



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:58 PM UTC

PDB ID : 1K8T / pdb_00001k8t
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

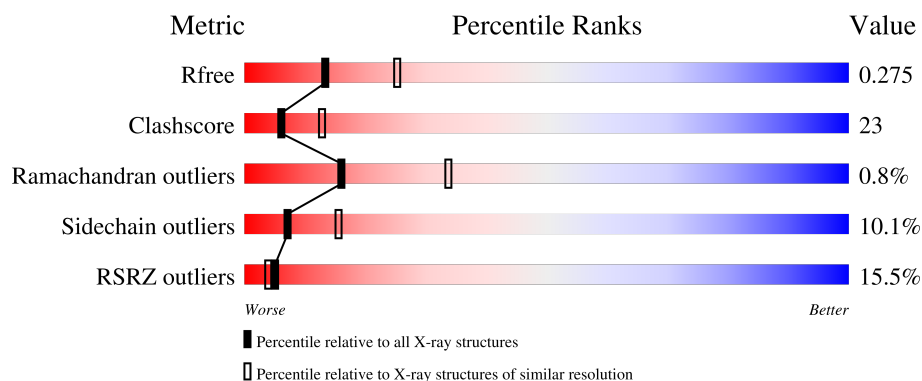
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	510	

2 Entry composition [i](#)

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
1	A	498	Total	C	N	O	S	0	0	0
			4025	2574	685	763	3			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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 (CCD ID: NI) (formula: Ni).

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

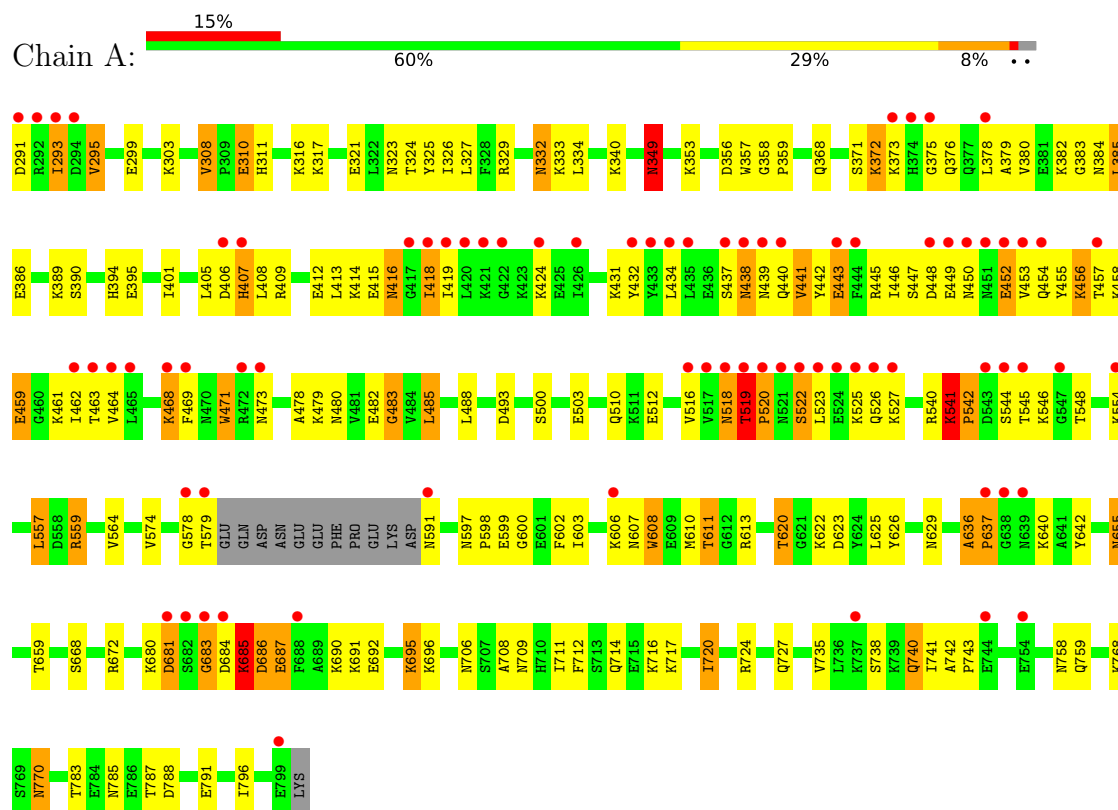
- Molecule 4 is water.

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: CALMODULIN-SENSITIVE ADENYLATE CYCLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 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 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.60) 98.1 (30.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	2365 reflections (9.89%)	wwPDB-VP
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 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.67	1/4101 (0.0%)	1.11	37/5519 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	637	PRO	N-CA	8.87	1.57	1.47

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	519	THR	CA-C-N	11.48	134.19	119.84
1	A	519	THR	C-N-CA	11.48	134.19	119.84
1	A	418	ILE	N-CA-C	10.52	121.67	111.67
1	A	683	GLY	N-CA-C	-8.46	93.13	113.18
1	A	636	ALA	CA-C-N	7.89	128.35	119.83
1	A	636	ALA	C-N-CA	7.89	128.35	119.83
1	A	637	PRO	N-CA-C	7.71	122.91	111.03
1	A	541	LYS	CA-C-N	7.45	126.99	119.24
1	A	541	LYS	C-N-CA	7.45	126.99	119.24
1	A	527	LYS	N-CA-C	-7.42	104.03	113.23
1	A	522	SER	N-CA-C	7.39	119.02	110.97
1	A	329	ARG	N-CA-C	-7.08	99.78	110.39
1	A	685	LYS	N-CA-C	-6.89	97.34	109.06
1	A	471	TRP	N-CA-C	6.88	120.63	110.30
1	A	686	ASP	N-CA-C	-6.34	105.49	113.23
1	A	629	ASN	N-CA-C	-6.28	105.93	113.97
1	A	680	LYS	N-CA-C	6.28	122.01	113.97
1	A	743	PRO	N-CA-C	6.14	121.61	113.57
1	A	738	SER	N-CA-C	-6.12	105.30	112.89
1	A	349	ASN	N-CA-C	6.11	120.34	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	796	ILE	N-CA-C	5.80	116.44	110.36
1	A	659	THR	N-CA-C	-5.75	101.45	110.36
1	A	542	PRO	N-CA-C	5.71	123.03	113.78
1	A	706	ASN	N-CA-C	5.70	122.04	114.12
1	A	483	GLY	N-CA-C	-5.61	107.27	114.85
1	A	441	VAL	N-CA-C	5.60	119.97	113.42
1	A	295	VAL	CB-CA-C	-5.58	105.45	111.59
1	A	623	ASP	N-CA-C	5.26	119.00	112.58
1	A	712	PHE	N-CA-C	5.23	116.79	111.14
1	A	625	LEU	N-CA-C	5.22	117.25	108.96
1	A	455	TYR	N-CA-C	5.21	116.99	108.76
1	A	358	GLY	CA-C-N	5.17	126.31	119.84
1	A	358	GLY	C-N-CA	5.17	126.31	119.84
1	A	783	THR	N-CA-C	-5.12	106.53	112.89
1	A	608	TRP	N-CA-C	5.12	116.55	111.07
1	A	478	ALA	N-CA-C	5.11	116.96	109.24
1	A	606	LYS	N-CA-C	5.08	118.64	112.23

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	183	0
2	A	20	0	0	0	0
3	A	1	0	0	0	0
4	A	96	0	0	3	0
All	All	4142	0	4060	183	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 23.

All (183) 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:332:ASN:HD22	1:A:332:ASN:C	1.80	0.89
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: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:HD22	1:A:770:ASN:H	1.40	0.68
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:332:ASN:C	1:A:332:ASN:ND2	2.53	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:522:SER:C	1:A:523:LEU:HD12	2.23	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:655:ASN:C	1:A:655:ASN:HD22	2.08	0.61
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:HD22	1:A:416:ASN:N	1.98	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: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:380:VAL:HG12	1:A:384:ASN:HD21	1.70	0.57
1:A:559:ARG:NH2	4:A:55:HOH:O	2.37	0.57
1:A:525:LYS:CE	1:A:724:ARG:HH12	2.15	0.56
1:A:405:LEU:HG	1:A:453:VAL:HG21	1.87	0.56
1:A:685:LYS:O	1:A:686:ASP:HB2	2.03	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:459:GLU:H	1:A:459:GLU:CD	2.14	0.56
1:A:522:SER:O	1:A:523:LEU:HD12	2.06	0.55
1:A:480:ASN:C	1:A:480:ASN:HD22	2.15	0.54
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:295:VAL:HG12	1:A:610:MET:SD	2.48	0.53
1:A:720:ILE:O	1:A:724:ARG:HG2	2.09	0.53
1:A:681:ASP:CG	1:A:690:LYS:HZ1	2.17	0.53
1:A:457:THR:HG21	1:A:468:LYS:CB	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:THR:CG2	1:A:469:PHE:H	2.21	0.53
1:A:681:ASP:OD1	1:A:681:ASP:N	2.24	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:415:GLU:C	1:A:416:ASN:HD22	2.19	0.51
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:545:THR:O	1:A:546:LYS:C	2.53	0.51
1:A:371:SER:C	1:A:373:LYS:N	2.69	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:685:LYS:HD3	1:A:685:LYS:C	2.36	0.50
1:A:375:GLY:HA2	1:A:464:VAL:HG11	1.92	0.50
1:A:371:SER:C	1:A:373:LYS:H	2.18	0.50
1:A:687:GLU:O	1:A:691:LYS:HG3	2.11	0.50
1:A:291:ASP:C	1:A:293:ILE:H	2.19	0.50
1:A:293:ILE:O	1:A:610:MET:CE	2.60	0.50
1:A:683:GLY:O	1:A:684:ASP:C	2.55	0.50
1:A:692:GLU:HG3	1:A:696:LYS:HE3	1.93	0.49
1:A:655:ASN:C	1:A:655:ASN:ND2	2.69	0.49
1:A:310:GLU:H	1:A:310:GLU:CD	2.20	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:293:ILE:O	1:A:610:MET:SD	2.71	0.48
1:A:735:VAL:HG13	1:A:741:ILE:HD11	1.94	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:523:LEU:C	1:A:716:LYS:HZ1	2.22	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:N	1:A:416:ASN:ND2	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LYS:HA	1:A:461:LYS:HD2	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:462:ILE:HG22	1:A:463:THR:O	2.16	0.46
1:A:591:ASN:HD22	1:A:591:ASN:C	2.24	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:437:SER:C	1:A:439:ASN:H	2.25	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:353:LYS:HB3	1:A:372:LYS:HD3	1.98	0.45
1:A:770:ASN:HD22	1:A:770:ASN:N	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:681:ASP:CG	1:A:690:LYS:NZ	2.75	0.44
1:A:602:PHE:C	1:A:603:ILE:HG13	2.41	0.43
1:A:770:ASN:H	1:A:770:ASN:ND2	2.12	0.43
1:A:357:TRP:HH2	1:A:439:ASN:ND2	2.16	0.43
1:A:408:LEU:O	1:A:412:GLU:HG3	2.18	0.43
1:A:541:LYS:H	1:A:541:LYS:HG2	1.48	0.43
1:A:446:ILE:CG1	1:A:447:SER:N	2.81	0.43
1:A:457:THR:HG22	1:A:469:PHE:O	2.19	0.42
1:A:523:LEU:HB3	1:A:716:LYS:CE	2.49	0.42
1:A:349:ASN:HB3	1:A:394:HIS:CE1	2.54	0.42
1:A:413:LEU:HB3	1:A:419:ILE:HG12	2.01	0.42
1:A:687:GLU:N	1:A:687:GLU:OE1	2.52	0.42
1:A:385:LEU:HD22	1:A:389:LYS:HE2	2.01	0.42
1:A:450:ASN:HD22	1:A:452:GLU:CD	2.27	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:293:ILE:CB	4:A:90:HOH:O	2.68	0.41
1:A:564:VAL:HG11	1:A:574:VAL:HG11	2.01	0.41
1:A:768:LYS:HG2	1:A:770:ASN:ND2	2.35	0.41
1:A:324:THR:HG22	1:A:325:TYR:O	2.21	0.41
1:A:418:ILE:O	1:A:419:ILE:CG2	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:406:ASP:HB2	1:A:407:HIS:HD2	1.86	0.41
1:A:640:LYS:H	1:A:640:LYS:HG2	1.57	0.41
1:A:443:GLU:HB2	1:A:456:LYS:CE	2.50	0.41
1:A:540:ARG:CZ	1:A:544:SER:HB2	2.50	0.41
1:A:687:GLU:H	1:A:687:GLU:CD	2.27	0.41
1:A:326:ILE:C	1:A:327:LEU:HD12	2.46	0.41
1:A:382:LYS:O	1:A:386:GLU:HG3	2.21	0.41
1:A:299:GLU:HG3	1:A:303:LYS:HD3	2.03	0.40
1:A:359:PRO:CB	1:A:405:LEU:HD11	2.50	0.40
1:A:447:SER:HB3	1:A:450:ASN:O	2.21	0.40
1:A:512:GLU:O	1:A:516:VAL:HG23	2.20	0.40
1:A:526:GLN:NE2	1:A:711:ILE:HG13	2.35	0.40
1:A:359:PRO:HB3	1:A:405:LEU:HD11	2.02	0.40
1:A:613:ARG:CZ	1:A:636:ALA:HB2	2.51	0.40
1:A:787:THR:CG2	1:A:788:ASP:N	2.84	0.40
1:A:401:ILE:HG21	1:A:485:LEU:HB3	2.03	0.40
1:A:482:GLU:O	1:A:482:GLU:HG3	2.22	0.40
1:A:711:ILE:O	1:A:717:LYS:HE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	16	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	520	PRO
1	A	438	ASN
1	A	518	ASN

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Mol	Chain	Res	Type
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%)	393 (90%)	44 (10%)	7 15

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	308	VAL
1	A	310	GLU
1	A	332	ASN
1	A	340	LYS
1	A	349	ASN
1	A	372	LYS
1	A	378	LEU
1	A	385	LEU
1	A	395	GLU
1	A	407	HIS
1	A	414	LYS
1	A	416	ASN
1	A	424	LYS
1	A	434	LEU
1	A	438	ASN
1	A	443	GLU
1	A	449	GLU
1	A	452	GLU
1	A	456	LYS
1	A	459	GLU
1	A	468	LYS
1	A	485	LEU
1	A	493	ASP
1	A	510	GLN
1	A	519	THR

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Mol	Chain	Res	Type
1	A	541	LYS
1	A	542	PRO
1	A	554	LYS
1	A	557	LEU
1	A	559	ARG
1	A	599	GLU
1	A	611	THR
1	A	620	THR
1	A	622	LYS
1	A	655	ASN
1	A	668	SER
1	A	672	ARG
1	A	681	ASP
1	A	685	LYS
1	A	687	GLU
1	A	695	LYS
1	A	720	ILE
1	A	740	GLN
1	A	770	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	ASN
1	A	332	ASN
1	A	368	GLN
1	A	376	GLN
1	A	377	GLN
1	A	384	ASN
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	551	ASN
1	A	553	GLN
1	A	591	ASN
1	A	629	ASN
1	A	655	ASN
1	A	709	ASN

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Mol	Chain	Res	Type
1	A	727	GLN
1	A	758	ASN
1	A	767	GLN
1	A	770	ASN

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 oligosaccharides 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	1004	-	4,4,4	0.94	0	6,6,6	0.49	0
2	SO4	A	1001	-	4,4,4	0.77	0	6,6,6	0.40	0
2	SO4	A	1002	-	4,4,4	0.82	0	6,6,6	0.48	0
2	SO4	A	1003	-	4,4,4	0.85	0	6,6,6	0.45	0

There are no bond length outliers.

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 [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, 95th 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%)	0.66	77 (15%) 5 4	23, 53, 97, 100	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	683	GLY	5.6
1	A	293	ILE	5.2
1	A	294	ASP	4.9
1	A	420	LEU	4.7
1	A	439	ASN	4.6
1	A	433	TYR	4.6
1	A	525	LYS	4.2
1	A	579	THR	4.2
1	A	451	ASN	4.2
1	A	544	SER	4.2
1	A	519	THR	4.1
1	A	450	ASN	4.0
1	A	638	GLY	3.9
1	A	523	LEU	3.9
1	A	521	ASN	3.8
1	A	520	PRO	3.6
1	A	449	GLU	3.5
1	A	454	GLN	3.5
1	A	464	VAL	3.5
1	A	526	GLN	3.4
1	A	682	SER	3.4
1	A	545	THR	3.4
1	A	444	PHE	3.4
1	A	681	ASP	3.3
1	A	291	ASP	3.2
1	A	452	GLU	3.1
1	A	434	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	527	LYS	3.1
1	A	462	ILE	3.1
1	A	448	ASP	3.0
1	A	517	VAL	3.0
1	A	522	SER	2.9
1	A	419	ILE	2.9
1	A	426	ILE	2.9
1	A	424	LYS	2.9
1	A	518	ASN	2.8
1	A	418	ILE	2.8
1	A	543	ASP	2.7
1	A	744	GLU	2.7
1	A	473	ASN	2.7
1	A	524	GLU	2.7
1	A	799	GLU	2.7
1	A	406	ASP	2.6
1	A	684	ASP	2.6
1	A	468	LYS	2.6
1	A	463	THR	2.6
1	A	417	GLY	2.6
1	A	432	TYR	2.6
1	A	639	ASN	2.6
1	A	469	PHE	2.5
1	A	407	HIS	2.5
1	A	438	ASN	2.5
1	A	554	LYS	2.4
1	A	547	GLY	2.4
1	A	421	LYS	2.4
1	A	606	LYS	2.3
1	A	375	GLY	2.3
1	A	292	ARG	2.3
1	A	688	PHE	2.3
1	A	374	HIS	2.3
1	A	378	LEU	2.3
1	A	591	ASN	2.2
1	A	437	SER	2.2
1	A	578	GLY	2.2
1	A	465	LEU	2.2
1	A	457	THR	2.2
1	A	754	GLU	2.2
1	A	637	PRO	2.2
1	A	440	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	737	LYS	2.2
1	A	373	LYS	2.2
1	A	422	GLY	2.2
1	A	453	VAL	2.2
1	A	472	ARG	2.1
1	A	435	LEU	2.1
1	A	516	VAL	2.0
1	A	443	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
2	SO4	A	1004	5/5	0.72	0.13	99,100,100,100	0
2	SO4	A	1003	5/5	0.83	0.21	96,97,97,98	0
2	SO4	A	1002	5/5	0.85	0.16	84,84,86,87	0
2	SO4	A	1001	5/5	0.94	0.10	61,62,65,65	0
3	NI	A	2001	1/1	0.94	0.06	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.