



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 06:49 am BST

PDB ID : 5F5P  
Title : Molecular Basis for Shroom2 Recognition by Rock1  
Authors : Zalewski, J.K.; VanDemark, A.P.; Heroux, A.  
Deposited on : 2015-12-04  
Resolution : 3.57 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

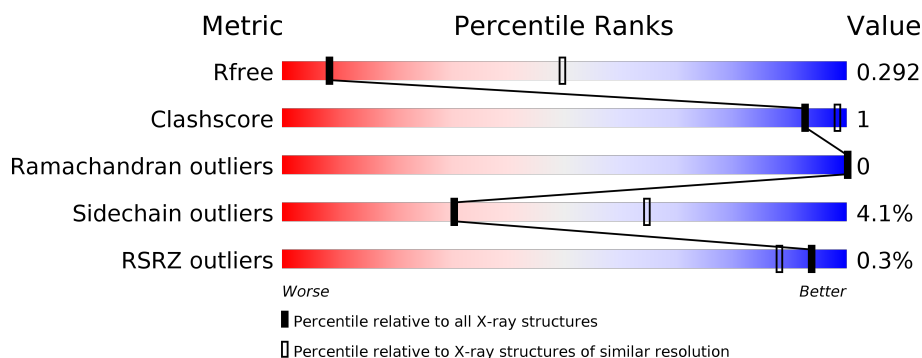
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.57 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	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	217	
1	B	217	
1	G	217	
1	H	217	
2	C	86	
2	D	86	

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Mol	Chain	Length	Quality of chain
2	E	86	
2	F	86	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	1701	-	-	-	X
3	CL	B	1701	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15406 atoms, of which 7771 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 Protein Shroom2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	181	Total	C	H	N	O	S	0	0	0
			2935	907	1482	255	287	4			
1	B	171	Total	C	H	N	O	S	0	0	0
			2816	871	1427	244	270	4			
1	G	180	Total	C	H	N	O	S	0	0	0
			2938	908	1487	254	285	4			
1	H	171	Total	C	H	N	O	S	0	0	0
			2811	869	1426	243	269	4			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1421	GLY	-	expression tag	UNP Q13796
A	1422	ILE	-	expression tag	UNP Q13796
A	1423	ASP	-	expression tag	UNP Q13796
A	1424	PRO	-	expression tag	UNP Q13796
A	1425	PHE	-	expression tag	UNP Q13796
A	1426	THR	-	expression tag	UNP Q13796
A	1611	HIS	-	expression tag	UNP Q13796
A	1612	SER	-	expression tag	UNP Q13796
A	1613	LYS	-	expression tag	UNP Q13796
A	1614	ARG	-	expression tag	UNP Q13796
A	1615	ALA	-	expression tag	UNP Q13796
A	1616	SER	-	expression tag	UNP Q13796
A	1617	SER	-	expression tag	UNP Q13796
A	1618	ASP	-	expression tag	UNP Q13796
A	1619	PRO	-	expression tag	UNP Q13796
A	1620	ALA	-	expression tag	UNP Q13796
A	1621	ALA	-	expression tag	UNP Q13796
A	1622	ASN	-	expression tag	UNP Q13796
A	1623	LYS	-	expression tag	UNP Q13796
A	1624	ALA	-	expression tag	UNP Q13796
A	1625	ARG	-	expression tag	UNP Q13796

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1626	LYS	-	expression tag	UNP Q13796
A	1627	GLU	-	expression tag	UNP Q13796
A	1628	ALA	-	expression tag	UNP Q13796
A	1629	GLU	-	expression tag	UNP Q13796
A	1630	LEU	-	expression tag	UNP Q13796
A	1631	ALA	-	expression tag	UNP Q13796
A	1632	ALA	-	expression tag	UNP Q13796
A	1633	ALA	-	expression tag	UNP Q13796
A	1634	THR	-	expression tag	UNP Q13796
A	1635	ALA	-	expression tag	UNP Q13796
A	1636	GLU	-	expression tag	UNP Q13796
A	1637	GLN	-	expression tag	UNP Q13796
B	1421	GLY	-	expression tag	UNP Q13796
B	1422	ILE	-	expression tag	UNP Q13796
B	1423	ASP	-	expression tag	UNP Q13796
B	1424	PRO	-	expression tag	UNP Q13796
B	1425	PHE	-	expression tag	UNP Q13796
B	1426	THR	-	expression tag	UNP Q13796
B	1611	HIS	-	expression tag	UNP Q13796
B	1612	SER	-	expression tag	UNP Q13796
B	1613	LYS	-	expression tag	UNP Q13796
B	1614	ARG	-	expression tag	UNP Q13796
B	1615	ALA	-	expression tag	UNP Q13796
B	1616	SER	-	expression tag	UNP Q13796
B	1617	SER	-	expression tag	UNP Q13796
B	1618	ASP	-	expression tag	UNP Q13796
B	1619	PRO	-	expression tag	UNP Q13796
B	1620	ALA	-	expression tag	UNP Q13796
B	1621	ALA	-	expression tag	UNP Q13796
B	1622	ASN	-	expression tag	UNP Q13796
B	1623	LYS	-	expression tag	UNP Q13796
B	1624	ALA	-	expression tag	UNP Q13796
B	1625	ARG	-	expression tag	UNP Q13796
B	1626	LYS	-	expression tag	UNP Q13796
B	1627	GLU	-	expression tag	UNP Q13796
B	1628	ALA	-	expression tag	UNP Q13796
B	1629	GLU	-	expression tag	UNP Q13796
B	1630	LEU	-	expression tag	UNP Q13796
B	1631	ALA	-	expression tag	UNP Q13796
B	1632	ALA	-	expression tag	UNP Q13796
B	1633	ALA	-	expression tag	UNP Q13796
B	1634	THR	-	expression tag	UNP Q13796

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1635	ALA	-	expression tag	UNP Q13796
B	1636	GLU	-	expression tag	UNP Q13796
B	1637	GLN	-	expression tag	UNP Q13796
G	1421	GLY	-	expression tag	UNP Q13796
G	1422	ILE	-	expression tag	UNP Q13796
G	1423	ASP	-	expression tag	UNP Q13796
G	1424	PRO	-	expression tag	UNP Q13796
G	1425	PHE	-	expression tag	UNP Q13796
G	1426	THR	-	expression tag	UNP Q13796
G	1611	HIS	-	expression tag	UNP Q13796
G	1612	SER	-	expression tag	UNP Q13796
G	1613	LYS	-	expression tag	UNP Q13796
G	1614	ARG	-	expression tag	UNP Q13796
G	1615	ALA	-	expression tag	UNP Q13796
G	1616	SER	-	expression tag	UNP Q13796
G	1617	SER	-	expression tag	UNP Q13796
G	1618	ASP	-	expression tag	UNP Q13796
G	1619	PRO	-	expression tag	UNP Q13796
G	1620	ALA	-	expression tag	UNP Q13796
G	1621	ALA	-	expression tag	UNP Q13796
G	1622	ASN	-	expression tag	UNP Q13796
G	1623	LYS	-	expression tag	UNP Q13796
G	1624	ALA	-	expression tag	UNP Q13796
G	1625	ARG	-	expression tag	UNP Q13796
G	1626	LYS	-	expression tag	UNP Q13796
G	1627	GLU	-	expression tag	UNP Q13796
G	1628	ALA	-	expression tag	UNP Q13796
G	1629	GLU	-	expression tag	UNP Q13796
G	1630	LEU	-	expression tag	UNP Q13796
G	1631	ALA	-	expression tag	UNP Q13796
G	1632	ALA	-	expression tag	UNP Q13796
G	1633	ALA	-	expression tag	UNP Q13796
G	1634	THR	-	expression tag	UNP Q13796
G	1635	ALA	-	expression tag	UNP Q13796
G	1636	GLU	-	expression tag	UNP Q13796
G	1637	GLN	-	expression tag	UNP Q13796
H	1421	GLY	-	expression tag	UNP Q13796
H	1422	ILE	-	expression tag	UNP Q13796
H	1423	ASP	-	expression tag	UNP Q13796
H	1424	PRO	-	expression tag	UNP Q13796
H	1425	PHE	-	expression tag	UNP Q13796
H	1426	THR	-	expression tag	UNP Q13796

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1611	HIS	-	expression tag	UNP Q13796
H	1612	SER	-	expression tag	UNP Q13796
H	1613	LYS	-	expression tag	UNP Q13796
H	1614	ARG	-	expression tag	UNP Q13796
H	1615	ALA	-	expression tag	UNP Q13796
H	1616	SER	-	expression tag	UNP Q13796
H	1617	SER	-	expression tag	UNP Q13796
H	1618	ASP	-	expression tag	UNP Q13796
H	1619	PRO	-	expression tag	UNP Q13796
H	1620	ALA	-	expression tag	UNP Q13796
H	1621	ALA	-	expression tag	UNP Q13796
H	1622	ASN	-	expression tag	UNP Q13796
H	1623	LYS	-	expression tag	UNP Q13796
H	1624	ALA	-	expression tag	UNP Q13796
H	1625	ARG	-	expression tag	UNP Q13796
H	1626	LYS	-	expression tag	UNP Q13796
H	1627	GLU	-	expression tag	UNP Q13796
H	1628	ALA	-	expression tag	UNP Q13796
H	1629	GLU	-	expression tag	UNP Q13796
H	1630	LEU	-	expression tag	UNP Q13796
H	1631	ALA	-	expression tag	UNP Q13796
H	1632	ALA	-	expression tag	UNP Q13796
H	1633	ALA	-	expression tag	UNP Q13796
H	1634	THR	-	expression tag	UNP Q13796
H	1635	ALA	-	expression tag	UNP Q13796
H	1636	GLU	-	expression tag	UNP Q13796
H	1637	GLN	-	expression tag	UNP Q13796

- Molecule 2 is a protein called Rho-associated protein kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	55	Total	C	H	N	O	S	0	0	0
			931	288	464	79	99	1			
2	D	61	Total	C	H	N	O	S	0	0	0
			1020	316	507	86	110	1			
2	E	57	Total	C	H	N	O	S	0	0	0
			968	300	485	80	102	1			
2	F	58	Total	C	H	N	O	S	0	0	0
			985	305	493	82	104	1			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	828	GLY	-	expression tag	UNP Q13464
C	829	ILE	-	expression tag	UNP Q13464
C	830	ASP	-	expression tag	UNP Q13464
C	831	PRO	-	expression tag	UNP Q13464
C	832	PHE	-	expression tag	UNP Q13464
C	833	THR	-	expression tag	UNP Q13464
D	828	GLY	-	expression tag	UNP Q13464
D	829	ILE	-	expression tag	UNP Q13464
D	830	ASP	-	expression tag	UNP Q13464
D	831	PRO	-	expression tag	UNP Q13464
D	832	PHE	-	expression tag	UNP Q13464
D	833	THR	-	expression tag	UNP Q13464
E	828	GLY	-	expression tag	UNP Q13464
E	829	ILE	-	expression tag	UNP Q13464
E	830	ASP	-	expression tag	UNP Q13464
E	831	PRO	-	expression tag	UNP Q13464
E	832	PHE	-	expression tag	UNP Q13464
E	833	THR	-	expression tag	UNP Q13464
F	828	GLY	-	expression tag	UNP Q13464
F	829	ILE	-	expression tag	UNP Q13464
F	830	ASP	-	expression tag	UNP Q13464
F	831	PRO	-	expression tag	UNP Q13464
F	832	PHE	-	expression tag	UNP Q13464
F	833	THR	-	expression tag	UNP Q13464

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0

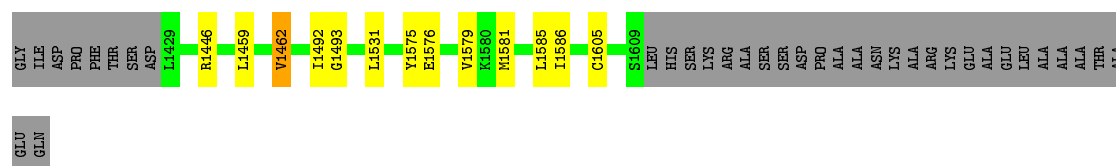


### 3 Residue-property plots [i](#)

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.

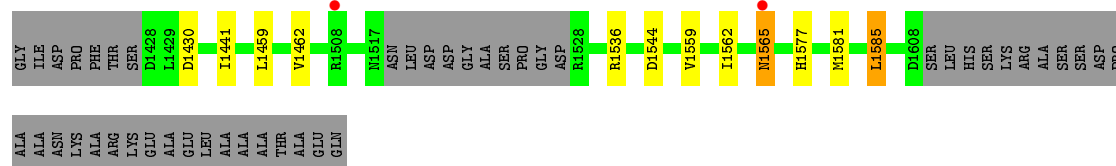
#### • Molecule 1: Protein Shroom2

Chain A: 



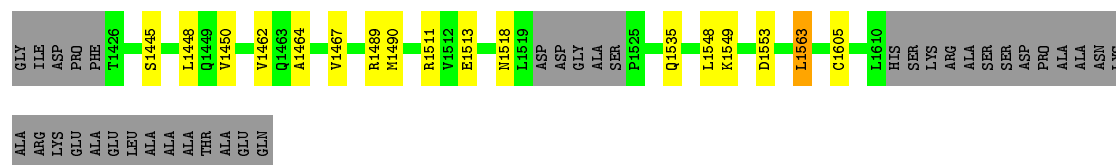
#### • Molecule 1: Protein Shroom2

Chain B: 



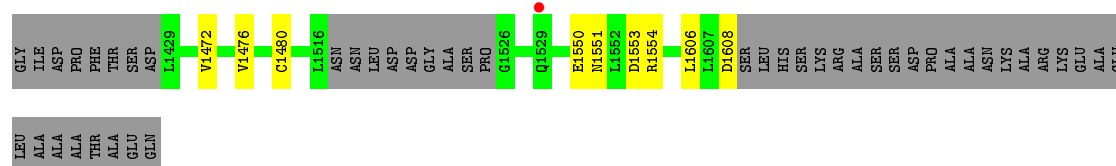
#### • Molecule 1: Protein Shroom2

Chain G: 



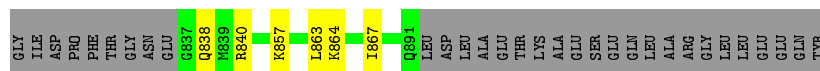
#### • Molecule 1: Protein Shroom2

Chain H: 



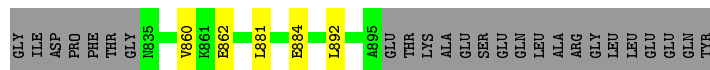
- Molecule 2: Rho-associated protein kinase 1

Chain C:  57% 7% 36%



- Molecule 2: Rho-associated protein kinase 1

Chain D:  65% 6% 29%



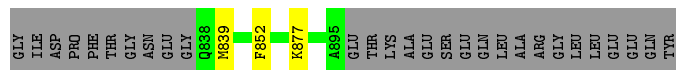
- Molecule 2: Rho-associated protein kinase 1

Chain E:  59% 7% 34%



- Molecule 2: Rho-associated protein kinase 1

Chain F:  64% 0% 33%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.59Å 133.79Å 135.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 3.57 47.67 – 3.57	Depositor EDS
% Data completeness (in resolution range)	96.8 (19.91-3.57) 85.9 (47.67-3.57)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 3.57Å)	Xtriage
Refinement program	PHENIX (dev_2219)	Depositor
R, $R_{free}$	0.271 , 0.287 0.281 , 0.292	Depositor DCC
$R_{free}$ test set	955 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	120.3	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 90.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15406	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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:  
CL

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	0.25	0/1465	0.42	0/1965
1	B	0.25	0/1399	0.41	0/1873
1	G	0.25	0/1462	0.41	0/1959
1	H	0.25	0/1395	0.40	0/1867
2	C	0.25	0/469	0.38	0/624
2	D	0.26	0/515	0.41	0/687
2	E	0.26	0/485	0.39	0/647
2	F	0.25	0/494	0.38	0/659
All	All	0.25	0/7684	0.41	0/10281

There are no bond length outliers.

There are no bond angle outliers.

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	1453	1482	1481	5	2
1	B	1389	1427	1427	7	0
1	G	1451	1487	1487	5	2
1	H	1385	1426	1424	2	0
2	C	467	464	464	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	513	507	507	0	0
2	E	483	485	484	2	0
2	F	492	493	492	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	7635	7771	7766	23	2

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 1.

The worst 5 of 23 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:G:1513:GLU:OE2	1:G:1535:GLN:NE2	2.27	0.68
2:C:838:GLN:OE1	2:C:838:GLN:N	2.42	0.53
1:B:1581:MET:O	1:B:1585:LEU:HB2	2.10	0.51
1:B:1459:LEU:O	1:B:1462:VAL:HG12	2.10	0.51
1:H:1472:VAL:O	1:H:1476:VAL:HG23	2.11	0.50

All (2) 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:1605:CYS:SG	1:G:1605:CYS:HG[4_545]	1.47	0.13
1:A:1605:CYS:HG	1:G:1605:CYS:SG[4_545]	1.58	0.02

## 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	179/217 (82%)	177 (99%)	2 (1%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	167/217 (77%)	166 (99%)	1 (1%)	0	100	100
1	G	176/217 (81%)	172 (98%)	4 (2%)	0	100	100
1	H	167/217 (77%)	164 (98%)	3 (2%)	0	100	100
2	C	53/86 (62%)	52 (98%)	1 (2%)	0	100	100
2	D	59/86 (69%)	59 (100%)	0	0	100	100
2	E	55/86 (64%)	55 (100%)	0	0	100	100
2	F	56/86 (65%)	55 (98%)	1 (2%)	0	100	100
All	All	912/1212 (75%)	900 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	163/189 (86%)	158 (97%)	5 (3%)	40	71
1	B	156/189 (82%)	151 (97%)	5 (3%)	39	70
1	G	164/189 (87%)	156 (95%)	8 (5%)	25	59
1	H	155/189 (82%)	150 (97%)	5 (3%)	39	70
2	C	52/77 (68%)	50 (96%)	2 (4%)	33	66
2	D	57/77 (74%)	52 (91%)	5 (9%)	10	40
2	E	54/77 (70%)	52 (96%)	2 (4%)	34	67
2	F	55/77 (71%)	52 (94%)	3 (6%)	21	56
All	All	856/1064 (80%)	821 (96%)	35 (4%)	30	64

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	884	GLU
2	F	839	MET

*Continued on next page...*

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Mol	Chain	Res	Type
1	H	1551	ASN
2	D	892	LEU
2	E	882	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	1551	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 [i](#)

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	181/217 (83%)	-0.10	0 100 100	87, 127, 166, 200	0
1	B	171/217 (78%)	-0.08	2 (1%) 79 65	85, 142, 189, 203	0
1	G	180/217 (82%)	-0.04	0 100 100	113, 163, 202, 230	0
1	H	171/217 (78%)	-0.05	1 (0%) 89 80	106, 142, 197, 217	0
2	C	55/86 (63%)	-0.24	0 100 100	97, 153, 196, 206	0
2	D	61/86 (70%)	-0.25	0 100 100	100, 154, 199, 209	0
2	E	57/86 (66%)	-0.15	0 100 100	120, 171, 219, 229	0
2	F	58/86 (67%)	-0.20	0 100 100	111, 163, 197, 203	0
All	All	934/1212 (77%)	-0.10	3 (0%) 94 88	85, 147, 198, 230	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1508	ARG	2.5
1	H	1529	GLN	2.5
1	B	1565	ASN	2.2

### 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 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	CL	B	1701	1/1	0.21	1.03	167,167,167,167	0
3	CL	A	1701	1/1	0.44	0.84	139,139,139,139	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.