Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 02:23 PM EDT

PDB ID	:	6ACN
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	:	2.50 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 (i) 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 (i)) were used in the production of this report:

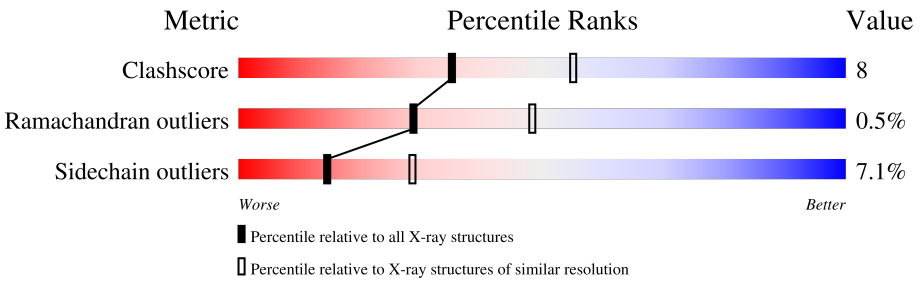
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	754	71% 23% 5% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6255 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.

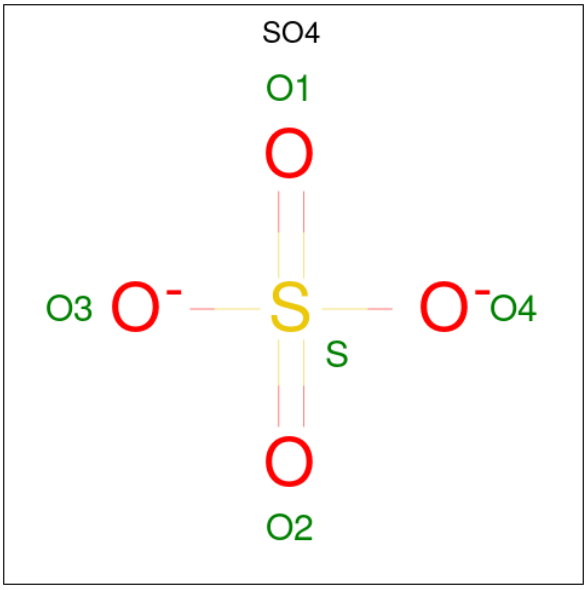
- Molecule 1 is a protein called ACONITASE.

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

There is a discrepancy between the modelled and reference sequences:

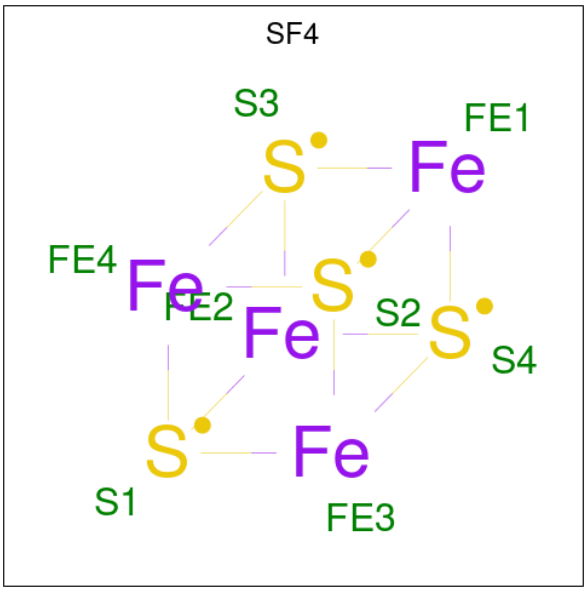
Chain	Residue	Modelled	Actual	Comment	Reference
A	647	SER	ARG	conflict	UNP P16276

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



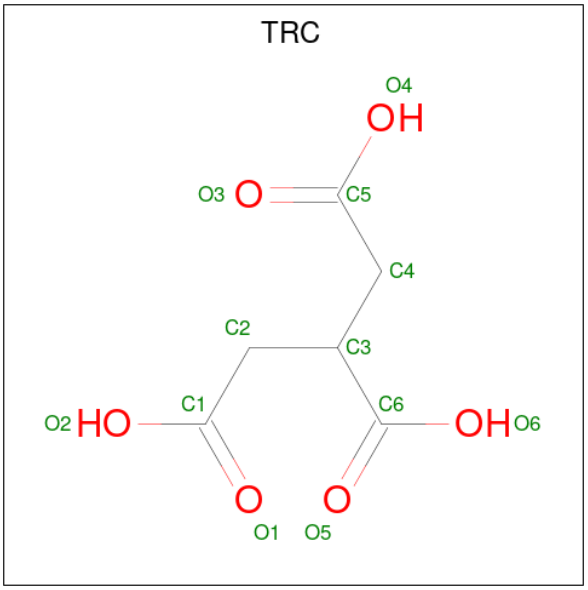
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 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
			Total	O		
5	A	407	407	407	0	0

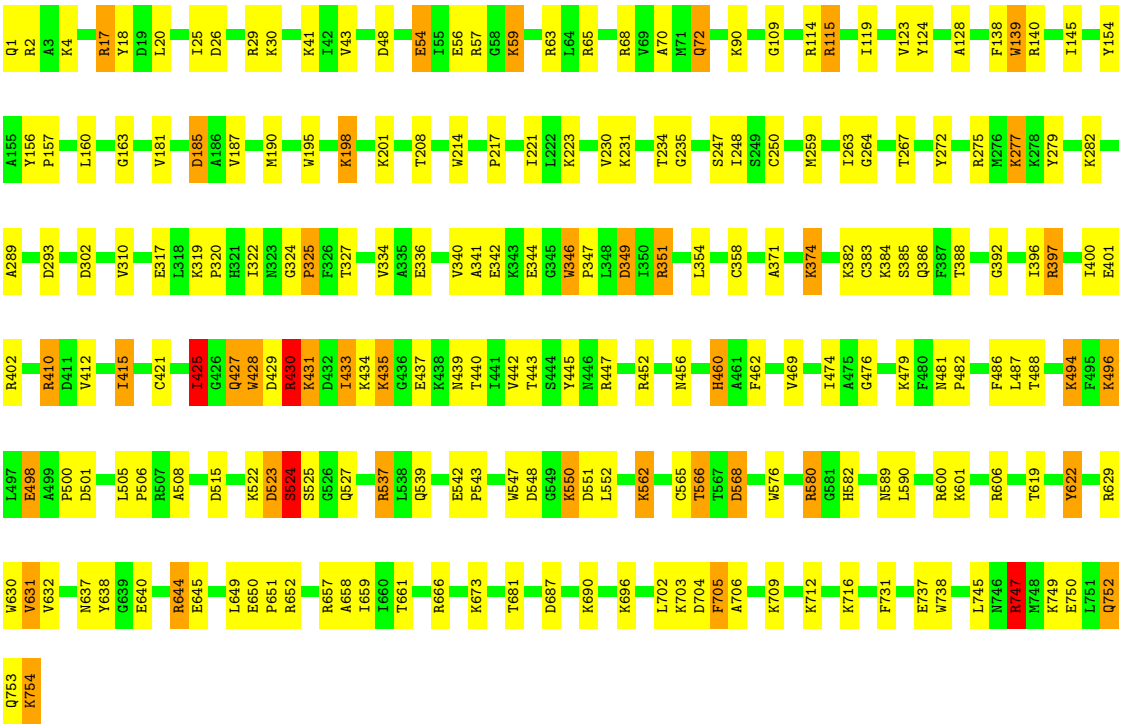
3 Residue-property plots (i)

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. 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. 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: 71% 23% 5% •



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore 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 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.187 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6255	wwPDB-VP
Average B, all atoms ($Å^2$)	17.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, SF4, PCA, TRC

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	0.96	1/5943 (0.0%)	1.72	113/8053 (1.4%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	488	THR	CA-CB	5.07	1.66	1.53

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	447	ARG	NE-CZ-NH2	16.52	128.56	120.30
1	A	447	ARG	NE-CZ-NH1	-15.06	112.77	120.30
1	A	410	ARG	NE-CZ-NH1	-14.09	113.25	120.30
1	A	410	ARG	NE-CZ-NH2	11.92	126.26	120.30
1	A	195	TRP	CD1-CG-CD2	10.88	115.01	106.30
1	A	402	ARG	NE-CZ-NH1	-10.32	115.14	120.30
1	A	666	ARG	NE-CZ-NH1	-9.60	115.50	120.30
1	A	115	ARG	NE-CZ-NH2	9.24	124.92	120.30
1	A	397	ARG	NE-CZ-NH1	-9.20	115.70	120.30
1	A	139	TRP	CD1-CG-CD2	9.17	113.64	106.30
1	A	17	ARG	NE-CZ-NH2	8.79	124.69	120.30
1	A	65	ARG	NE-CZ-NH1	-8.56	116.02	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	195	TRP	CE2-CD2-CG	-8.53	100.48	107.30
1	A	576	TRP	CD1-CG-CD2	8.43	113.04	106.30
1	A	195	TRP	CG-CD1-NE1	-8.40	101.70	110.10
1	A	629	ARG	NE-CZ-NH1	-8.39	116.11	120.30
1	A	346	TRP	CD1-CG-CD2	8.26	112.91	106.30
1	A	72	GLN	N-CA-CB	-8.07	96.07	110.60
1	A	738	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	A	551	ASP	CB-CG-OD1	8.04	125.53	118.30
1	A	402	ARG	NE-CZ-NH2	7.93	124.27	120.30
1	A	622	TYR	CB-CG-CD2	-7.91	116.25	121.00
1	A	547	TRP	CD1-CG-CD2	7.89	112.61	106.30
1	A	576	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	A	17	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	A	346	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	A	606	ARG	NE-CZ-NH1	-7.61	116.50	120.30
1	A	705	PHE	CB-CG-CD1	-7.50	115.55	120.80
1	A	139	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	A	606	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	A	498	GLU	CA-CB-CG	7.31	129.48	113.40
1	A	428	TRP	CD1-CG-CD2	7.27	112.11	106.30
1	A	190	MET	CG-SD-CE	7.24	111.78	100.20
1	A	195	TRP	CG-CD2-CE3	7.21	140.39	133.90
1	A	630	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	A	428	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	A	430	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	A	18	TYR	CB-CG-CD2	-7.02	116.79	121.00
1	A	214	TRP	CE2-CD2-CG	-6.98	101.72	107.30
1	A	72	GLN	CA-CB-CG	6.96	128.72	113.40
1	A	630	TRP	CD1-CG-CD2	6.95	111.86	106.30
1	A	275	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	A	195	TRP	CB-CG-CD1	-6.72	118.27	127.00
1	A	185	ASP	CB-CG-OD2	6.69	124.32	118.30
1	A	208	THR	N-CA-CB	-6.65	97.66	110.30
1	A	124	TYR	CB-CG-CD2	-6.63	117.02	121.00
1	A	214	TRP	CD1-CG-CD2	6.59	111.57	106.30
1	A	547	TRP	CE2-CD2-CG	-6.48	102.11	107.30
1	A	738	TRP	CE2-CD2-CG	-6.45	102.14	107.30
1	A	644	ARG	CA-CB-CG	6.43	127.55	113.40
1	A	666	ARG	NE-CZ-NH2	6.39	123.49	120.30
1	A	346	TRP	CG-CD2-CE3	6.37	139.63	133.90
1	A	57	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	A	374	LYS	CB-CG-CD	6.26	127.89	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	657	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	A	139	TRP	CG-CD1-NE1	-6.23	103.87	110.10
1	A	747	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	A	351	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	A	382	LYS	N-CA-CB	-6.10	99.62	110.60
1	A	63	ARG	N-CA-CB	-6.00	99.80	110.60
1	A	631	VAL	CG1-CB-CG2	-5.96	101.36	110.90
1	A	445	TYR	CB-CG-CD2	-5.96	117.43	121.00
1	A	43	VAL	CG1-CB-CG2	-5.95	101.38	110.90
1	A	630	TRP	CG-CD2-CE3	5.94	139.24	133.90
1	A	72	GLN	CB-CA-C	5.91	122.22	110.40
1	A	548	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	325	PRO	CA-C-N	5.68	129.70	117.20
1	A	632	VAL	CG1-CB-CG2	-5.66	101.84	110.90
1	A	114	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	A	140	ARG	N-CA-CB	-5.64	100.44	110.60
1	A	547	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	A	59	LYS	CA-C-N	5.60	129.51	117.20
1	A	302	ASP	CB-CG-OD2	5.58	123.33	118.30
1	A	428	TRP	CG-CD2-CE3	5.57	138.91	133.90
1	A	123	VAL	CA-CB-CG2	-5.56	102.56	110.90
1	A	630	TRP	CB-CG-CD1	-5.56	119.78	127.00
1	A	644	ARG	N-CA-CB	-5.55	100.60	110.60
1	A	156	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	A	580	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	A	293	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	566	THR	N-CA-CB	-5.53	99.80	110.30
1	A	346	TRP	CG-CD1-NE1	-5.52	104.58	110.10
1	A	310	VAL	CG1-CB-CG2	-5.51	102.09	110.90
1	A	195	TRP	CD1-NE1-CE2	5.49	113.94	109.00
1	A	738	TRP	CG-CD1-NE1	-5.48	104.62	110.10
1	A	447	ARG	N-CA-CB	-5.46	100.76	110.60
1	A	48	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	282	LYS	CB-CG-CD	5.46	125.79	111.60
1	A	425	ILE	CB-CA-C	-5.40	100.79	111.60
1	A	652	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	712	LYS	CA-CB-CG	5.37	125.21	113.40
1	A	250	CYS	N-CA-CB	-5.36	100.96	110.60
1	A	59	LYS	O-C-N	-5.33	114.17	122.70
1	A	500	PRO	CA-C-N	-5.32	105.50	117.20
1	A	494	LYS	CG-CD-CE	-5.29	96.04	111.90
1	A	63	ARG	CA-CB-CG	5.26	124.98	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	54	GLU	CA-CB-CG	5.24	124.93	113.40
1	A	68	ARG	CA-CB-CG	5.21	124.86	113.40
1	A	433	ILE	CA-C-N	-5.20	105.75	117.20
1	A	374	LYS	CD-CE-NZ	5.20	123.65	111.70
1	A	447	ARG	CA-CB-CG	5.20	124.83	113.40
1	A	524	SER	N-CA-C	5.19	125.01	111.00
1	A	382	LYS	CA-CB-CG	5.17	124.77	113.40
1	A	342	GLU	CA-C-N	5.16	128.55	117.20
1	A	346	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	A	524	SER	CA-C-N	-5.14	105.90	117.20
1	A	548	ASP	CA-CB-CG	5.13	124.68	113.40
1	A	601	LYS	CA-CB-CG	5.09	124.59	113.40
1	A	537	ARG	CG-CD-NE	-5.06	101.18	111.80
1	A	267	THR	CA-CB-CG2	5.03	119.44	112.40
1	A	565	CYS	CA-CB-SG	-5.00	104.99	114.00
1	A	160	LEU	N-CA-C	-5.00	97.49	111.00
1	A	139	TRP	CG-CD2-CE3	5.00	138.40	133.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	324	GLY	Peptide

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	95	0
2	A	5	0	0	0	0
3	A	8	0	0	1	0
4	A	12	0	5	1	0
5	A	407	0	0	10	0
All	All	6255	0	5816	96	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 8.

All (96) 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	1.57	0.85
1:A:371:ALA:HA	1:A:374:LYS:HD3	1.59	0.83
1:A:434:LYS:HB3	1:A:437:GLU:HG3	1.59	0.83
1:A:750:GLU:HA	1:A:754:LYS:HA	1.64	0.80
1:A:221:ILE:HG12	1:A:259:MET:HB3	1.66	0.77
1:A:277:LYS:HG2	1:A:289:ALA:HB1	1.69	0.73
3:A:999:SF4:FE4	5:A:806:HOH:O	1.44	0.70
1:A:198:LYS:HE2	5:A:823:HOH:O	1.91	0.69
1:A:640:GLU:HG2	5:A:970:HOH:O	1.95	0.66
1:A:384:LYS:HB2	1:A:474:ILE:O	1.98	0.64
1:A:752:GLN:HB2	1:A:753:GLN:HG2	1.80	0.64
1:A:354:LEU:HD13	1:A:443:THR:HG22	1.79	0.63
1:A:661:THR:O	1:A:681:THR:HA	2.00	0.61
1:A:145:ILE:HD12	1:A:392:GLY:HA2	1.84	0.58
1:A:54:GLU:HB2	5:A:1008:HOH:O	2.03	0.58
1:A:29:ARG:HH21	1:A:29:ARG:HG3	1.68	0.58
1:A:637:ASN:O	1:A:640:GLU:HB2	2.04	0.58
1:A:279:TYR:HD2	1:A:505:LEU:HD21	1.70	0.57
1:A:498:GLU:HB2	5:A:1118:HOH:O	2.03	0.56
1:A:428:TRP:CH2	1:A:430:ARG:HD3	2.42	0.55
1:A:745:LEU:O	1:A:749:LYS:HG3	2.07	0.55
1:A:631:VAL:HG22	1:A:658:ALA:HB3	1.88	0.55
1:A:496:LYS:NZ	1:A:496:LYS:HB2	2.22	0.54
1:A:139:TRP:HZ2	1:A:154:TYR:HH	1.53	0.54
1:A:341:ALA:HA	1:A:346:TRP:HB2	1.89	0.54
1:A:322:ILE:HG12	1:A:462:PHE:HB3	1.89	0.54
1:A:56:GLU:HB3	1:A:59:LYS:HB2	1.90	0.53
1:A:115:ARG:O	1:A:119:ILE:HG12	2.10	0.52
1:A:539:GLN:HB2	1:A:582:HIS:CD2	2.45	0.52
1:A:550:LYS:HA	1:A:703:LYS:NZ	2.24	0.52
1:A:487:LEU:O	1:A:494:LYS:HA	2.09	0.51
1:A:221:ILE:CG1	1:A:259:MET:HB3	2.39	0.51
1:A:524:SER:HB3	1:A:527:GLN:HB2	1.93	0.51
1:A:566:THR:HG22	1:A:568:ASP:H	1.75	0.51
1:A:70:ALA:O	1:A:163:GLY:HA2	2.13	0.49
1:A:322:ILE:CG1	1:A:462:PHE:HB3	2.42	0.49
1:A:706:ALA:HB3	1:A:709:LYS:HB2	1.95	0.49
1:A:347:PRO:HD2	1:A:460:HIS:CD2	2.48	0.48
1:A:430:ARG:HH12	1:A:439:ASN:HD21	1.61	0.48
1:A:371:ALA:CA	1:A:374:LYS:HD3	2.39	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:GLU:HB3	1:A:747:ARG:HD2	1.94	0.48
1:A:496:LYS:HB2	1:A:496:LYS:HZ2	1.78	0.48
1:A:479:LYS:HD2	1:A:479:LYS:HA	1.60	0.48
1:A:427:GLN:HE21	1:A:427:GLN:HA	1.79	0.47
1:A:320:PRO:HB2	1:A:334:VAL:CG2	2.45	0.47
1:A:230:VAL:HA	1:A:263:ILE:HA	1.97	0.46
1:A:388:THR:HG22	1:A:415:ILE:HG23	1.97	0.46
1:A:481:ASN:HA	1:A:482:PRO:HD3	1.83	0.46
1:A:25:ILE:O	1:A:29:ARG:HB2	2.15	0.45
1:A:349:ASP:OD2	1:A:384:LYS:NZ	2.49	0.45
1:A:645:GLU:HG3	1:A:649:LEU:HD12	1.98	0.45
1:A:562:LYS:NZ	5:A:941:HOH:O	2.48	0.45
1:A:590:LEU:HD11	1:A:651:PRO:HG3	1.97	0.45
1:A:749:LYS:HB3	1:A:749:LYS:HE3	1.85	0.44
1:A:217:PRO:HG3	1:A:248:ILE:HG23	1.98	0.44
1:A:673:LYS:HG2	1:A:731:PHE:CZ	2.52	0.44
1:A:41:LYS:NZ	5:A:1067:HOH:O	2.51	0.43
1:A:235:GLY:HA2	4:A:899:TRC:O3	2.17	0.43
1:A:351:ARG:NH1	1:A:433:ILE:HG22	2.33	0.43
1:A:562:LYS:O	1:A:562:LYS:HE2	2.18	0.43
1:A:619:THR:O	1:A:622:TYR:HB3	2.17	0.43
1:A:181:VAL:HB	1:A:185:ASP:HB2	2.00	0.43
1:A:54:GLU:H	1:A:54:GLU:CD	2.22	0.43
1:A:435:LYS:HE2	1:A:456:ASN:HB2	2.00	0.43
1:A:231:LYS:NZ	5:A:1159:HOH:O	2.48	0.43
1:A:650:GLU:HB2	1:A:651:PRO:HD3	2.00	0.43
1:A:340:VAL:O	1:A:344:GLU:HB2	2.19	0.43
1:A:354:LEU:O	1:A:443:THR:HA	2.19	0.43
1:A:638:TYR:CE2	1:A:659:ILE:HG21	2.54	0.43
1:A:687:ASP:HA	1:A:690:LYS:HD3	2.00	0.42
1:A:157:PRO:HG2	1:A:272:TYR:CD1	2.54	0.42
1:A:397:ARG:NH1	5:A:1130:HOH:O	2.51	0.42
1:A:486:PHE:HB3	1:A:494:LYS:HB3	2.01	0.42
1:A:552:LEU:HG	1:A:702:LEU:HD11	2.01	0.42
1:A:506:PRO:HB2	1:A:508:ALA:O	2.19	0.42
1:A:234:THR:HA	1:A:264:GLY:O	2.20	0.42
1:A:659:ILE:HG22	1:A:661:THR:HG23	2.02	0.42
1:A:26:ASP:OD1	1:A:30:LYS:NZ	2.53	0.42
1:A:145:ILE:HG21	1:A:358:CYS:HB3	2.01	0.42
1:A:320:PRO:HB2	1:A:334:VAL:HG22	2.02	0.41
1:A:550:LYS:HA	1:A:703:LYS:HZ2	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ARG:NH2	5:A:995:HOH:O	2.54	0.41
1:A:442:VAL:HG12	1:A:469:VAL:HG22	2.03	0.41
1:A:383:CYS:HB3	1:A:385:SER:O	2.20	0.41
1:A:440:THR:HA	1:A:460:HIS:O	2.21	0.41
1:A:542:GLU:HA	1:A:543:PRO:HD3	1.91	0.41
1:A:702:LEU:O	1:A:705:PHE:HB2	2.21	0.41
1:A:29:ARG:HH21	1:A:29:ARG:CG	2.33	0.41
1:A:396:ILE:O	1:A:400:ILE:HG12	2.20	0.41
1:A:429:ASP:OD1	1:A:431:LYS:NZ	2.54	0.41
1:A:29:ARG:HG3	1:A:29:ARG:NH2	2.36	0.40
1:A:128:ALA:HB2	1:A:138:PHE:CE2	2.57	0.40
1:A:401:GLU:CD	1:A:410:ARG:HH12	2.24	0.40
1:A:696:LYS:HA	1:A:696:LYS:HD3	1.89	0.40
1:A:421:CYS:HB2	1:A:425:ILE:HD11	2.04	0.40
1:A:1:PCA:HG3	1:A:17:ARG:HD2	2.03	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%)	709 (94%)	39 (5%)	4 (0%)	29 48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	523	ASP
1	A	524	SER
1	A	109	GLY
1	A	644	ARG

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%)	578 (93%)	44 (7%)	14 28

All (44) 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	90	LYS
1	A	187	VAL
1	A	198	LYS
1	A	201	LYS
1	A	223	LYS
1	A	247	SER
1	A	277	LYS
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	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	501	ASP
1	A	515	ASP
1	A	522	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	523	ASP
1	A	525	SER
1	A	537	ARG
1	A	550	LYS
1	A	562	LYS
1	A	568	ASP
1	A	580	ARG
1	A	589	ASN
1	A	600	ARG
1	A	704	ASP
1	A	716	LYS
1	A	747	ARG
1	A	752	GLN
1	A	754	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	653	HIS
1	A	671	ASN
1	A	752	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	0.96	0	9,10,12	0.80	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 monosaccharides 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	$\#\|Z\| > 2$
2	SO4	A	998	-	4,4,4	0.78	0	6,6,6	0.53	0
3	SF4	A	999	1	0,12,12	-	-	-		
4	TRC	A	899	-	11,11,11	1.92	2 (18%)	14,14,14	1.10	1 (7%)

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	-	-	2/12/12/12	-
3	SF4	A	999	1	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	899	TRC	C3-C6	3.91	1.58	1.51
4	A	899	TRC	C2-C3	2.48	1.58	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	899	TRC	O4-C5-C4	2.39	121.74	114.07

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	899	TRC	C3-C4-C5-O3
4	A	899	TRC	C3-C4-C5-O4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	SF4	1	0
4	A	899	TRC	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.