



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:31 am GMT

PDB ID : 4DBL  
Title : Crystal structure of E159Q mutant of BtuCDF  
Authors : Korkhov, V.M.; Mireku, S.M.; Hvorup, R.N.; Locher, K.P.  
Deposited on : 2012-01-16  
Resolution : 3.49 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

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

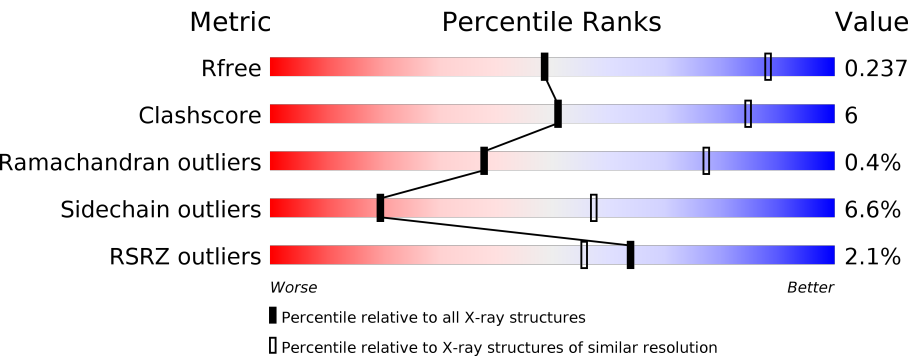
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.49 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	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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. 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	349	<div><div>3%</div><div><div></div><div>71%</div><div>19%</div><div>• 7%</div></div></div>
1	B	349	<div><div>%</div><div><div></div><div>72%</div><div>18%</div><div>• 7%</div></div></div>
1	F	349	<div><div>3%</div><div><div></div><div>73%</div><div>17%</div><div>• 7%</div></div></div>
1	G	349	<div><div>%</div><div><div></div><div>73%</div><div>17%</div><div>• 7%</div></div></div>
2	C	249	<div><div>%</div><div><div></div><div>85%</div><div>12%</div><div>•</div></div></div>
2	D	249	<div><div></div><div><div></div><div>84%</div><div>13%</div><div>•</div></div></div>

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Mol	Chain	Length	Quality of chain
2	H	249	 % 84% 12% •
2	I	249	 85% 12% •
3	E	255	 5% 78% 18% • •
3	J	255	 4% 78% 18% • •

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
4	PO4	C	301	-	-	X	-
4	PO4	H	301	-	-	X	-
5	SO4	I	303	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21230 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 Vitamin B12 import system permease protein BtuC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2441	1611	418	400	12			
1	B	324	Total	C	N	O	S	0	0	0
			2441	1611	418	400	12			
1	F	324	Total	C	N	O	S	0	0	0
			2441	1611	418	400	12			
1	G	324	Total	C	N	O	S	0	0	0
			2441	1611	418	400	12			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP P06609
A	-21	GLY	-	EXPRESSION TAG	UNP P06609
A	-20	HIS	-	EXPRESSION TAG	UNP P06609
A	-19	HIS	-	EXPRESSION TAG	UNP P06609
A	-18	HIS	-	EXPRESSION TAG	UNP P06609
A	-17	HIS	-	EXPRESSION TAG	UNP P06609
A	-16	HIS	-	EXPRESSION TAG	UNP P06609
A	-15	HIS	-	EXPRESSION TAG	UNP P06609
A	-14	HIS	-	EXPRESSION TAG	UNP P06609
A	-13	HIS	-	EXPRESSION TAG	UNP P06609
A	-12	HIS	-	EXPRESSION TAG	UNP P06609
A	-11	HIS	-	EXPRESSION TAG	UNP P06609
A	-10	SER	-	EXPRESSION TAG	UNP P06609
A	-9	SER	-	EXPRESSION TAG	UNP P06609
A	-8	GLY	-	EXPRESSION TAG	UNP P06609
A	-7	GLU	-	EXPRESSION TAG	UNP P06609
A	-6	ASN	-	EXPRESSION TAG	UNP P06609
A	-5	LEU	-	EXPRESSION TAG	UNP P06609
A	-4	TYR	-	EXPRESSION TAG	UNP P06609
A	-3	PHE	-	EXPRESSION TAG	UNP P06609
A	-2	GLN	-	EXPRESSION TAG	UNP P06609

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P06609
A	0	HIS	-	EXPRESSION TAG	UNP P06609
A	18	SER	CYS	ENGINEERED MUTATION	UNP P06609
A	32	SER	CYS	ENGINEERED MUTATION	UNP P06609
A	120	SER	CYS	ENGINEERED MUTATION	UNP P06609
A	156	SER	CYS	ENGINEERED MUTATION	UNP P06609
A	205	SER	CYS	ENGINEERED MUTATION	UNP P06609
A	206	SER	CYS	ENGINEERED MUTATION	UNP P06609
A	267	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	-22	MET	-	EXPRESSION TAG	UNP P06609
B	-21	GLY	-	EXPRESSION TAG	UNP P06609
B	-20	HIS	-	EXPRESSION TAG	UNP P06609
B	-19	HIS	-	EXPRESSION TAG	UNP P06609
B	-18	HIS	-	EXPRESSION TAG	UNP P06609
B	-17	HIS	-	EXPRESSION TAG	UNP P06609
B	-16	HIS	-	EXPRESSION TAG	UNP P06609
B	-15	HIS	-	EXPRESSION TAG	UNP P06609
B	-14	HIS	-	EXPRESSION TAG	UNP P06609
B	-13	HIS	-	EXPRESSION TAG	UNP P06609
B	-12	HIS	-	EXPRESSION TAG	UNP P06609
B	-11	HIS	-	EXPRESSION TAG	UNP P06609
B	-10	SER	-	EXPRESSION TAG	UNP P06609
B	-9	SER	-	EXPRESSION TAG	UNP P06609
B	-8	GLY	-	EXPRESSION TAG	UNP P06609
B	-7	GLU	-	EXPRESSION TAG	UNP P06609
B	-6	ASN	-	EXPRESSION TAG	UNP P06609
B	-5	LEU	-	EXPRESSION TAG	UNP P06609
B	-4	TYR	-	EXPRESSION TAG	UNP P06609
B	-3	PHE	-	EXPRESSION TAG	UNP P06609
B	-2	GLN	-	EXPRESSION TAG	UNP P06609
B	-1	GLY	-	EXPRESSION TAG	UNP P06609
B	0	HIS	-	EXPRESSION TAG	UNP P06609
B	18	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	32	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	120	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	156	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	205	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	206	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	267	SER	CYS	ENGINEERED MUTATION	UNP P06609
F	-22	MET	-	EXPRESSION TAG	UNP P06609
F	-21	GLY	-	EXPRESSION TAG	UNP P06609
F	-20	HIS	-	EXPRESSION TAG	UNP P06609

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	HIS	-	EXPRESSION TAG	UNP P06609
F	-18	HIS	-	EXPRESSION TAG	UNP P06609
F	-17	HIS	-	EXPRESSION TAG	UNP P06609
F	-16	HIS	-	EXPRESSION TAG	UNP P06609
F	-15	HIS	-	EXPRESSION TAG	UNP P06609
F	-14	HIS	-	EXPRESSION TAG	UNP P06609
F	-13	HIS	-	EXPRESSION TAG	UNP P06609
F	-12	HIS	-	EXPRESSION TAG	UNP P06609
F	-11	HIS	-	EXPRESSION TAG	UNP P06609
F	-10	SER	-	EXPRESSION TAG	UNP P06609
F	-9	SER	-	EXPRESSION TAG	UNP P06609
F	-8	GLY	-	EXPRESSION TAG	UNP P06609
F	-7	GLU	-	EXPRESSION TAG	UNP P06609
F	-6	ASN	-	EXPRESSION TAG	UNP P06609
F	-5	LEU	-	EXPRESSION TAG	UNP P06609
F	-4	TYR	-	EXPRESSION TAG	UNP P06609
F	-3	PHE	-	EXPRESSION TAG	UNP P06609
F	-2	GLN	-	EXPRESSION TAG	UNP P06609
F	-1	GLY	-	EXPRESSION TAG	UNP P06609
F	0	HIS	-	EXPRESSION TAG	UNP P06609
F	18	SER	CYS	ENGINEERED MUTATION	UNP P06609
F	32	SER	CYS	ENGINEERED MUTATION	UNP P06609
F	120	SER	CYS	ENGINEERED MUTATION	UNP P06609
F	156	SER	CYS	ENGINEERED MUTATION	UNP P06609
F	205	SER	CYS	ENGINEERED MUTATION	UNP P06609
F	206	SER	CYS	ENGINEERED MUTATION	UNP P06609
F	267	SER	CYS	ENGINEERED MUTATION	UNP P06609
G	-22	MET	-	EXPRESSION TAG	UNP P06609
G	-21	GLY	-	EXPRESSION TAG	UNP P06609
G	-20	HIS	-	EXPRESSION TAG	UNP P06609
G	-19	HIS	-	EXPRESSION TAG	UNP P06609
G	-18	HIS	-	EXPRESSION TAG	UNP P06609
G	-17	HIS	-	EXPRESSION TAG	UNP P06609
G	-16	HIS	-	EXPRESSION TAG	UNP P06609
G	-15	HIS	-	EXPRESSION TAG	UNP P06609
G	-14	HIS	-	EXPRESSION TAG	UNP P06609
G	-13	HIS	-	EXPRESSION TAG	UNP P06609
G	-12	HIS	-	EXPRESSION TAG	UNP P06609
G	-11	HIS	-	EXPRESSION TAG	UNP P06609
G	-10	SER	-	EXPRESSION TAG	UNP P06609
G	-9	SER	-	EXPRESSION TAG	UNP P06609
G	-8	GLY	-	EXPRESSION TAG	UNP P06609

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLU	-	EXPRESSION TAG	UNP P06609
G	-6	ASN	-	EXPRESSION TAG	UNP P06609
G	-5	LEU	-	EXPRESSION TAG	UNP P06609
G	-4	TYR	-	EXPRESSION TAG	UNP P06609
G	-3	PHE	-	EXPRESSION TAG	UNP P06609
G	-2	GLN	-	EXPRESSION TAG	UNP P06609
G	-1	GLY	-	EXPRESSION TAG	UNP P06609
G	0	HIS	-	EXPRESSION TAG	UNP P06609
G	18	SER	CYS	ENGINEERED MUTATION	UNP P06609
G	32	SER	CYS	ENGINEERED MUTATION	UNP P06609
G	120	SER	CYS	ENGINEERED MUTATION	UNP P06609
G	156	SER	CYS	ENGINEERED MUTATION	UNP P06609
G	205	SER	CYS	ENGINEERED MUTATION	UNP P06609
G	206	SER	CYS	ENGINEERED MUTATION	UNP P06609
G	267	SER	CYS	ENGINEERED MUTATION	UNP P06609

- Molecule 2 is a protein called Vitamin B12 import ATP-binding protein BtuD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	248	Total	C	N	O	S	0	0	0
			1893	1184	352	349	8			
2	D	248	Total	C	N	O	S	0	0	0
			1893	1184	352	349	8			
2	H	248	Total	C	N	O	S	0	0	0
			1893	1184	352	349	8			
2	I	248	Total	C	N	O	S	0	0	0
			1893	1184	352	349	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	159	GLN	GLU	ENGINEERED MUTATION	UNP P06611
C	180	SER	CYS	ENGINEERED MUTATION	UNP P06611
D	159	GLN	GLU	ENGINEERED MUTATION	UNP P06611
D	180	SER	CYS	ENGINEERED MUTATION	UNP P06611
H	159	GLN	GLU	ENGINEERED MUTATION	UNP P06611
H	180	SER	CYS	ENGINEERED MUTATION	UNP P06611
I	159	GLN	GLU	ENGINEERED MUTATION	UNP P06611
I	180	SER	CYS	ENGINEERED MUTATION	UNP P06611

- Molecule 3 is a protein called Vitamin B12-binding protein.

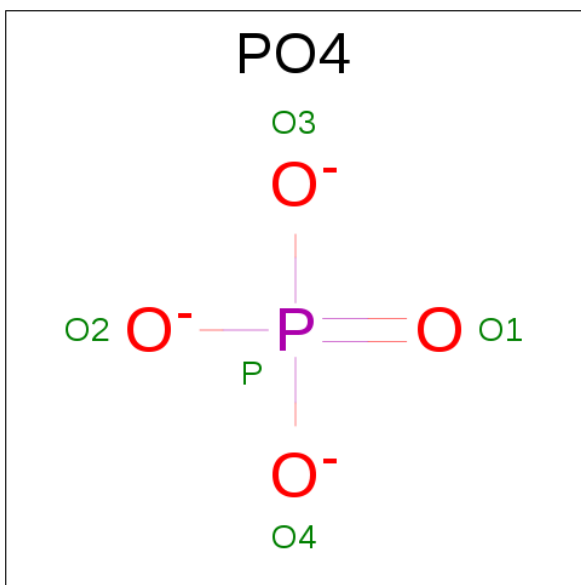
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	245	Total 1907	C 1216	N 332	O 355	S 4	0	0	0
3	J	245	Total 1907	C 1216	N 332	O 355	S 4	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	21	MET	-	INITIATING METHIONINE	UNP P37028
E	267	SER	-	EXPRESSION TAG	UNP P37028
E	268	GLY	-	EXPRESSION TAG	UNP P37028
E	269	SER	-	EXPRESSION TAG	UNP P37028
E	270	HIS	-	EXPRESSION TAG	UNP P37028
E	271	HIS	-	EXPRESSION TAG	UNP P37028
E	272	HIS	-	EXPRESSION TAG	UNP P37028
E	273	HIS	-	EXPRESSION TAG	UNP P37028
E	274	HIS	-	EXPRESSION TAG	UNP P37028
E	275	HIS	-	EXPRESSION TAG	UNP P37028
J	21	MET	-	INITIATING METHIONINE	UNP P37028
J	267	SER	-	EXPRESSION TAG	UNP P37028
J	268	GLY	-	EXPRESSION TAG	UNP P37028
J	269	SER	-	EXPRESSION TAG	UNP P37028
J	270	HIS	-	EXPRESSION TAG	UNP P37028
J	271	HIS	-	EXPRESSION TAG	UNP P37028
J	272	HIS	-	EXPRESSION TAG	UNP P37028
J	273	HIS	-	EXPRESSION TAG	UNP P37028
J	274	HIS	-	EXPRESSION TAG	UNP P37028
J	275	HIS	-	EXPRESSION TAG	UNP P37028

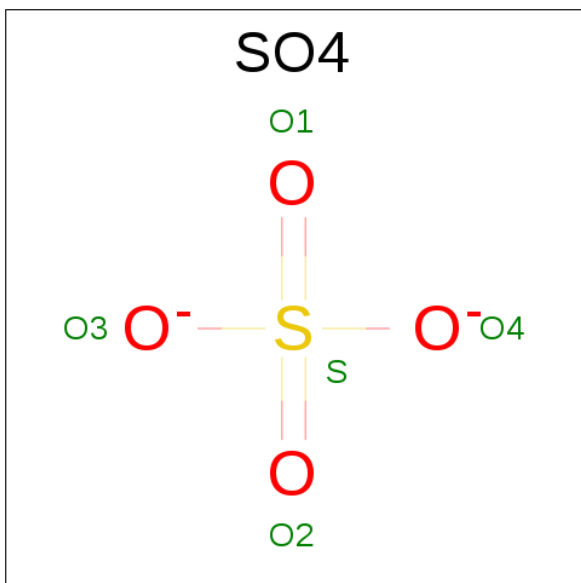
- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		
4	I	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

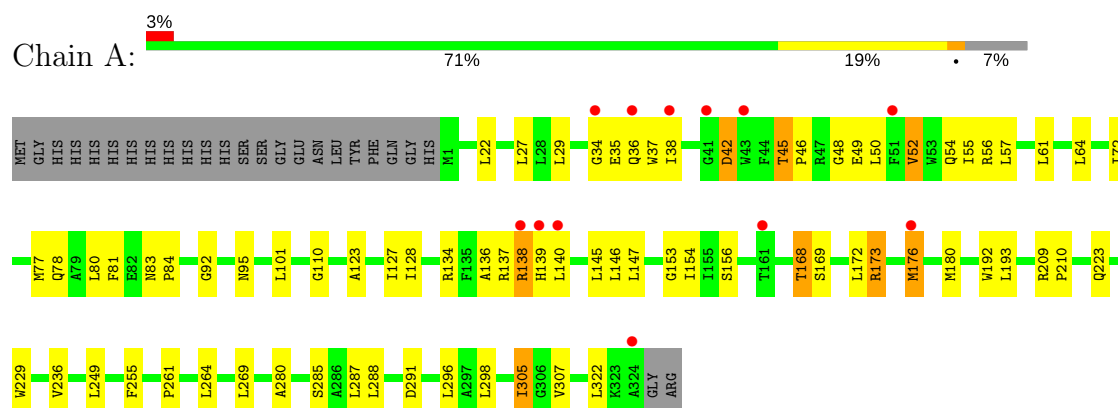


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		

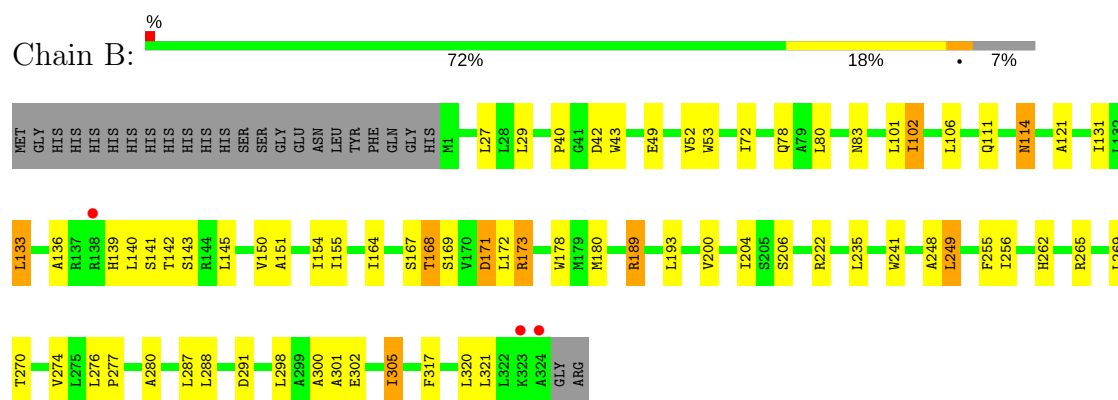
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

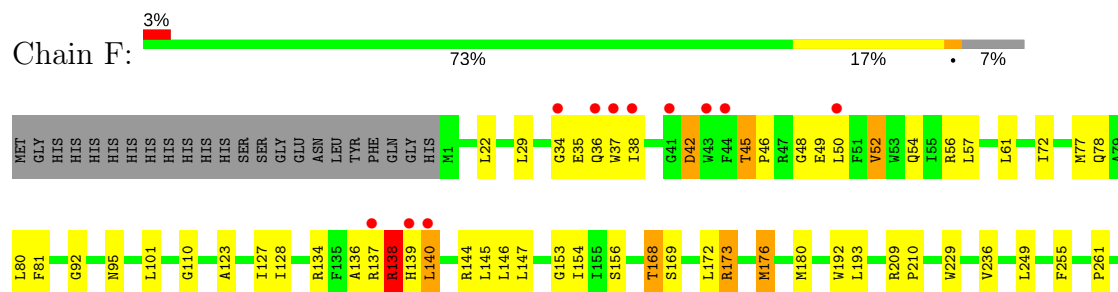
- Molecule 1: Vitamin B12 import system permease protein BtuC



- Molecule 1: Vitamin B12 import system permease protein BtuC

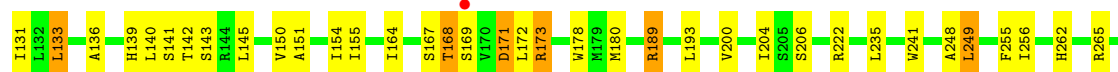
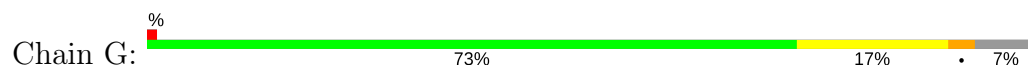


- Molecule 1: Vitamin B12 import system permease protein BtuC

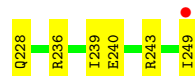
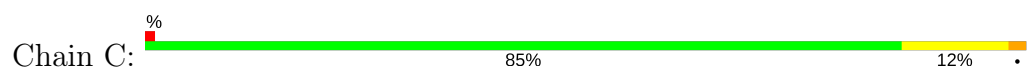




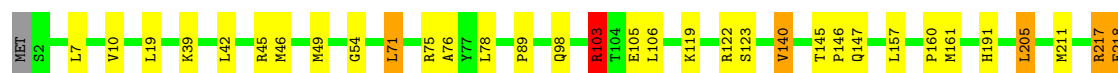
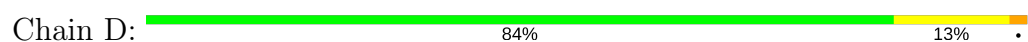
- Molecule 1: Vitamin B12 import system permease protein BtuC



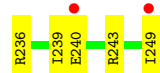
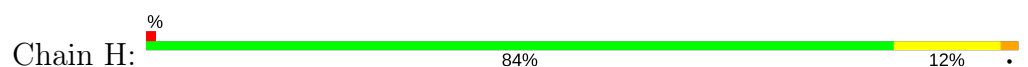
- Molecule 2: Vitamin B12 import ATP-binding protein BtuD



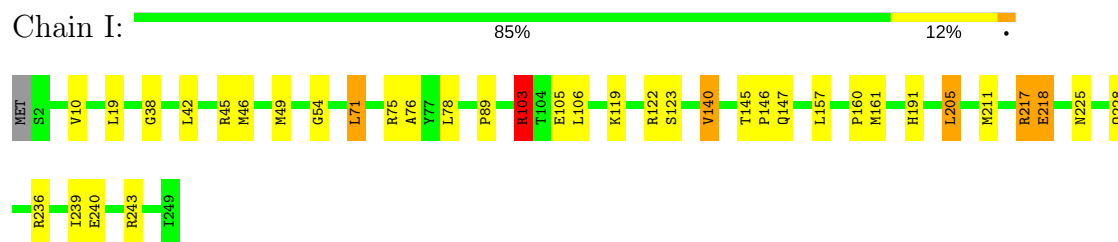
- Molecule 2: Vitamin B12 import ATP-binding protein BtuD



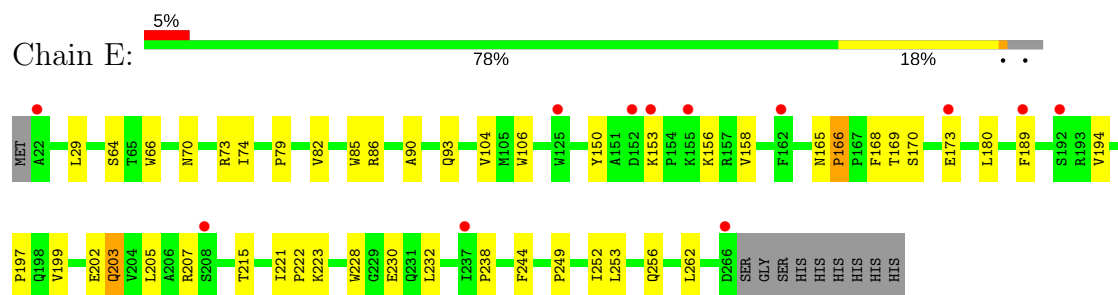
- Molecule 2: Vitamin B12 import ATP-binding protein BtuD



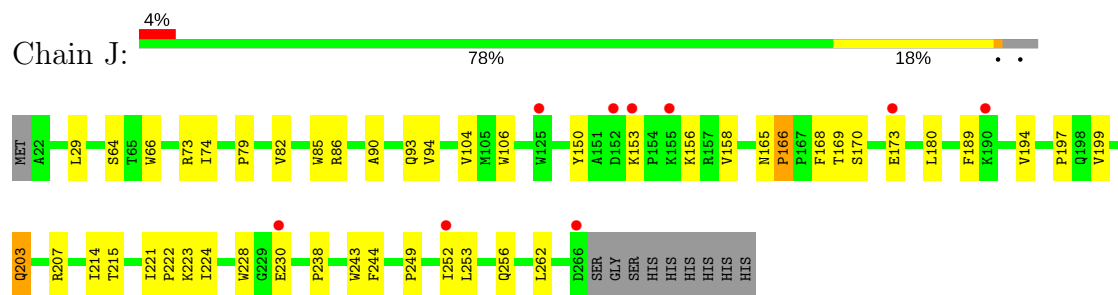
- Molecule 2: Vitamin B12 import ATP-binding protein BtuD



• Molecule 3: Vitamin B12-binding protein



• Molecule 3: Vitamin B12-binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.65Å 166.93Å 132.82Å 90.00° 119.76° 90.00°	Depositor
Resolution (Å)	30.02 – 3.49 30.02 – 3.49	Depositor EDS
% Data completeness (in resolution range)	92.5 (30.02-3.49) 92.6 (30.02-3.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 3.47Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.214 , 0.251 0.199 , 0.237	Depositor DCC
$R_{free}$ test set	2016 reflections (3.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 16.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.005 for l,k,-h-l 0.005 for -h-l,k,h 0.418 for -h-l,-k,l 0.015 for h,-k,-h-l 0.012 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	21230	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: PO4, SO4

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	0.27	0/2495	0.59	3/3408 (0.1%)
1	B	0.24	0/2495	0.41	0/3408
1	F	0.27	0/2495	0.52	3/3408 (0.1%)
1	G	0.24	0/2495	0.41	0/3408
2	C	0.24	0/1927	0.65	6/2611 (0.2%)
2	D	0.25	0/1927	0.65	6/2611 (0.2%)
2	H	0.24	0/1927	0.65	6/2611 (0.2%)
2	I	0.24	0/1927	0.64	6/2611 (0.2%)
3	E	0.22	0/1951	0.41	0/2661
3	J	0.22	0/1951	0.41	0/2661
All	All	0.25	0/21590	0.54	30/29398 (0.1%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	ARG	NE-CZ-NH2	15.78	128.19	120.30
1	A	138	ARG	NE-CZ-NH1	-15.16	112.72	120.30
2	H	45	ARG	NE-CZ-NH2	-13.07	113.77	120.30
2	C	45	ARG	NE-CZ-NH2	-12.95	113.83	120.30
2	D	45	ARG	NE-CZ-NH1	-12.68	113.96	120.30
2	I	45	ARG	NE-CZ-NH1	-12.65	113.98	120.30
2	D	103	ARG	NE-CZ-NH1	-12.47	114.06	120.30
2	H	103	ARG	NE-CZ-NH2	-12.42	114.09	120.30
2	C	103	ARG	NE-CZ-NH2	-12.31	114.14	120.30
2	I	103	ARG	NE-CZ-NH1	-12.28	114.16	120.30
2	D	103	ARG	NE-CZ-NH2	12.21	126.41	120.30
2	I	103	ARG	NE-CZ-NH2	11.78	126.19	120.30
2	H	45	ARG	NE-CZ-NH1	11.58	126.09	120.30
2	H	103	ARG	NE-CZ-NH1	11.53	126.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	45	ARG	NE-CZ-NH1	11.48	126.04	120.30
2	C	103	ARG	NE-CZ-NH1	11.46	126.03	120.30
2	I	45	ARG	NE-CZ-NH2	11.11	125.86	120.30
2	D	45	ARG	NE-CZ-NH2	11.11	125.85	120.30
1	F	138	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	F	138	ARG	NE-CZ-NH1	10.07	125.33	120.30
1	A	138	ARG	CD-NE-CZ	6.98	133.37	123.60
2	D	103	ARG	CD-NE-CZ	6.25	132.35	123.60
2	I	103	ARG	CD-NE-CZ	6.05	132.07	123.60
1	F	140	LEU	CB-CG-CD2	5.99	121.17	111.00
2	H	45	ARG	CD-NE-CZ	5.92	131.89	123.60
2	C	45	ARG	CD-NE-CZ	5.86	131.81	123.60
2	H	103	ARG	CD-NE-CZ	5.83	131.76	123.60
2	C	103	ARG	CD-NE-CZ	5.81	131.73	123.60
2	D	45	ARG	CD-NE-CZ	5.78	131.69	123.60
2	I	45	ARG	CD-NE-CZ	5.76	131.67	123.60

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	2441	0	2606	41	0
1	B	2441	0	2606	42	0
1	F	2441	0	2606	39	0
1	G	2441	0	2606	41	0
2	C	1893	0	1927	22	0
2	D	1893	0	1927	24	0
2	H	1893	0	1927	22	0
2	I	1893	0	1927	25	0
3	E	1907	0	1924	28	0
3	J	1907	0	1924	27	0
4	C	5	0	0	2	0
4	D	5	0	0	1	0
4	H	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	5	0	0	1	0
5	C	15	0	0	0	0
5	D	15	0	0	0	0
5	H	15	0	0	0	0
5	I	15	0	0	2	0
All	All	21230	0	21980	280	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 6.

All (280) 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:F:110:GLY:O	3:J:223:LYS:NZ	2.12	0.83
1:G:173:ARG:NH2	3:J:66:TRP:O	2.15	0.79
1:A:110:GLY:O	3:E:223:LYS:NZ	2.16	0.77
1:B:173:ARG:NH2	3:E:66:TRP:O	2.18	0.77
1:A:38:ILE:HD13	1:A:48:GLY:HA2	1.71	0.72
1:F:38:ILE:HD13	1:F:48:GLY:HA2	1.71	0.71
2:C:119:LYS:HG2	2:C:122:ARG:HH21	1.56	0.70
2:H:119:LYS:HG2	2:H:122:ARG:HH21	1.56	0.70
2:D:119:LYS:HG2	2:D:122:ARG:HH21	1.56	0.70
1:F:173:ARG:NH2	1:G:167:SER:O	2.25	0.69
1:F:147:LEU:HB3	1:G:321:LEU:HD13	1.73	0.69
1:G:140:LEU:HD13	1:G:145:LEU:HB2	1.73	0.69
2:C:239:ILE:HD13	2:D:239:ILE:HD13	1.75	0.69
1:B:140:LEU:HD13	1:B:145:LEU:HB2	1.73	0.69
2:I:119:LYS:HG2	2:I:122:ARG:HH21	1.56	0.68
1:G:78:GLN:OE1	1:G:265:ARG:NH2	2.28	0.67
2:H:239:ILE:HD13	2:I:239:ILE:HD13	1.76	0.67
1:B:78:GLN:OE1	1:B:265:ARG:NH2	2.28	0.66
1:F:147:LEU:HD13	1:G:321:LEU:HD22	1.77	0.66
1:A:173:ARG:NH2	1:B:167:SER:O	2.28	0.66
1:A:147:LEU:HB3	1:B:321:LEU:HD13	1.77	0.65
1:B:101:LEU:HD11	1:B:248:ALA:HA	1.79	0.65
1:G:101:LEU:HD11	1:G:248:ALA:HA	1.79	0.65
1:B:141:SER:O	1:B:143:SER:N	2.30	0.64
3:J:165:ASN:HB3	3:J:166:PRO:HD3	1.80	0.62
1:F:146:LEU:HD23	1:G:143:SER:HB3	1.81	0.62
1:A:95:ASN:HB3	1:A:156:SER:HB3	1.82	0.62
1:G:141:SER:O	1:G:143:SER:N	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:36:GLY:N	4:C:301:PO4:O4	2.33	0.61
3:E:165:ASN:HB3	3:E:166:PRO:HD3	1.81	0.61
1:F:95:ASN:HB3	1:F:156:SER:HB3	1.82	0.61
1:A:147:LEU:HD13	1:B:321:LEU:HD22	1.82	0.60
1:B:49:GLU:OE1	1:F:273:ARG:NH2	2.34	0.60
1:A:146:LEU:HD23	1:B:143:SER:HB3	1.82	0.60
3:J:156:LYS:NZ	3:J:262:LEU:O	2.28	0.60
2:H:38:GLY:N	4:H:301:PO4:O3	2.32	0.59
1:B:270:THR:HG21	2:D:89:PRO:HD2	1.84	0.59
2:I:217:ARG:NH2	5:I:303:SO4:O1	2.35	0.59
1:F:22:LEU:HD22	1:F:285:SER:HB3	1.85	0.59
1:A:22:LEU:HD22	1:A:285:SER:HB3	1.85	0.58
3:E:156:LYS:NZ	3:E:262:LEU:O	2.28	0.58
2:I:243:ARG:NH1	5:I:303:SO4:O1	2.33	0.58
3:J:169:THR:OG1	3:J:170:SER:N	2.37	0.58
3:E:169:THR:OG1	3:E:170:SER:N	2.36	0.57
2:H:45:ARG:NH2	2:H:53:LYS:O	2.38	0.57
1:B:83:ASN:HD22	1:B:145:LEU:HD23	1.70	0.56
1:G:200:VAL:HG21	1:G:241:TRP:CD2	2.40	0.56
1:G:83:ASN:HD22	1:G:145:LEU:HD23	1.70	0.56
1:G:270:THR:HG21	2:I:89:PRO:HD2	1.86	0.56
1:B:200:VAL:HG21	1:B:241:TRP:CD2	2.40	0.56
3:J:221:ILE:H	3:J:222:PRO:HD2	1.71	0.56
3:E:221:ILE:H	3:E:222:PRO:HD2	1.71	0.55
3:J:82:VAL:HB	3:J:104:VAL:HG22	1.89	0.55
2:D:71:LEU:HD13	2:D:75:ARG:HH21	1.72	0.54
2:H:71:LEU:HD13	2:H:75:ARG:HH21	1.72	0.54
2:C:45:ARG:NH2	2:C:53:LYS:O	2.38	0.54
2:D:76:ALA:HB1	2:D:140:VAL:HG22	1.89	0.54
2:I:76:ALA:HB1	2:I:140:VAL:HG22	1.89	0.54
2:H:76:ALA:HB1	2:H:140:VAL:HG22	1.90	0.54
3:E:82:VAL:HB	3:E:104:VAL:HG22	1.89	0.54
2:C:71:LEU:HD13	2:C:75:ARG:HH21	1.72	0.53
2:I:38:GLY:N	4:I:301:PO4:O2	2.41	0.53
1:G:40:PRO:HA	1:G:43:TRP:CD2	2.44	0.53
1:B:262:HIS:ND1	1:B:320:LEU:HD11	2.24	0.53
2:I:71:LEU:HD13	2:I:75:ARG:HH21	1.72	0.53
2:C:76:ALA:HB1	2:C:140:VAL:HG22	1.90	0.52
1:F:264:LEU:HB3	1:F:269:LEU:HD12	1.92	0.52
2:C:39:LYS:N	4:C:301:PO4:O1	2.26	0.52
3:E:90:ALA:HB3	3:E:93:GLN:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:262:HIS:ND1	1:G:320:LEU:HD11	2.24	0.52
1:G:72:ILE:HD11	1:G:280:ALA:HB2	1.91	0.52
1:B:40:PRO:HA	1:B:43:TRP:CD2	2.44	0.52
1:F:136:ALA:HB2	1:F:145:LEU:HD21	1.92	0.52
3:E:194:VAL:HB	3:E:197:PRO:HB3	1.92	0.52
2:H:161:MET:HG3	2:H:191:HIS:CE1	2.45	0.52
3:J:194:VAL:HB	3:J:197:PRO:HB3	1.92	0.51
2:D:161:MET:HG3	2:D:191:HIS:CE1	2.46	0.51
2:I:161:MET:HG3	2:I:191:HIS:CE1	2.45	0.51
1:B:72:ILE:HD11	1:B:280:ALA:HB2	1.92	0.51
1:B:193:LEU:HB3	1:B:249:LEU:HD22	1.92	0.51
2:C:161:MET:HG3	2:C:191:HIS:CE1	2.46	0.51
1:G:151:ALA:O	1:G:155:ILE:HG13	2.10	0.51
1:G:193:LEU:HB3	1:G:249:LEU:HD22	1.92	0.50
2:I:103:ARG:NH1	2:I:147:GLN:O	2.44	0.50
1:A:264:LEU:HB3	1:A:269:LEU:HD12	1.92	0.50
2:D:103:ARG:NH1	2:D:147:GLN:O	2.44	0.50
2:C:89:PRO:HA	2:C:123:SER:HA	1.94	0.50
3:E:249:PRO:O	3:E:252:ILE:HG12	2.12	0.50
1:B:151:ALA:O	1:B:155:ILE:HG13	2.10	0.50
3:J:90:ALA:HB3	3:J:93:GLN:HB2	1.92	0.50
2:H:89:PRO:HA	2:H:123:SER:HA	1.94	0.50
1:F:255:PHE:CE1	1:G:155:ILE:HG12	2.47	0.49
1:A:34:GLY:H	1:A:296:LEU:HD21	1.77	0.49
1:F:34:GLY:H	1:F:296:LEU:HD21	1.77	0.49
3:J:189:PHE:CE2	3:J:199:VAL:HG11	2.48	0.49
3:E:189:PHE:CE2	3:E:199:VAL:HG11	2.48	0.49
2:H:37:ALA:N	4:H:301:PO4:O3	2.45	0.49
2:D:89:PRO:HA	2:D:123:SER:HA	1.95	0.49
3:E:221:ILE:N	3:E:222:PRO:HD2	2.27	0.49
3:J:221:ILE:N	3:J:222:PRO:HD2	2.27	0.48
1:A:136:ALA:HB2	1:A:145:LEU:HD21	1.94	0.48
1:A:255:PHE:CE1	1:B:155:ILE:HG12	2.48	0.48
2:I:89:PRO:HA	2:I:123:SER:HA	1.94	0.48
1:B:222:ARG:HH12	2:D:49:MET:HG3	1.79	0.48
1:F:42:ASP:O	1:F:45:THR:HB	2.14	0.48
3:J:249:PRO:O	3:J:252:ILE:HG12	2.12	0.48
1:A:255:PHE:CZ	1:B:155:ILE:HG12	2.49	0.48
1:A:36:GLN:HB3	1:A:56:ARG:HH22	1.79	0.48
1:A:42:ASP:O	1:A:45:THR:HB	2.14	0.48
2:C:46:MET:HB2	2:C:46:MET:HE2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:203:GLN:O	3:J:207:ARG:HG2	2.15	0.47
1:B:298:LEU:HB2	1:B:301:ALA:HB3	1.97	0.47
1:F:36:GLN:HB3	1:F:56:ARG:HH22	1.79	0.47
2:H:19:LEU:HD22	2:H:211:MET:HB2	1.97	0.47
1:A:138:ARG:O	1:A:139:HIS:HB2	2.15	0.47
3:E:203:GLN:O	3:E:207:ARG:HG2	2.15	0.47
2:H:217:ARG:HE	2:H:218:GLU:HG3	1.80	0.47
3:J:29:LEU:HD22	3:J:64:SER:HB2	1.96	0.47
3:E:29:LEU:HD22	3:E:64:SER:HB2	1.96	0.47
1:G:291:ASP:HB2	1:G:305:ILE:HD11	1.97	0.47
2:I:217:ARG:HE	2:I:218:GLU:HG3	1.80	0.47
3:J:199:VAL:HB	3:J:203:GLN:HG3	1.97	0.47
1:B:291:ASP:HB2	1:B:305:ILE:HD11	1.97	0.47
1:G:43:TRP:CD1	1:G:52:VAL:HG21	2.50	0.46
1:F:255:PHE:CZ	1:G:155:ILE:HG12	2.49	0.46
3:J:158:VAL:HG11	3:J:180:LEU:HD11	1.97	0.46
1:B:288:LEU:HA	1:B:288:LEU:HD23	1.73	0.46
2:C:19:LEU:HD22	2:C:211:MET:HB2	1.97	0.46
2:D:217:ARG:HE	2:D:218:GLU:HG3	1.80	0.46
2:I:239:ILE:HG22	2:I:240:GLU:HG3	1.98	0.46
2:C:239:ILE:HG22	2:C:240:GLU:HG3	1.98	0.46
2:D:239:ILE:HG22	2:D:240:GLU:HG3	1.98	0.46
2:D:39:LYS:N	4:D:301:PO4:O4	2.37	0.46
2:D:19:LEU:HD22	2:D:211:MET:HB2	1.97	0.46
2:I:19:LEU:HD22	2:I:211:MET:HB2	1.97	0.46
3:E:203:GLN:HG2	3:E:203:GLN:H	1.43	0.46
3:E:221:ILE:HD11	3:E:238:PRO:HD3	1.98	0.46
1:G:222:ARG:HH12	2:I:49:MET:HG3	1.81	0.46
2:H:239:ILE:HG22	2:H:240:GLU:HG3	1.98	0.46
3:J:221:ILE:HD11	3:J:238:PRO:HD3	1.98	0.46
1:B:43:TRP:CD1	1:B:52:VAL:HG21	2.51	0.45
2:C:217:ARG:HE	2:C:218:GLU:HG3	1.80	0.45
1:F:322:LEU:HD21	1:G:131:ILE:HG23	1.98	0.45
1:G:298:LEU:HB2	1:G:301:ALA:HB3	1.97	0.45
3:E:158:VAL:HG11	3:E:180:LEU:HD11	1.97	0.45
1:F:80:LEU:HD21	1:F:236:VAL:HG23	1.98	0.45
1:A:80:LEU:HD21	1:A:236:VAL:HG23	1.98	0.45
1:A:322:LEU:HD21	1:B:131:ILE:HG23	1.97	0.45
1:B:269:LEU:HD22	1:B:274:VAL:HG11	1.99	0.45
1:B:317:PHE:CZ	1:B:321:LEU:HD11	2.52	0.45
2:C:42:LEU:O	2:C:46:MET:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:10:VAL:HA	2:D:54:GLY:HA3	1.99	0.45
1:A:72:ILE:HD11	1:A:280:ALA:HB2	1.99	0.45
2:C:236:ARG:NH2	2:C:243:ARG:HD3	2.32	0.45
2:H:236:ARG:NH2	2:H:243:ARG:HD3	2.32	0.45
2:H:10:VAL:HA	2:H:54:GLY:HA3	1.99	0.45
3:E:199:VAL:HB	3:E:203:GLN:HG3	1.98	0.44
1:G:287:LEU:HD23	1:G:287:LEU:HA	1.78	0.44
1:B:102:ILE:HD13	1:B:178:TRP:HE3	1.83	0.44
1:G:269:LEU:HD22	1:G:274:VAL:HG11	1.99	0.44
1:A:138:ARG:O	1:A:138:ARG:HG3	2.17	0.44
2:C:10:VAL:HA	2:C:54:GLY:HA3	1.99	0.44
1:F:192:TRP:CE2	1:F:193:LEU:HG	2.52	0.44
2:H:42:LEU:O	2:H:46:MET:HG3	2.18	0.44
1:F:72:ILE:HD11	1:F:280:ALA:HB2	1.99	0.44
2:C:157:LEU:HB3	2:C:160:PRO:HB3	2.00	0.44
3:J:252:ILE:HG13	3:J:253:LEU:H	1.82	0.44
3:J:86:ARG:HG2	3:J:106:TRP:CE3	2.53	0.44
1:B:133:LEU:HD23	1:B:133:LEU:HA	1.79	0.44
2:D:42:LEU:O	2:D:46:MET:HG3	2.18	0.44
2:I:145:THR:HA	2:I:146:PRO:HD3	1.90	0.44
1:A:192:TRP:CE2	1:A:193:LEU:HG	2.52	0.44
1:F:138:ARG:O	1:F:139:HIS:HB2	2.17	0.44
1:G:171:ASP:N	1:G:171:ASP:OD1	2.51	0.44
2:I:218:GLU:HB3	2:I:236:ARG:HH22	1.83	0.44
2:D:157:LEU:HB3	2:D:160:PRO:HB3	2.00	0.43
1:G:317:PHE:CZ	1:G:321:LEU:HD11	2.52	0.43
2:I:10:VAL:HA	2:I:54:GLY:HA3	2.00	0.43
2:D:236:ARG:NH2	2:D:243:ARG:HD3	2.33	0.43
1:G:102:ILE:HD13	1:G:178:TRP:HE3	1.83	0.43
2:H:157:LEU:HB3	2:H:160:PRO:HB3	2.00	0.43
2:I:236:ARG:NH2	2:I:243:ARG:HD3	2.32	0.43
3:E:252:ILE:HG13	3:E:253:LEU:H	1.82	0.43
2:H:218:GLU:HB3	2:H:236:ARG:HH22	1.84	0.43
1:G:101:LEU:HG	1:G:121:ALA:HB2	2.01	0.43
2:H:71:LEU:HA	2:H:71:LEU:HD23	1.89	0.43
2:D:98:GLN:HB3	2:D:98:GLN:HE21	1.71	0.43
1:G:168:THR:HG22	1:G:169:SER:H	1.84	0.43
2:I:42:LEU:O	2:I:46:MET:HG3	2.18	0.43
1:F:146:LEU:HA	1:F:146:LEU:HD12	1.90	0.43
1:F:291:ASP:HA	1:F:305:ILE:HD11	2.01	0.43
1:F:45:THR:O	1:F:49:GLU:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:218:GLU:HB3	2:C:236:ARG:HH22	1.83	0.43
1:F:168:THR:HG22	1:F:169:SER:H	1.84	0.43
1:A:78:GLN:HE22	1:A:261:PRO:HG2	1.84	0.42
1:A:223:GLN:NE2	2:C:143:GLN:OE1	2.44	0.42
1:A:55:ILE:HG21	3:E:202:GLU:HB2	2.01	0.42
1:A:52:VAL:O	1:A:57:LEU:HB2	2.19	0.42
1:B:114:ASN:HD21	1:B:189:ARG:HH12	1.66	0.42
2:D:145:THR:HA	2:D:146:PRO:HD3	1.89	0.42
1:G:136:ALA:HA	1:G:140:LEU:HD11	2.01	0.42
1:A:291:ASP:HA	1:A:305:ILE:HD11	2.01	0.42
3:J:74:ILE:O	3:J:79:PRO:HD3	2.18	0.42
2:D:218:GLU:HB3	2:D:236:ARG:HH22	1.83	0.42
3:E:74:ILE:O	3:E:79:PRO:HD3	2.18	0.42
2:I:217:ARG:HD3	2:I:217:ARG:H	1.84	0.42
1:B:171:ASP:N	1:B:171:ASP:OD1	2.51	0.42
3:E:86:ARG:HG2	3:E:106:TRP:CE3	2.53	0.42
2:I:217:ARG:HD3	2:I:217:ARG:N	2.35	0.42
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.77	0.42
1:B:101:LEU:HG	1:B:121:ALA:HB2	2.01	0.42
1:B:150:VAL:O	1:B:154:ILE:HG13	2.20	0.42
2:D:217:ARG:HD3	2:D:217:ARG:H	1.84	0.42
2:H:145:THR:HA	2:H:146:PRO:HD3	1.89	0.42
1:B:80:LEU:HD13	1:B:235:LEU:HB2	2.02	0.42
3:E:156:LYS:HD2	3:E:262:LEU:HG	2.02	0.42
1:G:150:VAL:O	1:G:154:ILE:HG13	2.20	0.42
3:J:150:TYR:HA	3:J:153:LYS:HD3	2.02	0.42
3:J:189:PHE:CE1	3:J:199:VAL:HG21	2.55	0.42
2:D:217:ARG:N	2:D:217:ARG:HD3	2.35	0.42
1:F:123:ALA:O	1:F:127:ILE:HG12	2.20	0.42
1:F:52:VAL:O	1:F:57:LEU:HB2	2.19	0.42
1:G:102:ILE:O	1:G:106:LEU:HG	2.20	0.42
1:G:114:ASN:HD21	1:G:189:ARG:HH12	1.66	0.42
2:H:217:ARG:H	2:H:217:ARG:HD3	1.84	0.42
2:I:157:LEU:HB3	2:I:160:PRO:HB3	2.01	0.42
1:A:123:ALA:O	1:A:127:ILE:HG12	2.20	0.42
1:A:168:THR:HG22	1:A:169:SER:H	1.84	0.42
2:D:46:MET:HB2	2:D:46:MET:HE2	1.78	0.42
3:J:168:PHE:HB2	3:J:197:PRO:O	2.20	0.42
1:B:136:ALA:HA	1:B:140:LEU:HD11	2.01	0.41
3:E:150:TYR:HA	3:E:153:LYS:HD3	2.02	0.41
1:F:145:LEU:HD23	1:F:145:LEU:HA	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:LEU:O	1:F:176:MET:HB2	2.20	0.41
1:B:168:THR:HG22	1:B:169:SER:H	1.84	0.41
1:A:154:ILE:HG21	1:B:255:PHE:CZ	2.55	0.41
1:A:172:LEU:O	1:A:176:MET:HB2	2.20	0.41
2:D:205:LEU:HD12	2:D:225:ASN:HB3	2.03	0.41
1:F:154:ILE:HG21	1:G:255:PHE:CZ	2.56	0.41
1:G:276:LEU:HB2	1:G:277:PRO:HD3	2.02	0.41
1:A:154:ILE:HG21	1:B:255:PHE:HZ	1.85	0.41
2:C:217:ARG:HD3	2:C:217:ARG:H	1.85	0.41
1:G:114:ASN:N	1:G:114:ASN:OD1	2.52	0.41
1:F:81:PHE:HE2	1:F:145:LEU:HB3	1.86	0.41
1:G:133:LEU:HD23	1:G:133:LEU:HA	1.79	0.41
2:C:205:LEU:HD12	2:C:225:ASN:HB3	2.03	0.41
3:E:168:PHE:HB2	3:E:197:PRO:O	2.20	0.41
1:F:78:GLN:HE22	1:F:261:PRO:HG2	1.85	0.41
1:A:134:ARG:O	1:A:137:ARG:HG2	2.20	0.41
1:A:27:LEU:HD21	1:A:64:LEU:HD11	2.03	0.41
1:A:36:GLN:O	1:A:38:ILE:HG13	2.21	0.41
1:A:92:GLY:HA3	1:A:153:GLY:HA2	2.03	0.41
3:E:189:PHE:CE1	3:E:199:VAL:HG21	2.55	0.41
3:J:214:ILE:HD13	3:J:224:ILE:HG13	2.03	0.41
1:B:276:LEU:HB2	1:B:277:PRO:HD3	2.03	0.41
1:F:140:LEU:HD13	1:F:144:ARG:HB2	2.03	0.41
1:F:176:MET:O	1:F:180:MET:HG3	2.21	0.41
2:H:217:ARG:N	2:H:217:ARG:HD3	2.36	0.41
1:A:176:MET:O	1:A:180:MET:HG3	2.21	0.41
2:H:205:LEU:HD12	2:H:225:ASN:HB3	2.03	0.41
2:C:217:ARG:HD3	2:C:217:ARG:N	2.36	0.41
1:B:300:ALA:HA	3:E:70:ASN:HB2	2.03	0.41
1:G:80:LEU:HD13	1:G:235:LEU:HB2	2.03	0.41
2:I:205:LEU:HD12	2:I:225:ASN:HB3	2.03	0.41
3:J:156:LYS:HD2	3:J:262:LEU:HG	2.01	0.41
3:E:205:LEU:HD23	3:E:232:LEU:HD22	2.02	0.40
1:F:209:ARG:HB3	1:F:210:PRO:HD3	2.03	0.40
1:G:288:LEU:HA	1:G:288:LEU:HD23	1.74	0.40
1:A:81:PHE:HE2	1:A:145:LEU:HB3	1.86	0.40
1:F:134:ARG:O	1:F:137:ARG:HG2	2.21	0.40
1:F:46:PRO:HA	1:F:49:GLU:HG2	2.03	0.40
1:A:209:ARG:HB3	1:A:210:PRO:HD3	2.03	0.40
1:B:102:ILE:O	1:B:106:LEU:HG	2.21	0.40
3:J:94:VAL:CG1	3:J:104:VAL:HG11	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PRO:HA	1:A:49:GLU:HG2	2.03	0.40
1:A:83:ASN:HA	1:A:84:PRO:HD3	1.91	0.40
1:F:36:GLN:HB3	1:F:56:ARG:NH2	2.36	0.40
2:I:46:MET:HE2	2:I:46:MET:HB2	1.80	0.40
3:J:243:TRP:CZ2	3:J:253:LEU:HD13	2.56	0.40
1:F:92:GLY:HA3	1:F:153:GLY:HA2	2.03	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	322/349 (92%)	309 (96%)	13 (4%)	0	100	100
1	B	322/349 (92%)	306 (95%)	14 (4%)	2 (1%)	28	70
1	F	322/349 (92%)	309 (96%)	13 (4%)	0	100	100
1	G	322/349 (92%)	306 (95%)	14 (4%)	2 (1%)	28	70
2	C	246/249 (99%)	242 (98%)	3 (1%)	1 (0%)	38	77
2	D	246/249 (99%)	243 (99%)	2 (1%)	1 (0%)	38	77
2	H	246/249 (99%)	242 (98%)	3 (1%)	1 (0%)	38	77
2	I	246/249 (99%)	242 (98%)	3 (1%)	1 (0%)	38	77
3	E	243/255 (95%)	225 (93%)	16 (7%)	2 (1%)	22	65
3	J	243/255 (95%)	225 (93%)	16 (7%)	2 (1%)	22	65
All	All	2758/2902 (95%)	2649 (96%)	97 (4%)	12 (0%)	38	77

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	103	ARG

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Mol	Chain	Res	Type
2	H	103	ARG
1	B	139	HIS
1	B	142	THR
2	D	103	ARG
3	E	230	GLU
1	G	139	HIS
1	G	142	THR
2	I	103	ARG
3	J	230	GLU
3	E	166	PRO
3	J	166	PRO

### 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	249/270 (92%)	227 (91%)	22 (9%)	12	43
1	B	249/270 (92%)	227 (91%)	22 (9%)	12	43
1	F	249/270 (92%)	227 (91%)	22 (9%)	12	43
1	G	249/270 (92%)	227 (91%)	22 (9%)	12	43
2	C	200/201 (100%)	189 (94%)	11 (6%)	25	62
2	D	200/201 (100%)	190 (95%)	10 (5%)	28	65
2	H	200/201 (100%)	189 (94%)	11 (6%)	25	62
2	I	200/201 (100%)	191 (96%)	9 (4%)	32	69
3	E	205/214 (96%)	197 (96%)	8 (4%)	37	72
3	J	205/214 (96%)	197 (96%)	8 (4%)	37	72
All	All	2206/2312 (95%)	2061 (93%)	145 (7%)	19	57

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	35	GLU

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Mol	Chain	Res	Type
1	A	37	TRP
1	A	42	ASP
1	A	45	THR
1	A	50	LEU
1	A	52	VAL
1	A	54	GLN
1	A	61	LEU
1	A	77	MET
1	A	101	LEU
1	A	128	ILE
1	A	140	LEU
1	A	168	THR
1	A	173	ARG
1	A	176	MET
1	A	229	TRP
1	A	249	LEU
1	A	287	LEU
1	A	298	LEU
1	A	305	ILE
1	A	307	VAL
1	B	27	LEU
1	B	29	LEU
1	B	42	ASP
1	B	53	TRP
1	B	102	ILE
1	B	111	GLN
1	B	114	ASN
1	B	133	LEU
1	B	164	ILE
1	B	168	THR
1	B	171	ASP
1	B	172	LEU
1	B	173	ARG
1	B	180	MET
1	B	189	ARG
1	B	204	ILE
1	B	206	SER
1	B	249	LEU
1	B	256	ILE
1	B	287	LEU
1	B	302	GLU
1	B	305	ILE

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Mol	Chain	Res	Type
2	C	45	ARG
2	C	71	LEU
2	C	78	LEU
2	C	105	GLU
2	C	106	LEU
2	C	140	VAL
2	C	205	LEU
2	C	217	ARG
2	C	218	GLU
2	C	228	GLN
2	C	249	ILE
2	D	7	LEU
2	D	71	LEU
2	D	78	LEU
2	D	105	GLU
2	D	106	LEU
2	D	140	VAL
2	D	205	LEU
2	D	217	ARG
2	D	218	GLU
2	D	228	GLN
3	E	73	ARG
3	E	85	TRP
3	E	173	GLU
3	E	203	GLN
3	E	215	THR
3	E	228	TRP
3	E	244	PHE
3	E	256	GLN
1	F	29	LEU
1	F	35	GLU
1	F	37	TRP
1	F	42	ASP
1	F	45	THR
1	F	50	LEU
1	F	52	VAL
1	F	54	GLN
1	F	61	LEU
1	F	77	MET
1	F	101	LEU
1	F	128	ILE
1	F	138	ARG

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Mol	Chain	Res	Type
1	F	168	THR
1	F	173	ARG
1	F	176	MET
1	F	229	TRP
1	F	249	LEU
1	F	287	LEU
1	F	298	LEU
1	F	305	ILE
1	F	307	VAL
1	G	27	LEU
1	G	29	LEU
1	G	42	ASP
1	G	53	TRP
1	G	102	ILE
1	G	111	GLN
1	G	114	ASN
1	G	133	LEU
1	G	164	ILE
1	G	168	THR
1	G	171	ASP
1	G	172	LEU
1	G	173	ARG
1	G	180	MET
1	G	189	ARG
1	G	204	ILE
1	G	206	SER
1	G	249	LEU
1	G	256	ILE
1	G	287	LEU
1	G	302	GLU
1	G	305	ILE
2	H	45	ARG
2	H	71	LEU
2	H	78	LEU
2	H	105	GLU
2	H	106	LEU
2	H	140	VAL
2	H	205	LEU
2	H	217	ARG
2	H	218	GLU
2	H	228	GLN
2	H	249	ILE

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Mol	Chain	Res	Type
2	I	71	LEU
2	I	78	LEU
2	I	105	GLU
2	I	106	LEU
2	I	140	VAL
2	I	205	LEU
2	I	217	ARG
2	I	218	GLU
2	I	228	GLN
3	J	73	ARG
3	J	85	TRP
3	J	173	GLU
3	J	203	GLN
3	J	215	THR
3	J	228	TRP
3	J	244	PHE
3	J	256	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	HIS
2	C	195	HIS
2	C	199	HIS
2	D	97	HIS
2	D	195	HIS
2	D	199	HIS
3	E	62	GLN
1	F	272	HIS
2	H	195	HIS
2	H	199	HIS
2	I	97	HIS
2	I	195	HIS
2	I	199	HIS
3	J	62	GLN

### 5.3.3 RNA ⓘ

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](#)

16 ligands 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	$\# Z  > 2$
4	PO4	C	301	-	4,4,4	0.98	0	6,6,6	0.59	0
5	SO4	C	302	-	4,4,4	0.11	0	6,6,6	0.05	0
5	SO4	C	303	-	4,4,4	0.11	0	6,6,6	0.05	0
5	SO4	C	304	-	4,4,4	0.11	0	6,6,6	0.04	0
4	PO4	D	301	-	4,4,4	0.93	0	6,6,6	0.49	0
5	SO4	D	302	-	4,4,4	0.10	0	6,6,6	0.05	0
5	SO4	D	303	-	4,4,4	0.11	0	6,6,6	0.06	0
5	SO4	D	304	-	4,4,4	0.11	0	6,6,6	0.04	0
4	PO4	H	301	-	4,4,4	0.87	0	6,6,6	0.42	0
5	SO4	H	302	-	4,4,4	0.11	0	6,6,6	0.04	0
5	SO4	H	303	-	4,4,4	0.11	0	6,6,6	0.05	0
5	SO4	H	304	-	4,4,4	0.11	0	6,6,6	0.04	0
4	PO4	I	301	-	4,4,4	0.78	0	6,6,6	0.44	0
5	SO4	I	302	-	4,4,4	0.12	0	6,6,6	0.04	0
5	SO4	I	303	-	4,4,4	0.11	0	6,6,6	0.05	0
5	SO4	I	304	-	4,4,4	0.11	0	6,6,6	0.05	0

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
4	PO4	C	301	-	-	0/0/0/0	0/0/0/0
5	SO4	C	302	-	-	0/0/0/0	0/0/0/0
5	SO4	C	303	-	-	0/0/0/0	0/0/0/0
5	SO4	C	304	-	-	0/0/0/0	0/0/0/0
4	PO4	D	301	-	-	0/0/0/0	0/0/0/0
5	SO4	D	302	-	-	0/0/0/0	0/0/0/0
5	SO4	D	303	-	-	0/0/0/0	0/0/0/0
5	SO4	D	304	-	-	0/0/0/0	0/0/0/0
4	PO4	H	301	-	-	0/0/0/0	0/0/0/0
5	SO4	H	302	-	-	0/0/0/0	0/0/0/0
5	SO4	H	303	-	-	0/0/0/0	0/0/0/0
5	SO4	H	304	-	-	0/0/0/0	0/0/0/0
4	PO4	I	301	-	-	0/0/0/0	0/0/0/0
5	SO4	I	302	-	-	0/0/0/0	0/0/0/0
5	SO4	I	303	-	-	0/0/0/0	0/0/0/0
5	SO4	I	304	-	-	0/0/0/0	0/0/0/0

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.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	301	PO4	2	0
4	D	301	PO4	1	0
4	H	301	PO4	2	0
4	I	301	PO4	1	0
5	I	303	SO4	2	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, 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	324/349 (92%)	0.14	12 (3%) 42 35	16, 52, 148, 268	0
1	B	324/349 (92%)	0.10	3 (0%) 84 77	15, 46, 114, 241	0
1	F	324/349 (92%)	0.16	12 (3%) 42 35	15, 50, 144, 254	0
1	G	324/349 (92%)	0.09	5 (1%) 74 66	16, 45, 117, 237	0
2	C	248/249 (99%)	0.07	2 (0%) 86 79	17, 52, 115, 165	0
2	D	248/249 (99%)	0.07	0 100 100	12, 35, 96, 159	0
2	H	248/249 (99%)	0.12	2 (0%) 86 79	16, 53, 113, 202	0
2	I	248/249 (99%)	0.06	0 100 100	12, 36, 93, 183	0
3	E	245/255 (96%)	0.36	12 (4%) 30 24	42, 98, 160, 208	0
3	J	245/255 (96%)	0.33	9 (3%) 42 35	46, 95, 165, 224	0
All	All	2778/2902 (95%)	0.15	57 (2%) 64 55	12, 53, 138, 268	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	323	LYS	9.2
1	F	36	GLN	7.8
1	G	323	LYS	7.8
1	G	324	ALA	6.6
1	A	36	GLN	5.6
1	B	324	ALA	5.4
3	J	155	LYS	4.6
1	A	34	GLY	4.2
1	A	324	ALA	4.0
3	E	155	LYS	4.0
1	F	34	GLY	4.0
1	F	324	ALA	3.7
1	F	139	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	38	ILE	3.5
1	F	38	ILE	3.4
1	F	43	TRP	3.2
2	H	249	ILE	3.2
1	A	139	HIS	3.2
1	A	138	ARG	3.2
1	A	43	TRP	3.0
3	J	173	GLU	2.9
1	A	51	PHE	2.9
3	E	189	PHE	2.9
3	J	125	TRP	2.8
1	F	140	LEU	2.8
3	E	266	ASP	2.7
1	A	161	THR	2.7
1	F	41	GLY	2.7
3	J	153	LYS	2.6
3	J	266	ASP	2.6
1	G	47	ARG	2.5
3	E	152	ASP	2.5
3	E	153	LYS	2.4
3	J	152	ASP	2.4
3	J	230	GLU	2.4
3	E	208	SER	2.4
1	B	138	ARG	2.4
3	E	192	SER	2.4
1	A	41	GLY	2.4
3	E	162	PHE	2.3
1	A	176	MET	2.3
3	E	173	GLU	2.3
1	F	50	LEU	2.3
2	C	249	ILE	2.3
3	J	252	ILE	2.2
1	F	137	ARG	2.2
1	G	36	GLN	2.2
3	J	190	LYS	2.2
1	F	44	PHE	2.2
1	G	169	SER	2.1
2	H	240	GLU	2.1
3	E	22	ALA	2.1
1	F	37	TRP	2.1
3	E	237	ILE	2.1
2	C	117	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	125	TRP	2.1
1	A	140	LEU	2.0

## 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	PO4	D	301	5/5	0.98	0.18	-0.19	28,29,30,30	0
4	PO4	I	301	5/5	0.97	0.16	-0.70	34,35,36,36	0
4	PO4	C	301	5/5	0.95	0.16	-0.84	39,40,40,41	0
4	PO4	H	301	5/5	0.97	0.16	-1.26	41,42,42,43	0
5	SO4	C	303	5/5	0.79	0.47	-	139,139,140,140	0
5	SO4	I	302	5/5	0.82	0.18	-	152,153,153,155	0
5	SO4	H	304	5/5	0.83	0.19	-	153,153,153,155	0
5	SO4	D	303	5/5	0.91	0.15	-	144,144,144,145	0
5	SO4	D	304	5/5	0.79	0.35	-	142,142,143,143	0
5	SO4	H	302	5/5	0.82	0.26	-	146,146,147,148	0
5	SO4	I	304	5/5	0.92	0.43	-	159,159,160,162	0
5	SO4	D	302	5/5	0.80	0.18	-	145,145,146,146	0
5	SO4	C	302	5/5	0.90	0.15	-	142,142,143,143	0
5	SO4	H	303	5/5	0.82	0.45	-	143,143,143,145	0
5	SO4	C	304	5/5	0.83	0.15	-	145,145,146,146	0
5	SO4	I	303	5/5	0.86	0.24	-	157,157,158,159	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.