Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:03 PM GMT

PDB ID	:	5ACN
Title	:	STRUCTURE OF ACTIVATED ACONITASE. FORMATION OF THE (4FE-4S) CLUSTER IN THE CRYSTAL
Authors	:	Robbins, A.H.; Stout, C.D.
Deposited on	:	1990-01-16
Resolution	:	2.10 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 (i)) were used in the production of this report:

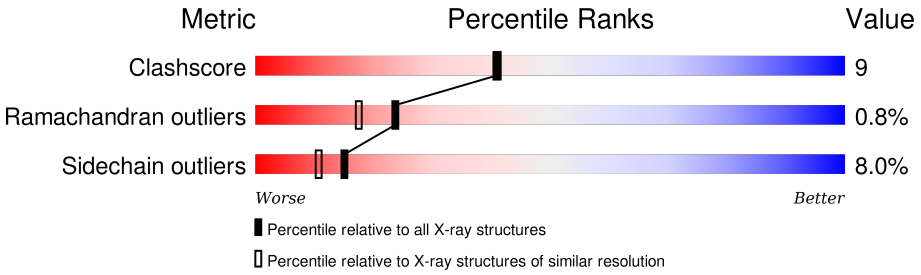
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.10 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	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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	70% 24% 5% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6254 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.

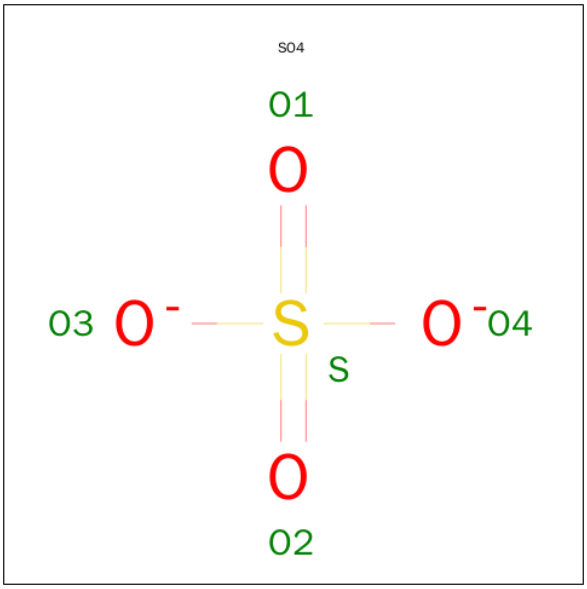
- Molecule 1 is a protein called ACONITASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	754	Total	C	N	O	S	0	0	0
			5823	3671	1035	1095	22			

There is a discrepancy between the modelled and reference sequences:

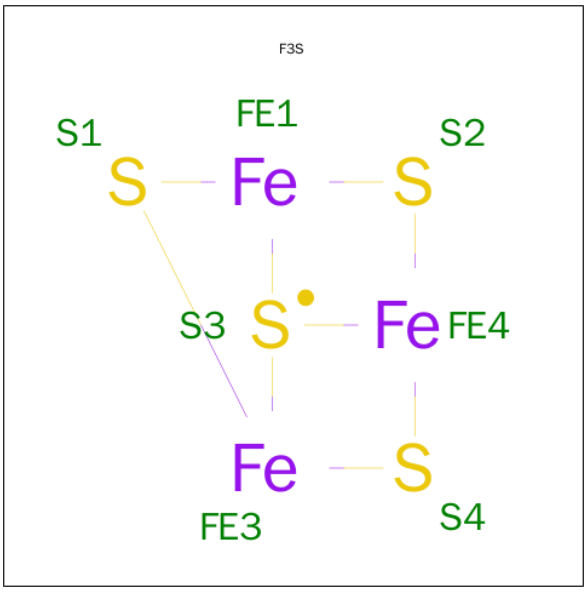
Chain	Residue	Modelled	Actual	Comment	Reference
A	647	SER	ARG	CONFLICT	UNP P16276

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



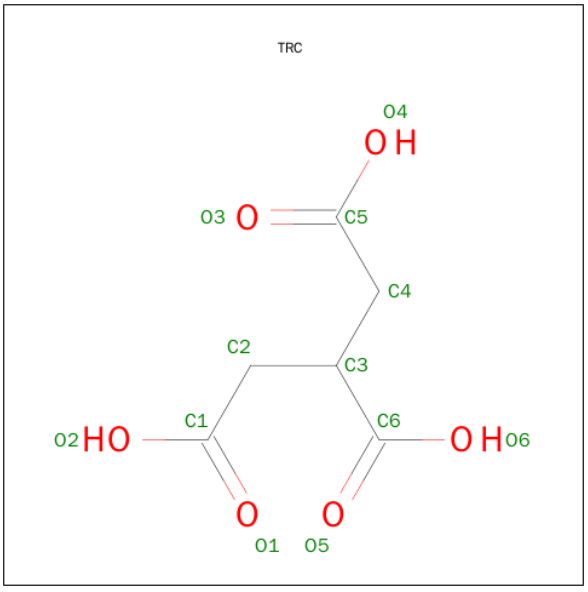
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 7 3 4	0	0

- Molecule 4 is TRICARBALLYLIC ACID (three-letter code: TRC) (formula: $C_6H_8O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 12 6 6	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	407	Total	O	0	0
			407	407		

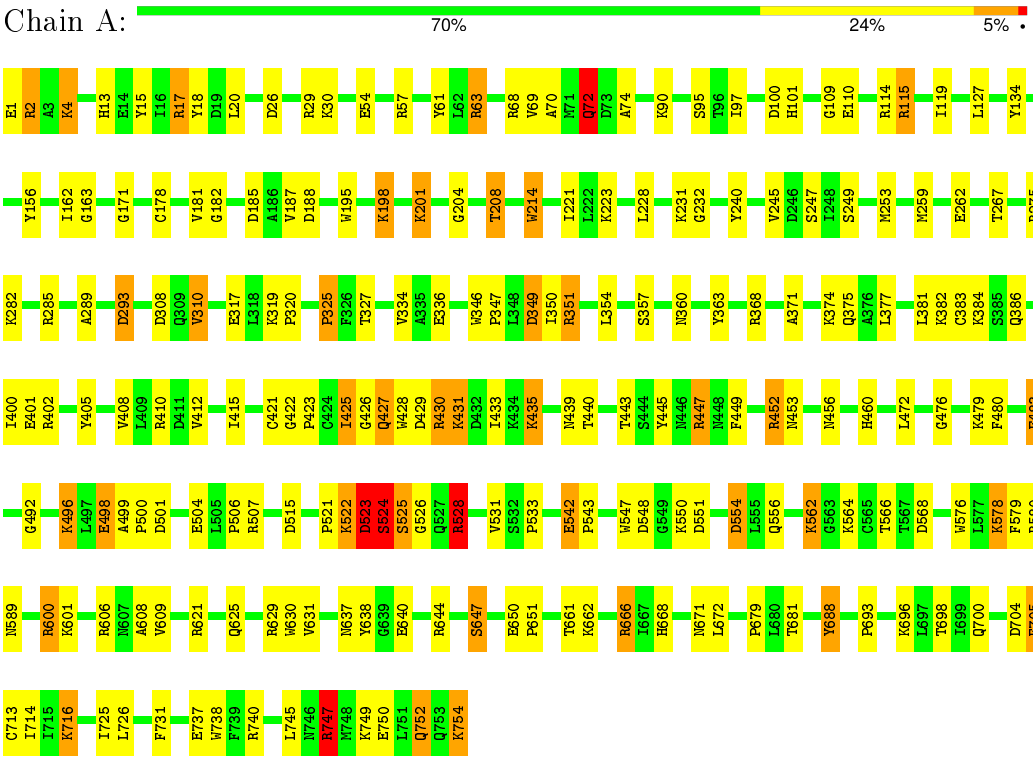
3 Residue-property plots (i)

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	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	173.60Å 72.00Å 72.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.215 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6254	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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: TRC, F3S, PCA, 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	0.98	1/5943 (0.0%)	1.73	110/8053 (1.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	647	SER	CA-CB	-6.88	1.42	1.52

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	447	ARG	NE-CZ-NH1	-15.50	112.55	120.30
1	A	666	ARG	NE-CZ-NH1	-13.57	113.52	120.30
1	A	447	ARG	NE-CZ-NH2	11.64	126.12	120.30
1	A	195	TRP	CD1-CG-CD2	11.05	115.14	106.30
1	A	275	ARG	NE-CZ-NH1	-10.87	114.87	120.30
1	A	405	TYR	CB-CG-CD2	-10.78	114.53	121.00
1	A	72	GLN	CA-CB-CG	10.30	136.05	113.40
1	A	368	ARG	NE-CZ-NH2	10.14	125.37	120.30
1	A	402	ARG	NE-CZ-NH1	-9.97	115.31	120.30
1	A	410	ARG	NE-CZ-NH1	-9.68	115.46	120.30
1	A	606	ARG	NE-CZ-NH2	9.22	124.91	120.30
1	A	738	TRP	CD1-CG-CD2	8.93	113.44	106.30
1	A	275	ARG	NE-CZ-NH2	8.82	124.71	120.30
1	A	72	GLN	N-CA-CB	-8.77	94.82	110.60
1	A	17	ARG	NE-CZ-NH2	8.69	124.64	120.30
1	A	114	ARG	NE-CZ-NH1	-8.61	115.99	120.30
1	A	195	TRP	CE2-CD2-CG	-8.61	100.42	107.30
1	A	195	TRP	CG-CD1-NE1	-8.60	101.50	110.10
1	A	139	TRP	CD1-CG-CD2	8.55	113.14	106.30
1	A	498	GLU	CA-CB-CG	8.44	131.96	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	576	TRP	CD1-CG-CD2	8.39	113.01	106.30
1	A	445	TYR	CB-CG-CD2	-8.24	116.06	121.00
1	A	134	TYR	CB-CG-CD2	-8.24	116.06	121.00
1	A	346	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	A	17	ARG	NE-CZ-NH1	-7.98	116.31	120.30
1	A	139	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	A	576	TRP	CE2-CD2-CG	-7.72	101.12	107.30
1	A	606	ARG	NE-CZ-NH1	-7.65	116.47	120.30
1	A	140	ARG	NE-CZ-NH1	-7.60	116.50	120.30
1	A	410	ARG	NE-CZ-NH2	7.57	124.08	120.30
1	A	214	TRP	CD1-CG-CD2	7.55	112.34	106.30
1	A	57	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	A	630	TRP	CE2-CD2-CG	-7.37	101.40	107.30
1	A	18	TYR	CB-CG-CD2	-7.25	116.65	121.00
1	A	738	TRP	CE2-CD2-CG	-7.24	101.50	107.30
1	A	666	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	A	547	TRP	CD1-CG-CD2	7.14	112.01	106.30
1	A	630	TRP	CG-CD2-CE3	7.14	140.32	133.90
1	A	630	TRP	CD1-CG-CD2	7.08	111.96	106.30
1	A	551	ASP	CB-CG-OD1	7.08	124.67	118.30
1	A	214	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	A	631	VAL	CG1-CB-CG2	-7.03	99.65	110.90
1	A	368	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	A	188	ASP	CB-CG-OD2	7.01	124.61	118.30
1	A	528	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	A	428	TRP	CD1-CG-CD2	6.93	111.85	106.30
1	A	705	PHE	CB-CG-CD1	-6.90	115.97	120.80
1	A	428	TRP	CE2-CD2-CG	-6.87	101.81	107.30
1	A	547	TRP	CE2-CD2-CG	-6.87	101.81	107.30
1	A	638	TYR	CB-CG-CD2	-6.85	116.89	121.00
1	A	240	TYR	CB-CG-CD1	-6.71	116.98	121.00
1	A	383	CYS	CA-CB-SG	-6.70	101.95	114.00
1	A	72	GLN	CB-CA-C	6.64	123.67	110.40
1	A	195	TRP	CB-CG-CD1	-6.60	118.42	127.00
1	A	293	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	61	TYR	CB-CG-CD2	-6.46	117.12	121.00
1	A	346	TRP	CE2-CD2-CG	-6.43	102.16	107.30
1	A	688	TYR	CB-CG-CD2	-6.39	117.16	121.00
1	A	507	ARG	CA-CB-CG	6.31	127.28	113.40
1	A	638	TYR	CB-CG-CD1	6.25	124.75	121.00
1	A	452	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	A	325	PRO	CA-C-N	6.18	130.81	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	195	TRP	CG-CD2-CE3	6.12	139.41	133.90
1	A	531	VAL	CG1-CB-CG2	-6.10	101.14	110.90
1	A	63	ARG	N-CA-CB	-6.08	99.66	110.60
1	A	504	GLU	OE1-CD-OE2	-6.07	116.02	123.30
1	A	114	ARG	NE-CZ-NH2	6.01	123.31	120.30
1	A	629	ARG	CB-CG-CD	-6.00	95.99	111.60
1	A	156	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	A	310	VAL	CG1-CB-CG2	-5.95	101.37	110.90
1	A	580	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	A	523	ASP	CA-CB-CG	5.93	126.44	113.40
1	A	747	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	A	110	GLU	CA-CB-CG	5.90	126.37	113.40
1	A	585	ASN	CB-CG-ND2	5.86	130.76	116.70
1	A	278	LYS	CA-CB-CG	5.85	126.28	113.40
1	A	140	ARG	N-CA-CB	-5.84	100.08	110.60
1	A	195	TRP	CD1-NE1-CE2	5.81	114.23	109.00
1	A	483	GLU	CA-CB-CG	5.77	126.09	113.40
1	A	547	TRP	CG-CD2-CE3	5.74	139.07	133.90
1	A	630	TRP	CB-CG-CD1	-5.70	119.59	127.00
1	A	54	GLU	CB-CG-CD	5.69	129.56	114.20
1	A	408	VAL	CG1-CB-CG2	-5.65	101.86	110.90
1	A	90	LYS	CA-CB-CG	5.59	125.71	113.40
1	A	57	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	A	428	TRP	CG-CD2-CE3	5.53	138.88	133.90
1	A	115	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	A	346	TRP	CG-CD1-NE1	-5.51	104.59	110.10
1	A	600	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	A	738	TRP	CG-CD1-NE1	-5.49	104.61	110.10
1	A	500	PRO	CA-C-N	-5.46	105.18	117.20
1	A	600	ARG	CA-CB-CG	5.45	125.40	113.40
1	A	498	GLU	N-CA-CB	-5.44	100.81	110.60
1	A	100	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	566	THR	N-CA-CB	-5.33	100.16	110.30
1	A	208	THR	N-CA-CB	-5.33	100.17	110.30
1	A	698	THR	CA-CB-CG2	5.33	119.86	112.40
1	A	267	THR	CA-CB-CG2	5.32	119.85	112.40
1	A	644	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	A	524	SER	N-CA-C	5.25	125.19	111.00
1	A	601	LYS	CA-CB-CG	5.16	124.74	113.40
1	A	740	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	A	542	GLU	CB-CG-CD	-5.14	100.33	114.20
1	A	547	TRP	CG-CD1-NE1	-5.13	104.97	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	708	GLY	CA-C-N	5.10	128.42	117.20
1	A	245	VAL	CA-CB-CG2	-5.09	103.26	110.90
1	A	548	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	68	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	282	LYS	CB-CG-CD	5.04	124.72	111.60
1	A	285	ARG	NE-CZ-NH1	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

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	5823	0	5811	100	0
2	A	5	0	0	0	0
3	A	7	0	0	1	0
4	A	12	0	5	0	0
5	A	407	0	0	11	0
All	All	6254	0	5816	100	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 9.

All (100) 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:384:LYS:HD2	1:A:476:GLY:HA3	1.63	0.80
1:A:750:GLU:HA	1:A:754:LYS:HA	1.62	0.80
1:A:521:PRO:HB2	1:A:523:ASP:HB2	1.63	0.79
1:A:430:ARG:HH12	1:A:439:ASN:HD21	1.34	0.75
1:A:371:ALA:HA	1:A:374:LYS:HD3	1.68	0.75
1:A:640:GLU:HG2	5:A:970:HOH:O	1.90	0.72
1:A:496:LYS:HB2	1:A:496:LYS:HZ2	1.58	0.69
1:A:447:ARG:HG3	1:A:449:PHE:HD2	1.62	0.64
1:A:431:LYS:HA	1:A:431:LYS:HE3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:LYS:NZ	1:A:496:LYS:HB2	2.14	0.62
1:A:430:ARG:HH12	1:A:439:ASN:ND2	1.97	0.61
1:A:447:ARG:HG2	1:A:452:ARG:HG2	1.82	0.61
1:A:277:LYS:HG2	1:A:289:ALA:HB1	1.83	0.61
1:A:29:ARG:HG3	1:A:29:ARG:HH21	1.66	0.61
1:A:354:LEU:HD13	1:A:443:THR:HG22	1.82	0.60
1:A:562:LYS:HE2	1:A:562:LYS:O	2.01	0.59
1:A:374:LYS:HG2	1:A:375:GLN:N	2.18	0.58
1:A:737:GLU:HB3	1:A:747:ARG:HD2	1.85	0.58
1:A:621:ARG:O	1:A:625:GLN:HG2	2.02	0.58
1:A:182:GLY:HA3	1:A:671:ASN:HD21	1.69	0.57
1:A:754:LYS:HB3	1:A:754:LYS:NZ	2.21	0.56
1:A:745:LEU:O	1:A:749:LYS:HG3	2.06	0.56
1:A:661:THR:O	1:A:681:THR:HA	2.05	0.55
1:A:522:LYS:O	1:A:522:LYS:HD2	2.06	0.55
1:A:564:LYS:NZ	5:A:966:HOH:O	2.36	0.55
1:A:347:PRO:HD2	1:A:440:THR:OG1	2.07	0.54
1:A:221:ILE:HG12	1:A:259:MET:HB3	1.90	0.54
1:A:357:SER:HB2	3:A:999:F3S:S3	2.47	0.53
1:A:228:LEU:HB3	1:A:232:GLY:HA3	1.90	0.52
1:A:447:ARG:HG3	1:A:449:PHE:CD2	2.43	0.52
1:A:351:ARG:NH1	1:A:433:ILE:HG22	2.25	0.51
1:A:672:LEU:HB2	1:A:679:PRO:HG3	1.92	0.51
1:A:1:PCA:HG3	1:A:17:ARG:HD2	1.93	0.51
1:A:427:GLN:HG2	5:A:1013:HOH:O	2.11	0.50
1:A:749:LYS:O	1:A:752:GLN:HG2	2.12	0.50
1:A:397:ARG:HD2	5:A:877:HOH:O	2.12	0.50
1:A:29:ARG:HG3	1:A:29:ARG:NH2	2.26	0.49
1:A:371:ALA:CA	1:A:374:LYS:HD3	2.41	0.49
1:A:13:HIS:H	1:A:13:HIS:CD2	2.30	0.49
1:A:498:GLU:HB2	5:A:1118:HOH:O	2.12	0.49
1:A:162:ILE:HD12	1:A:181:VAL:HG21	1.93	0.48
1:A:198:LYS:HE2	5:A:823:HOH:O	2.12	0.48
1:A:181:VAL:HB	1:A:185:ASP:HB2	1.94	0.48
1:A:479:LYS:HA	1:A:479:LYS:HD2	1.68	0.48
1:A:2:ARG:HD3	1:A:2:ARG:H	1.78	0.48
1:A:637:ASN:O	1:A:640:GLU:HB2	2.14	0.48
1:A:483:GLU:HA	5:A:1031:HOH:O	2.12	0.47
1:A:384:LYS:HD3	5:A:812:HOH:O	2.15	0.47
1:A:374:LYS:HE2	1:A:375:GLN:HG3	1.95	0.47
1:A:320:PRO:HB2	1:A:334:VAL:HG22	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:PRO:HB2	1:A:334:VAL:CG2	2.44	0.47
1:A:63:ARG:NH2	5:A:1172:HOH:O	2.48	0.47
1:A:662:LYS:HE3	1:A:688:TYR:CG	2.50	0.47
1:A:72:GLN:OE1	1:A:74:ALA:HB3	2.14	0.47
1:A:700:GLN:OE1	1:A:714:ILE:HD11	2.14	0.47
1:A:650:GLU:HB2	1:A:651:PRO:HD3	1.97	0.47
1:A:204:GLY:O	1:A:310:VAL:HA	2.13	0.47
1:A:69:VAL:O	1:A:95:SER:HA	2.15	0.47
1:A:144:GLY:HA3	1:A:393:SER:HA	1.96	0.46
1:A:435:LYS:HD2	1:A:456:ASN:HA	1.97	0.46
1:A:480:PHE:CE2	1:A:485:ASP:HB2	2.50	0.46
1:A:350:ILE:CD1	1:A:472:LEU:HB3	2.45	0.46
1:A:578:LYS:HE3	1:A:579:PHE:CZ	2.51	0.46
1:A:588:ASN:OD1	1:A:621:ARG:NH1	2.48	0.46
1:A:26:ASP:OD2	1:A:30:LYS:NZ	2.49	0.46
1:A:713:CYS:HB3	1:A:725:ILE:HG13	1.98	0.46
1:A:72:GLN:HG2	1:A:101:HIS:CE1	2.51	0.45
1:A:381:LEU:HD21	1:A:489:GLY:HA2	1.99	0.45
1:A:679:PRO:HD2	1:A:731:PHE:CE2	2.51	0.45
1:A:426:GLY:HA2	1:A:453:ASN:O	2.17	0.45
1:A:704:ASP:OD1	1:A:709:LYS:NZ	2.51	0.44
1:A:422:GLY:HA3	1:A:423:PRO:HD3	1.85	0.44
1:A:363:TYR:CE1	1:A:506:PRO:HG3	2.53	0.44
1:A:171:GLY:HA3	1:A:178:CYS:SG	2.58	0.44
1:A:542:GLU:HA	1:A:543:PRO:HD3	1.87	0.44
1:A:528:ARG:HB2	5:A:919:HOH:O	2.17	0.43
1:A:562:LYS:HE2	1:A:562:LYS:C	2.38	0.43
1:A:70:ALA:O	1:A:163:GLY:HA2	2.19	0.43
1:A:349:ASP:OD2	1:A:384:LYS:NZ	2.52	0.43
1:A:214:TRP:CE2	1:A:499:ALA:HA	2.53	0.43
1:A:524:SER:O	1:A:526:GLY:N	2.52	0.43
1:A:435:LYS:HD3	1:A:435:LYS:HA	1.75	0.43
1:A:249:SER:O	1:A:253:MET:HG3	2.19	0.42
1:A:97:ILE:HG21	1:A:127:LEU:HD13	2.01	0.42
1:A:29:ARG:CG	1:A:29:ARG:HH21	2.27	0.42
1:A:554:ASP:OD1	1:A:716:LYS:NZ	2.52	0.42
1:A:4:LYS:HG3	1:A:15:TYR:CZ	2.55	0.42
1:A:382:LYS:NZ	5:A:1073:HOH:O	2.52	0.42
1:A:115:ARG:O	1:A:119:ILE:HG12	2.20	0.42
1:A:277:LYS:HZ1	1:A:293:ASP:CG	2.23	0.41
1:A:421:CYS:HB2	1:A:425:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:SER:HB3	1:A:668:HIS:CE1	2.56	0.41
1:A:429:ASP:OD1	1:A:431:LYS:NZ	2.54	0.41
1:A:400:ILE:HG13	1:A:401:GLU:N	2.36	0.41
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.83	0.41
1:A:231:LYS:HB3	1:A:231:LYS:HE3	1.92	0.41
1:A:201:LYS:HG3	1:A:308:ASP:OD1	2.21	0.40
1:A:430:ARG:CZ	1:A:433:ILE:HG12	2.52	0.40
1:A:374:LYS:NZ	1:A:501:ASP:OD1	2.55	0.40
1:A:556:GLN:NE2	1:A:608:ALA:HB2	2.35	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	752/754 (100%)	705 (94%)	41 (6%)	6 (1%)	24 17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	523	ASP
1	A	524	SER
1	A	109	GLY
1	A	525	SER
1	A	492	GLY
1	A	554	ASP

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	622/622 (100%)	572 (92%)	50 (8%)	15 11

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	4	LYS
1	A	20	LEU
1	A	72	GLN
1	A	187	VAL
1	A	198	LYS
1	A	201	LYS
1	A	208	THR
1	A	223	LYS
1	A	247	SER
1	A	262	GLU
1	A	317	GLU
1	A	319	LYS
1	A	325	PRO
1	A	327	THR
1	A	336	GLU
1	A	349	ASP
1	A	351	ARG
1	A	360	ASN
1	A	386	GLN
1	A	412	VAL
1	A	415	ILE
1	A	425	ILE
1	A	427	GLN
1	A	430	ARG
1	A	431	LYS
1	A	435	LYS
1	A	460	HIS
1	A	496	LYS
1	A	515	ASP
1	A	522	LYS
1	A	525	SER
1	A	528	ARG
1	A	533	PRO

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Mol	Chain	Res	Type
1	A	550	LYS
1	A	562	LYS
1	A	568	ASP
1	A	578	LYS
1	A	589	ASN
1	A	600	ARG
1	A	609	VAL
1	A	666	ARG
1	A	693	PRO
1	A	696	LYS
1	A	705	PHE
1	A	716	LYS
1	A	726	LEU
1	A	747	ARG
1	A	752	GLN
1	A	754	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	106	GLN
1	A	309	GLN
1	A	439	ASN
1	A	589	ASN
1	A	653	HIS
1	A	671	ASN
1	A	722	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	PCA	A	1	1	7,8,9	0.89	0	9,10,12	1.32	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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	PCA	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\|>2$
4	TRC	A	899	-	2,11,11	2.33	1 (50%)	4,14,14	2.79	1 (25%)
2	SO4	A	998	-	4,4,4	1.71	1 (25%)	6,6,6	0.41	0
3	F3S	A	999	1	0,9,9	0.00	-	0,15,15	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
4	TRC	A	899	-	-	0/4/12/12	0/0/0/0
2	SO4	A	998	-	-	0/0/0/0	0/0/0/0
3	F3S	A	999	1	-	0/0/24/24	0/0/3/3

All (2) 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
4	A	899	TRC	C2-C3	2.94	1.58	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	899	TRC	C5-C4-C3	5.30	122.12	113.87

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
3	A	999	F3S	1	0

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

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.