



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 04:11 PM GMT

PDB ID : 3BEZ
Title : Crystal structure of Escherichia coli Signal peptide peptidase (SppA), SeMet crystals
Authors : Paetzel, M.
Deposited on : 2007-11-20
Resolution : 2.76 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

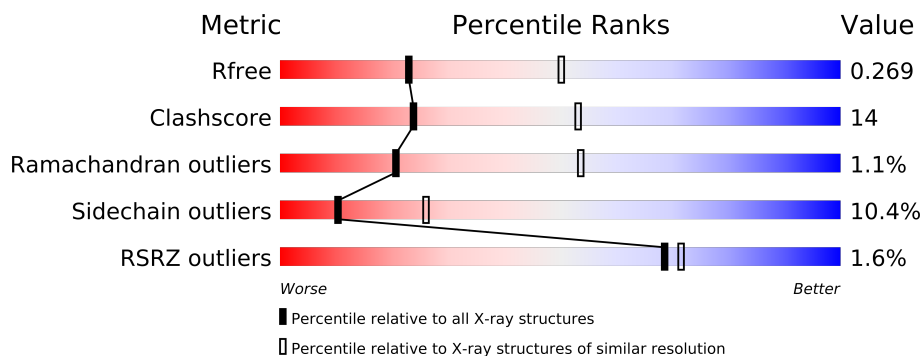
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.76 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}	66092	2406 (2.80-2.72)
Clashscore	79885	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (2.80-2.72)
RSRZ outliers	66119	2409 (2.80-2.72)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	593	
1	B	593	
1	C	593	
1	D	593	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14989 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Protease 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	Se	0	0	0
			3576	2257	610	701	8			
1	B	473	Total	C	N	O	Se	0	0	0
			3572	2254	609	701	8			
1	C	476	Total	C	N	O	Se	0	0	0
			3597	2269	616	704	8			
1	D	479	Total	C	N	O	Se	0	0	0
			3617	2279	619	711	8			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MSE	-	EXPRESSION TAG	UNP P08395
A	27	GLY	-	EXPRESSION TAG	UNP P08395
A	28	SER	-	EXPRESSION TAG	UNP P08395
A	29	SER	-	EXPRESSION TAG	UNP P08395
A	30	HIS	-	EXPRESSION TAG	UNP P08395
A	31	HIS	-	EXPRESSION TAG	UNP P08395
A	32	HIS	-	EXPRESSION TAG	UNP P08395
A	33	HIS	-	EXPRESSION TAG	UNP P08395
A	34	HIS	-	EXPRESSION TAG	UNP P08395
A	35	HIS	-	EXPRESSION TAG	UNP P08395
A	36	SER	-	EXPRESSION TAG	UNP P08395
A	37	SER	-	EXPRESSION TAG	UNP P08395
A	38	GLY	-	EXPRESSION TAG	UNP P08395
A	39	LEU	-	EXPRESSION TAG	UNP P08395
A	40	VAL	-	EXPRESSION TAG	UNP P08395
A	41	PRO	-	EXPRESSION TAG	UNP P08395
A	42	ARG	-	EXPRESSION TAG	UNP P08395
A	43	GLY	-	EXPRESSION TAG	UNP P08395
A	44	SER	-	EXPRESSION TAG	UNP P08395
A	45	HIS	-	EXPRESSION TAG	UNP P08395
A	46	MSE	-	EXPRESSION TAG	UNP P08395

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	MSE	-	EXPRESSION TAG	UNP P08395
B	27	GLY	-	EXPRESSION TAG	UNP P08395
B	28	SER	-	EXPRESSION TAG	UNP P08395
B	29	SER	-	EXPRESSION TAG	UNP P08395
B	30	HIS	-	EXPRESSION TAG	UNP P08395
B	31	HIS	-	EXPRESSION TAG	UNP P08395
B	32	HIS	-	EXPRESSION TAG	UNP P08395
B	33	HIS	-	EXPRESSION TAG	UNP P08395
B	34	HIS	-	EXPRESSION TAG	UNP P08395
B	35	HIS	-	EXPRESSION TAG	UNP P08395
B	36	SER	-	EXPRESSION TAG	UNP P08395
B	37	SER	-	EXPRESSION TAG	UNP P08395
B	38	GLY	-	EXPRESSION TAG	UNP P08395
B	39	LEU	-	EXPRESSION TAG	UNP P08395
B	40	VAL	-	EXPRESSION TAG	UNP P08395
B	41	PRO	-	EXPRESSION TAG	UNP P08395
B	42	ARG	-	EXPRESSION TAG	UNP P08395
B	43	GLY	-	EXPRESSION TAG	UNP P08395
B	44	SER	-	EXPRESSION TAG	UNP P08395
B	45	HIS	-	EXPRESSION TAG	UNP P08395
B	46	MSE	-	EXPRESSION TAG	UNP P08395
C	26	MSE	-	EXPRESSION TAG	UNP P08395
C	27	GLY	-	EXPRESSION TAG	UNP P08395
C	28	SER	-	EXPRESSION TAG	UNP P08395
C	29	SER	-	EXPRESSION TAG	UNP P08395
C	30	HIS	-	EXPRESSION TAG	UNP P08395
C	31	HIS	-	EXPRESSION TAG	UNP P08395
C	32	HIS	-	EXPRESSION TAG	UNP P08395
C	33	HIS	-	EXPRESSION TAG	UNP P08395
C	34	HIS	-	EXPRESSION TAG	UNP P08395
C	35	HIS	-	EXPRESSION TAG	UNP P08395
C	36	SER	-	EXPRESSION TAG	UNP P08395
C	37	SER	-	EXPRESSION TAG	UNP P08395
C	38	GLY	-	EXPRESSION TAG	UNP P08395
C	39	LEU	-	EXPRESSION TAG	UNP P08395
C	40	VAL	-	EXPRESSION TAG	UNP P08395
C	41	PRO	-	EXPRESSION TAG	UNP P08395
C	42	ARG	-	EXPRESSION TAG	UNP P08395
C	43	GLY	-	EXPRESSION TAG	UNP P08395
C	44	SER	-	EXPRESSION TAG	UNP P08395
C	45	HIS	-	EXPRESSION TAG	UNP P08395
C	46	MSE	-	EXPRESSION TAG	UNP P08395

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Chain	Residue	Modelled	Actual	Comment	Reference
D	26	MSE	-	EXPRESSION TAG	UNP P08395
D	27	GLY	-	EXPRESSION TAG	UNP P08395
D	28	SER	-	EXPRESSION TAG	UNP P08395
D	29	SER	-	EXPRESSION TAG	UNP P08395
D	30	HIS	-	EXPRESSION TAG	UNP P08395
D	31	HIS	-	EXPRESSION TAG	UNP P08395
D	32	HIS	-	EXPRESSION TAG	UNP P08395
D	33	HIS	-	EXPRESSION TAG	UNP P08395
D	34	HIS	-	EXPRESSION TAG	UNP P08395
D	35	HIS	-	EXPRESSION TAG	UNP P08395
D	36	SER	-	EXPRESSION TAG	UNP P08395
D	37	SER	-	EXPRESSION TAG	UNP P08395
D	38	GLY	-	EXPRESSION TAG	UNP P08395
D	39	LEU	-	EXPRESSION TAG	UNP P08395
D	40	VAL	-	EXPRESSION TAG	UNP P08395
D	41	PRO	-	EXPRESSION TAG	UNP P08395
D	42	ARG	-	EXPRESSION TAG	UNP P08395
D	43	GLY	-	EXPRESSION TAG	UNP P08395
D	44	SER	-	EXPRESSION TAG	UNP P08395
D	45	HIS	-	EXPRESSION TAG	UNP P08395
D	46	MSE	-	EXPRESSION TAG	UNP P08395

- Molecule 2 is water.

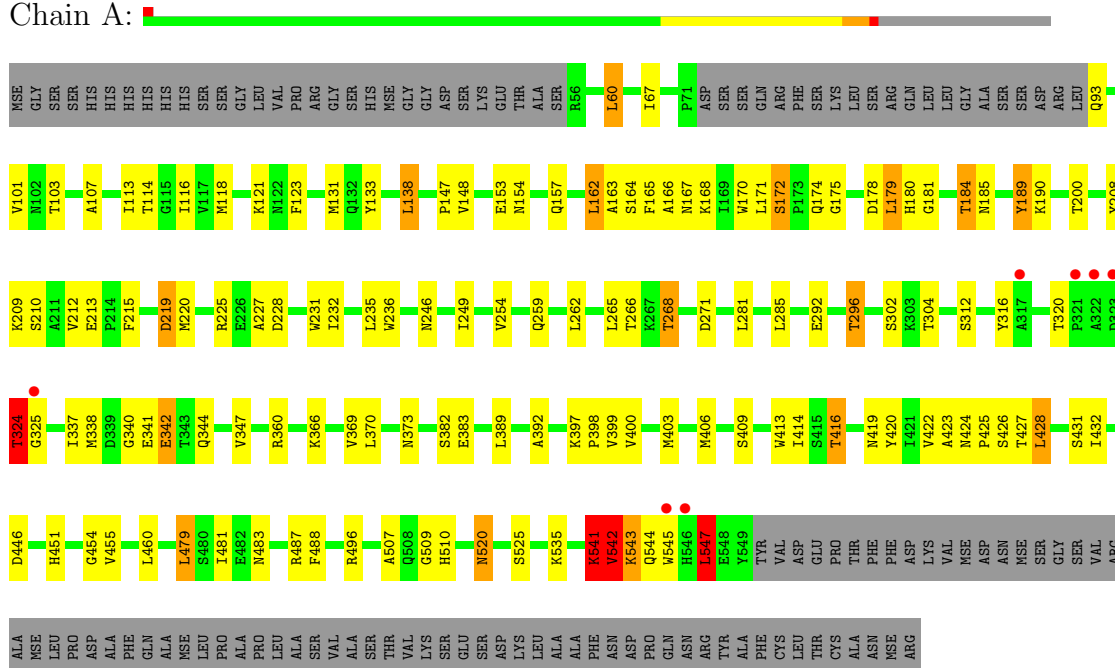
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	149	Total	O	0	0
			149	149		
2	B	166	Total	O	0	0
			166	166		
2	C	139	Total	O	0	0
			139	139		
2	D	173	Total	O	0	0
			173	173		

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 errors 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.

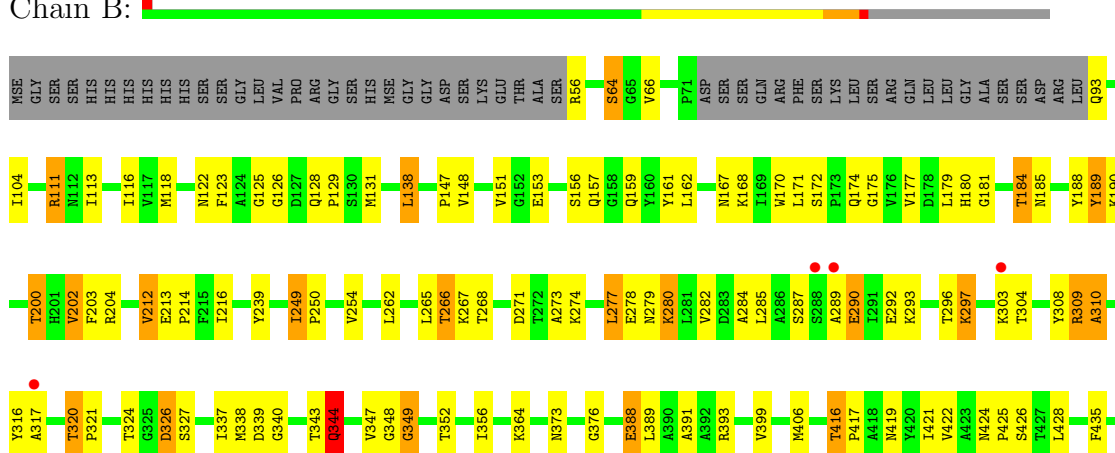
• Molecule 1: Protease 4

Chain A:



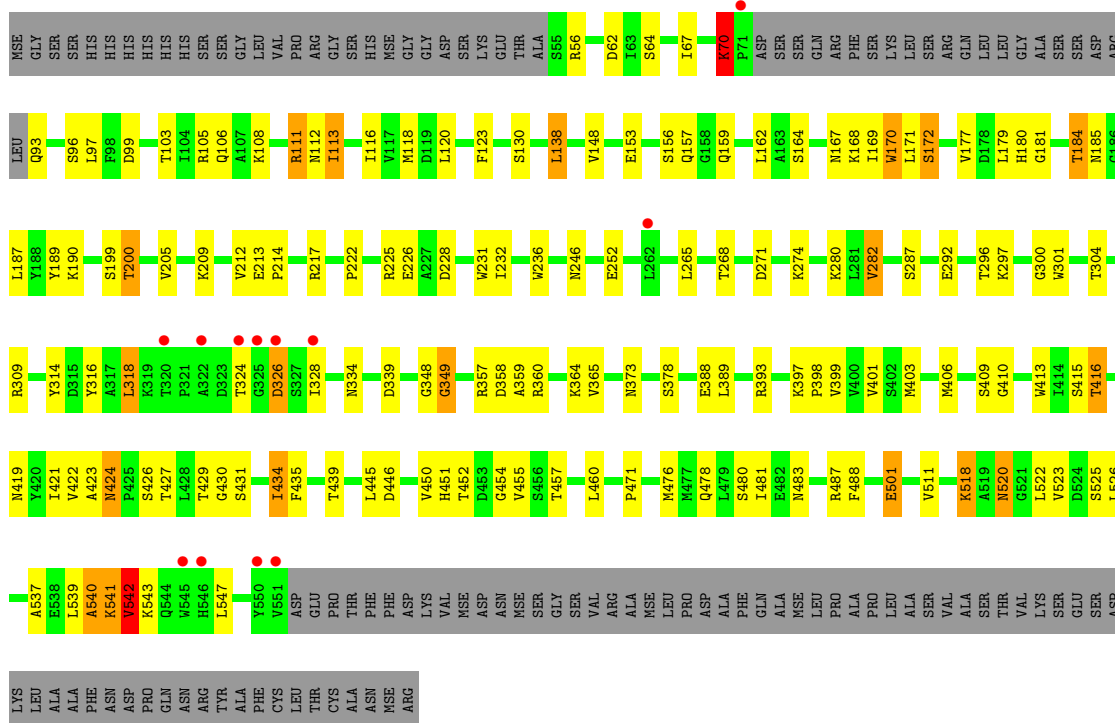
• Molecule 1: Protease 4

Chain B:



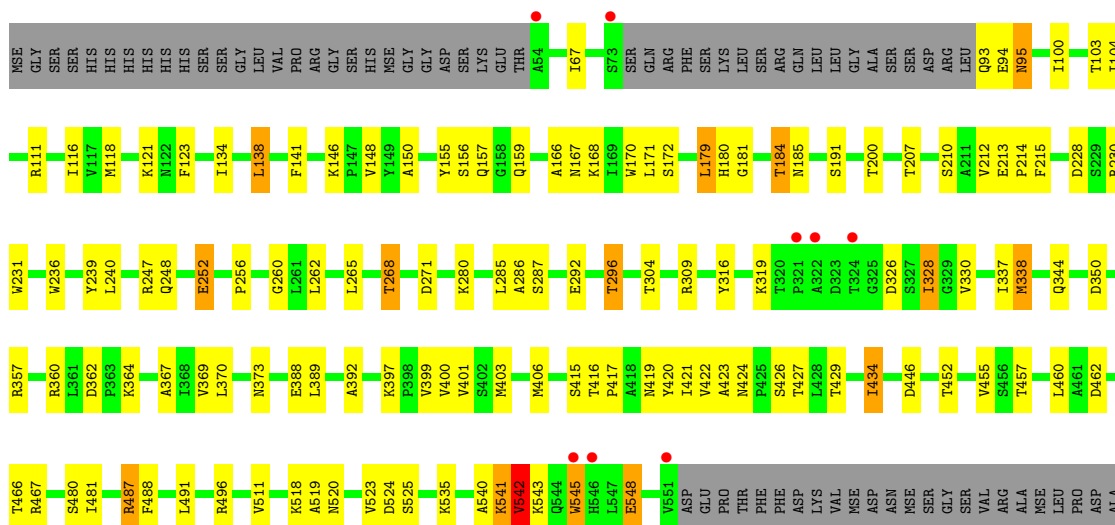
- Molecule 1: Protease 4

Chain C:



- Molecule 1: Protease 4

Chain D:



PHE	GLN	ALA	MSE	LEU	PRO	ALA	PRO	LEU	ALA	SER	VAL	ALA	SER	THR	VAL	LYS	SER	GLU	SER	ASP	LYS	LEU	ALA	ALA	PHE	ASN	ASP	PRO	GLN	ASN	ARG	TYR	ALA	PHE	CYS	LEU	THR	CYS	ALA	ASN	MSE	ARG
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.02Å 153.04Å 100.21Å 90.00° 104.17° 90.00°	Depositor
Resolution (Å)	46.63 – 2.76 46.85 – 2.76	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.63-2.76) 98.6 (46.85-2.76)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.259 0.201 , 0.269	Depositor DCC
R_{free} test set	3501 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 16.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 69169 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14989	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

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	0.80	1/3635 (0.0%)	0.85	5/4922 (0.1%)
1	B	0.81	1/3631 (0.0%)	0.87	1/4918 (0.0%)
1	C	0.81	0/3656	0.88	2/4950 (0.0%)
1	D	0.80	2/3676 (0.1%)	0.86	2/4977 (0.0%)
All	All	0.80	4/14598 (0.0%)	0.86	10/19767 (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	2
1	B	0	2
1	C	0	2
1	D	0	1
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	542	VAL	CA-CB	6.76	1.69	1.54
1	A	542	VAL	CA-CB	6.10	1.67	1.54
1	D	542	VAL	CA-CB	5.75	1.66	1.54
1	D	545	TRP	CE3-CZ3	5.07	1.47	1.38

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	350	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	547	LEU	CA-CB-CG	5.94	128.96	115.30
1	A	219	ASP	CB-CG-OD1	5.83	123.55	118.30
1	C	542	VAL	N-CA-C	5.72	126.43	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ASP	CB-CG-OD2	-5.30	113.53	118.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	541	LYS	Peptide
1	A	544	GLN	Peptide
1	B	340	GLY	Peptide
1	B	541	LYS	Peptide
1	C	70	LYS	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3576	0	3537	106	0
1	B	3572	0	3526	110	0
1	C	3597	0	3554	127	0
1	D	3617	0	3571	93	0
2	A	149	0	0	0	0
2	B	166	0	0	6	0
2	C	139	0	0	5	0
2	D	173	0	0	2	0
All	All	14989	0	14188	409	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 409 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:123:PHE:CZ	1:B:131:MSE:HE2	1.73	1.21
1:A:403:MSE:HE2	1:A:423:ALA:HB2	1.27	1.17
1:C:403:MSE:HE2	1:C:423:ALA:HB2	1.28	1.15
1:A:541:LYS:HD3	1:A:542:VAL:HG23	1.24	1.14

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:121:LYS:HE2	2:D:691:HOH:O	1.55	1.05

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	469/593 (79%)	426 (91%)	39 (8%)	4 (1%)	25 60
1	B	469/593 (79%)	428 (91%)	32 (7%)	9 (2%)	12 34
1	C	472/593 (80%)	433 (92%)	33 (7%)	6 (1%)	18 47
1	D	475/593 (80%)	437 (92%)	37 (8%)	1 (0%)	56 87
All	All	1885/2372 (80%)	1724 (92%)	141 (8%)	20 (1%)	21 53

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	542	VAL
1	B	326	ASP
1	B	344	GLN
1	B	542	VAL
1	C	326	ASP

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	373/460 (81%)	340 (91%)	33 (9%)	14 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	372/460 (81%)	328 (88%)	44 (12%)	8	20
1	C	374/460 (81%)	333 (89%)	41 (11%)	9	24
1	D	377/460 (82%)	339 (90%)	38 (10%)	11	28
All	All	1496/1840 (81%)	1340 (90%)	156 (10%)	10	26

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	511	VAL
1	C	252	GLU
1	D	446	ASP
1	B	525	SER
1	C	111	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	424	ASN
1	C	167	ASN
1	D	346	ASN
1	B	483	ASN
1	C	128	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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, 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	473/593 (79%)	-0.28	7 (1%) 70 73	9, 25, 46, 60	0
1	B	473/593 (79%)	-0.28	4 (0%) 83 85	11, 23, 50, 62	0
1	C	476/593 (80%)	-0.24	12 (2%) 54 58	9, 21, 43, 60	0
1	D	479/593 (80%)	-0.25	8 (1%) 67 70	10, 23, 45, 55	0
All	All	1901/2372 (80%)	-0.26	31 (1%) 68 71	9, 23, 47, 62	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	322	ALA	5.0
1	C	324	THR	4.4
1	C	545	TRP	4.3
1	D	551	VAL	4.0
1	C	546	HIS	4.0

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 carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.