W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 03:00 am GMT

PDB ID	:	4MVN
Title	:	Crystal structure of the staphylococcal serine protease SplA in complex with a specific phosphonate inhibitor
Authors	:	Zdzalik, M.; Burchacka, E.; Niemczyk, J.S.; Pustelny, K.; Popowicz, G.M.; Wladyka, B.; Dubin, A.; Potempa, J.; Sienczyk, M.; Dubin, G.; Oleksyszyn, J.
Deposited on	:	2013-09-24
Resolution	:	1.70 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:

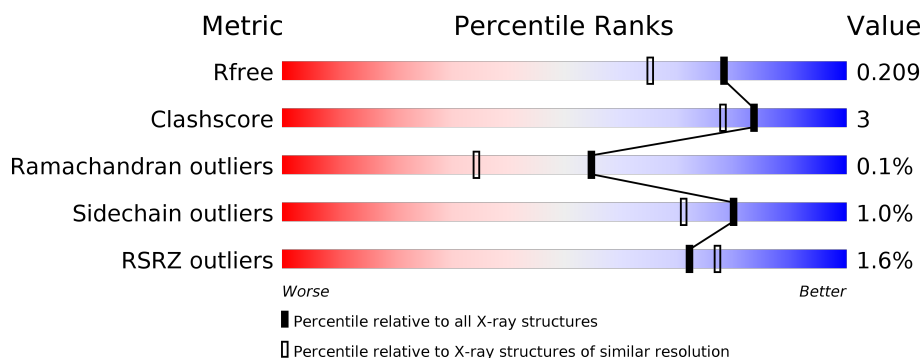|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	Percentile Ranks	Value
Rfree		0.209
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		1.0%
RSRZ outliers		1.6%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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.

| Mol	Chain	Length	Quality of chain
1	A	200	96% · ··
1	B	200	6% / 89% 10% ··
1	C	200	% / 93% 6% ··
1	D	200	% / 92% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7077 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 Serine protease splA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	5	1
			1524	970	254	298	2			
1	B	199	Total	C	N	O	S	0	6	1
			1505	956	247	299	3			
1	C	197	Total	C	N	O	S	0	2	1
			1503	951	248	302	2			
1	D	200	Total	C	N	O	S	0	8	0
			1562	989	262	309	2			

- Molecule 2 is [(1S)-1-{[(BENZYLOXY)CARBONYL]AMINO}-2-PHENYLETHYL]PHOSPHONIC ACID (three-letter code: I1S) (formula: $C_{16}H_{18}NO_5P$).
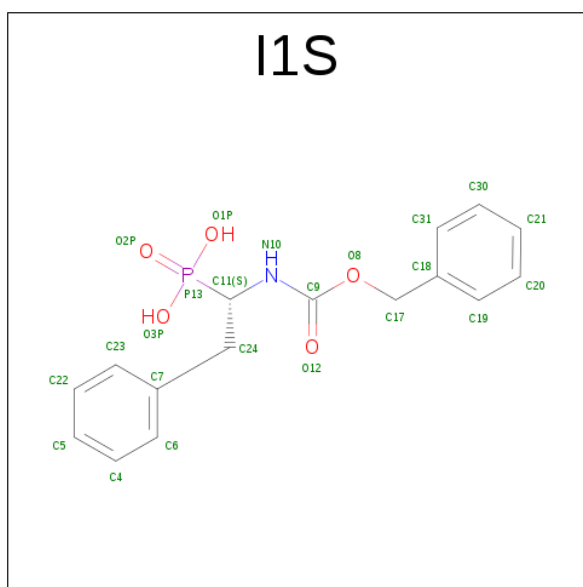
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	16	1	4	1		
2	B	1	Total	C	N	O	P	0	0
			22	16	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 44	C 32	N 2	O 8	P 2	0	1
2	D	1	Total 22	C 16	N 1	O 4	P 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	224	Total 224	O 224	0	0
3	B	146	Total 146	O 146	0	0
3	C	219	Total 219	O 219	0	0
3	D	284	Total 284	O 284	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
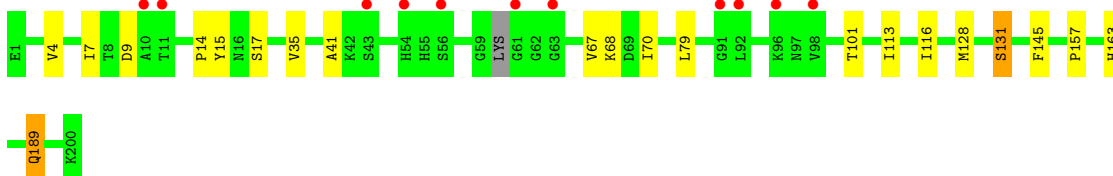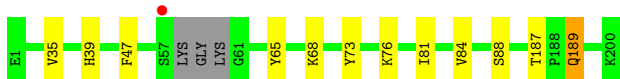
• Molecule 1: Serine protease splA

Chain A:

• Molecule 1: Serine protease splA

Chain B:

• Molecule 1: Serine protease splA

Chain C:

• Molecule 1: Serine protease splA

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.13Å 81.63Å 133.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.70	Depositor
	39.14 – 1.70	EDS
% Data completeness	96.9 (25.00-1.70)	Depositor
(in resolution range)	96.9 (39.14-1.70)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.83 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.165 , 0.209	Depositor
	0.164 , 0.209	DCC
R_{free} test set	4356 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	16.2	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.1	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	0.96	EDS
Total number of atoms	7077	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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:
I1S

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	1.24	3/1566 (0.2%)	1.04	2/2116 (0.1%)
1	B	1.05	2/1553 (0.1%)	0.95	0/2105
1	C	1.22	3/1539 (0.2%)	1.07	0/2080
1	D	1.33	4/1614 (0.2%)	1.17	2/2178 (0.1%)
All	All	1.22	12/6272 (0.2%)	1.06	4/8479 (0.0%)

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	D	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	ALA	C-O	7.38	1.37	1.23
1	C	73	TYR	CD2-CE2	7.14	1.50	1.39
1	A	145	PHE	CE2-CZ	6.54	1.49	1.37
1	C	84	VAL	CB-CG2	6.40	1.66	1.52
1	D	62	GLY	N-CA	6.17	1.55	1.46
1	D	170	TYR	CD2-CE2	6.13	1.48	1.39
1	A	145	PHE	CD2-CE2	5.37	1.50	1.39
1	D	62	GLY	CA-C	5.32	1.60	1.51
1	B	113	ILE	CA-CB	5.27	1.67	1.54
1	D	130	GLU	CB-CG	5.03	1.61	1.52
1	B	145	PHE	CE2-CZ	5.02	1.46	1.37
1	C	47	PHE	CE2-CZ	5.00	1.46	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	112	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	D	112	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	22[A]	VAL	N-CA-C	5.11	124.79	111.00
1	A	22[B]	VAL	N-CA-C	5.11	124.79	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	GLY	Peptide
1	D	60	LYS	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	1524	0	1471	5	0
1	B	1505	0	1411	13	0
1	C	1503	0	1419	9	0
1	D	1562	0	1519	7	0
2	A	22	0	16	0	0
2	B	22	0	16	0	0
2	C	44	0	32	0	0
2	D	22	0	16	0	0
3	A	224	0	0	3	0
3	B	146	0	0	2	0
3	C	219	0	0	5	0
3	D	284	0	0	0	0
All	All	7077	0	5900	34	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 3.

All (34) 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:189[A]:GLN:HG3	3:C:444:HOH:O	1.56	1.04
1:A:5:LYS:HE3	3:A:517:HOH:O	1.68	0.93
1:B:15:TYR:HB3	1:B:128[A]:MET:HE1	1.64	0.77
1:C:187:THR:OG1	1:C:189[A]:GLN:HG2	1.96	0.66
1:C:35:VAL:HG12	1:C:81:ILE:HD12	1.78	0.64
1:C:189[A]:GLN:CG	3:C:444:HOH:O	2.27	0.61
1:C:39:HIS:HE1	3:C:464:HOH:O	1.83	0.61
1:B:7:ILE:HB	1:B:128[A]:MET:HG2	1.85	0.59
1:B:15:TYR:CB	1:B:128[A]:MET:HE1	2.33	0.58
1:B:4:VAL:HG22	1:B:131[A]:SER:HB3	1.86	0.57
1:A:5:LYS:CE	3:A:517:HOH:O	2.36	0.57
1:D:86:GLU:HG2	1:D:93:ASN:ND2	2.20	0.56
1:B:41:ALA:HB1	1:B:70[A]:ILE:HD12	1.87	0.55
1:D:9:ASP:OD1	1:D:11:THR:HG23	2.06	0.54
1:B:35[A]:VAL:HG13	1:B:79:LEU:HD11	1.89	0.54
1:D:37[B]:ASN:HD22	1:D:168:ILE:HD12	1.76	0.51
1:B:17:SER:HG	1:B:101:THR:HG1	1.59	0.50
1:D:37[B]:ASN:ND2	1:D:168:ILE:HD12	2.27	0.50
1:B:189[A]:GLN:OE1	3:B:502:HOH:O	2.20	0.47
1:A:20:ALA:HB2	1:A:118:TYR:CE2	2.50	0.46
1:C:68:LYS:HE3	3:C:445:HOH:O	2.15	0.46
1:A:39:HIS:HD2	3:A:488:HOH:O	1.98	0.46
1:D:86:GLU:HG2	1:D:93:ASN:HD21	1.83	0.43
1:D:104:ALA:O	1:D:105:ASP:HB2	2.19	0.43
1:C:76:LYS:HG3	3:C:512:HOH:O	2.18	0.43
1:B:67:VAL:HG11	1:B:70[A]:ILE:HD11	2.00	0.43
1:C:35:VAL:HG12	1:C:81:ILE:CD1	2.48	0.42
1:C:65:TYR:CE1	1:C:88:SER:HB3	2.55	0.42
1:B:9:ASP:O	3:B:469:HOH:O	2.22	0.41
1:B:68:LYS:HB3	1:B:68:LYS:HE2	1.94	0.41
1:D:89:THR:HG22	1:D:89:THR:O	2.20	0.41
1:B:14:PRO:HG3	1:B:163:HIS:HB3	2.02	0.40
1:A:20:ALA:HB2	1:A:118:TYR:CZ	2.56	0.40
1:B:116:ILE:O	1:B:157:PRO:HD2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	200/200 (100%)	195 (98%)	4 (2%)	1 (0%)	32	15
1	B	201/200 (100%)	196 (98%)	5 (2%)	0	100	100
1	C	195/200 (98%)	191 (98%)	4 (2%)	0	100	100
1	D	206/200 (103%)	203 (98%)	3 (2%)	0	100	100
All	All	802/800 (100%)	785 (98%)	16 (2%)	1 (0%)	55	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	GLY

5.3.2 Protein sidechains ⓘ

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	160/168 (95%)	160 (100%)	0	100	100
1	B	155/168 (92%)	151 (97%)	4 (3%)	51	31
1	C	157/168 (94%)	155 (99%)	2 (1%)	73	60
1	D	168/168 (100%)	165 (98%)	3 (2%)	64	47
All	All	640/672 (95%)	631 (99%)	9 (1%)	80	58

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	131[A]	SER
1	B	131[B]	SER
1	B	189[A]	GLN
1	B	189[B]	GLN
1	C	189[A]	GLN
1	C	189[B]	GLN
1	D	47	PHE
1	D	90	GLU
1	D	200	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	123	GLN
1	B	196	ASN
1	C	39	HIS
1	C	136	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

5 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	I1S	A	301	1	18,23,24	1.41	1 (5%)	21,29,32	1.82	5 (23%)
2	I1S	B	301	1	18,23,24	1.52	1 (5%)	21,29,32	1.60	3 (14%)
2	I1S	C	301[A]	1	18,23,24	1.13	1 (5%)	21,29,32	2.07	4 (19%)
2	I1S	C	301[B]	1	18,23,24	1.51	1 (5%)	21,29,32	1.28	2 (9%)
2	I1S	D	301	1	18,23,24	1.61	2 (11%)	21,29,32	1.50	3 (14%)

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
2	I1S	A	301	1	-	0/12/17/19	0/2/2/2
2	I1S	B	301	1	-	0/12/17/19	0/2/2/2
2	I1S	C	301[A]	1	-	0/12/17/19	0/2/2/2
2	I1S	C	301[B]	1	-	0/12/17/19	0/2/2/2
2	I1S	D	301	1	-	0/12/17/19	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301[A]	I1S	O8-C9	3.29	1.41	1.35
2	D	301	I1S	O12-C9	3.96	1.29	1.21
2	D	301	I1S	O8-C9	4.12	1.43	1.35
2	A	301	I1S	O8-C9	4.75	1.44	1.35
2	B	301	I1S	O8-C9	4.98	1.45	1.35
2	C	301[B]	I1S	O8-C9	5.27	1.45	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301[A]	I1S	O8-C9-O12	-6.65	110.86	124.22
2	A	301	I1S	O8-C9-O12	-4.74	114.69	124.22
2	B	301	I1S	O8-C9-O12	-4.17	115.85	124.22
2	D	301	I1S	O8-C9-O12	-3.61	116.96	124.22
2	C	301[B]	I1S	O8-C9-O12	-2.52	119.16	124.22
2	C	301[A]	I1S	C22-C23-C7	-2.43	116.94	120.64
2	B	301	I1S	O8-C17-C18	-2.20	103.94	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	I1S	C5-C22-C23	-2.13	117.28	120.21
2	A	301	I1S	O8-C17-C18	2.23	114.95	109.41
2	A	301	I1S	C22-C23-C7	2.33	124.18	120.64
2	D	301	I1S	O12-C9-N10	2.39	128.98	124.87
2	C	301[A]	I1S	O12-C9-N10	2.49	129.16	124.87
2	B	301	I1S	O8-C9-N10	2.55	116.02	110.54
2	D	301	I1S	C31-C18-C19	2.66	122.37	118.16
2	C	301[B]	I1S	O8-C17-C18	3.61	118.38	109.41
2	A	301	I1S	O8-C9-N10	3.84	118.79	110.54
2	C	301[A]	I1S	O8-C9-N10	4.39	119.97	110.54

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 (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 ⓘ

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, 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	199/200 (99%)	-0.38	0	100	100	8, 16, 31, 47	4 (2%)
1	B	199/200 (99%)	0.19	11 (5%)	26	29	15, 25, 42, 47	6 (3%)
1	C	197/200 (98%)	-0.47	1 (0%)	90	93	7, 16, 26, 43	2 (1%)
1	D	200/200 (100%)	-0.46	1 (0%)	90	93	6, 12, 21, 33	3 (1%)
All	All	795/800 (99%)	-0.28	13 (1%)	72	77	6, 17, 36, 47	15 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	92	LEU	3.6
1	B	98	VAL	2.9
1	B	63	GLY	2.8
1	B	54	HIS	2.8
1	C	57	SER	2.7
1	B	91	GLY	2.7
1	B	43	SER	2.7
1	B	61	GLY	2.6
1	B	10	ALA	2.5
1	B	11	THR	2.4
1	D	61[A]	GLY	2.4
1	B	56	SER	2.1
1	B	96	LYS	2.0

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

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

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6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	I1S	A	301	22/23	0.92	0.13	1.04	18,24,37,41	0
2	I1S	C	301[B]	22/23	0.98	0.10	1.02	10,13,21,22	22
2	I1S	C	301[A]	22/23	0.98	0.10	0.99	6,12,24,26	22
2	I1S	B	301	22/23	0.94	0.11	0.70	17,23,38,38	0
2	I1S	D	301	22/23	0.97	0.09	0.60	9,13,23,24	0

6.5 Other polymers (i)

There are no such residues in this entry.