
1	A	740	GLN
1	A	770	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	ASN
1	A	368	GLN
1	A	376	GLN
1	A	377	GLN
1	A	394	HIS
1	A	407	HIS
1	A	416	ASN
1	A	473	ASN
1	A	480	ASN
1	A	526	GLN
1	A	531	ASN
1	A	553	GLN
1	A	591	ASN
1	A	655	ASN
1	A	709	ASN
1	A	727	GLN
1	A	758	ASN
1	A	767	GLN
1	A	770	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	1001	-	4,4,4	1.71	1 (25%)	6,6,6	0.48	0
2	SO4	A	1002	-	4,4,4	1.77	2 (50%)	6,6,6	0.52	0
2	SO4	A	1003	-	4,4,4	1.82	2 (50%)	6,6,6	0.49	0
2	SO4	A	1004	-	4,4,4	1.95	2 (50%)	6,6,6	0.48	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	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1004	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	SO4	O4-S	2.58	1.56	1.47
2	A	1004	SO4	O3-S	2.57	1.56	1.47
2	A	1002	SO4	O3-S	2.34	1.55	1.47
2	A	1001	SO4	O3-S	2.33	1.55	1.47
2	A	1004	SO4	O4-S	2.33	1.55	1.47
2	A	1002	SO4	O4-S	2.26	1.55	1.47
2	A	1003	SO4	O3-S	2.20	1.54	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 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	498/510 (97%)	0.72	70 (14%) <b>3</b> <b>2</b>	23, 53, 97, 100	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	433	TYR	6.2
1	A	544	SER	6.0
1	A	639	ASN	5.8
1	A	638	GLY	5.6
1	A	683	GLY	5.5
1	A	462	ILE	5.2
1	A	465	LEU	5.0
1	A	521	ASN	5.0
1	A	293	ILE	4.8
1	A	420	LEU	4.8
1	A	684	ASP	4.7
1	A	522	SER	4.6
1	A	449	GLU	4.5
1	A	525	LYS	4.3
1	A	464	VAL	4.1
1	A	520	PRO	4.1
1	A	519	THR	4.0
1	A	523	LEU	4.0
1	A	682	SER	3.8
1	A	518	ASN	3.8
1	A	439	ASN	3.6
1	A	378	LEU	3.6
1	A	461	LYS	3.5
1	A	421	LYS	3.3
1	A	460	GLY	3.3
1	A	434	LEU	3.3
1	A	527	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	444	PHE	3.2
1	A	424	LYS	3.1
1	A	418	ILE	3.1
1	A	291	ASP	3.1
1	A	543	ASP	3.1
1	A	423	LYS	3.0
1	A	526	GLN	3.0
1	A	459	GLU	3.0
1	A	681	ASP	3.0
1	A	545	THR	2.9
1	A	546	LYS	2.9
1	A	468	LYS	2.8
1	A	688	PHE	2.7
1	A	737	LYS	2.7
1	A	606	LYS	2.7
1	A	417	GLY	2.7
1	A	422	GLY	2.6
1	A	738	SER	2.6
1	A	457	THR	2.5
1	A	469	PHE	2.5
1	A	472	ARG	2.5
1	A	451	ASN	2.5
1	A	579	THR	2.5
1	A	438	ASN	2.5
1	A	374	HIS	2.4
1	A	454	GLN	2.4
1	A	432	TYR	2.4
1	A	637	PRO	2.4
1	A	419	ILE	2.3
1	A	517	VAL	2.3
1	A	641	ALA	2.3
1	A	548	THR	2.3
1	A	458	LYS	2.3
1	A	443	GLU	2.2
1	A	426	ILE	2.2
1	A	744	GLU	2.1
1	A	377	GLN	2.1
1	A	740	GLN	2.1
1	A	415	GLU	2.1
1	A	450	ASN	2.1
1	A	612	GLY	2.1
1	A	651	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	754	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	A	1003	5/5	0.21	0.40	96,97,97,98	0
2	SO4	A	1001	5/5	0.20	0.04	61,62,65,65	0
2	SO4	A	1004	5/5	0.15	-0.97	99,100,100,100	0
2	SO4	A	1002	5/5	0.15	-1.05	84,84,86,87	0
3	NI	A	2001	1/1	0.12	-2.76	79,79,79,79	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.