Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:26 PM 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.; Grabarek, Z.; Bohm, A.; Tang, W.-J.
Deposited on	:	2001-10-25
Resolution	:	2.60 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

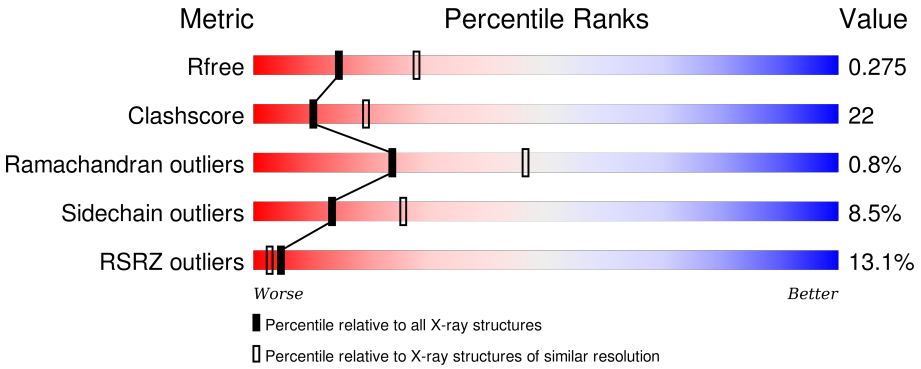
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 >=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 <=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	510	13% 65% 27% 6% •

2 Entry composition

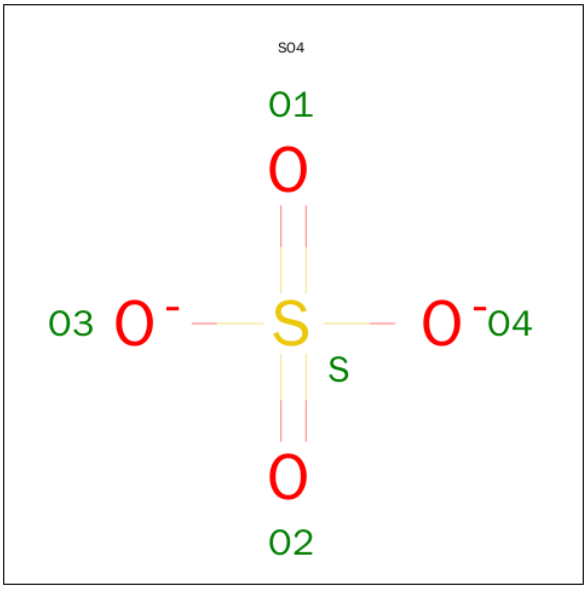
There are 4 unique types of molecules in this entry. The entry contains 4142 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CALMODULIN-SENSITIVE ADENYLATE CYCLASE.

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

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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

- Molecule 4 is water.

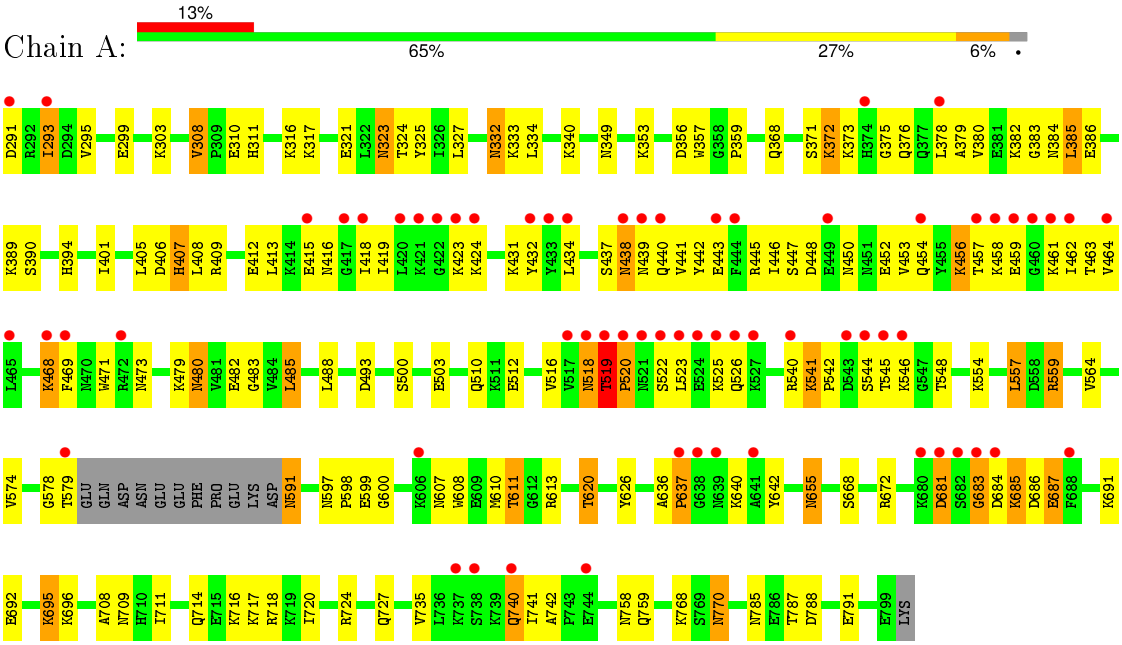
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	96	Total O 96 96	0	0

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 (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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	4.94 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.229 , 0.276 0.229 , 0.275	Depositor DCC
R_{free} test set	2364 reflections (9.89%)	DCC
Wilson B-factor (Å^2)	52.2	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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(^{o})	Ideal(^{o})
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 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	4025	0	4060	176	0
2	A	20	0	0	0	0
3	A	1	0	0	0	0
4	A	96	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4142	0	4060	176	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 22.

All (176) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ASN:HD22	1:A:333:LYS:N	2.05	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	24 46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	520	PRO

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Mol	Chain	Res	Type
1	A	438	ASN
1	A	518	ASN
1	A	293	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	437/455 (96%)	400 (92%)	37 (8%)	13 25

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

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Mol	Chain	Res	Type
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
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 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 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	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	A	1002	-	4,4,4	1.65	2 (50%)	6,6,6	0.53	0
2	SO4	A	1003	-	4,4,4	1.71	2 (50%)	6,6,6	0.50	0
2	SO4	A	1004	-	4,4,4	1.83	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	O3-S	2.06	1.54	1.47
2	A	1002	SO4	O4-S	2.12	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1004	SO4	O4-S	2.18	1.55	1.47
2	A	1001	SO4	O3-S	2.19	1.55	1.47
2	A	1002	SO4	O3-S	2.20	1.55	1.47
2	A	1004	SO4	O3-S	2.42	1.56	1.47
2	A	1003	SO4	O4-S	2.43	1.56	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} 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^2)	Q<0.9
1	A	498/510 (97%)	0.68	65 (13%) 5 3	23, 53, 97, 100	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	462	ILE	5.8
1	A	433	TYR	5.7
1	A	293	ILE	5.3
1	A	544	SER	5.2
1	A	638	GLY	5.2
1	A	683	GLY	4.9
1	A	639	ASN	4.9
1	A	420	LEU	4.8
1	A	684	ASP	4.8
1	A	519	THR	4.4
1	A	449	GLU	4.3
1	A	521	ASN	4.3
1	A	464	VAL	4.3
1	A	525	LYS	4.2
1	A	522	SER	4.2
1	A	465	LEU	4.2
1	A	523	LEU	4.1
1	A	520	PRO	4.0
1	A	682	SER	4.0
1	A	518	ASN	3.9
1	A	434	LEU	3.9
1	A	421	LYS	3.4
1	A	461	LYS	3.4
1	A	439	ASN	3.4
1	A	641	ALA	3.1
1	A	460	GLY	3.1
1	A	444	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	291	ASP	3.1
1	A	459	GLU	2.9
1	A	681	ASP	2.8
1	A	543	ASP	2.8
1	A	546	LYS	2.8
1	A	545	THR	2.8
1	A	526	GLN	2.8
1	A	468	LYS	2.7
1	A	424	LYS	2.7
1	A	527	LYS	2.7
1	A	579	THR	2.7
1	A	688	PHE	2.6
1	A	606	LYS	2.6
1	A	423	LYS	2.6
1	A	378	LEU	2.6
1	A	418	ILE	2.6
1	A	443	GLU	2.5
1	A	458	LYS	2.5
1	A	517	VAL	2.5
1	A	469	PHE	2.4
1	A	637	PRO	2.4
1	A	422	GLY	2.4
1	A	737	LYS	2.3
1	A	438	ASN	2.3
1	A	738	SER	2.3
1	A	680	LYS	2.3
1	A	417	GLY	2.2
1	A	740	GLN	2.2
1	A	457	THR	2.2
1	A	415	GLU	2.2
1	A	440	GLN	2.2
1	A	540	ARG	2.2
1	A	432	TYR	2.1
1	A	744	GLU	2.1
1	A	374	HIS	2.1
1	A	454	GLN	2.1
1	A	472	ARG	2.0
1	A	524	GLU	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^{th} 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^2)	Q<0.9
2	SO4	A	1001	5/5	0.97	0.18	-0.10	61,62,65,65	0
2	SO4	A	1003	5/5	0.85	0.20	-0.17	96,97,97,98	0
2	SO4	A	1002	5/5	0.95	0.16	-1.05	84,84,86,87	0
2	SO4	A	1004	5/5	0.86	0.16	-1.06	99,100,100,100	0
3	NI	A	2001	1/1	0.93	0.11	-	79,79,79,79	0

6.5 Other polymers (i)

There are no such residues in this entry.