



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:36 am GMT

PDB ID : 4A34
Title : Crystal structure of the fucose mutarotase in complex with L-fucose from *Streptococcus pneumoniae*
Authors : Higgins, M.A.; Boraston, A.B.
Deposited on : 2011-09-29
Resolution : 2.50 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

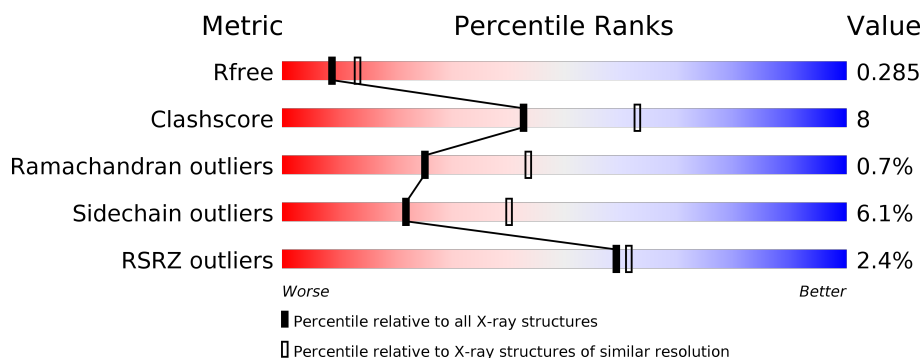
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	147	
1	B	147	
1	C	147	
1	D	147	
1	E	147	
1	F	147	

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Mol	Chain	Length	Quality of chain
1	G	147	
1	H	147	
1	I	147	
1	J	147	
1	K	147	
1	L	147	
1	M	147	
1	N	147	
1	O	147	
1	P	147	
1	Q	147	
1	R	147	
1	S	147	
1	T	147	

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
2	FUL	J	1142	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22775 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 RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	0	0
			1087	694	178	208	7			
1	B	140	Total	C	N	O	S	0	0	0
			1080	690	178	205	7			
1	C	140	Total	C	N	O	S	0	0	0
			1073	685	177	204	7			
1	D	140	Total	C	N	O	S	0	1	0
			1095	699	178	211	7			
1	E	139	Total	C	N	O	S	0	0	0
			1075	685	175	208	7			
1	F	140	Total	C	N	O	S	0	0	0
			1073	686	176	204	7			
1	G	140	Total	C	N	O	S	0	0	0
			1098	702	180	209	7			
1	H	140	Total	C	N	O	S	0	0	0
			1089	696	178	208	7			
1	I	142	Total	C	N	O	S	0	0	0
			1100	702	180	211	7			
1	J	140	Total	C	N	O	S	0	0	0
			1076	687	177	205	7			
1	K	140	Total	C	N	O	S	0	0	0
			1086	693	177	209	7			
1	L	140	Total	C	N	O	S	0	0	0
			1098	702	180	209	7			
1	M	140	Total	C	N	O	S	0	0	0
			1094	699	179	209	7			
1	N	140	Total	C	N	O	S	0	0	0
			1075	689	174	205	7			
1	O	140	Total	C	N	O	S	0	0	0
			1079	689	177	206	7			
1	P	140	Total	C	N	O	S	0	0	0
			1080	689	177	207	7			

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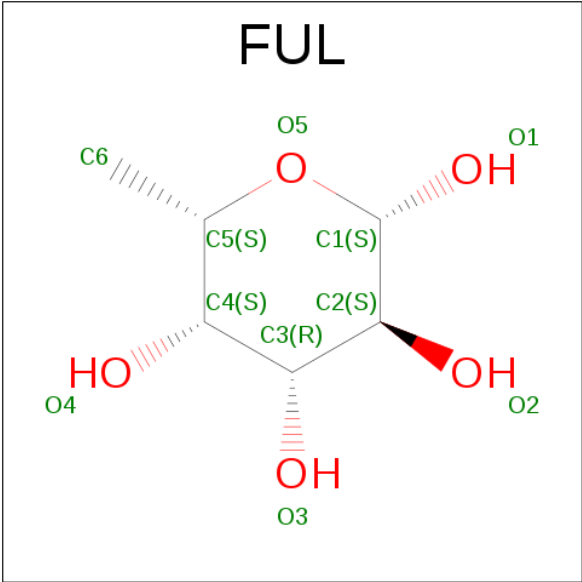
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	140	Total	C	N	O	S	0	0	0
			1084	692	177	208	7			
1	R	140	Total	C	N	O	S	0	0	0
			1080	691	175	207	7			
1	S	140	Total	C	N	O	S	0	0	0
			1094	702	180	205	7			
1	T	140	Total	C	N	O	S	0	0	0
			1079	690	177	205	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	GLN	-	EXPRESSION TAG	UNP Q04I09
B	147	GLN	-	EXPRESSION TAG	UNP Q04I09
C	147	GLN	-	EXPRESSION TAG	UNP Q04I09
D	147	GLN	-	EXPRESSION TAG	UNP Q04I09
E	147	GLN	-	EXPRESSION TAG	UNP Q04I09
F	147	GLN	-	EXPRESSION TAG	UNP Q04I09
G	147	GLN	-	EXPRESSION TAG	UNP Q04I09
H	147	GLN	-	EXPRESSION TAG	UNP Q04I09
I	147	GLN	-	EXPRESSION TAG	UNP Q04I09
J	147	GLN	-	EXPRESSION TAG	UNP Q04I09
K	147	GLN	-	EXPRESSION TAG	UNP Q04I09
L	147	GLN	-	EXPRESSION TAG	UNP Q04I09
M	147	GLN	-	EXPRESSION TAG	UNP Q04I09
N	147	GLN	-	EXPRESSION TAG	UNP Q04I09
O	147	GLN	-	EXPRESSION TAG	UNP Q04I09
P	147	GLN	-	EXPRESSION TAG	UNP Q04I09
Q	147	GLN	-	EXPRESSION TAG	UNP Q04I09
R	147	GLN	-	EXPRESSION TAG	UNP Q04I09
S	147	GLN	-	EXPRESSION TAG	UNP Q04I09
T	147	GLN	-	EXPRESSION TAG	UNP Q04I09

- Molecule 2 is SUGAR (BETA-L-FUCOSE) (three-letter code: FUL) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	C	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			11	6	5		
2	E	1	Total	C	O	0	0
			11	6	5		
2	F	1	Total	C	O	0	0
			11	6	5		
2	G	1	Total	C	O	0	0
			11	6	5		
2	H	1	Total	C	O	0	0
			11	6	5		
2	I	1	Total	C	O	0	0
			11	6	5		
2	J	1	Total	C	O	0	0
			11	6	5		
2	K	1	Total	C	O	0	0
			11	6	5		
2	L	1	Total	C	O	0	0
			11	6	5		
2	M	1	Total	C	O	0	0
			11	6	5		
2	N	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	C	O	0	0
			11	6	5		
2	P	1	Total	C	O	0	0
			11	6	5		
2	Q	1	Total	C	O	0	0
			11	6	5		
2	R	1	Total	C	O	0	0
			11	6	5		
2	S	1	Total	C	O	0	0
			11	6	5		
2	T	1	Total	C	O	0	0
			11	6	5		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	1	Total	K	0	0
			1	1		
3	Q	1	Total	K	0	0
			1	1		
3	D	1	Total	K	0	0
			1	1		
3	K	1	Total	K	0	0
			1	1		
3	E	1	Total	K	0	0
			1	1		
3	B	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		
3	N	1	Total	K	0	0
			1	1		
3	L	1	Total	K	0	0
			1	1		
3	S	1	Total	K	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	49	Total	O	0	0
			49	49		
4	C	46	Total	O	0	0
			46	46		
4	D	38	Total	O	0	0
			38	38		
4	E	58	Total	O	0	0
			58	58		
4	F	44	Total	O	0	0
			44	44		
4	G	28	Total	O	0	0
			28	28		
4	H	41	Total	O	0	0
			41	41		
4	I	30	Total	O	0	0
			30	30		
4	J	22	Total	O	0	0
			22	22		
4	K	56	Total	O	0	0
			56	56		
4	L	31	Total	O	0	0
			31	31		
4	M	46	Total	O	0	0
			46	46		
4	N	50	Total	O	0	0
			50	50		
4	O	44	Total	O	0	0
			44	44		
4	P	55	Total	O	0	0
			55	55		
4	Q	27	Total	O	0	0
			27	27		
4	R	34	Total	O	0	0
			34	34		
4	S	48	Total	O	0	0
			48	48		
4	T	45	Total	O	0	0
			45	45		

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.

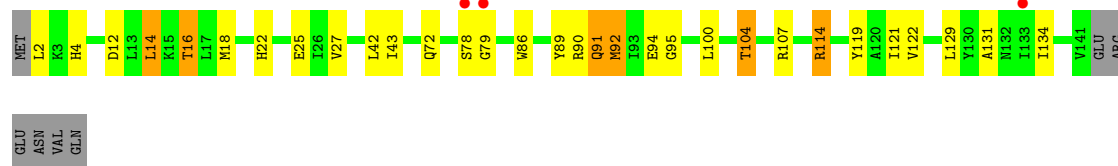
• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

Chain A: 




• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

Chain B: 



• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

Chain C: 



• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

Chain D: 



• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

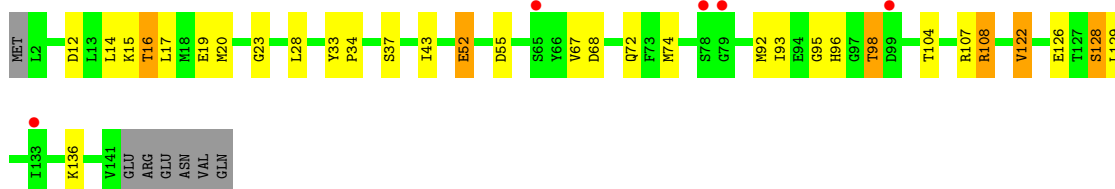
Chain E: 



GLU
ARG
GLU
ASN
VAL
GLN

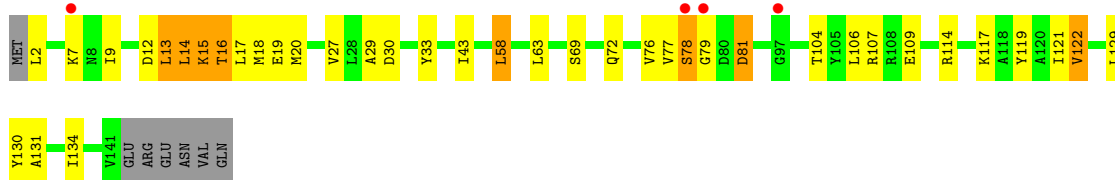
• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

Chain F: 3% 73% 18% 5%



• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

Chain G: 3% 69% 21% 5% 5%



• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

Chain H: % 82% 10% 5%



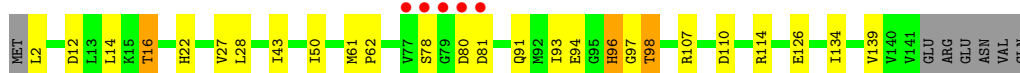
• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

Chain I: 3% 80% 14% . .



• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

Chain J: 3% 78% 16% 5%

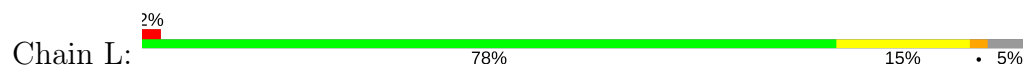


• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

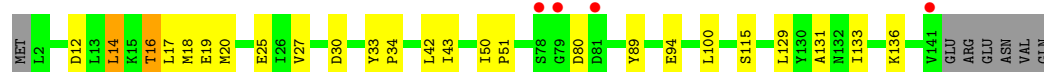
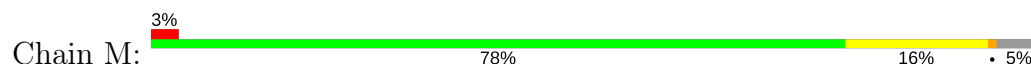
Chain K: % 77% 15% 5%



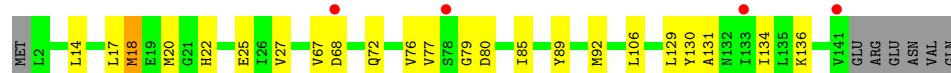
• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN



• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN



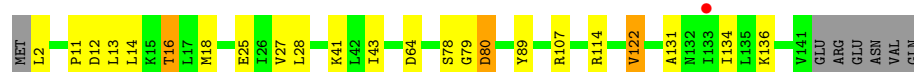
• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN



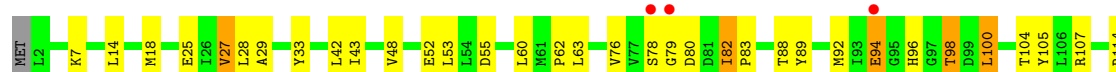
• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN



• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

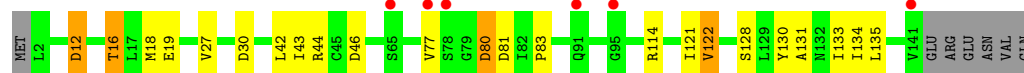
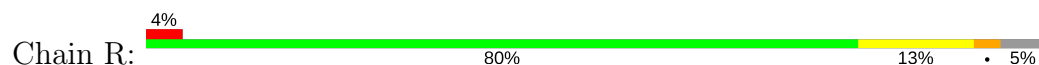


• Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN

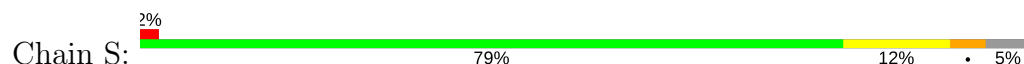




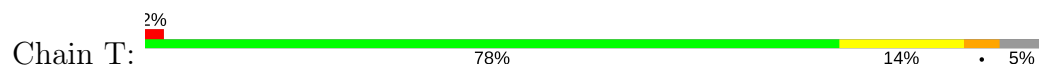
- Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN



- Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN



- Molecule 1: RBSD/FUCU TRANSPORT PROTEIN FAMILY PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.32Å 144.16Å 165.46Å 90.00° 97.51° 90.00°	Depositor
Resolution (Å)	19.97 – 2.50 19.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.97-2.50) 99.6 (19.97-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.225 , 0.292 0.220 , 0.285	Depositor DCC
R_{free} test set	5139 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22775	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.10% 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

5.1 Standard geometry

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

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	0.42	0/1107	0.59	0/1502
1	B	0.42	0/1100	0.59	0/1492
1	C	0.43	0/1093	0.57	0/1485
1	D	0.41	0/1115	0.58	0/1513
1	E	0.42	0/1095	0.58	0/1488
1	F	0.41	0/1093	0.57	0/1485
1	G	0.43	0/1118	0.62	0/1514
1	H	0.40	0/1109	0.59	0/1505
1	I	0.41	0/1120	0.57	0/1520
1	J	0.43	0/1096	0.60	0/1489
1	K	0.40	0/1106	0.61	0/1502
1	L	0.41	0/1118	0.57	0/1514
1	M	0.43	0/1114	0.59	0/1510
1	N	0.43	0/1095	0.63	0/1488
1	O	0.41	0/1099	0.61	0/1493
1	P	0.42	0/1100	0.59	0/1494
1	Q	0.40	0/1104	0.59	0/1498
1	R	0.40	0/1100	0.58	0/1494
1	S	0.44	0/1114	0.63	0/1506
1	T	0.43	0/1099	0.61	0/1493
All	All	0.42	0/22095	0.59	0/29985

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	1087	0	1084	11	0
1	B	1080	0	1076	20	0
1	C	1073	0	1058	17	0
1	D	1095	0	1093	16	0
1	E	1075	0	1063	22	0
1	F	1073	0	1064	23	0
1	G	1098	0	1116	29	0
1	H	1089	0	1091	14	0
1	I	1100	0	1098	17	0
1	J	1076	0	1068	18	0
1	K	1086	0	1083	18	0
1	L	1098	0	1116	16	0
1	M	1094	0	1105	14	0
1	N	1075	0	1070	15	0
1	O	1079	0	1069	26	0
1	P	1080	0	1072	24	0
1	Q	1084	0	1081	24	0
1	R	1080	0	1079	12	0
1	S	1094	0	1116	16	0
1	T	1079	0	1077	20	0
2	A	11	0	12	0	0
2	B	11	0	12	0	0
2	C	11	0	12	1	0
2	D	11	0	12	0	0
2	E	11	0	12	1	0
2	F	11	0	12	2	0
2	G	11	0	12	0	0
2	H	11	0	12	0	0
2	I	11	0	12	2	0
2	J	11	0	12	0	0
2	K	11	0	12	0	0
2	L	11	0	12	0	0
2	M	11	0	12	0	0
2	N	11	0	12	0	0
2	O	11	0	12	0	0
2	P	11	0	12	0	0
2	Q	11	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	11	0	12	0	0
2	S	11	0	12	0	0
2	T	11	0	12	1	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	N	1	0	0	0	0
3	Q	1	0	0	0	0
3	S	1	0	0	0	0
4	A	58	0	0	0	0
4	B	49	0	0	3	0
4	C	46	0	0	2	0
4	D	38	0	0	1	0
4	E	58	0	0	1	0
4	F	44	0	0	1	0
4	G	28	0	0	1	0
4	H	41	0	0	0	0
4	I	30	0	0	1	0
4	J	22	0	0	0	0
4	K	56	0	0	0	0
4	L	31	0	0	2	0
4	M	46	0	0	0	0
4	N	50	0	0	0	0
4	O	44	0	0	5	0
4	P	55	0	0	0	0
4	Q	27	0	0	1	0
4	R	34	0	0	0	0
4	S	48	0	0	0	0
4	T	45	0	0	0	0
All	All	22775	0	21919	343	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 8.

The worst 5 of 343 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:S:80:ASP:CB	1:S:81:ASP:HA	1.71	1.19
1:S:80:ASP:HB3	1:S:81:ASP:HA	1.20	1.18
1:O:79:GLY:HA2	1:O:80:ASP:HB2	1.22	1.11
1:J:96:HIS:H	1:J:97:GLY:CA	1.63	1.10
1:J:96:HIS:N	1:J:97:GLY:HA2	1.65	1.09

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	138/147 (94%)	134 (97%)	4 (3%)	0	100	100
1	B	138/147 (94%)	131 (95%)	6 (4%)	1 (1%)	25	43
1	C	138/147 (94%)	134 (97%)	3 (2%)	1 (1%)	25	43
1	D	139/147 (95%)	131 (94%)	8 (6%)	0	100	100
1	E	137/147 (93%)	131 (96%)	6 (4%)	0	100	100
1	F	138/147 (94%)	131 (95%)	6 (4%)	1 (1%)	25	43
1	G	138/147 (94%)	130 (94%)	7 (5%)	1 (1%)	25	43
1	H	138/147 (94%)	133 (96%)	5 (4%)	0	100	100
1	I	140/147 (95%)	137 (98%)	3 (2%)	0	100	100
1	J	138/147 (94%)	125 (91%)	11 (8%)	2 (1%)	13	23
1	K	138/147 (94%)	132 (96%)	3 (2%)	3 (2%)	8	12
1	L	138/147 (94%)	135 (98%)	2 (1%)	1 (1%)	25	43
1	M	138/147 (94%)	135 (98%)	3 (2%)	0	100	100
1	N	138/147 (94%)	133 (96%)	5 (4%)	0	100	100
1	O	138/147 (94%)	131 (95%)	5 (4%)	2 (1%)	13	23
1	P	138/147 (94%)	131 (95%)	6 (4%)	1 (1%)	25	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	138/147 (94%)	132 (96%)	6 (4%)	0	100	100
1	R	138/147 (94%)	133 (96%)	4 (3%)	1 (1%)	25	43
1	S	138/147 (94%)	130 (94%)	6 (4%)	2 (1%)	13	23
1	T	138/147 (94%)	130 (94%)	4 (3%)	4 (3%)	5	7
All	All	2762/2940 (94%)	2639 (96%)	103 (4%)	20 (1%)	25	43

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	78	SER
1	K	79	GLY
1	K	80	ASP
1	O	80	ASP
1	S	78	SER

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	119/130 (92%)	115 (97%)	4 (3%)	42	69
1	B	117/130 (90%)	108 (92%)	9 (8%)	15	28
1	C	115/130 (88%)	110 (96%)	5 (4%)	33	58
1	D	121/130 (93%)	113 (93%)	8 (7%)	19	36
1	E	118/130 (91%)	110 (93%)	8 (7%)	18	34
1	F	116/130 (89%)	108 (93%)	8 (7%)	18	34
1	G	123/130 (95%)	110 (89%)	13 (11%)	8	15
1	H	120/130 (92%)	113 (94%)	7 (6%)	23	43
1	I	121/130 (93%)	115 (95%)	6 (5%)	28	51
1	J	117/130 (90%)	111 (95%)	6 (5%)	28	50
1	K	120/130 (92%)	113 (94%)	7 (6%)	23	43
1	L	123/130 (95%)	118 (96%)	5 (4%)	35	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	122/130 (94%)	116 (95%)	6 (5%)	29	52
1	N	117/130 (90%)	113 (97%)	4 (3%)	42	69
1	O	117/130 (90%)	112 (96%)	5 (4%)	33	58
1	P	118/130 (91%)	112 (95%)	6 (5%)	28	50
1	Q	119/130 (92%)	105 (88%)	14 (12%)	6	11
1	R	119/130 (92%)	112 (94%)	7 (6%)	23	42
1	S	123/130 (95%)	112 (91%)	11 (9%)	11	22
1	T	118/130 (91%)	111 (94%)	7 (6%)	23	42
All	All	2383/2600 (92%)	2237 (94%)	146 (6%)	22	40

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	117	LYS
1	L	14	LEU
1	S	102	THR
1	I	122	VAL
1	K	16	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	96	HIS
1	T	4	HIS
1	Q	96	HIS
1	F	96	HIS
1	S	4	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 for Mogul analysis.

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	FUL	A	1142	-	11,11,11	0.60	0	15,16,16	1.23	2 (13%)
2	FUL	B	1142	-	11,11,11	0.68	0	15,16,16	0.75	0
2	FUL	C	1142	-	11,11,11	0.53	0	15,16,16	1.03	1 (6%)
2	FUL	D	1142	-	11,11,11	0.61	0	15,16,16	0.82	1 (6%)
2	FUL	E	1141	-	11,11,11	0.62	0	15,16,16	0.99	1 (6%)
2	FUL	F	1142	-	11,11,11	0.53	0	15,16,16	0.67	0
2	FUL	G	1142	-	11,11,11	0.56	0	15,16,16	0.66	0
2	FUL	H	1142	-	11,11,11	0.66	0	15,16,16	0.93	1 (6%)
2	FUL	I	1144	-	11,11,11	0.60	0	15,16,16	1.10	1 (6%)
2	FUL	J	1142	-	11,11,11	0.59	0	15,16,16	0.94	1 (6%)
2	FUL	K	1142	-	11,11,11	0.53	0	15,16,16	1.03	1 (6%)
2	FUL	L	1142	-	11,11,11	0.56	0	15,16,16	0.90	0
2	FUL	M	1142	-	11,11,11	0.61	0	15,16,16	0.93	1 (6%)
2	FUL	N	1142	-	11,11,11	0.57	0	15,16,16	0.96	1 (6%)
2	FUL	O	1142	-	11,11,11	0.64	0	15,16,16	0.79	0
2	FUL	P	1142	-	11,11,11	0.62	0	15,16,16	0.93	1 (6%)
2	FUL	Q	1142	-	11,11,11	0.61	0	15,16,16	0.92	0
2	FUL	R	1142	-	11,11,11	0.57	0	15,16,16	1.22	2 (13%)
2	FUL	S	1142	-	11,11,11	0.60	0	15,16,16	0.82	0
2	FUL	T	1142	-	11,11,11	0.74	0	15,16,16	0.98	1 (6%)

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	FUL	A	1142	-	-	0/0/20/20	0/1/1/1
2	FUL	B	1142	-	-	0/0/20/20	0/1/1/1
2	FUL	C	1142	-	-	0/0/20/20	0/1/1/1
2	FUL	D	1142	-	-	0/0/20/20	0/1/1/1
2	FUL	E	1141	-	-	0/0/20/20	0/1/1/1
2	FUL	F	1142	-	-	0/0/20/20	0/1/1/1
2	FUL	G	1142	-	-	0/0/20/20	0/1/1/1
2	FUL	H	1142	-	-	0/0/20/20	0/1/1/1
2	FUL	I	1144	-	-	0/0/20/20	0/1/1/1
2	FUL	J	1142	-	-	0/0/20/20	0/1/1/1
2	FUL	K	1142	-	-	0/0/20/20	0/1/1/1
2	FUL	L	1142	-	-	0/0/20/20	0/1/1/1
2	FUL	M	1142	-	-	0/0/20/20	0/1/1/1
2	FUL	N	1142	-	-	0/0/20/20	0/1/1/1
2	FUL	O	1142	-	-	0/0/20/20	0/1/1/1
2	FUL	P	1142	-	-	0/0/20/20	0/1/1/1
2	FUL	Q	1142	-	-	0/0/20/20	0/1/1/1
2	FUL	R	1142	-	-	0/0/20/20	0/1/1/1
2	FUL	S	1142	-	-	0/0/20/20	0/1/1/1
2	FUL	T	1142	-	-	0/0/20/20	0/1/1/1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1142	FUL	O5-C5-C4	-2.46	105.57	109.62
2	C	1142	FUL	C6-C5-C4	-2.21	109.14	113.07
2	N	1142	FUL	C6-C5-C4	-2.05	109.42	113.07
2	T	1142	FUL	O5-C5-C4	-2.05	106.25	109.62
2	R	1142	FUL	O5-C5-C4	-2.02	106.30	109.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1142	FUL	1	0
2	E	1141	FUL	1	0
2	F	1142	FUL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1144	FUL	2	0
2	T	1142	FUL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	140/147 (95%)	-0.20	0 100 100	26, 35, 46, 52	0
1	B	140/147 (95%)	-0.06	3 (2%) 64 66	27, 36, 54, 59	0
1	C	140/147 (95%)	-0.07	3 (2%) 64 66	28, 37, 57, 59	0
1	D	140/147 (95%)	-0.12	2 (1%) 75 76	27, 35, 51, 55	0
1	E	139/147 (94%)	-0.08	3 (2%) 62 64	24, 33, 49, 57	0
1	F	140/147 (95%)	0.12	5 (3%) 43 45	29, 41, 61, 64	0
1	G	140/147 (95%)	0.06	4 (2%) 52 55	29, 39, 56, 62	0
1	H	140/147 (95%)	0.03	1 (0%) 87 88	25, 40, 56, 58	0
1	I	142/147 (96%)	-0.12	5 (3%) 44 47	28, 36, 51, 55	0
1	J	140/147 (95%)	0.09	5 (3%) 43 45	27, 38, 63, 68	0
1	K	140/147 (95%)	-0.12	2 (1%) 75 76	25, 36, 52, 56	0
1	L	140/147 (95%)	0.10	3 (2%) 64 66	30, 43, 64, 66	0
1	M	140/147 (95%)	-0.07	4 (2%) 52 55	26, 35, 50, 59	0
1	N	140/147 (95%)	-0.13	4 (2%) 52 55	24, 35, 46, 48	0
1	O	140/147 (95%)	0.02	5 (3%) 43 45	27, 37, 58, 60	0
1	P	140/147 (95%)	-0.23	1 (0%) 87 88	25, 34, 44, 48	0
1	Q	140/147 (95%)	0.15	4 (2%) 52 55	30, 41, 66, 70	0
1	R	140/147 (95%)	0.06	6 (4%) 36 38	28, 39, 61, 62	0
1	S	140/147 (95%)	-0.15	3 (2%) 64 66	23, 32, 49, 57	0
1	T	140/147 (95%)	-0.27	3 (2%) 64 66	22, 30, 47, 52	0
All	All	2801/2940 (95%)	-0.05	66 (2%) 59 61	22, 36, 57, 70	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	79	GLY	5.4
1	E	79	GLY	5.3
1	T	79	GLY	5.2
1	C	79	GLY	4.8
1	C	78	SER	4.3

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FUL	J	1142	11/11	0.91	0.22	2.17	48,49,50,51	0
2	FUL	M	1142	11/11	0.90	0.19	1.60	42,44,45,46	0
2	FUL	S	1142	11/11	0.92	0.21	1.51	33,35,37,38	0
2	FUL	A	1142	11/11	0.91	0.17	1.32	27,29,30,30	0
2	FUL	I	1144	11/11	0.94	0.18	1.28	43,43,44,45	0
2	FUL	K	1142	11/11	0.93	0.20	0.99	39,40,42,43	0
2	FUL	L	1142	11/11	0.91	0.20	0.94	41,44,45,46	0
2	FUL	Q	1142	11/11	0.89	0.21	0.78	47,49,49,49	0
2	FUL	C	1142	11/11	0.91	0.16	0.75	35,38,39,39	0
2	FUL	E	1141	11/11	0.92	0.17	0.74	33,34,35,35	0
2	FUL	D	1142	11/11	0.95	0.16	0.74	37,37,38,40	0
2	FUL	H	1142	11/11	0.92	0.16	0.62	33,36,38,38	0
2	FUL	T	1142	11/11	0.95	0.16	0.51	37,37,38,40	0
2	FUL	N	1142	11/11	0.92	0.16	0.28	33,35,35,35	0
2	FUL	O	1142	11/11	0.94	0.17	0.06	40,40,41,41	0
2	FUL	F	1142	11/11	0.93	0.15	-0.13	46,46,46,46	0
2	FUL	P	1142	11/11	0.96	0.14	-0.25	36,38,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FUL	R	1142	11/11	0.94	0.15	-0.37	33,34,36,36	0
2	FUL	B	1142	11/11	0.95	0.13	-0.47	40,41,42,42	0
2	FUL	G	1142	11/11	0.94	0.14	-0.65	40,41,41,41	0
3	K	C	1143	1/1	0.94	0.08	-0.80	58,58,58,58	0
3	K	L	1143	1/1	0.98	0.04	-3.82	46,46,46,46	0
3	K	N	1143	1/1	0.98	0.05	-	47,47,47,47	0
3	K	J	1143	1/1	0.98	0.10	-	47,47,47,47	0
3	K	K	1143	1/1	0.95	0.05	-	47,47,47,47	0
3	K	S	1143	1/1	0.94	0.07	-	59,59,59,59	0
3	K	B	1143	1/1	0.97	0.09	-	36,36,36,36	0
3	K	Q	1143	1/1	0.96	0.06	-	44,44,44,44	0
3	K	E	1142	1/1	0.95	0.07	-	56,56,56,56	0
3	K	D	1143	1/1	0.98	0.05	-	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.