Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 09:06 PM GMT

PDB ID	:	1NIT
Title	:	CRYSTAL STRUCTURE OF ACONITASE WITH TRANS-ACONITATE AND NITROCITRATE BOUND
Authors	:	Lauble, H.; Kennedy, M.C.; Beinert, H.; Stout, C.D.
Deposited on	:	1993-01-17
Resolution	:	2.05 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 ⓘ symbol.

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

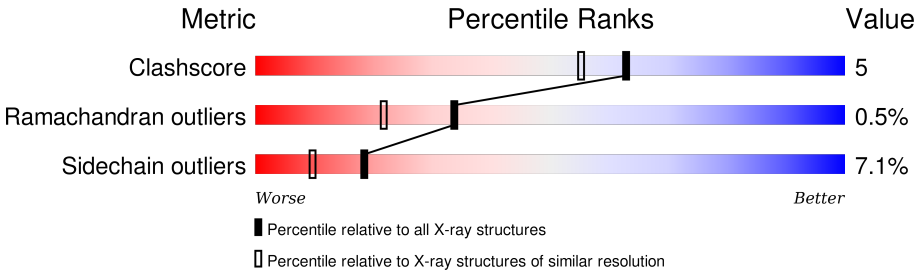
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.05 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))
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	754	79% 16%

2 Entry composition

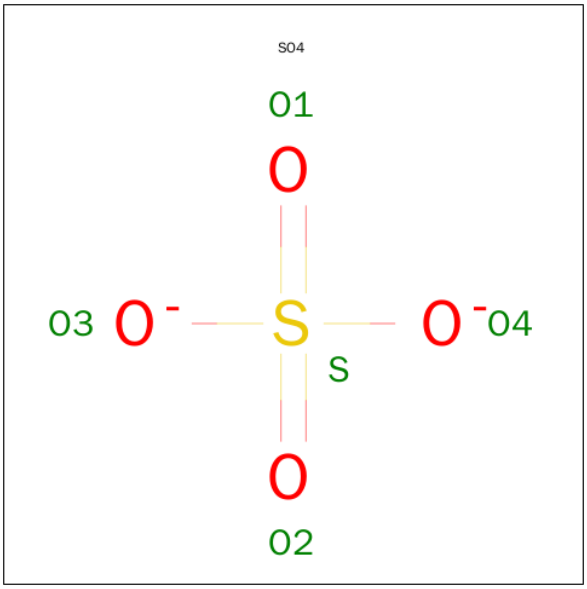
There are 4 unique types of molecules in this entry. The entry contains 6116 atoms, of which 1 is hydrogen and 0 are deuteriums.

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 ACONITASE.

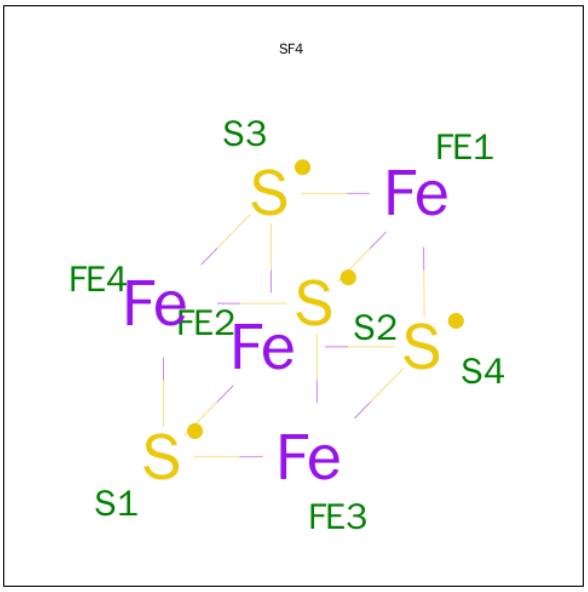
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	753	5812	3664	1031	1095	22	0	0	0

- 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

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	8	4	4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
4	A	290	291	1	290	0	0

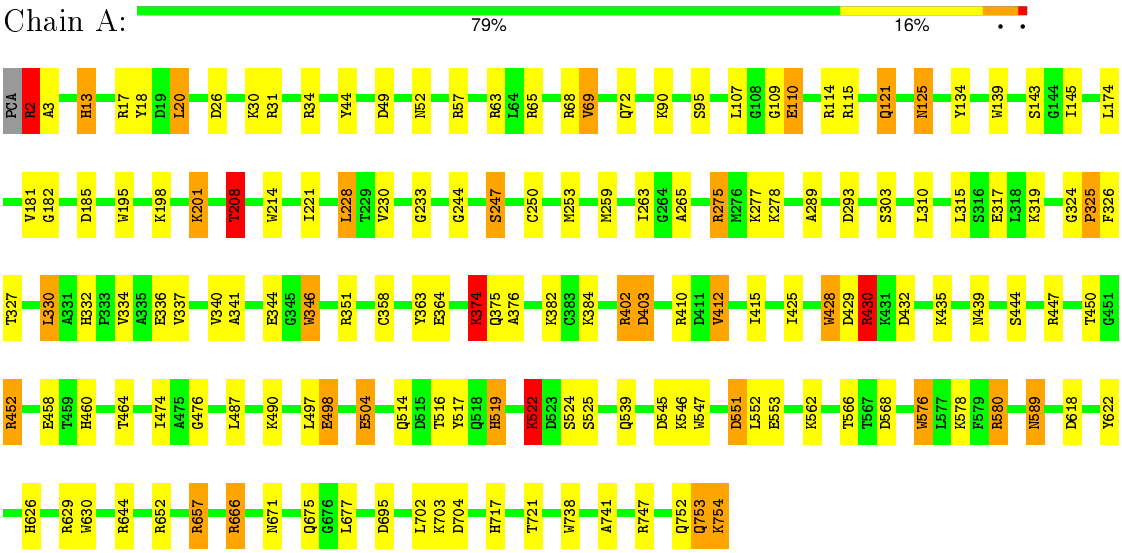
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: ACONITASE

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, α, β, γ	185.50Å 72.00Å 73.00Å 90.00° 90.00° 77.70°	Depositor
Resolution (Å)	8.00 – 2.05	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.05)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6116	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 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	0.86	0/5938	1.59	80/8044 (1.0%)

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	3

There are no bond length outliers.

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	402	ARG	NE-CZ-NH2	-21.50	109.55	120.30
1	A	430	ARG	NE-CZ-NH2	-15.17	112.72	120.30
1	A	402	ARG	NE-CZ-NH1	15.12	127.86	120.30
1	A	666	ARG	NE-CZ-NH2	-14.66	112.97	120.30
1	A	115	ARG	NE-CZ-NH2	-14.23	113.18	120.30
1	A	430	ARG	NE-CZ-NH1	13.84	127.22	120.30
1	A	580	ARG	NE-CZ-NH2	-13.79	113.41	120.30
1	A	580	ARG	NE-CZ-NH1	12.88	126.74	120.30
1	A	410	ARG	NE-CZ-NH2	-12.73	113.93	120.30
1	A	410	ARG	NE-CZ-NH1	12.45	126.53	120.30
1	A	63	ARG	NE-CZ-NH2	-11.01	114.80	120.30
1	A	666	ARG	NE-CZ-NH1	10.73	125.66	120.30
1	A	346	TRP	CD1-CG-CD2	10.08	114.36	106.30
1	A	31	ARG	NE-CZ-NH2	-9.89	115.36	120.30
1	A	139	TRP	CD1-CG-CD2	9.57	113.95	106.30
1	A	275	ARG	NE-CZ-NH1	9.43	125.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	63	ARG	NE-CZ-NH1	9.15	124.87	120.30
1	A	195	TRP	CD1-CG-CD2	9.06	113.55	106.30
1	A	44	TYR	CB-CG-CD2	-8.80	115.72	121.00
1	A	65	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	A	630	TRP	CD1-CG-CD2	8.63	113.20	106.30
1	A	738	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	A	346	TRP	CE2-CD2-CG	-8.03	100.88	107.30
1	A	139	TRP	CE2-CD2-CG	-7.99	100.91	107.30
1	A	452	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	57	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	547	TRP	CD1-CG-CD2	7.64	112.41	106.30
1	A	630	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	A	325	PRO	CA-C-N	7.60	133.92	117.20
1	A	498	GLU	CA-CB-CG	7.60	130.12	113.40
1	A	576	TRP	CD1-CG-CD2	7.52	112.31	106.30
1	A	65	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	34	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	A	195	TRP	CG-CD1-NE1	-7.07	103.03	110.10
1	A	576	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	A	195	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	A	547	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	A	351	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	A	115	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	A	214	TRP	CD1-CG-CD2	6.79	111.73	106.30
1	A	428	TRP	CD1-CG-CD2	6.77	111.71	106.30
1	A	214	TRP	CE2-CD2-CG	-6.76	101.89	107.30
1	A	31	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	A	139	TRP	CG-CD2-CE3	6.62	139.86	133.90
1	A	293	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	403	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	738	TRP	CE2-CD2-CG	-6.59	102.03	107.30
1	A	346	TRP	CG-CD1-NE1	-6.57	103.53	110.10
1	A	666	ARG	CG-CD-NE	-6.55	98.04	111.80
1	A	351	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	657	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	522	LYS	CA-C-N	-6.47	102.96	117.20
1	A	428	TRP	CE2-CD2-CG	-6.46	102.14	107.30
1	A	519	HIS	CB-CG-ND1	6.32	139.01	123.20
1	A	139	TRP	CB-CG-CD1	-6.21	118.93	127.00
1	A	18	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	A	139	TRP	CG-CD1-NE1	-6.09	104.01	110.10
1	A	504	GLU	OE1-CD-OE2	-5.99	116.11	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	458	GLU	OE1-CD-OE2	-5.96	116.14	123.30
1	A	13	HIS	CB-CA-C	-5.74	98.92	110.40
1	A	412	VAL	CB-CA-C	-5.63	100.69	111.40
1	A	551	ASP	CB-CG-OD1	5.63	123.36	118.30
1	A	374	LYS	CA-CB-CG	5.45	125.38	113.40
1	A	695	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	738	TRP	CG-CD1-NE1	-5.38	104.72	110.10
1	A	415	ILE	CG1-CB-CG2	-5.38	99.57	111.40
1	A	753	GLN	N-CA-C	5.38	125.52	111.00
1	A	630	TRP	CB-CG-CD1	-5.35	120.04	127.00
1	A	630	TRP	CG-CD1-NE1	-5.30	104.80	110.10
1	A	545	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	208	THR	N-CA-CB	-5.25	100.33	110.30
1	A	2	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	A	325	PRO	O-C-N	-5.20	114.39	122.70
1	A	618	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	539	GLN	CG-CD-NE2	5.18	129.13	116.70
1	A	429	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	410	ARG	CG-CD-NE	-5.07	101.15	111.80
1	A	57	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	363	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	A	69	VAL	CG1-CB-CG2	-5.01	102.89	110.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	324	GLY	Peptide
1	A	580	ARG	Sidechain
1	A	68	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5812	0	5793	62	0
2	A	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	0	0	0	0
4	A	290	1	0	3	0
All	All	6115	1	5793	62	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 5.

All (62) 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:430:ARG:HH22	1:A:439:ASN:HD21	1.29	0.78
1:A:566:THR:HG22	1:A:568:ASP:H	1.53	0.73
1:A:228:LEU:HD23	1:A:263:ILE:HD12	1.74	0.70
1:A:430:ARG:HH22	1:A:439:ASN:ND2	1.91	0.69
1:A:384:LYS:HD3	1:A:476:GLY:HA3	1.78	0.65
1:A:546:LYS:HD3	1:A:741:ALA:O	2.01	0.60
1:A:277:LYS:HG3	1:A:289:ALA:HB1	1.85	0.59
1:A:49:ASP:OD2	1:A:52:ASN:HB2	2.03	0.57
1:A:336:GLU:O	1:A:340:VAL:HG23	2.04	0.57
1:A:430:ARG:HD2	1:A:432:ASP:OD1	2.04	0.57
1:A:402:ARG:HD2	1:A:403:ASP:OD1	2.05	0.56
1:A:2:ARG:HE	1:A:3:ALA:N	2.04	0.55
1:A:752:GLN:O	1:A:754:LYS:HG3	2.08	0.53
1:A:17:ARG:NH2	1:A:20:LEU:HD23	2.24	0.53
1:A:552:LEU:HD23	1:A:629:ARG:HH21	1.75	0.51
1:A:428:TRP:CZ2	1:A:430:ARG:HD3	2.47	0.50
1:A:2:ARG:HE	1:A:3:ALA:H	1.59	0.50
1:A:275:ARG:NH2	4:A:1055:HOH:O	2.44	0.49
1:A:644:ARG:HB3	2:A:998:SO4:O1	2.13	0.49
1:A:622:TYR:O	1:A:626:HIS:HD2	1.96	0.49
1:A:233:GLY:O	1:A:265:ALA:HA	2.12	0.49
1:A:2:ARG:NE	1:A:3:ALA:H	2.10	0.48
1:A:244:GLY:O	1:A:247:SER:HB3	2.14	0.48
1:A:374:LYS:HD2	1:A:375:GLN:HG3	1.96	0.48
1:A:341:ALA:HA	1:A:346:TRP:CE3	2.49	0.48
1:A:145:ILE:HG21	1:A:358:CYS:HB3	1.96	0.48
1:A:110:GLU:O	1:A:114:ARG:HG3	2.15	0.47
1:A:230:VAL:HA	1:A:263:ILE:HA	1.97	0.47
1:A:444:SER:HA	1:A:464:THR:O	2.15	0.47
1:A:13:HIS:CD2	1:A:13:HIS:H	2.31	0.47
1:A:717:HIS:HD2	1:A:721:THR:HB	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ARG:NH2	4:A:1059:HOH:O	2.36	0.46
1:A:430:ARG:NH2	1:A:439:ASN:HD21	2.05	0.46
1:A:250:CYS:HA	1:A:253:MET:CE	2.45	0.46
1:A:69:VAL:O	1:A:95:SER:HA	2.16	0.46
1:A:121:GLN:O	1:A:125:ASN:HB2	2.15	0.45
1:A:182:GLY:HA3	1:A:671:ASN:HD21	1.80	0.45
1:A:452:ARG:NH2	4:A:1288:HOH:O	2.49	0.45
1:A:143:SER:HB3	1:A:516:THR:HB	1.97	0.45
1:A:652:ARG:HD3	1:A:677:LEU:HG	1.98	0.45
1:A:208:THR:O	1:A:315:LEU:HB2	2.17	0.45
1:A:551:ASP:H	1:A:703:LYS:HZ2	1.63	0.44
1:A:754:LYS:HZ2	1:A:754:LYS:C	2.20	0.44
1:A:522:LYS:CE	1:A:522:LYS:HA	2.48	0.43
1:A:675:GLN:HA	1:A:675:GLN:NE2	2.34	0.43
1:A:326:PHE:HD2	1:A:450:THR:HG1	1.66	0.43
1:A:2:ARG:CD	1:A:3:ALA:H	2.32	0.42
1:A:522:LYS:HE3	1:A:522:LYS:HA	2.01	0.42
1:A:275:ARG:NE	1:A:278:LYS:HZ1	2.18	0.42
1:A:576:TRP:CE2	1:A:589:ASN:HB3	2.55	0.41
1:A:250:CYS:HA	1:A:253:MET:HE2	2.02	0.41
1:A:589:ASN:C	1:A:589:ASN:HD22	2.24	0.41
1:A:376:ALA:HB2	1:A:474:ILE:HD13	2.03	0.41
1:A:26:ASP:O	1:A:30:LYS:HD3	2.21	0.41
1:A:330:LEU:HD22	1:A:332:HIS:CE1	2.56	0.41
1:A:334:VAL:O	1:A:337:VAL:HG12	2.20	0.41
1:A:181:VAL:HB	1:A:185:ASP:HB2	2.03	0.41
1:A:201:LYS:HA	1:A:201:LYS:HD2	1.90	0.41
1:A:221:ILE:HG12	1:A:259:MET:HB3	2.02	0.40
1:A:90:LYS:HD2	1:A:134:TYR:O	2.21	0.40
1:A:517:TYR:OH	1:A:519:HIS:HD2	2.05	0.40
1:A:364:GLU:HB2	1:A:504:GLU:HA	2.04	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	751/754 (100%)	714 (95%)	33 (4%)	4 (0%)	34 22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	SER
1	A	525	SER
1	A	753	GLN
1	A	109	GLY

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	621/622 (100%)	577 (93%)	44 (7%)	18 10

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

Mol	Chain	Res	Type
1	A	2	ARG
1	A	20	LEU
1	A	72	GLN
1	A	107	LEU
1	A	110	GLU
1	A	121	GLN
1	A	125	ASN
1	A	174	LEU
1	A	198	LYS
1	A	201	LYS
1	A	208	THR
1	A	228	LEU
1	A	247	SER
1	A	303	SER
1	A	310	LEU

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Mol	Chain	Res	Type
1	A	317	GLU
1	A	319	LYS
1	A	325	PRO
1	A	327	THR
1	A	330	LEU
1	A	344	GLU
1	A	374	LYS
1	A	382	LYS
1	A	412	VAL
1	A	425	ILE
1	A	430	ARG
1	A	435	LYS
1	A	460	HIS
1	A	487	LEU
1	A	490	LYS
1	A	497	LEU
1	A	498	GLU
1	A	514	GLN
1	A	522	LYS
1	A	553	GLU
1	A	562	LYS
1	A	578	LYS
1	A	589	ASN
1	A	657	ARG
1	A	666	ARG
1	A	702	LEU
1	A	704	ASP
1	A	747	ARG
1	A	754	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	321	HIS
1	A	395	GLN
1	A	439	ASN
1	A	514	GLN
1	A	519	HIS
1	A	536	GLN
1	A	585	ASN
1	A	589	ASN

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Mol	Chain	Res	Type
1	A	637	ASN
1	A	671	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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	998	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
3	SF4	A	999	1,4	0,12,12	0.00	-	0,24,24	0.00	-

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	998	-	-	0/0/0/0	0/0/0/0
3	SF4	A	999	1,4	-	0/0/48/48	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	998	SO4	O1-S	-2.18	1.39	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	998	SO4	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.