



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:55 am BST

PDB ID : 6QSZ  
Title : Crystal structure of the Sir4 H-BRCT domain in complex with Esc1 pS1450 peptide  
Authors : Deshpande, I.; Keusch, J.J.; Challa, K.; Iesmantavicius, V.; Gasser, S.M.; Gut, H.  
Deposited on : 2019-02-22  
Resolution : 2.50 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](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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

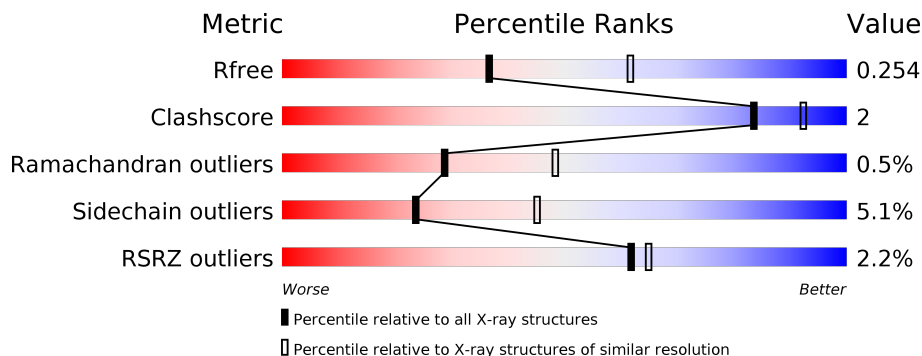
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	127	
1	C	127	
1	E	127	
1	G	127	
1	I	127	
1	K	127	

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Mol	Chain	Length	Quality of chain
1	M	127	<p>2% 80% 9% 10%</p>
1	O	127	<p>6% 77% 9% 13%</p>
2	B	16	<p>56% 44%</p>
2	D	16	<p>50% 6% 44%</p>
2	F	16	<p>50% 6% 44%</p>
2	H	16	<p>69% 31%</p>
2	J	16	<p>31% 13% 56%</p>
2	L	16	<p>56% 6% 38%</p>
2	N	16	<p>56% 6% 38%</p>
2	P	16	<p>63% 38%</p>

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 8262 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 Regulatory protein SIR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	112	Total 945	C 604	N 156	O 179	Se 6	0	2	0
1	C	113	Total 937	C 600	N 155	O 178	Se 4	0	0	0
1	E	113	Total 938	C 599	N 156	O 179	Se 4	0	0	0
1	G	114	Total 943	C 602	N 157	O 180	Se 4	0	0	0
1	I	112	Total 931	C 595	N 155	O 177	Se 4	0	0	0
1	K	114	Total 949	C 606	N 158	O 181	Se 4	0	0	0
1	M	114	Total 951	C 607	N 157	O 183	Se 4	0	1	0
1	O	111	Total 922	C 589	N 153	O 176	Se 4	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	959	GLY	-	expression tag	UNP P11978
A	960	PRO	-	expression tag	UNP P11978
C	959	GLY	-	expression tag	UNP P11978
C	960	PRO	-	expression tag	UNP P11978
E	959	GLY	-	expression tag	UNP P11978
E	960	PRO	-	expression tag	UNP P11978
G	959	GLY	-	expression tag	UNP P11978
G	960	PRO	-	expression tag	UNP P11978
I	959	GLY	-	expression tag	UNP P11978
I	960	PRO	-	expression tag	UNP P11978
K	959	GLY	-	expression tag	UNP P11978
K	960	PRO	-	expression tag	UNP P11978
M	959	GLY	-	expression tag	UNP P11978

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Chain	Residue	Modelled	Actual	Comment	Reference
M	960	PRO	-	expression tag	UNP P11978
O	959	GLY	-	expression tag	UNP P11978
O	960	PRO	-	expression tag	UNP P11978

- Molecule 2 is a protein called Silent chromatin protein ESC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	P	0	0	0
			68	39	9	19	1			
2	D	9	Total	C	N	O	P	0	0	0
			68	39	9	19	1			
2	F	9	Total	C	N	O	P	0	0	0
			68	39	9	19	1			
2	H	11	Total	C	N	O	P	0	0	0
			82	46	11	24	1			
2	J	7	Total	C	N	O	P	0	0	0
			55	32	7	15	1			
2	L	10	Total	C	N	O	P	0	0	0
			74	42	10	21	1			
2	N	10	Total	C	N	O	P	0	0	0
			74	42	10	21	1			
2	P	10	Total	C	N	O	P	0	0	0
			74	42	10	21	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	B	8	Total	O	0	0
			8	8		
4	C	28	Total	O	0	0
			28	28		
4	D	5	Total	O	0	0
			5	5		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	E	12	Total O 12 12	0	0
4	F	1	Total O 1 1	0	0
4	G	35	Total O 35 35	0	0
4	H	4	Total O 4 4	0	0
4	I	23	Total O 23 23	0	0
4	J	3	Total O 3 3	0	0
4	K	16	Total O 16 16	0	0
4	L	3	Total O 3 3	0	0
4	M	9	Total O 9 9	0	0
4	N	3	Total O 3 3	0	0
4	O	8	Total O 8 8	0	0
4	P	3	Total O 3 3	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: Regulatory protein SIR4

Chain A: 




- Molecule 1: Regulatory protein SIR4

Chain C: 




- Molecule 1: Regulatory protein SIR4

Chain E: 




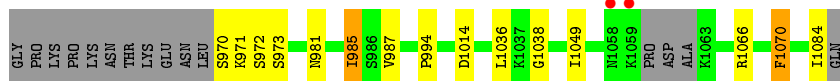
- Molecule 1: Regulatory protein SIR4

Chain G: 

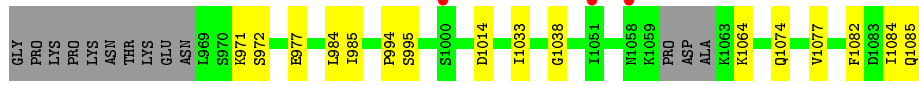
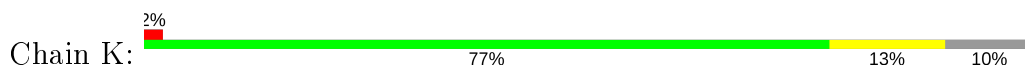


- Molecule 1: Regulatory protein SIR4

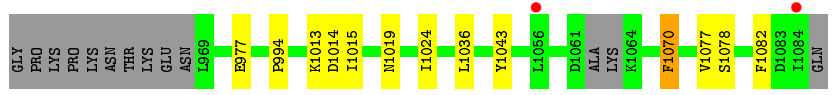
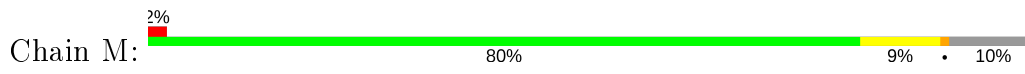
Chain I: 



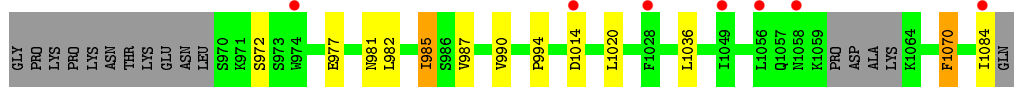
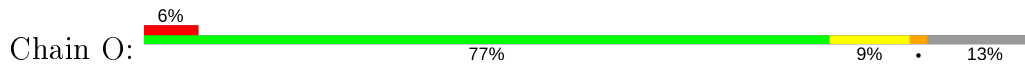
- Molecule 1: Regulatory protein SIR4



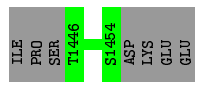
• Molecule 1: Regulatory protein SIR4



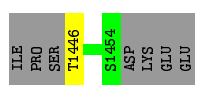
• Molecule 1: Regulatory protein SIR4



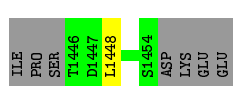
• Molecule 2: Silent chromatin protein ESC1



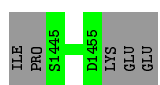
• Molecule 2: Silent chromatin protein ESC1



• Molecule 2: Silent chromatin protein ESC1



• Molecule 2: Silent chromatin protein ESC1

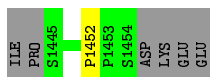




## ● Molecule 2: Silent chromatin protein ESC1

Chain J: 

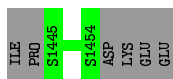
## ● Molecule 2: Silent chromatin protein ESC1

Chain L: 

## ● Molecule 2: Silent chromatin protein ESC1

Chain N: 

## ● Molecule 2: Silent chromatin protein ESC1

Chain P: 

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.06Å 68.34Å 77.81Å 72.61° 84.10° 87.41°	Depositor
Resolution (Å)	46.58 – 2.50 46.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (46.58-2.50) 96.6 (46.58-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 2.51Å)	Xtrriage
Refinement program	BUSTER 2.11.5	Depositor
R, $R_{free}$	0.189 , 0.234 0.209 , 0.254	Depositor DCC
$R_{free}$ test set	2124 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.8	Xtrriage
Anisotropy	0.428	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 52.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8262	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SEP

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	0.51	0/958	0.71	0/1277
1	C	0.52	0/950	0.66	0/1268
1	E	0.45	0/950	0.64	0/1267
1	G	0.53	0/955	0.68	0/1274
1	I	0.47	0/943	0.70	0/1256
1	K	0.46	0/961	0.66	0/1279
1	M	0.48	0/964	0.65	0/1287
1	O	0.44	0/934	0.63	0/1245
2	B	0.59	0/59	0.76	0/81
2	D	0.68	0/59	0.81	0/81
2	F	0.54	0/59	0.70	0/81
2	H	0.64	0/73	0.78	0/100
2	J	0.51	0/46	0.75	0/63
2	L	0.62	0/65	0.76	0/89
2	N	0.72	0/65	0.78	0/89
2	P	0.59	0/65	0.86	0/89
All	All	0.49	0/8106	0.68	0/10826

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

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	945	0	939	3	0
1	C	937	0	934	4	0
1	E	938	0	933	7	0
1	G	943	0	938	5	0
1	I	931	0	929	5	0
1	K	949	0	948	7	0
1	M	951	0	942	5	0
1	O	922	0	916	4	0
2	B	68	0	55	0	0
2	D	68	0	55	0	0
2	F	68	0	55	1	0
2	H	82	0	64	0	0
2	J	55	0	43	1	0
2	L	74	0	60	1	0
2	N	74	0	60	1	0
2	P	74	0	60	0	0
3	C	1	0	0	0	0
4	A	21	0	0	0	0
4	B	8	0	0	0	0
4	C	28	0	0	0	0
4	D	5	0	0	0	0
4	E	12	0	0	0	0
4	F	1	0	0	0	0
4	G	35	0	0	0	0
4	H	4	0	0	0	0
4	I	23	0	0	0	0
4	J	3	0	0	0	0
4	K	16	0	0	0	0
4	L	3	0	0	0	0
4	M	9	0	0	0	0
4	N	3	0	0	1	0
4	O	8	0	0	0	0
4	P	3	0	0	0	0
All	All	8262	0	7931	39	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 2.

All (39) 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:K:1074:GLN:HG2	1:K:1084:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1015:ILE:HA	1:M:1019:ASN:HD22	1.67	0.58
1:K:1077:VAL:HG12	1:K:1082:PHE:O	2.04	0.58
1:G:985:ILE:HD11	1:G:987:VAL:HG22	1.89	0.54
1:I:985:ILE:HD11	1:I:987:VAL:HG22	1.90	0.53
1:C:983:LYS:NZ	1:E:1026:ASN:HD22	2.06	0.53
1:M:1013:LYS:HE2	1:M:1024:ILE:HG21	1.91	0.53
1:C:985:ILE:HD11	1:C:987:VAL:HG22	1.93	0.51
1:O:985:ILE:HD11	1:O:987:VAL:HG22	1.93	0.51
1:G:969:LEU:HD22	1:G:973:SER:HB3	1.92	0.50
1:K:994:PRO:HG3	1:K:1038:GLY:HA3	1.92	0.50
1:I:970:SER:HB3	2:J:1453:PRO:HG3	1.94	0.48
1:E:982:LEU:HA	1:E:985:ILE:HG12	1.96	0.48
1:E:977:GLU:HG2	2:F:1448:LEU:HD13	1.98	0.46
1:A:990:VAL:HG22	1:A:1036:LEU:HA	1.98	0.45
1:M:1077:VAL:HG12	1:M:1082:PHE:O	2.16	0.45
1:O:981:ASN:O	1:O:985:ILE:HG23	2.17	0.45
1:E:969:LEU:HD21	1:E:974:TRP:HB2	1.99	0.44
1:G:1009:MSE:HB3	1:K:984:LEU:HD22	1.99	0.44
1:M:1036:LEU:O	1:M:1070:PHE:HB3	2.17	0.44
1:G:981:ASN:O	1:G:985:ILE:HG23	2.18	0.43
1:E:1036:LEU:O	1:E:1070:PHE:HB3	2.19	0.43
1:I:1036:LEU:O	1:I:1070:PHE:HB3	2.19	0.43
1:I:981:ASN:O	1:I:985:ILE:HG23	2.19	0.43
2:N:1447:ASP:HB2	4:N:1503:HOH:O	2.17	0.43
1:K:971:LYS:HD3	2:L:1452:PRO:HB3	2.01	0.43
1:C:981:ASN:O	1:C:985:ILE:HG23	2.18	0.42
1:A:988:SER:HB2	1:A:1031:SER:OG	2.18	0.42
1:M:994:PRO:HB3	1:M:1043:TYR:CD1	2.54	0.42
1:A:1074:GLN:NE2	1:A:1084:ILE:HD11	2.34	0.42
1:G:1008:LYS:HD2	1:G:1070:PHE:HE2	1.84	0.42
1:E:987:VAL:HG21	1:E:1016:PHE:CD2	2.55	0.41
1:K:1077:VAL:CG1	1:K:1082:PHE:O	2.67	0.41
1:C:988:SER:HB2	1:C:1031:SER:OG	2.20	0.41
1:I:994:PRO:HG3	1:I:1038:GLY:HA3	2.03	0.41
1:O:982:LEU:HD13	1:O:1020:LEU:HB3	2.03	0.41
1:K:985:ILE:HG21	1:K:1033:ILE:HD12	2.03	0.40
1:O:1036:LEU:O	1:O:1070:PHE:HB3	2.21	0.40
1:E:981:ASN:O	1:E:985:ILE:HG23	2.21	0.40

There are no symmetry-related clashes.

## 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	110/127 (87%)	109 (99%)	1 (1%)	0	100	100
1	C	109/127 (86%)	107 (98%)	2 (2%)	0	100	100
1	E	109/127 (86%)	106 (97%)	2 (2%)	1 (1%)	17	31
1	G	110/127 (87%)	107 (97%)	3 (3%)	0	100	100
1	I	108/127 (85%)	104 (96%)	3 (3%)	1 (1%)	17	31
1	K	110/127 (87%)	106 (96%)	2 (2%)	2 (2%)	8	14
1	M	111/127 (87%)	107 (96%)	4 (4%)	0	100	100
1	O	107/127 (84%)	104 (97%)	2 (2%)	1 (1%)	17	31
2	B	6/16 (38%)	5 (83%)	1 (17%)	0	100	100
2	D	6/16 (38%)	6 (100%)	0	0	100	100
2	F	6/16 (38%)	5 (83%)	1 (17%)	0	100	100
2	H	8/16 (50%)	7 (88%)	1 (12%)	0	100	100
2	J	4/16 (25%)	4 (100%)	0	0	100	100
2	L	7/16 (44%)	6 (86%)	1 (14%)	0	100	100
2	N	7/16 (44%)	6 (86%)	1 (14%)	0	100	100
2	P	7/16 (44%)	5 (71%)	2 (29%)	0	100	100
All	All	925/1144 (81%)	894 (97%)	26 (3%)	5 (0%)	29	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	994	PRO
1	O	994	PRO
1	I	971	LYS
1	K	995	SER
1	K	1064	LYS

### 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	108/115 (94%)	103 (95%)	5 (5%)	27	50
1	C	107/115 (93%)	102 (95%)	5 (5%)	26	49
1	E	107/115 (93%)	101 (94%)	6 (6%)	21	40
1	G	107/115 (93%)	101 (94%)	6 (6%)	21	40
1	I	106/115 (92%)	98 (92%)	8 (8%)	13	26
1	K	108/115 (94%)	104 (96%)	4 (4%)	34	60
1	M	109/115 (95%)	105 (96%)	4 (4%)	34	60
1	O	105/115 (91%)	98 (93%)	7 (7%)	16	31
2	B	8/15 (53%)	8 (100%)	0	100	100
2	D	8/15 (53%)	7 (88%)	1 (12%)	4	8
2	F	8/15 (53%)	8 (100%)	0	100	100
2	H	10/15 (67%)	10 (100%)	0	100	100
2	J	6/15 (40%)	5 (83%)	1 (17%)	2	4
2	L	9/15 (60%)	9 (100%)	0	100	100
2	N	9/15 (60%)	9 (100%)	0	100	100
2	P	9/15 (60%)	9 (100%)	0	100	100
All	All	924/1040 (89%)	877 (95%)	47 (5%)	24	45

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1000	SER
1	A	1014	ASP
1	A	1064	LYS
1	A	1077	VAL
1	A	1083	ASP
1	C	985	ILE
1	C	1014	ASP
1	C	1047	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	1070	PHE
1	C	1083	ASP
2	D	1446	THR
1	E	969	LEU
1	E	985	ILE
1	E	988	SER
1	E	996	GLU
1	E	1014	ASP
1	E	1070	PHE
1	G	972	SER
1	G	977	GLU
1	G	985	ILE
1	G	1014	ASP
1	G	1072	LYS
1	G	1084	ILE
1	I	972	SER
1	I	973	SER
1	I	985	ILE
1	I	1014	ASP
1	I	1049	ILE
1	I	1066	ARG
1	I	1070	PHE
1	I	1084	ILE
2	J	1447	ASP
1	K	972	SER
1	K	977	GLU
1	K	1014	ASP
1	K	1085	GLN
1	M	977	GLU
1	M	1014	ASP
1	M	1070	PHE
1	M	1078	SER
1	O	972	SER
1	O	977	GLU
1	O	985	ILE
1	O	990	VAL
1	O	1014	ASP
1	O	1070	PHE
1	O	1084	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:



Mol	Chain	Res	Type
1	E	1026	ASN
1	M	1019	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](#)

8 non-standard protein/DNA/RNA residues 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	SEP	F	1450	2	8,9,10	1.15	1 (12%)	8,12,14	2.32	2 (25%)
2	SEP	D	1450	2	8,9,10	1.07	1 (12%)	8,12,14	1.85	2 (25%)
2	SEP	P	1450	2	8,9,10	1.06	0	8,12,14	2.04	2 (25%)
2	SEP	J	1450	2	8,9,10	1.36	1 (12%)	8,12,14	2.06	2 (25%)
2	SEP	H	1450	2	8,9,10	0.81	0	8,12,14	2.26	3 (37%)
2	SEP	N	1450	2	8,9,10	1.52	1 (12%)	8,12,14	2.16	1 (12%)
2	SEP	L	1450	2	8,9,10	0.92	0	8,12,14	2.28	2 (25%)
2	SEP	B	1450	2	8,9,10	0.74	0	8,12,14	2.48	2 (25%)

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	SEP	F	1450	2	-	1/5/8/10	-
2	SEP	D	1450	2	-	1/5/8/10	-
2	SEP	P	1450	2	-	1/5/8/10	-
2	SEP	J	1450	2	-	2/5/8/10	-
2	SEP	H	1450	2	-	2/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	N	1450	2	-	1/5/8/10	-
2	SEP	L	1450	2	-	1/5/8/10	-
2	SEP	B	1450	2	-	2/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	1450	SEP	P-OG	-3.70	1.48	1.60
2	J	1450	SEP	P-OG	-2.96	1.50	1.60
2	F	1450	SEP	P-OG	-2.52	1.52	1.60
2	D	1450	SEP	P-OG	-2.20	1.53	1.60

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1450	SEP	OG-CB-CA	5.77	113.76	108.14
2	N	1450	SEP	OG-CB-CA	5.39	113.39	108.14
2	B	1450	SEP	OG-CB-CA	5.35	113.35	108.14
2	L	1450	SEP	OG-CB-CA	5.19	113.19	108.14
2	H	1450	SEP	OG-CB-CA	4.84	112.86	108.14
2	P	1450	SEP	OG-CB-CA	4.58	112.60	108.14
2	J	1450	SEP	O2P-P-OG	4.10	117.65	106.73
2	D	1450	SEP	OG-CB-CA	3.95	111.98	108.14
2	B	1450	SEP	OG-P-O1P	3.50	116.29	106.47
2	J	1450	SEP	OG-CB-CA	3.33	111.39	108.14
2	L	1450	SEP	O2P-P-OG	2.89	114.44	106.73
2	F	1450	SEP	OG-P-O1P	2.60	113.75	106.47
2	H	1450	SEP	OG-P-O1P	2.44	113.33	106.47
2	D	1450	SEP	O2P-P-OG	2.41	113.14	106.73
2	H	1450	SEP	O2P-P-OG	-2.34	100.51	106.73
2	P	1450	SEP	OG-P-O1P	2.18	112.59	106.47

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1450	SEP	CB-OG-P-O2P
2	F	1450	SEP	CA-CB-OG-P
2	D	1450	SEP	CA-CB-OG-P
2	P	1450	SEP	CA-CB-OG-P
2	J	1450	SEP	CA-CB-OG-P

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Mol	Chain	Res	Type	Atoms
2	H	1450	SEP	CA-CB-OG-P
2	N	1450	SEP	CA-CB-OG-P
2	L	1450	SEP	CA-CB-OG-P
2	B	1450	SEP	CA-CB-OG-P
2	J	1450	SEP	CB-OG-P-O2P
2	H	1450	SEP	CB-OG-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 [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, 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	108/127 (85%)	0.25	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	39, 61, 91, 127	0
1	C	109/127 (85%)	0.11	2 (1%) <span style="border: 1px solid blue; padding: 0 2px;">68</span> <span style="border: 1px solid blue; padding: 0 2px;">71</span>	44, 61, 100, 140	0
1	E	109/127 (85%)	0.26	5 (4%) <span style="border: 1px solid red; padding: 0 2px;">32</span> <span style="border: 1px solid red; padding: 0 2px;">34</span>	44, 66, 119, 160	0
1	G	110/127 (86%)	0.02	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	38, 56, 92, 107	0
1	I	108/127 (85%)	0.14	2 (1%) <span style="border: 1px solid blue; padding: 0 2px;">66</span> <span style="border: 1px solid blue; padding: 0 2px;">69</span>	44, 66, 107, 133	0
1	K	110/127 (86%)	0.17	3 (2%) <span style="border: 1px solid blue; padding: 0 2px;">54</span> <span style="border: 1px solid blue; padding: 0 2px;">58</span>	44, 67, 108, 120	0
1	M	110/127 (86%)	0.21	2 (1%) <span style="border: 1px solid blue; padding: 0 2px;">68</span> <span style="border: 1px solid blue; padding: 0 2px;">71</span>	46, 74, 123, 157	0
1	O	107/127 (84%)	0.36	7 (6%) <span style="border: 1px solid red; padding: 0 2px;">18</span> <span style="border: 1px solid red; padding: 0 2px;">19</span>	48, 79, 118, 151	0
2	B	8/16 (50%)	0.27	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	69, 77, 99, 100	0
2	D	8/16 (50%)	-0.04	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	75, 87, 95, 120	0
2	F	8/16 (50%)	0.44	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	65, 72, 94, 111	0
2	H	10/16 (62%)	0.29	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	51, 60, 87, 89	0
2	J	6/16 (37%)	0.57	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	83, 89, 94, 96	0
2	L	9/16 (56%)	0.12	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	74, 81, 97, 129	0
2	N	9/16 (56%)	0.37	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	76, 82, 92, 115	0
2	P	9/16 (56%)	0.76	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	88, 93, 108, 130	0
All	All	938/1144 (81%)	0.20	21 (2%) <span style="border: 1px solid blue; padding: 0 2px;">62</span> <span style="border: 1px solid blue; padding: 0 2px;">65</span>	38, 67, 111, 160	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	1059	LYS	3.7
1	O	1056	LEU	3.6
1	O	1084	ILE	3.4
1	K	1051	ILE	3.3
1	C	1058	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	O	1058	ASN	2.9
1	E	1084	ILE	2.7
1	E	1056	LEU	2.7
1	E	1049	ILE	2.6
1	M	1056	LEU	2.5
1	E	1053	TYR	2.5
1	O	1014	ASP	2.5
1	K	1058	ASN	2.5
1	C	971	LYS	2.5
1	O	1049	ILE	2.3
1	O	1028	PHE	2.2
1	M	1084	ILE	2.2
1	E	1058	ASN	2.2
1	I	1058	ASN	2.2
1	O	974	TRP	2.1
1	K	1000	SER	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
2	SEP	J	1450	10/11	0.95	0.15	74,77,84,85	0
2	SEP	P	1450	10/11	0.96	0.11	83,85,86,87	0
2	SEP	D	1450	10/11	0.96	0.13	68,70,75,77	0
2	SEP	F	1450	10/11	0.97	0.16	62,64,65,67	0
2	SEP	N	1450	10/11	0.97	0.13	73,73,77,78	0
2	SEP	B	1450	10/11	0.97	0.18	65,66,70,71	0
2	SEP	L	1450	10/11	0.98	0.13	69,73,74,74	0
2	SEP	H	1450	10/11	0.98	0.15	49,53,57,58	0

## 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	C	1101	1/1	0.85	0.15	95,95,95,95	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.