



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:11 AM UTC

PDB ID : 6QSZ / pdb_00006qsz
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

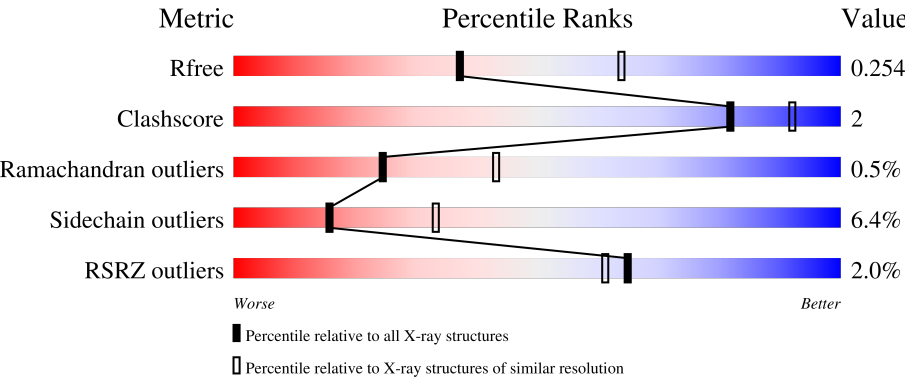
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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 $\leq 5\%$. 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	2% 76% 11% • 12%
1	C	127	2% 78% 9% • 11%
1	E	127	% 76% 10% •• 11%
1	G	127	2% 76% 13% • 10%
1	I	127	% 73% 13% •• 12%

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Mol	Chain	Length	Quality of chain
1	K	127	 77% 11% 10%
1	M	127	 78% 11% 10%
1	O	127	 77% 9% 13%
2	B	16	 50% 6% 44%
2	D	16	 44% 12% 44%
2	F	16	 44% 12% 44%
2	H	16	 62% 6% 31%
2	J	16	 25% 19% 56%
2	L	16	 50% 12% 38%
2	N	16	 50% 12% 38%
2	P	16	 44% 19% 38%

2 Entry composition

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

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 (CCD ID: 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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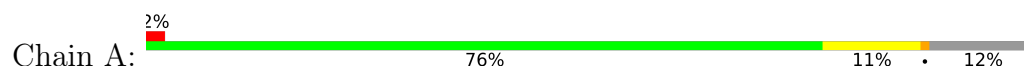
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	12	Total 12	O 12	0	0
4	F	1	Total 1	O 1	0	0
4	G	35	Total 35	O 35	0	0
4	H	4	Total 4	O 4	0	0
4	I	23	Total 23	O 23	0	0
4	J	3	Total 3	O 3	0	0
4	K	16	Total 16	O 16	0	0
4	L	3	Total 3	O 3	0	0
4	M	9	Total 9	O 9	0	0
4	N	3	Total 3	O 3	0	0
4	O	8	Total 8	O 8	0	0
4	P	3	Total 3	O 3	0	0

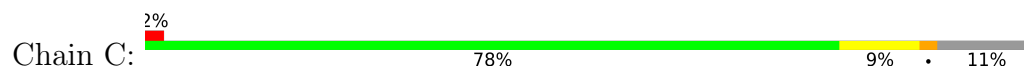
3 Residue-property plots [i](#)

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.

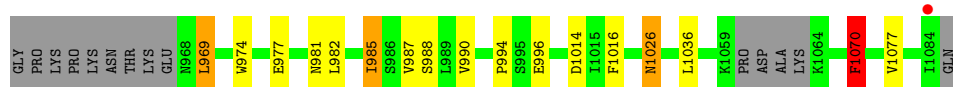
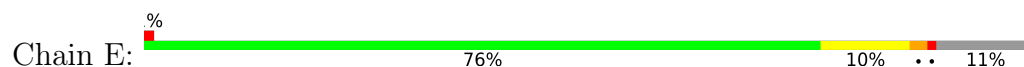
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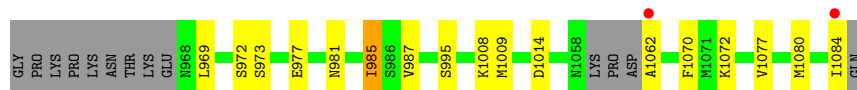
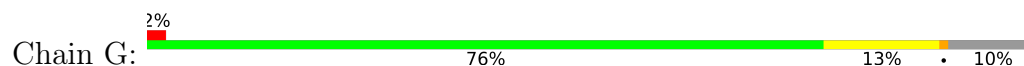
- Molecule 1: Regulatory protein SIR4



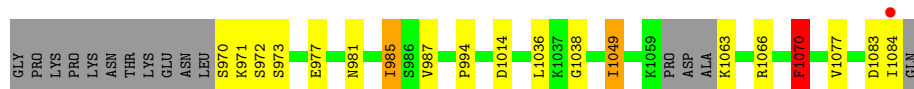
- Molecule 1: Regulatory protein SIR4



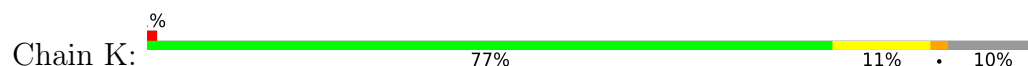
- Molecule 1: Regulatory protein SIR4



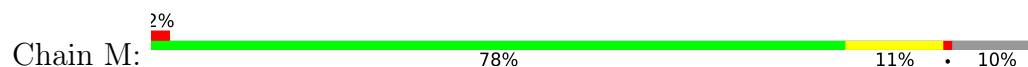
- Molecule 1: Regulatory protein SIR4



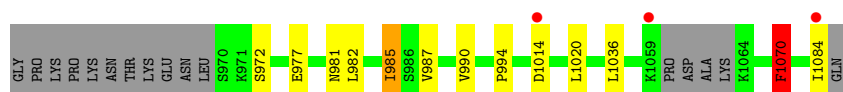
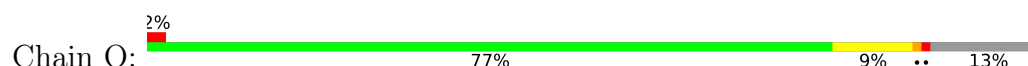
- Molecule 1: Regulatory protein SIR4



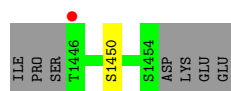
- Molecule 1: Regulatory protein SIR4



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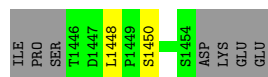
- Molecule 2: Silent chromatin protein ESC1



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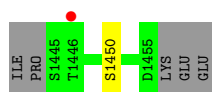


- Molecule 2: Silent chromatin protein ESC1

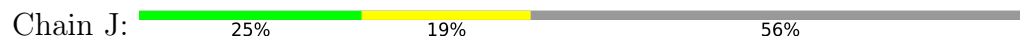


- Molecule 2: Silent chromatin protein ESC1

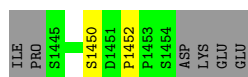




- Molecule 2: Silent chromatin protein ESC1



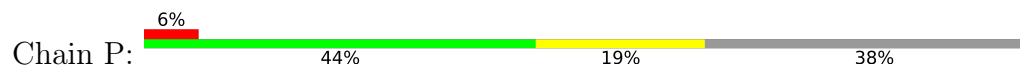
- Molecule 2: Silent chromatin protein ESC1



- Molecule 2: Silent chromatin protein ESC1



- Molecule 2: Silent chromatin protein ESC1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.51Å)	Xtriage
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 ²)	52.8	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8262	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 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	0.86	0/958	1.42	8/1277 (0.6%)
1	C	0.89	1/950 (0.1%)	1.38	5/1268 (0.4%)
1	E	0.75	0/950	1.28	1/1267 (0.1%)
1	G	0.88	2/955 (0.2%)	1.36	5/1274 (0.4%)
1	I	0.81	0/943	1.40	5/1256 (0.4%)
1	K	0.79	0/961	1.35	2/1279 (0.2%)
1	M	0.80	0/964	1.38	3/1287 (0.2%)
1	O	0.75	0/934	1.32	1/1245 (0.1%)
2	B	0.92	0/59	1.05	0/81
2	D	1.03	0/59	1.26	0/81
2	F	0.83	0/59	0.98	0/81
2	H	1.01	0/73	1.10	0/100
2	J	0.78	0/46	0.95	0/63
2	L	0.99	0/65	1.08	0/89
2	N	1.14	0/65	1.12	0/89
2	P	0.97	0/65	1.31	2/89 (2.2%)
All	All	0.83	3/8106 (0.0%)	1.35	32/10826 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1080	MSE	SE-CE	-5.52	1.78	1.95
1	C	1080	MSE	SE-CE	-5.10	1.80	1.95
1	G	995	SER	CA-C	5.05	1.58	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1070	PHE	CA-CB-CG	7.44	121.24	113.80
1	O	1070	PHE	CA-CB-CG	7.43	121.23	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	1070	PHE	CA-CB-CG	7.31	121.11	113.80
1	M	1070	PHE	CA-CB-CG	7.27	121.07	113.80
1	E	1070	PHE	CA-CB-CG	6.59	120.39	113.80
1	I	1083	ASP	CA-CB-CG	6.49	119.09	112.60
1	I	1049	ILE	N-CA-CB	6.06	120.69	110.56
1	A	1064	LYS	CA-C-N	5.91	129.68	120.75
1	A	1064	LYS	C-N-CA	5.91	129.68	120.75
1	C	1047	SER	CA-C-N	5.85	128.11	120.28
1	C	1047	SER	C-N-CA	5.85	128.11	120.28
2	P	1445	SER	CA-C-N	5.63	132.30	121.54
2	P	1445	SER	C-N-CA	5.63	132.30	121.54
1	A	1073	THR	CA-C-N	5.62	127.81	120.28
1	A	1073	THR	C-N-CA	5.62	127.81	120.28
1	I	1063	LYS	CA-C-N	5.56	131.23	122.78
1	I	1063	LYS	C-N-CA	5.56	131.23	122.78
1	A	1072	LYS	CA-C-N	5.54	127.64	120.44
1	A	1072	LYS	C-N-CA	5.54	127.64	120.44
1	C	999	ASP	CA-C-N	5.52	127.61	120.44
1	C	999	ASP	C-N-CA	5.52	127.61	120.44
1	A	973	SER	CA-C-N	5.33	127.42	120.28
1	A	973	SER	C-N-CA	5.33	127.42	120.28
1	K	1084	ILE	CA-C-N	5.30	131.25	121.70
1	K	1084	ILE	C-N-CA	5.30	131.25	121.70
1	G	995	SER	CA-C-N	5.29	131.65	121.54
1	G	995	SER	C-N-CA	5.29	131.65	121.54
1	G	1062	ALA	CA-C-N	5.28	128.58	120.82
1	G	1062	ALA	C-N-CA	5.28	128.58	120.82
1	G	995	SER	N-CA-C	5.12	116.90	110.24
1	M	1047	SER	CA-C-N	5.06	127.31	120.38
1	M	1047	SER	C-N-CA	5.06	127.31	120.38

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	5	0
1	E	938	0	933	8	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	40	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 (40) 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:981:ASN:O	1:I:985:ILE:HG23	2.19	0.43
1:I:1036:LEU:O	1:I:1070:PHE:HB3	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:C:983:LYS:HZ3	1:E:1026:ASN:HD22	1.68	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

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	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%)	14	27
1	G	110/127 (87%)	107 (97%)	3 (3%)	0	100	100
1	I	108/127 (85%)	104 (96%)	3 (3%)	1 (1%)	14	27
1	K	110/127 (87%)	106 (96%)	2 (2%)	2 (2%)	6	12
1	M	111/127 (87%)	107 (96%)	4 (4%)	0	100	100
1	O	107/127 (84%)	104 (97%)	2 (2%)	1 (1%)	14	27
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%)	24	43

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 ⓘ

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%)	102 (94%)	6 (6%)	19	39
1	C	107/115 (93%)	100 (94%)	7 (6%)	15	32
1	E	107/115 (93%)	98 (92%)	9 (8%)	10	22
1	G	107/115 (93%)	100 (94%)	7 (6%)	15	32
1	I	106/115 (92%)	96 (91%)	10 (9%)	8	18
1	K	108/115 (94%)	103 (95%)	5 (5%)	24	48
1	M	109/115 (95%)	104 (95%)	5 (5%)	24	48
1	O	105/115 (91%)	98 (93%)	7 (7%)	15	31
2	B	8/15 (53%)	8 (100%)	0	100	100
2	D	8/15 (53%)	7 (88%)	1 (12%)	4	9
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%)	8 (89%)	1 (11%)	6	12
All	All	924/1040 (89%)	865 (94%)	59 (6%)	16	33

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	985	ILE
1	A	992	GLU
1	A	1000	SER
1	A	1014	ASP
1	A	1064	LYS
1	A	1077	VAL
1	C	969	LEU
1	C	985	ILE

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Mol	Chain	Res	Type
1	C	1014	ASP
1	C	1026	ASN
1	C	1047	SER
1	C	1070	PHE
1	C	1077	VAL
2	D	1446	THR
1	E	969	LEU
1	E	985	ILE
1	E	988	SER
1	E	990	VAL
1	E	996	GLU
1	E	1014	ASP
1	E	1026	ASN
1	E	1070	PHE
1	E	1077	VAL
1	G	972	SER
1	G	977	GLU
1	G	985	ILE
1	G	1014	ASP
1	G	1072	LYS
1	G	1077	VAL
1	G	1084	ILE
1	I	972	SER
1	I	973	SER
1	I	977	GLU
1	I	985	ILE
1	I	1014	ASP
1	I	1049	ILE
1	I	1066	ARG
1	I	1070	PHE
1	I	1077	VAL
1	I	1084	ILE
2	J	1447	ASP
1	K	972	SER
1	K	977	GLU
1	K	1014	ASP
1	K	1077	VAL
1	K	1085	GLN
1	M	977	GLU
1	M	985	ILE
1	M	1014	ASP
1	M	1070	PHE

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Mol	Chain	Res	Type
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
2	P	1446	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1058	ASN
1	E	1026	ASN
1	E	1058	ASN
1	I	1058	ASN
1	K	1058	ASN
1	M	1019	ASN
1	M	1058	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1.18	1 (12%)	7,12,14	2.48	2 (28%)
2	SEP	P	1450	2	8,9,10	1.10	0	7,12,14	2.16	3 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SEP	H	1450	2	8,9,10	0.83	0	7,12,14	2.43	3 (42%)
2	SEP	B	1450	2	8,9,10	0.76	0	7,12,14	2.67	2 (28%)
2	SEP	N	1450	2	8,9,10	1.56	1 (12%)	7,12,14	2.31	1 (14%)
2	SEP	J	1450	2	8,9,10	1.41	1 (12%)	7,12,14	2.18	2 (28%)
2	SEP	L	1450	2	8,9,10	0.95	0	7,12,14	2.41	2 (28%)
2	SEP	D	1450	2	8,9,10	1.11	1 (12%)	7,12,14	1.90	2 (28%)

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	-	1/6/8/10	-
2	SEP	P	1450	2	-	1/6/8/10	-
2	SEP	H	1450	2	-	2/6/8/10	-
2	SEP	B	1450	2	-	2/6/8/10	-
2	SEP	N	1450	2	-	1/6/8/10	-
2	SEP	J	1450	2	-	2/6/8/10	-
2	SEP	L	1450	2	-	1/6/8/10	-
2	SEP	D	1450	2	-	1/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	1450	SEP	P-OG	-3.81	1.48	1.60
2	J	1450	SEP	P-OG	-3.05	1.50	1.60
2	F	1450	SEP	P-OG	-2.60	1.52	1.60
2	D	1450	SEP	P-OG	-2.27	1.53	1.60

All (17) 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	4.21	117.65	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1450	SEP	OG-CB-CA	3.95	111.98	108.14
2	B	1450	SEP	OG-P-O1P	3.64	116.29	106.44
2	J	1450	SEP	OG-CB-CA	3.33	111.39	108.14
2	L	1450	SEP	O2P-P-OG	2.98	114.44	106.67
2	F	1450	SEP	OG-P-O1P	2.71	113.75	106.44
2	H	1450	SEP	OG-P-O1P	2.55	113.33	106.44
2	D	1450	SEP	O2P-P-OG	2.48	113.14	106.67
2	H	1450	SEP	O2P-P-OG	-2.36	100.51	106.67
2	P	1450	SEP	OG-P-O1P	2.27	112.59	106.44
2	P	1450	SEP	O3P-P-OG	2.07	112.05	106.67

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	B	1450	SEP	CA-CB-OG-P
2	D	1450	SEP	CA-CB-OG-P
2	F	1450	SEP	CA-CB-OG-P
2	H	1450	SEP	CA-CB-OG-P
2	J	1450	SEP	CA-CB-OG-P
2	L	1450	SEP	CA-CB-OG-P
2	N	1450	SEP	CA-CB-OG-P
2	P	1450	SEP	CA-CB-OG-P
2	H	1450	SEP	CB-OG-P-O2P
2	J	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 oligosaccharides 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

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, 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	108/127 (85%)	0.02	2 (1%) 66 62	39, 61, 91, 127	0
1	C	109/127 (85%)	0.00	3 (2%) 55 50	44, 60, 100, 140	0
1	E	109/127 (85%)	0.11	1 (0%) 81 78	44, 66, 119, 160	0
1	G	110/127 (86%)	-0.09	2 (1%) 67 64	38, 56, 92, 107	0
1	I	108/127 (85%)	0.06	1 (0%) 81 78	44, 66, 107, 133	0
1	K	110/127 (86%)	0.03	1 (0%) 81 78	44, 67, 108, 120	0
1	M	110/127 (86%)	0.19	3 (2%) 56 51	24, 74, 123, 157	1 (0%)
1	O	107/127 (84%)	0.25	3 (2%) 55 50	48, 79, 118, 151	0
2	B	8/16 (50%)	0.87	1 (12%) 8 6	69, 77, 99, 100	0
2	D	8/16 (50%)	0.83	0 100 100	75, 87, 95, 120	0
2	F	8/16 (50%)	0.65	0 100 100	65, 72, 94, 111	0
2	H	10/16 (62%)	0.62	1 (10%) 12 10	51, 60, 87, 89	0
2	J	6/16 (37%)	0.81	0 100 100	83, 89, 94, 96	0
2	L	9/16 (56%)	0.74	0 100 100	74, 81, 97, 129	0
2	N	9/16 (56%)	0.77	0 100 100	76, 82, 92, 116	0
2	P	9/16 (56%)	1.09	1 (11%) 10 8	88, 93, 108, 130	0
All	All	938/1144 (81%)	0.12	19 (2%) 65 61	24, 67, 111, 160	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	1084	ILE	6.0
1	M	1084	ILE	5.1
1	G	1084	ILE	4.2
1	K	969	LEU	3.5
1	M	1061	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	1062	ALA	2.9
1	A	1084	ILE	2.9
1	O	1059	LYS	2.8
1	E	1084	ILE	2.8
1	C	1060	PRO	2.7
1	M	1060	PRO	2.7
1	C	1084	ILE	2.6
1	O	1084	ILE	2.6
1	A	1060	PRO	2.5
2	H	1446	THR	2.4
2	B	1446	THR	2.3
2	P	1446	THR	2.2
1	C	969	LEU	2.2
1	O	1014	ASP	2.0

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, 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	B-factors(Å ²)	Q<0.9
2	SEP	J	1450	10/11	0.91	0.10	74,77,84,85	0
2	SEP	P	1450	10/11	0.92	0.08	83,85,86,87	0
2	SEP	D	1450	10/11	0.94	0.08	68,70,75,77	0
2	SEP	L	1450	10/11	0.94	0.09	69,73,74,74	0
2	SEP	N	1450	10/11	0.94	0.10	73,73,77,78	0
2	SEP	F	1450	10/11	0.94	0.08	62,64,65,67	0
2	SEP	B	1450	10/11	0.97	0.07	65,66,70,71	0
2	SEP	H	1450	10/11	0.97	0.07	49,53,57,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	C	1101	1/1	0.85	0.19	95,95,95,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.