Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2023 – 10:13 PM EDT

PDB ID	:	3AWE
Title	:	Crystal structure of Pten-like domain of Ci-VSP (248-576)
Authors	:	Matsuda, M.; Sakata, S.; Takeshita, K.; Suzuki, M.; Yamashita, E.; Okamura, Y.; Nakagawa, A.
Deposited on	:	2011-03-19
Resolution	:	2.77 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:

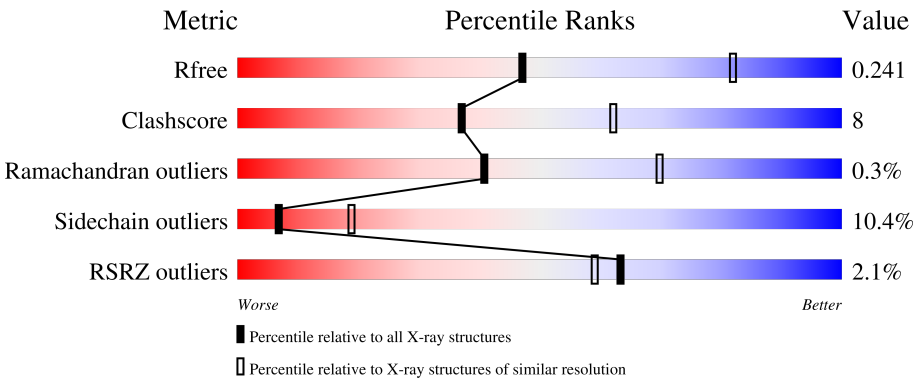
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	2% 74% 14% • 9%
1	B	334	2% 73% 15% • 8%
1	C	334	2% 67% 19% 5% 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7587 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.

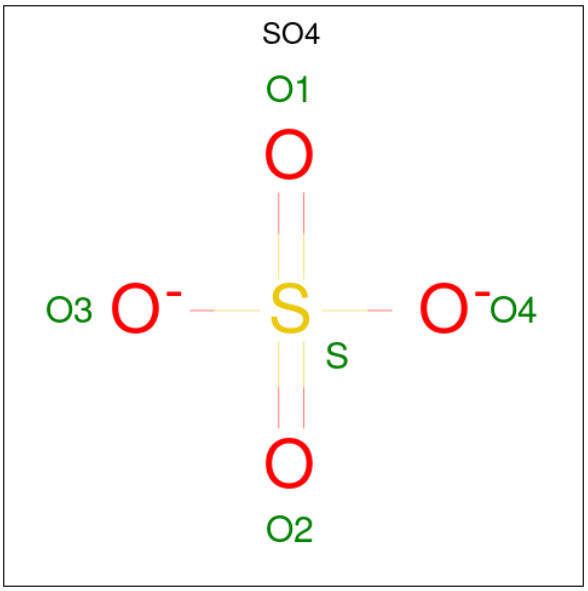
- Molecule 1 is a protein called Voltage-sensor containing phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	305	2442	1554	413	461	14	0	0	0
1	B	307	2472	1573	421	464	14	0	0	0
1	C	308	2483	1579	425	465	14	0	0	0

There are 15 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
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
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

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

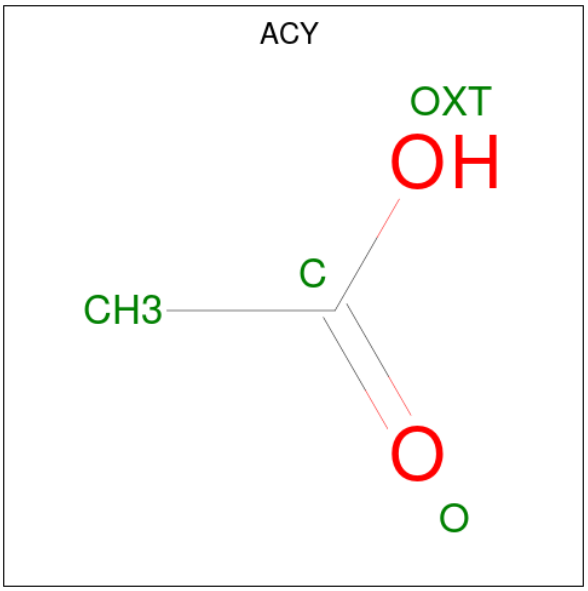


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	C	1	4	2	2	0	0

- Molecule 5 is water.

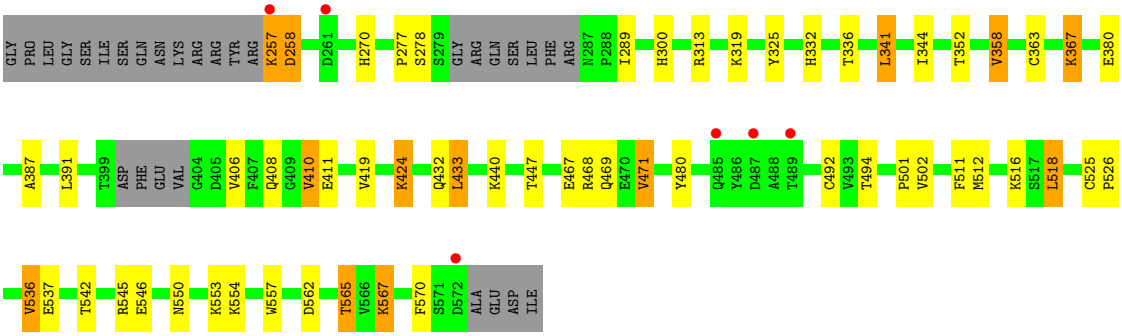
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	63	63	63	0	0
			Total	O		
5	B	48	48	48	0	0
			Total	O		
5	C	39	39	39	0	0

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.

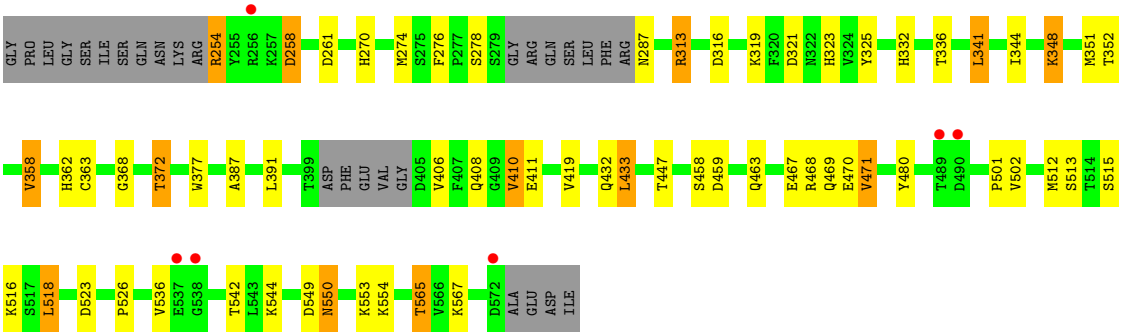
• Molecule 1: Voltage-sensor containing phosphatase

Chain A:



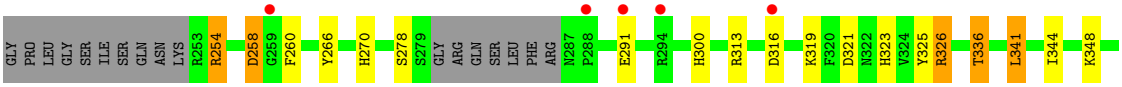
• Molecule 1: Voltage-sensor containing phosphatase

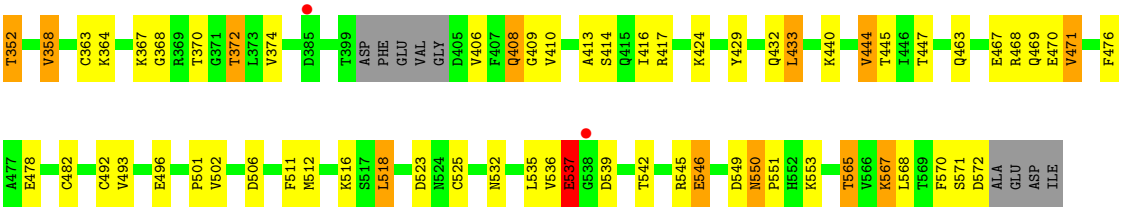
Chain B:



• Molecule 1: Voltage-sensor containing phosphatase

Chain C:




T352
V358
C363
K364
K367
G368
R369
T370
G371
T372
L373
V374
D385
T399
ASP
PHE
GLU
VAL
GLY
D405
V406
F407
Q408
G409
V410
A413
S414
Q415
I416
R417
K424
Y429
Q432
L433
K440
V444
T445
I446
T447
Q463
E467
R468
Q469
E470
V471
F476
A477
E478
C482
C492
V493
E496
P501
V502
D506
F511
M512
K516
S517
L518
D523
N524
C525
N532
L535
V536
E537
G538
D539
T542
R545
E546
D549
N550
P551
H552
K553
T565
V566
K567
L568
T569
F570
S571
D572
ALA
GLU
ASP
ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	131.21Å 176.53Å 50.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.13 – 2.77 44.13 – 2.77	Depositor EDS
% Data completeness (in resolution range)	97.6 (44.13-2.77) 97.7 (44.13-2.77)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.52 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.5.0071	Depositor
R, R_{free}	0.208 , 0.253 0.199 , 0.241	Depositor DCC
R_{free} test set	1533 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7587	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SO4, ACY

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	0.95	7/2497 (0.3%)	0.84	2/3369 (0.1%)
1	B	0.95	2/2528 (0.1%)	0.80	1/3410 (0.0%)
1	C	0.98	4/2539 (0.2%)	0.88	5/3424 (0.1%)
All	All	0.96	13/7564 (0.2%)	0.84	8/10203 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	TYR	CD1-CE1	-7.08	1.28	1.39
1	C	537	GLU	CB-CG	-6.49	1.39	1.52
1	B	536	VAL	CB-CG2	-6.35	1.39	1.52
1	A	492	CYS	CB-SG	-5.90	1.72	1.81
1	A	325	TYR	CD2-CE2	-5.79	1.30	1.39
1	A	325	TYR	CE2-CZ	-5.77	1.31	1.38
1	A	410	VAL	CB-CG1	-5.40	1.41	1.52
1	B	325	TYR	CE2-CZ	-5.38	1.31	1.38
1	C	363	CYS	CB-SG	5.18	1.91	1.82
1	C	325	TYR	CE2-CZ	-5.15	1.31	1.38
1	A	536	VAL	CB-CG2	-5.14	1.42	1.52
1	C	266	TYR	CE2-CZ	-5.14	1.31	1.38
1	A	325	TYR	CG-CD1	-5.04	1.32	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	363	CYS	CA-CB-SG	7.55	127.60	114.00
1	C	363	CYS	CA-CB-SG	7.10	126.78	114.00
1	C	545	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	C	409	GLY	O-C-N	-5.30	114.22	122.70
1	B	363	CYS	CA-CB-SG	5.19	123.34	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	545	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	C	417	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	539	ASP	CB-CG-OD1	5.03	122.83	118.30

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	2442	0	2391	31	1
1	B	2472	0	2423	33	0
1	C	2483	0	2436	51	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	15	0	0	0	0
3	A	1	0	0	0	0
4	C	4	0	3	1	0
5	A	63	0	0	1	0
5	B	48	0	0	1	0
5	C	39	0	0	2	1
All	All	7587	0	7253	115	1

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 (115) 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:CG	1.82	0.92
1:B:332:HIS:HD2	1:B:411:GLU:OE2	1.67	0.77
1:C:326:ARG:HH11	1:C:326:ARG:HG3	1.49	0.77
1:B:447:THR:OG1	1:B:565:THR:HB	1.86	0.74
1:B:471:VAL:HG13	1:B:501:PRO:CG	2.18	0.74
1:B:332:HIS:CD2	1:B:411:GLU:OE2	2.41	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:VAL:HG13	1:A:501:PRO:CG	2.19	0.71
1:A:447:THR:OG1	1:A:565:THR:HB	1.89	0.71
1:B:368:GLY:O	1:B:372:THR:HG22	1.90	0.71
1:C:471:VAL:HG13	1:C:501:PRO:CG	2.20	0.70
1:A:332:HIS:HD2	1:A:411:GLU:OE2	1.75	0.70
1:C:368:GLY:O	1:C:372:THR:HG22	1.93	0.69
1:A:471:VAL:HG13	1:A:501:PRO:HG2	1.74	0.67
1:C:326:ARG:CG	1:C:326:ARG:NH1	2.50	0.67
1:A:542:THR:OG1	1:A:567:LYS:HG3	1.94	0.66
1:B:341:LEU:CD2	1:B:433:LEU:HD13	2.26	0.66
1:C:326:ARG:HH11	1:C:326:ARG:HG2	1.61	0.65
1:B:471:VAL:HG13	1:B:501:PRO:HG2	1.79	0.65
1:A:332:HIS:CD2	1:A:411:GLU:OE2	2.50	0.65
1:A:467:GLU:O	1:A:468:ARG:HB2	1.97	0.64
1:C:447:THR:OG1	1:C:565:THR:HB	1.98	0.64
1:B:313:ARG:NH2	5:B:33:HOH:O	2.29	0.64
1:B:471:VAL:HG13	1:B:501:PRO:HG3	1.80	0.63
1:B:254:ARG:CG	1:B:254:ARG:HH11	2.11	0.63
1:A:341:LEU:CD2	1:A:433:LEU:HD13	2.28	0.62
1:C:471:VAL:HG13	1:C:501:PRO:HG2	1.81	0.62
1:C:326:ARG:NH1	1:C:326:ARG:HG2	2.14	0.61
1:C:542:THR:OG1	1:C:567:LYS:HG3	2.00	0.60
1:B:341:LEU:HD22	1:B:433:LEU:HD13	1.83	0.60
1:C:471:VAL:HG13	1:C:501:PRO:HG3	1.82	0.60
1:C:341:LEU:CD2	1:C:433:LEU:HD13	2.32	0.60
1:C:341:LEU:HD22	1:C:433:LEU:HD13	1.84	0.59
1:C:254:ARG:CG	1:C:254:ARG:HH11	2.15	0.59
1:A:424:LYS:NZ	1:A:537:GLU:OE1	2.35	0.59
1:C:447:THR:HG22	1:C:492:CYS:SG	2.44	0.58
1:B:467:GLU:O	1:B:468:ARG:HB2	2.04	0.58
1:A:471:VAL:HG13	1:A:501:PRO:HG3	1.86	0.57
1:C:367:LYS:HE3	1:C:408:GLN:O	2.04	0.56
1:B:270:HIS:HA	1:B:358:VAL:HG22	1.88	0.56
1:C:367:LYS:HE2	1:C:410:VAL:O	2.06	0.56
1:B:391:LEU:HD22	1:B:410:VAL:HG13	1.88	0.55
1:C:270:HIS:HA	1:C:358:VAL:HG22	1.88	0.55
1:C:532:ASN:HB3	1:C:535:LEU:HD12	1.89	0.54
1:C:546:GLU:OE1	4:C:1:ACY:OXT	2.26	0.54
1:B:459:ASP:OD1	1:B:513:SER:OG	2.24	0.54
1:A:277:PRO:HB2	1:A:289:ILE:HG13	1.90	0.54
1:A:471:VAL:CG1	1:A:501:PRO:HG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:THR:OG1	1:B:567:LYS:HG3	2.09	0.53
1:B:549:ASP:O	1:B:550:ASN:HB2	2.09	0.52
1:A:270:HIS:HA	1:A:358:VAL:HG22	1.92	0.51
1:C:463:GLN:HG3	1:C:470:GLU:HG3	1.92	0.51
1:C:321:ASP:O	1:C:323:HIS:CD2	2.64	0.51
1:A:391:LEU:HD22	1:A:410:VAL:HG13	1.93	0.51
1:C:410:VAL:HG21	1:C:416:ILE:HG13	1.91	0.51
1:A:387:ALA:HB1	1:A:419:VAL:HG12	1.92	0.50
1:C:316:ASP:HB3	1:C:319:LYS:HD2	1.94	0.50
1:B:387:ALA:HB1	1:B:419:VAL:HG12	1.94	0.48
1:A:341:LEU:HD22	1:A:433:LEU:HD13	1.95	0.48
1:B:258:ASP:OD2	1:B:258:ASP:N	2.48	0.47
1:A:300:HIS:CE1	1:A:358:VAL:HG21	2.49	0.47
1:B:463:GLN:HG3	1:B:470:GLU:HG3	1.97	0.47
1:C:429:TYR:O	1:C:432:GLN:HB2	2.15	0.47
1:B:254:ARG:NH1	1:B:261:ASP:OD2	2.47	0.47
1:C:258:ASP:OD2	1:C:258:ASP:N	2.48	0.47
1:C:445:THR:HA	1:C:493:VAL:O	2.15	0.47
1:B:321:ASP:HB2	1:B:323:HIS:HD2	1.80	0.46
1:C:536:VAL:HG12	1:C:537:GLU:N	2.30	0.46
1:A:562:ASP:OD1	5:A:129:HOH:O	2.20	0.46
1:B:254:ARG:CG	1:B:254:ARG:NH1	2.76	0.46
1:C:336:THR:HG22	1:C:506:ASP:OD2	2.16	0.46
1:C:549:ASP:O	1:C:550:ASN:HB2	2.16	0.46
1:C:414:SER:HB2	5:C:14:HOH:O	2.15	0.46
1:C:413:ALA:HB1	5:C:99:HOH:O	2.16	0.45
1:C:300:HIS:CE1	1:C:358:VAL:HG21	2.51	0.45
1:C:348:LYS:O	1:C:352:THR:OG1	2.33	0.45
1:C:471:VAL:CG1	1:C:501:PRO:HG2	2.46	0.45
1:A:257:LYS:HB3	1:A:258:ASP:OD2	2.17	0.45
1:C:467:GLU:O	1:C:468:ARG:HB2	2.16	0.45
1:C:370:THR:O	1:C:374:VAL:HG23	2.15	0.45
1:B:391:LEU:CD2	1:B:410:VAL:HG13	2.47	0.45
1:C:254:ARG:HH11	1:C:254:ARG:HG2	1.79	0.45
1:B:518:LEU:HD13	1:B:526:PRO:CG	2.47	0.45
1:C:476:PHE:N	1:C:476:PHE:CD2	2.85	0.44
1:A:440:LYS:O	1:A:570:PHE:HA	2.17	0.44
1:C:254:ARG:CG	1:C:254:ARG:NH1	2.75	0.44
1:C:571:SER:O	1:C:572:ASP:CB	2.64	0.44
1:C:260:PHE:HA	1:C:291:GLU:OE2	2.18	0.43
1:C:518:LEU:HD23	1:C:518:LEU:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:CYS:HA	1:C:496:GLU:O	2.19	0.43
1:C:511:PHE:O	1:C:525:CYS:HB2	2.18	0.43
1:B:471:VAL:CG1	1:B:501:PRO:HG2	2.46	0.43
1:C:536:VAL:CG1	1:C:537:GLU:N	2.81	0.43
1:A:344:ILE:HG23	1:A:380:GLU:HG2	2.01	0.43
1:A:258:ASP:OD2	1:A:258:ASP:N	2.52	0.43
1:A:367:LYS:CE	1:A:411:GLU:HG3	2.49	0.43
1:B:274:MET:HG3	1:B:362:HIS:HB3	2.01	0.43
1:A:518:LEU:HD23	1:A:518:LEU:HA	1.86	0.42
1:A:391:LEU:CD2	1:A:410:VAL:HG13	2.49	0.42
1:C:444:VAL:HG13	1:C:568:LEU:HD23	2.02	0.42
1:A:536:VAL:HG12	1:A:537:GLU:N	2.34	0.42
1:C:410:VAL:CG2	1:C:416:ILE:HG13	2.50	0.42
1:B:351:MET:HG3	1:B:377:TRP:CZ2	2.56	0.41
1:B:513:SER:OG	1:B:515:SER:HB3	2.19	0.41
1:A:518:LEU:HD13	1:A:526:PRO:HB3	2.02	0.41
1:B:276:PHE:CZ	1:B:313:ARG:HB3	2.54	0.41
1:A:367:LYS:HE3	1:A:411:GLU:HG3	2.01	0.41
1:B:344:ILE:O	1:B:348:LYS:HB2	2.21	0.41
1:C:550:ASN:HB2	1:C:551:PRO:HD3	2.03	0.41
1:C:344:ILE:O	1:C:348:LYS:HB2	2.21	0.41
1:C:440:LYS:O	1:C:570:PHE:HA	2.21	0.41
1:B:433:LEU:HD12	1:B:433:LEU:HA	1.91	0.40
1:A:511:PHE:O	1:A:525:CYS:HB2	2.21	0.40
1:B:316:ASP:HB3	1:B:319:LYS:HD2	2.03	0.40
1:A:554:LYS:HA	1:A:557:TRP:CD2	2.57	0.40
1:A:387:ALA:CB	1:A:419:VAL:HG12	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:GLU:OE1	5:C:160:HOH:O[4_456]	1.94	0.26

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	299/334 (90%)	288 (96%)	10 (3%)	1 (0%)	41	70
1	B	301/334 (90%)	288 (96%)	12 (4%)	1 (0%)	41	70
1	C	302/334 (90%)	286 (95%)	15 (5%)	1 (0%)	41	70
All	All	902/1002 (90%)	862 (96%)	37 (4%)	3 (0%)	41	70

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	271/296 (92%)	244 (90%)	27 (10%)	7	20
1	B	274/296 (93%)	245 (89%)	29 (11%)	6	18
1	C	275/296 (93%)	246 (90%)	29 (10%)	7	18
All	All	820/888 (92%)	735 (90%)	85 (10%)	7	19

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	LYS
1	A	258	ASP
1	A	278	SER
1	A	313	ARG
1	A	319	LYS
1	A	336	THR

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Mol	Chain	Res	Type
1	A	341	LEU
1	A	352	THR
1	A	358	VAL
1	A	367	LYS
1	A	406	VAL
1	A	408	GLN
1	A	424	LYS
1	A	432	GLN
1	A	433	LEU
1	A	469	GLN
1	A	471	VAL
1	A	480	TYR
1	A	494	THR
1	A	502	VAL
1	A	512	MET
1	A	516	LYS
1	A	518	LEU
1	A	546	GLU
1	A	553	LYS
1	A	565	THR
1	A	567	LYS
1	B	254	ARG
1	B	258	ASP
1	B	278	SER
1	B	287	ASN
1	B	313	ARG
1	B	336	THR
1	B	341	LEU
1	B	348	LYS
1	B	352	THR
1	B	358	VAL
1	B	372	THR
1	B	406	VAL
1	B	408	GLN
1	B	410	VAL
1	B	432	GLN
1	B	433	LEU
1	B	458	SER
1	B	469	GLN
1	B	471	VAL
1	B	480	TYR
1	B	502	VAL

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Mol	Chain	Res	Type
1	B	512	MET
1	B	516	LYS
1	B	518	LEU
1	B	523	ASP
1	B	544	LYS
1	B	553	LYS
1	B	554	LYS
1	B	565	THR
1	C	254	ARG
1	C	258	ASP
1	C	278	SER
1	C	313	ARG
1	C	326	ARG
1	C	336	THR
1	C	341	LEU
1	C	352	THR
1	C	358	VAL
1	C	364	LYS
1	C	372	THR
1	C	406	VAL
1	C	408	GLN
1	C	424	LYS
1	C	433	LEU
1	C	444	VAL
1	C	469	GLN
1	C	471	VAL
1	C	478	GLU
1	C	502	VAL
1	C	512	MET
1	C	516	LYS
1	C	518	LEU
1	C	523	ASP
1	C	537	GLU
1	C	546	GLU
1	C	553	LYS
1	C	565	THR
1	C	567	LYS

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	322	ASN

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Mol	Chain	Res	Type
1	A	332	HIS
1	B	332	HIS
1	C	323	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	3	-	4,4,4	0.26	0	6,6,6	0.32	0
4	ACY	C	1	-	3,3,3	1.25	0	3,3,3	0.12	0
2	SO4	B	1	-	4,4,4	0.21	0	6,6,6	0.51	0
2	SO4	C	2	-	4,4,4	0.17	0	6,6,6	0.57	0
2	SO4	C	5	-	4,4,4	0.18	0	6,6,6	0.39	0
2	SO4	A	7	-	4,4,4	0.21	0	6,6,6	0.54	0
2	SO4	B	6	-	4,4,4	0.21	0	6,6,6	0.31	0
2	SO4	C	4	-	4,4,4	0.21	0	6,6,6	0.43	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1	ACY	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)

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	305/334 (91%)	0.07	6 (1%)	65	61	14, 25, 42, 50	0
1	B	307/334 (91%)	-0.02	6 (1%)	65	61	14, 25, 42, 52	0
1	C	308/334 (92%)	0.13	7 (2%)	60	55	14, 26, 42, 50	0
All	All	920/1002 (91%)	0.06	19 (2%)	63	59	14, 25, 42, 52	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	259	GLY	3.8
1	B	572	ASP	3.2
1	A	489	THR	3.1
1	B	538	GLY	2.8
1	B	537	GLU	2.6
1	A	487	ASP	2.6
1	C	291	GLU	2.6
1	C	538	GLY	2.5
1	C	385	ASP	2.5
1	C	316	ASP	2.5
1	A	572	ASP	2.5
1	B	489	THR	2.4
1	A	261	ASP	2.3
1	C	294	ARG	2.1
1	A	257	LYS	2.1
1	A	485	GLN	2.1
1	B	490	ASP	2.1
1	C	288	PRO	2.0
1	B	256	ARG	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 monosaccharides 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	C	5	5/5	0.63	0.28	75,75,77,78	0
2	SO4	C	4	5/5	0.85	0.19	80,80,81,81	0
2	SO4	A	7	5/5	0.90	0.18	78,78,78,79	0
4	ACY	C	1	4/4	0.93	0.15	12,14,15,15	0
2	SO4	B	6	5/5	0.94	0.15	48,50,51,52	0
2	SO4	C	2	5/5	0.95	0.14	46,47,48,50	0
3	NA	A	1	1/1	0.96	0.15	11,11,11,11	0
2	SO4	A	3	5/5	0.98	0.16	34,35,36,38	0
2	SO4	B	1	5/5	0.99	0.14	19,22,25,26	0

6.5 Other polymers (i)

There are no such residues in this entry.