Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 02:31 PM EDT

PDB ID	:	3AWG
Title	:	Crystal structure of Pten-like domain of Ci-VSP G356A mutant (248-576)
Authors	:	Matsuda, M.; Sakata, S.; Takeshita, K.; Suzuki, M.; Yamashita, E.; Okamura, Y.; Nakagawa, A.
Deposited on	:	2011-03-19
Resolution	:	2.39 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:

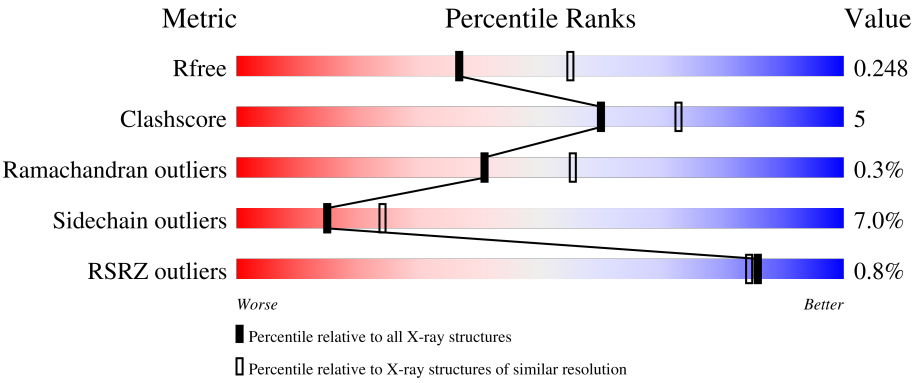
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.39 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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% 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	334	% 76% 12% • 8%
1	B	334	% 79% 11% • 8%
1	C	334	75% 16% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7707 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.

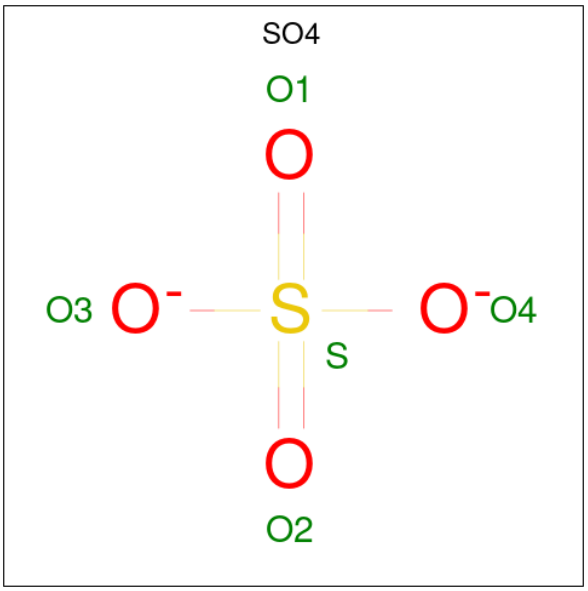
- Molecule 1 is a protein called Voltage-sensor containing phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2465	1570	420	461	14			
1	B	306	Total	C	N	O	S	0	0	0
			2465	1570	420	461	14			
1	C	308	Total	C	N	O	S	0	0	0
			2477	1576	422	465	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	GLY	-	expression tag	UNP Q4W8A1
A	244	PRO	-	expression tag	UNP Q4W8A1
A	245	LEU	-	expression tag	UNP Q4W8A1
A	246	GLY	-	expression tag	UNP Q4W8A1
A	247	SER	-	expression tag	UNP Q4W8A1
A	365	ALA	GLY	engineered mutation	UNP Q4W8A1
B	243	GLY	-	expression tag	UNP Q4W8A1
B	244	PRO	-	expression tag	UNP Q4W8A1
B	245	LEU	-	expression tag	UNP Q4W8A1
B	246	GLY	-	expression tag	UNP Q4W8A1
B	247	SER	-	expression tag	UNP Q4W8A1
B	365	ALA	GLY	engineered mutation	UNP Q4W8A1
C	243	GLY	-	expression tag	UNP Q4W8A1
C	244	PRO	-	expression tag	UNP Q4W8A1
C	245	LEU	-	expression tag	UNP Q4W8A1
C	246	GLY	-	expression tag	UNP Q4W8A1
C	247	SER	-	expression tag	UNP Q4W8A1
C	365	ALA	GLY	engineered mutation	UNP Q4W8A1

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	98	Total O 98 98	0	0
3	B	74	Total O 74 74	0	0

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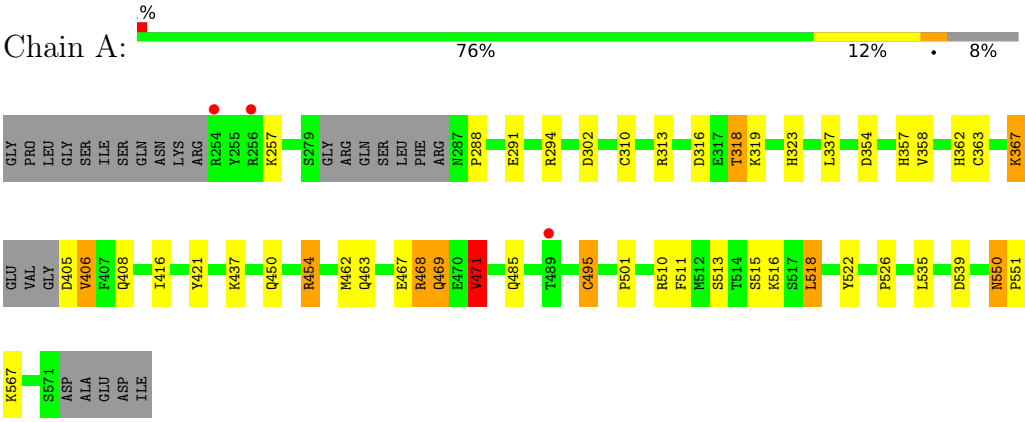
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	78	Total O 78 78	0	0

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.

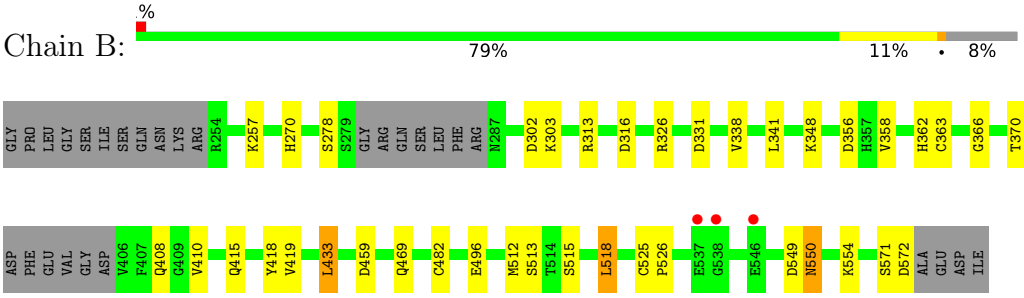
• Molecule 1: Voltage-sensor containing phosphatase

Chain A:



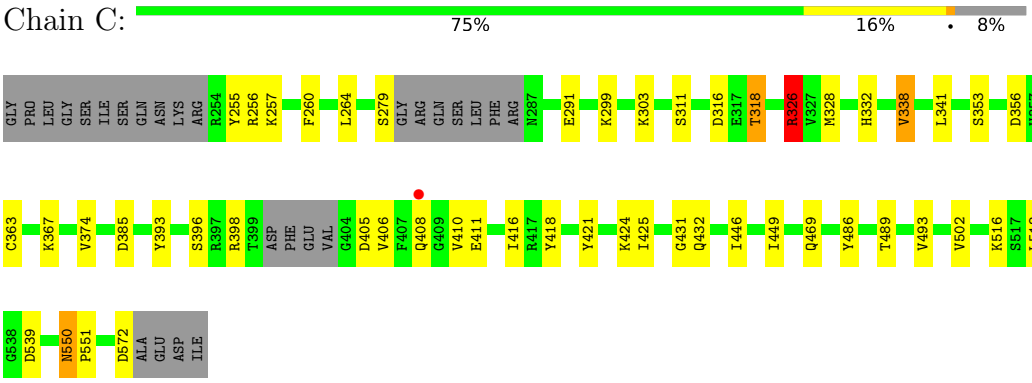
• Molecule 1: Voltage-sensor containing phosphatase

Chain B:



• Molecule 1: Voltage-sensor containing phosphatase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	131.15Å 176.49Å 50.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.39 48.91 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.91-2.39) 99.5 (48.91-2.39)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.63 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0071	Depositor
R, R_{free}	0.194 , 0.255 0.185 , 0.248	Depositor DCC
R_{free} test set	2426 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7707	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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, 0.333 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: 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	1.11	4/2521 (0.2%)	0.93	3/3401 (0.1%)
1	B	1.08	4/2521 (0.2%)	0.93	3/3401 (0.1%)
1	C	1.10	4/2533 (0.2%)	0.93	2/3417 (0.1%)
All	All	1.10	12/7575 (0.2%)	0.93	8/10219 (0.1%)

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
1	B	0	1
1	C	0	1
All	All	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	363	CYS	CB-SG	6.94	1.94	1.82
1	B	363	CYS	CB-SG	6.87	1.94	1.82
1	A	363	CYS	CB-SG	6.76	1.93	1.82
1	B	418	TYR	CD1-CE1	-6.73	1.29	1.39
1	B	418	TYR	CD2-CE2	-6.72	1.29	1.39
1	A	310	CYS	CB-SG	-6.62	1.71	1.82
1	C	418	TYR	CD2-CE2	-6.42	1.29	1.39
1	A	522	TYR	CE1-CZ	5.83	1.46	1.38
1	A	495	CYS	CB-SG	-5.81	1.72	1.81
1	B	338	VAL	CB-CG1	-5.69	1.40	1.52
1	C	421	TYR	CD2-CE2	-5.16	1.31	1.39
1	C	291	GLU	CG-CD	5.10	1.59	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	433	LEU	CA-CB-CG	5.73	128.47	115.30
1	A	539	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	326	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	454	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	316	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	331	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	471	VAL	CG1-CB-CG2	5.15	119.14	110.90
1	C	398	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	362	HIS	Peptide
1	B	362	HIS	Peptide
1	C	362	HIS	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	2465	0	2419	25	0
1	B	2465	0	2419	17	0
1	C	2477	0	2426	25	0
2	A	15	0	0	0	0
2	B	10	0	0	0	0
2	C	25	0	0	0	0
3	A	98	0	0	4	0
3	B	74	0	0	3	0
3	C	78	0	0	1	0
All	All	7707	0	7264	67	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 (67) 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:C:326:ARG:HH11	1:C:326:ARG:HG2	1.15	1.04
1:C:326:ARG:HH11	1:C:326:ARG:CG	1.89	0.84
1:C:326:ARG:HG2	1:C:326:ARG:NH1	1.80	0.80
1:B:370:THR:O	1:B:374:VAL:HG13	1.86	0.75
1:B:270:HIS:HA	1:B:358:VAL:HG22	1.71	0.71
1:C:316:ASP:OD1	1:C:318:THR:HB	1.90	0.70
1:B:571:SER:O	1:B:572:ASP:HB2	1.92	0.69
1:C:303:LYS:HD3	1:C:356:ASP:HB3	1.75	0.68
1:C:338:VAL:HG13	3:C:96:HOH:O	1.94	0.68
1:A:367:LYS:HD3	3:A:59:HOH:O	1.94	0.67
1:A:316:ASP:OD1	1:A:318:THR:HB	2.01	0.61
1:C:446:ILE:HB	1:C:493:VAL:HG22	1.85	0.59
1:C:449:ILE:HG21	1:C:493:VAL:HG13	1.85	0.58
1:C:446:ILE:HB	1:C:493:VAL:CG2	2.34	0.57
1:C:393:TYR:O	1:C:396:SER:HB2	2.04	0.57
1:A:421:TYR:CD2	1:A:535:LEU:HD13	2.39	0.57
1:A:406:VAL:HG13	1:A:416:ILE:HD13	1.87	0.56
1:B:326:ARG:HD3	3:B:112:HOH:O	2.05	0.55
1:C:361:ILE:HD12	1:C:374:VAL:HG22	1.88	0.55
1:C:326:ARG:CG	1:C:326:ARG:NH1	2.55	0.54
1:C:449:ILE:CG2	1:C:486:TYR:HE1	2.22	0.53
1:C:303:LYS:HD3	1:C:356:ASP:CB	2.38	0.53
1:A:405:ASP:HB3	1:A:408:GLN:HG2	1.91	0.53
1:B:512:MET:HE2	3:B:581:HOH:O	2.09	0.52
1:B:513:SER:OG	1:B:515:SER:HB3	2.09	0.52
1:B:370:THR:O	1:B:374:VAL:CG1	2.57	0.51
1:C:405:ASP:HB3	1:C:408:GLN:NE2	2.25	0.51
1:A:406:VAL:HG13	1:A:416:ILE:CD1	2.41	0.50
1:A:405:ASP:O	1:A:408:GLN:HG2	2.11	0.50
1:A:354:ASP:HB3	1:A:357:HIS:CG	2.47	0.49
1:C:332:HIS:HD2	1:C:411:GLU:OE2	1.95	0.49
1:B:512:MET:CE	3:B:581:HOH:O	2.61	0.48
1:B:518:LEU:HD13	1:B:526:PRO:HB3	1.95	0.48
1:A:471:VAL:HG13	1:A:501:PRO:HG2	1.96	0.48
1:A:291:GLU:OE2	1:A:294:ARG:NH2	2.45	0.46
1:A:467:GLU:C	1:A:468:ARG:HG3	2.35	0.46
1:C:449:ILE:CG2	1:C:486:TYR:CE1	2.98	0.46
1:A:550:ASN:HB2	1:A:551:PRO:HD3	1.98	0.46
1:C:410:VAL:HG21	1:C:416:ILE:HG13	1.98	0.45
1:A:323:HIS:HB3	3:A:220:HOH:O	2.15	0.45
1:B:303:LYS:HD3	1:B:356:ASP:HB2	1.99	0.45
1:A:511:PHE:O	1:A:526:PRO:HD2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:ARG:HA	1:C:260:PHE:O	2.17	0.44
1:A:469:GLN:HE21	1:A:469:GLN:HA	1.83	0.44
1:C:550:ASN:HB2	1:C:551:PRO:HD3	2.00	0.44
1:A:463:GLN:OE1	1:A:510:ARG:HD3	2.17	0.43
1:A:518:LEU:HD23	1:A:518:LEU:HA	1.79	0.43
1:C:535:LEU:HD23	1:C:535:LEU:HA	1.82	0.43
1:C:410:VAL:CG2	1:C:416:ILE:HG13	2.49	0.43
1:B:549:ASP:O	1:B:550:ASN:HB2	2.20	0.42
1:A:518:LEU:HD13	1:A:526:PRO:HB3	2.00	0.42
1:B:482:CYS:HA	1:B:496:GLU:O	2.20	0.42
1:A:535:LEU:HA	1:A:535:LEU:HD23	1.86	0.42
1:B:571:SER:O	1:B:572:ASP:CB	2.65	0.42
1:C:255:TYR:OH	1:C:299:LYS:HE3	2.20	0.41
1:B:366:GLY:HA3	1:B:398:ARG:HH21	1.86	0.41
1:B:415:GLN:O	1:B:419:VAL:HG23	2.20	0.41
1:A:288:PRO:HG2	1:A:291:GLU:HB2	2.02	0.41
1:A:513:SER:HB3	3:A:583:HOH:O	2.20	0.41
1:A:567:LYS:HE2	3:A:225:HOH:O	2.19	0.41
1:B:525:CYS:HB2	1:B:526:PRO:HD2	2.02	0.41
1:A:561:ARG:HH11	1:A:561:ARG:HD2	1.77	0.41
1:A:462:MET:HG3	1:A:511:PHE:CE2	2.57	0.40
1:A:563:ASN:OD1	1:A:563:ASN:N	2.53	0.40
1:C:425:ILE:HG22	1:C:431:GLY:HA2	2.03	0.40
1:B:459:ASP:O	1:B:513:SER:HA	2.22	0.40
1:C:264:LEU:HD23	1:C:264:LEU:C	2.42	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	300/334 (90%)	288 (96%)	11 (4%)	1 (0%)	41 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	300/334 (90%)	287 (96%)	12 (4%)	1 (0%)	41 55
1	C	302/334 (90%)	294 (97%)	7 (2%)	1 (0%)	41 55
All	All	902/1002 (90%)	869 (96%)	30 (3%)	3 (0%)	41 55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	550	ASN
1	B	550	ASN
1	C	550	ASN

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	273/296 (92%)	252 (92%)	21 (8%)	13 20
1	B	273/296 (92%)	260 (95%)	13 (5%)	25 41
1	C	274/296 (93%)	251 (92%)	23 (8%)	11 16
All	All	820/888 (92%)	763 (93%)	57 (7%)	15 24

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	LYS
1	A	302	ASP
1	A	313	ARG
1	A	318	THR
1	A	319	LYS
1	A	337	LEU
1	A	358	VAL
1	A	367	LYS
1	A	398	ARG
1	A	406	VAL
1	A	437	LYS

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Mol	Chain	Res	Type
1	A	450	GLN
1	A	454	ARG
1	A	468	ARG
1	A	469	GLN
1	A	471	VAL
1	A	485	GLN
1	A	495	CYS
1	A	515	SER
1	A	516	LYS
1	A	518	LEU
1	B	257	LYS
1	B	278	SER
1	B	302	ASP
1	B	313	ARG
1	B	341	LEU
1	B	348	LYS
1	B	374	VAL
1	B	408	GLN
1	B	410	VAL
1	B	433	LEU
1	B	469	GLN
1	B	518	LEU
1	B	554	LYS
1	C	257	LYS
1	C	279	SER
1	C	311	SER
1	C	318	THR
1	C	326	ARG
1	C	328	MET
1	C	338	VAL
1	C	341	LEU
1	C	353	SER
1	C	358	VAL
1	C	367	LYS
1	C	385	ASP
1	C	406	VAL
1	C	424	LYS
1	C	432	GLN
1	C	469	GLN
1	C	489	THR
1	C	502	VAL
1	C	516	LYS

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Mol	Chain	Res	Type
1	C	518	LEU
1	C	537	GLU
1	C	539	ASP
1	C	572	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	HIS
1	A	469	GLN
1	C	332	HIS
1	C	408	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

10 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	B	1	-	4,4,4	0.31	0	6,6,6	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	C	10	-	4,4,4	0.33	0	6,6,6	0.51	0
2	SO4	C	7	-	4,4,4	0.30	0	6,6,6	0.30	0
2	SO4	C	4	-	4,4,4	0.20	0	6,6,6	0.44	0
2	SO4	A	6	-	4,4,4	0.22	0	6,6,6	0.87	0
2	SO4	B	2	-	4,4,4	0.24	0	6,6,6	0.56	0
2	SO4	A	8	-	4,4,4	0.19	0	6,6,6	0.62	0
2	SO4	A	3	-	4,4,4	0.11	0	6,6,6	0.37	0
2	SO4	C	5	-	4,4,4	0.28	0	6,6,6	0.44	0
2	SO4	C	9	-	4,4,4	0.20	0	6,6,6	0.72	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

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	306/334 (91%)	-0.15	3 (0%)	82	80	14, 27, 46, 71	0
1	B	306/334 (91%)	-0.07	3 (0%)	82	80	20, 31, 49, 56	0
1	C	308/334 (92%)	-0.12	1 (0%)	94	93	18, 32, 48, 57	0
All	All	920/1002 (91%)	-0.11	7 (0%)	86	84	14, 30, 48, 71	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	ARG	3.0
1	B	546	GLU	2.9
1	C	408	GLN	2.5
1	A	254	ARG	2.2
1	A	489	THR	2.2
1	B	537	GLU	2.2
1	B	538	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 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	B-factors(Å^2)	Q<0.9
2	SO4	C	9	5/5	0.86	0.14	82,84,85,86	0
2	SO4	A	8	5/5	0.89	0.18	84,84,85,85	0
2	SO4	C	5	5/5	0.95	0.13	50,51,53,54	0
2	SO4	C	4	5/5	0.96	0.12	51,53,54,57	0
2	SO4	A	6	5/5	0.98	0.15	37,38,45,46	0
2	SO4	C	10	5/5	0.98	0.19	53,53,54,55	0
2	SO4	B	1	5/5	0.99	0.12	35,35,37,38	0
2	SO4	C	7	5/5	0.99	0.12	33,33,35,35	0
2	SO4	B	2	5/5	0.99	0.15	32,33,37,39	0
2	SO4	A	3	5/5	0.99	0.10	36,37,39,40	0

6.5 Other polymers (i)

There are no such residues in this entry.