Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 12:48 PM JST

PDB ID	:	4WXO
Title	:	SadC (300-487) from Pseudomonas aeruginosa PAO1
Authors	:	Liu, C.; Liu, S.; Gu, L.
Deposited on	:	2014-11-14
Resolution	:	2.81 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 (1)) were used in the production of this report:

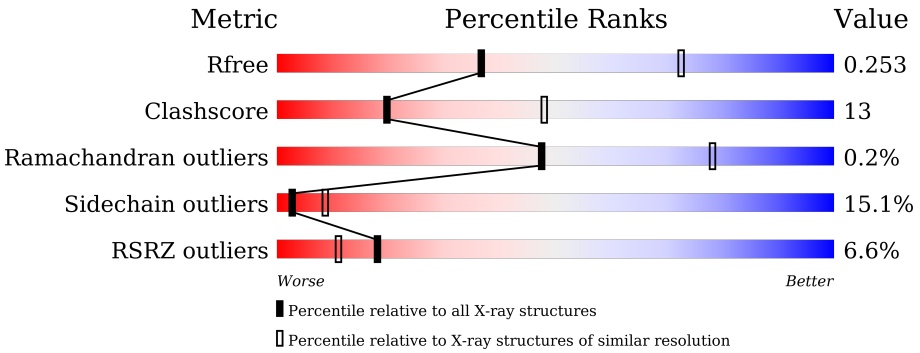
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.81 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	211	62% 21% · 14%
1	B	211	% 60% 25% •• 14%
1	C	211	15% 56% 25% 6% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4354 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	Se	0	1	0
			1447	890	276	272	4	5			
1	B	182	Total	C	N	O	S	Se	0	1	0
			1447	890	276	272	4	5			
1	C	182	Total	C	N	O	S	Se	0	1	0
			1447	890	276	272	4	5			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	MSE	-	expression tag	UNP Q9HW69
A	278	GLY	-	expression tag	UNP Q9HW69
A	279	SER	-	expression tag	UNP Q9HW69
A	280	SER	-	expression tag	UNP Q9HW69
A	281	HIS	-	expression tag	UNP Q9HW69
A	282	HIS	-	expression tag	UNP Q9HW69
A	283	HIS	-	expression tag	UNP Q9HW69
A	284	HIS	-	expression tag	UNP Q9HW69
A	285	HIS	-	expression tag	UNP Q9HW69
A	286	HIS	-	expression tag	UNP Q9HW69
A	287	SER	-	expression tag	UNP Q9HW69
A	288	GLN	-	expression tag	UNP Q9HW69
A	289	ASP	-	expression tag	UNP Q9HW69
A	290	LEU	-	expression tag	UNP Q9HW69
A	291	GLU	-	expression tag	UNP Q9HW69
A	292	VAL	-	expression tag	UNP Q9HW69
A	293	LEU	-	expression tag	UNP Q9HW69
A	294	PHE	-	expression tag	UNP Q9HW69
A	295	GLN	-	expression tag	UNP Q9HW69
A	296	GLY	-	expression tag	UNP Q9HW69
A	297	PRO	-	expression tag	UNP Q9HW69
A	298	GLY	-	expression tag	UNP Q9HW69
A	299	SER	-	expression tag	UNP Q9HW69

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Chain	Residue	Modelled	Actual	Comment	Reference
B	277	MSE	-	expression tag	UNP Q9HW69
B	278	GLY	-	expression tag	UNP Q9HW69
B	279	SER	-	expression tag	UNP Q9HW69
B	280	SER	-	expression tag	UNP Q9HW69
B	281	HIS	-	expression tag	UNP Q9HW69
B	282	HIS	-	expression tag	UNP Q9HW69
B	283	HIS	-	expression tag	UNP Q9HW69
B	284	HIS	-	expression tag	UNP Q9HW69
B	285	HIS	-	expression tag	UNP Q9HW69
B	286	HIS	-	expression tag	UNP Q9HW69
B	287	SER	-	expression tag	UNP Q9HW69
B	288	GLN	-	expression tag	UNP Q9HW69
B	289	ASP	-	expression tag	UNP Q9HW69
B	290	LEU	-	expression tag	UNP Q9HW69
B	291	GLU	-	expression tag	UNP Q9HW69
B	292	VAL	-	expression tag	UNP Q9HW69
B	293	LEU	-	expression tag	UNP Q9HW69
B	294	PHE	-	expression tag	UNP Q9HW69
B	295	GLN	-	expression tag	UNP Q9HW69
B	296	GLY	-	expression tag	UNP Q9HW69
B	297	PRO	-	expression tag	UNP Q9HW69
B	298	GLY	-	expression tag	UNP Q9HW69
B	299	SER	-	expression tag	UNP Q9HW69
C	277	MSE	-	expression tag	UNP Q9HW69
C	278	GLY	-	expression tag	UNP Q9HW69
C	279	SER	-	expression tag	UNP Q9HW69
C	280	SER	-	expression tag	UNP Q9HW69
C	281	HIS	-	expression tag	UNP Q9HW69
C	282	HIS	-	expression tag	UNP Q9HW69
C	283	HIS	-	expression tag	UNP Q9HW69
C	284	HIS	-	expression tag	UNP Q9HW69
C	285	HIS	-	expression tag	UNP Q9HW69
C	286	HIS	-	expression tag	UNP Q9HW69
C	287	SER	-	expression tag	UNP Q9HW69
C	288	GLN	-	expression tag	UNP Q9HW69
C	289	ASP	-	expression tag	UNP Q9HW69
C	290	LEU	-	expression tag	UNP Q9HW69
C	291	GLU	-	expression tag	UNP Q9HW69
C	292	VAL	-	expression tag	UNP Q9HW69
C	293	LEU	-	expression tag	UNP Q9HW69
C	294	PHE	-	expression tag	UNP Q9HW69
C	295	GLN	-	expression tag	UNP Q9HW69

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Chain	Residue	Modelled	Actual	Comment	Reference
C	296	GLY	-	expression tag	UNP Q9HW69
C	297	PRO	-	expression tag	UNP Q9HW69
C	298	GLY	-	expression tag	UNP Q9HW69
C	299	SER	-	expression tag	UNP Q9HW69

- Molecule 2 is water.

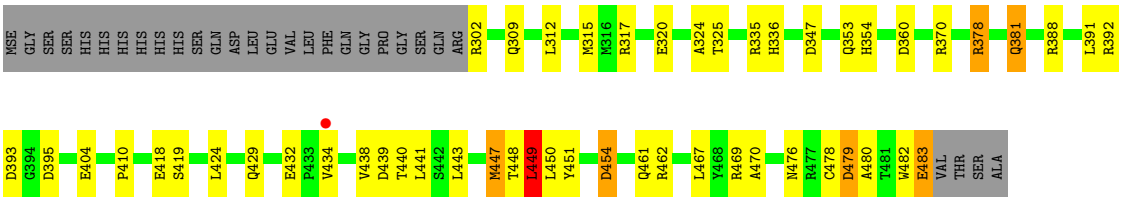
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total O 6 6	0	0
2	B	4	Total O 4 4	0	0
2	C	3	Total O 3 3	0	0

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.

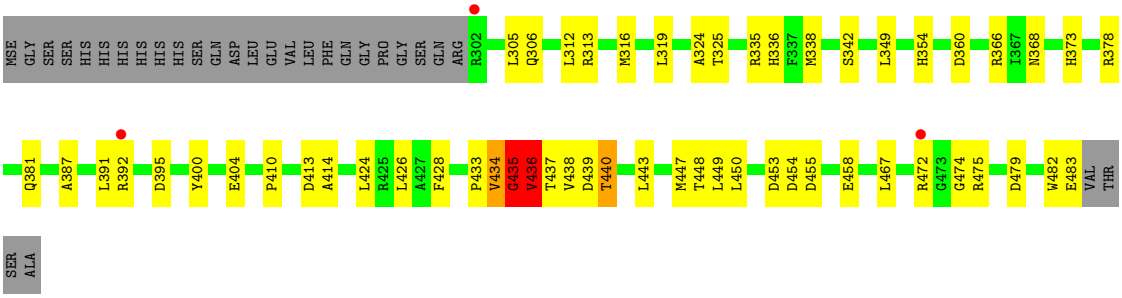
• Molecule 1: Uncharacterized protein

Chain A:



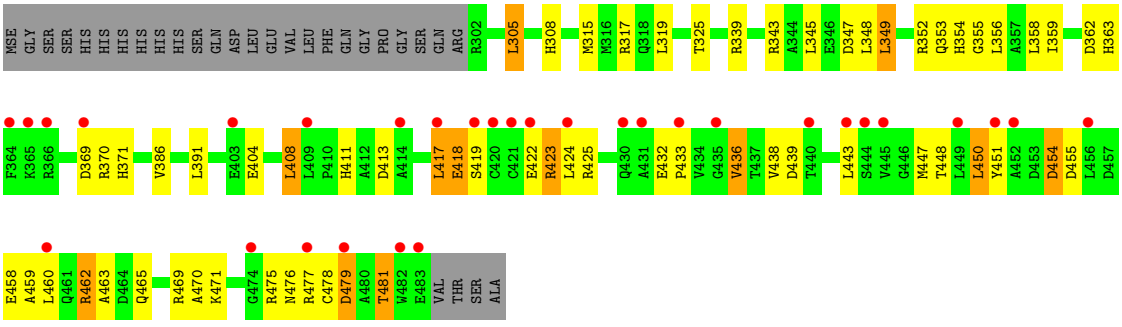
• Molecule 1: Uncharacterized protein

Chain B:



• Molecule 1: Uncharacterized protein

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	79.42Å 116.45Å 88.22Å 90.00° 110.19° 90.00°	Depositor
Resolution (Å)	39.46 – 2.81 39.46 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.46-2.81) 98.3 (39.46-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.66 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.200 , 0.254 0.203 , 0.253	Depositor DCC
R_{free} test set	935 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	62.8	Xtriage
Anisotropy	0.715	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 69.3	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	0.94	EDS
Total number of atoms	4354	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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

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	0.52	0/1466	0.65	1/1968 (0.1%)
1	B	0.56	0/1466	0.75	2/1968 (0.1%)
1	C	0.41	0/1466	0.56	0/1968
All	All	0.50	0/4398	0.66	3/5904 (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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	436	VAL	CB-CA-C	-7.38	97.39	111.40
1	B	435	GLY	N-CA-C	5.51	126.88	113.10
1	A	449	LEU	CB-CG-CD2	-5.23	102.11	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	435	GLY	Peptide

5.2 Too-close contacts

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	1447	0	1418	27	1
1	B	1447	0	1418	47	0
1	C	1447	0	1418	35	0
2	A	6	0	0	0	0
2	B	4	0	0	1	0
2	C	3	0	0	1	0
All	All	4354	0	4254	109	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 13.

All (109) 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:448:THR:C	1:A:449:LEU:HD23	1.59	1.22
1:A:449:LEU:HD23	1:A:449:LEU:N	1.61	1.10
1:B:436:VAL:O	1:B:436:VAL:HG13	1.29	1.09
1:B:435:GLY:CA	1:B:436:VAL:HB	1.90	1.02
1:B:435:GLY:N	1:B:436:VAL:CG1	2.29	0.95
1:B:436:VAL:O	1:B:436:VAL:CG1	2.06	0.94
1:B:435:GLY:H	1:B:436:VAL:HG12	1.30	0.93
1:B:435:GLY:N	1:B:436:VAL:HB	1.86	0.89
1:A:449:LEU:N	1:A:449:LEU:CD2	2.37	0.86
1:C:462:ARG:HB2	1:C:481:THR:HG21	1.58	0.85
1:A:448:THR:C	1:A:449:LEU:CD2	2.43	0.84
1:B:435:GLY:N	1:B:436:VAL:CB	2.40	0.83
1:B:436:VAL:O	1:B:438:VAL:HG23	1.79	0.82
1:A:447:MSE:CE	1:A:478:CYS:HB3	2.10	0.81
1:A:447:MSE:HE3	1:A:478:CYS:HB3	1.62	0.80
1:A:448:THR:O	1:A:449:LEU:CD2	2.29	0.79
1:B:435:GLY:H	1:B:436:VAL:CG1	1.92	0.79
1:B:435:GLY:HA3	1:B:436:VAL:HB	1.64	0.78
1:A:448:THR:O	1:A:449:LEU:HD23	1.84	0.77
1:B:435:GLY:CA	1:B:436:VAL:CB	2.65	0.73
1:B:435:GLY:N	1:B:436:VAL:HG12	1.97	0.71
1:A:360:ASP:HB2	1:A:467:LEU:HD21	1.78	0.66
1:C:447:MSE:HE2	1:C:478:CYS:HB3	1.80	0.64
1:B:360:ASP:HB2	1:B:467:LEU:HD21	1.79	0.64
1:B:439:ASP:O	1:B:440:THR:HG23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:ALA:HB2	1:C:479:ASP:HB2	1.81	0.62
1:A:451:TYR:O	1:A:454:ASP:HB2	2.02	0.60
1:A:482:TRP:O	1:A:483:GLU:HB2	2.02	0.60
1:B:475:ARG:NH1	2:B:502:HOH:O	2.22	0.59
1:C:356:LEU:HD21	1:C:460:LEU:HD23	1.84	0.59
1:B:387:ALA:HA	1:B:424:LEU:HD21	1.85	0.58
1:A:469:ARG:NH2	1:A:480:ALA:O	2.37	0.58
1:A:429:GLN:OE1	1:A:476:ASN:ND2	2.35	0.57
1:B:455:ASP:HB3	1:B:458:GLU:HB2	1.86	0.56
1:C:418:GLU:O	1:C:422:GLU:HG2	2.05	0.56
1:C:448:THR:HG22	1:C:463:ALA:HB2	1.86	0.56
1:A:317:ARG:O	1:A:320:GLU:HB3	2.06	0.55
1:B:439:ASP:OD1	1:B:440:THR:N	2.39	0.55
1:B:434:VAL:CA	1:B:436:VAL:HG11	2.35	0.55
1:A:448:THR:OG1	1:A:462:ARG:NH1	2.40	0.55
1:B:368:ASN:OD1	1:B:373:HIS:HA	2.07	0.55
1:C:308:HIS:ND1	2:C:501:HOH:O	2.33	0.55
1:A:378:ARG:HA	1:A:381:GLN:HG3	1.91	0.52
1:B:324:ALA:HB1	1:B:336:HIS:CG	2.45	0.52
1:C:354:HIS:HB2	1:C:450:LEU:HB3	1.92	0.51
1:A:448:THR:O	1:A:449:LEU:HD22	2.09	0.50
1:C:465:GLN:O	1:C:469:ARG:HG3	2.12	0.50
1:B:428:PHE:CD2	1:B:443:LEU:HD23	2.47	0.50
1:B:433:PRO:O	1:B:436:VAL:HG11	2.13	0.49
1:C:370:ARG:HG2	1:C:371:HIS:CE1	2.48	0.49
1:B:387:ALA:O	1:B:391:LEU:HG	2.13	0.49
1:C:339:ARG:O	1:C:343:ARG:HD3	2.12	0.48
1:C:391:LEU:HD21	1:C:424:LEU:HD11	1.95	0.48
1:C:417:LEU:HD21	1:C:447:MSE:HB3	1.95	0.48
1:B:436:VAL:O	1:B:438:VAL:CG2	2.59	0.48
1:B:437:THR:O	1:B:437:THR:OG1	2.30	0.48
1:B:424:LEU:HD23	1:B:424:LEU:HA	1.67	0.47
1:C:419[B]:SER:OG	1:C:423:ARG:NH2	2.44	0.47
1:C:447:MSE:CE	1:C:478:CYS:HB3	2.44	0.47
1:B:354:HIS:ND1	1:B:410:PRO:HA	2.29	0.47
1:B:434:VAL:C	1:B:436:VAL:CG1	2.83	0.46
1:A:447:MSE:HE2	1:A:478:CYS:HB3	1.95	0.46
1:C:348:LEU:HD12	1:C:348:LEU:HA	1.79	0.46
1:A:392:ARG:HG3	1:A:395:ASP:OD1	2.15	0.46
1:C:305:LEU:HD12	1:C:305:LEU:HA	1.56	0.46
1:C:425:ARG:NH1	1:C:476:ASN:OD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:PRO:HB2	1:C:436:VAL:HG23	1.97	0.46
1:A:443:LEU:C	1:A:443:LEU:HD12	2.36	0.45
1:C:471:LYS:HG3	1:C:475:ARG:NH1	2.32	0.45
1:B:434:VAL:C	1:B:436:VAL:HB	2.36	0.45
1:B:436:VAL:O	1:B:436:VAL:HG22	2.17	0.45
1:B:448:THR:OG1	1:B:449:LEU:N	2.50	0.45
1:A:429:GLN:HA	1:A:441:LEU:O	2.17	0.45
1:A:354:HIS:O	1:A:450:LEU:N	2.46	0.44
1:B:434:VAL:C	1:B:436:VAL:HG11	2.37	0.44
1:C:355:GLY:O	1:C:408:LEU:HA	2.17	0.44
1:B:454:ASP:OD1	1:B:455:ASP:N	2.51	0.44
1:C:319:LEU:HD23	1:C:319:LEU:HA	1.85	0.43
1:A:309:GLN:O	1:A:312:LEU:HB2	2.18	0.43
1:C:451:TYR:O	1:C:454:ASP:HB2	2.18	0.43
1:C:454:ASP:OD1	1:C:462:ARG:NH2	2.51	0.43
1:A:449:LEU:HD22	1:A:449:LEU:HA	1.54	0.43
1:C:459:ALA:HA	1:C:462:ARG:NE	2.34	0.43
1:C:349:LEU:HB2	1:C:352:ARG:HG3	2.01	0.43
1:B:414:ALA:HB1	1:B:483:GLU:HB3	2.01	0.43
1:B:433:PRO:C	1:B:436:VAL:HG11	2.40	0.42
1:B:474:GLY:O	1:B:475:ARG:HB2	2.20	0.42
1:A:324:ALA:HB1	1:A:336:HIS:CG	2.54	0.42
1:C:345:LEU:HD21	1:C:454:ASP:O	2.20	0.42
1:B:313:ARG:HA	1:B:316:MSE:HE3	2.01	0.42
1:B:447:MSE:HE2	1:B:447:MSE:HB2	1.78	0.42
1:B:319:LEU:HD23	1:B:319:LEU:HA	1.89	0.42
1:B:482:TRP:CD1	1:B:482:TRP:N	2.88	0.41
1:C:362:ASP:HB3	1:C:475:ARG:HD2	2.01	0.41
1:A:354:HIS:ND1	1:A:410:PRO:HA	2.35	0.41
1:C:369:ASP:N	1:C:369:ASP:OD1	2.52	0.41
1:C:476:ASN:O	1:C:477:ARG:HD2	2.20	0.41
1:B:338:MSE:HE1	1:B:400:TYR:HE2	1.85	0.41
1:C:354:HIS:CE1	1:C:411:HIS:H	2.38	0.41
1:B:305:LEU:HA	1:B:305:LEU:HD12	1.84	0.41
1:B:378:ARG:HA	1:B:378:ARG:HD3	1.80	0.41
1:B:426:LEU:HA	1:B:426:LEU:HD23	1.81	0.41
1:C:433:PRO:HB2	1:C:436:VAL:CG2	2.50	0.41
1:B:312:LEU:HD23	1:B:312:LEU:HA	1.92	0.41
1:C:359:ILE:HG23	1:C:443:LEU:HD13	2.01	0.41
1:A:470:ALA:HB2	1:A:479:ASP:HB2	2.03	0.40
1:B:392:ARG:HG2	1:B:395:ASP:OD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:LEU:HD23	1:C:358:LEU:HA	1.88	0.40
1:C:370:ARG:HG2	1:C:371:HIS:ND1	2.37	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:370:ARG:NH1	1:A:439:ASP:OD2[2_455]	2.16	0.04

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	181/211 (86%)	178 (98%)	3 (2%)	0	100 100
1	B	181/211 (86%)	176 (97%)	4 (2%)	1 (1%)	25 56
1	C	181/211 (86%)	176 (97%)	5 (3%)	0	100 100
All	All	543/633 (86%)	530 (98%)	12 (2%)	1 (0%)	47 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	436	VAL

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	149/167 (89%)	123 (83%)	26 (17%)	2 6
1	B	149/167 (89%)	133 (89%)	16 (11%)	6 20
1	C	149/167 (89%)	123 (83%)	26 (17%)	2 6
All	All	447/501 (89%)	379 (85%)	68 (15%)	3 8

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	ARG
1	A	315	MSE
1	A	325	THR
1	A	335	ARG
1	A	347	ASP
1	A	353	GLN
1	A	378	ARG
1	A	381	GLN
1	A	388	ARG
1	A	391	LEU
1	A	393	ASP
1	A	404	GLU
1	A	418	GLU
1	A	419[A]	SER
1	A	419[B]	SER
1	A	424	LEU
1	A	432	GLU
1	A	434	VAL
1	A	438	VAL
1	A	440	THR
1	A	447	MSE
1	A	449	LEU
1	A	454	ASP
1	A	461	GLN
1	A	479	ASP
1	A	483	GLU
1	B	306	GLN
1	B	325	THR
1	B	335	ARG
1	B	342	SER
1	B	349	LEU
1	B	366	ARG
1	B	381	GLN
1	B	404	GLU

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Mol	Chain	Res	Type
1	B	413	ASP
1	B	434	VAL
1	B	436	VAL
1	B	440	THR
1	B	450	LEU
1	B	453	ASP
1	B	472	ARG
1	B	479	ASP
1	C	305	LEU
1	C	315	MSE
1	C	317	ARG
1	C	325	THR
1	C	347	ASP
1	C	349	LEU
1	C	353	GLN
1	C	363	HIS
1	C	386	VAL
1	C	404	GLU
1	C	408	LEU
1	C	413	ASP
1	C	417	LEU
1	C	418	GLU
1	C	423	ARG
1	C	432	GLU
1	C	436	VAL
1	C	438	VAL
1	C	439	ASP
1	C	450	LEU
1	C	454	ASP
1	C	455	ASP
1	C	458	GLU
1	C	462	ARG
1	C	479	ASP
1	C	481	THR

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	353	GLN
1	A	381	GLN
1	B	381	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

There are no ligands in this entry.

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	177/211 (83%)	0.06	1 (0%) 89 86	42, 70, 120, 153	0
1	B	177/211 (83%)	0.15	3 (1%) 70 63	42, 71, 108, 128	0
1	C	177/211 (83%)	0.92	31 (17%) 1 1	42, 115, 164, 199	0
All	All	531/633 (83%)	0.38	35 (6%) 18 11	42, 79, 149, 199	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	420	CYS	5.0
1	C	483	GLU	4.8
1	C	482	TRP	4.4
1	C	451	TYR	4.1
1	C	365	LYS	3.7
1	C	424	LEU	3.7
1	C	443	LEU	3.7
1	C	479	ASP	3.7
1	C	421	CYS	3.3
1	C	456	LEU	3.2
1	C	460	LEU	3.2
1	C	474	GLY	3.2
1	C	417	LEU	3.0
1	C	445	VAL	3.0
1	C	422	GLU	3.0
1	B	392	ARG	2.9
1	C	431	ALA	2.8
1	B	302	ARG	2.7
1	C	433	PRO	2.7
1	C	369	ASP	2.7
1	C	440	THR	2.6
1	C	409	LEU	2.6
1	C	430	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	414	ALA	2.4
1	C	419[A]	SER	2.4
1	B	472	ARG	2.4
1	C	403	GLU	2.4
1	C	444	SER	2.3
1	A	434	VAL	2.1
1	C	452	ALA	2.1
1	C	435	GLY	2.1
1	C	364	PHE	2.1
1	C	449	LEU	2.1
1	C	366	ARG	2.1
1	C	477	ARG	2.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.