



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:46 AM GMT

PDB ID : 3PUX  
Title : Crystal Structure of an outward-facing MBP-Maltose transporter complex bound to ADP-BeF<sub>3</sub>  
Authors : Oldham, M.L.; Chen, J.  
Deposited on : 2010-12-06  
Resolution : 2.30 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

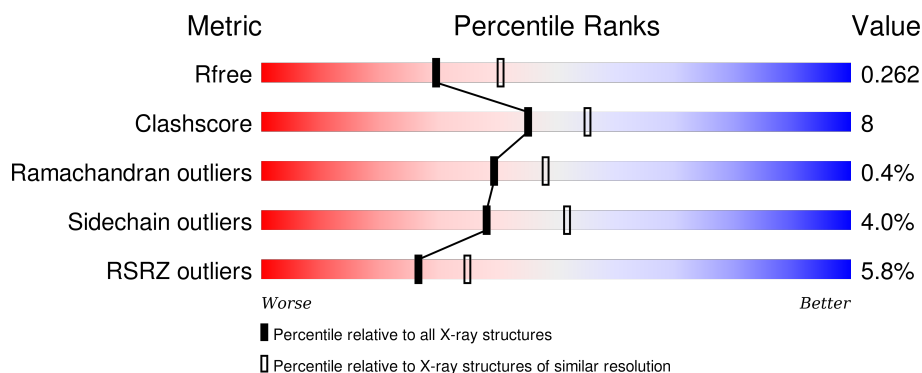
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	E	378	<div> <div>4%</div> <div>85%13%..</div> </div>
2	F	514	<div> <div>6%</div> <div>79%16%• 5%</div> </div>
3	G	296	<div> <div>5%</div> <div>83%15%..</div> </div>
4	A	381	<div> <div>4%</div> <div>75%20%• •</div> </div>
4	B	381	<div> <div>8%</div> <div>73%19%• 6%</div> </div>

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
7	PGV	F	4001	-	-	-	X
7	PGV	F	4010	-	-	-	X
7	PGV	G	4009	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15273 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 Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	374	Total	C	N	O	S	0	3	0
			2915	1879	474	556	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	371	ALA	-	EXPRESSION TAG	UNP P0AEX9
E	372	SER	-	EXPRESSION TAG	UNP P0AEX9
E	373	ALA	-	EXPRESSION TAG	UNP P0AEX9
E	374	SER	-	EXPRESSION TAG	UNP P0AEX9
E	375	HIS	-	EXPRESSION TAG	UNP P0AEX9
E	376	HIS	-	EXPRESSION TAG	UNP P0AEX9
E	377	HIS	-	EXPRESSION TAG	UNP P0AEX9
E	378	HIS	-	EXPRESSION TAG	UNP P0AEX9

- Molecule 2 is a protein called Maltose transport system permease protein malF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	490	Total	C	N	O	S	0	2	0
			3831	2520	608	685	18			

- Molecule 3 is a protein called Maltose transport system permease protein malG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	293	Total	C	N	O	S	0	2	0
			2270	1520	362	378	10			

- Molecule 4 is a protein called Maltose/maltodextrin import ATP-binding protein MalK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	371	Total	C	N	O	S	0	8	0
			2929	1856	522	536	15			

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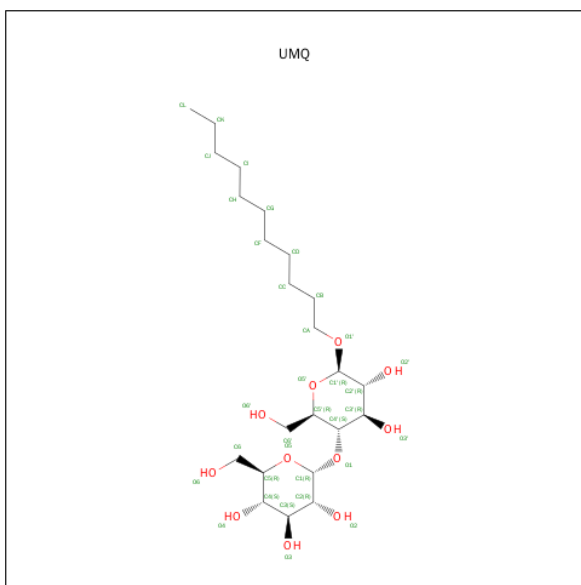
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	358	Total	C	N	O	S	0	4	0
			2816	1785	502	516	13			

There are 20 discrepancies between the modelled and reference sequences:

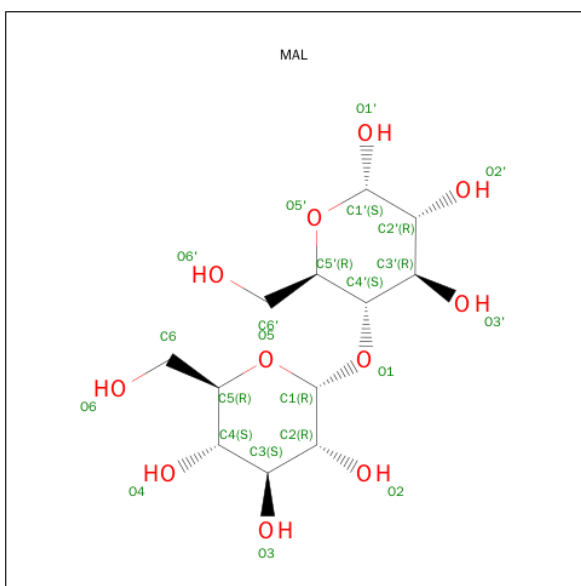
Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	EXPRESSION TAG	UNP P68187
A	373	SER	-	EXPRESSION TAG	UNP P68187
A	374	ALA	-	EXPRESSION TAG	UNP P68187
A	375	SER	-	EXPRESSION TAG	UNP P68187
A	376	HIS	-	EXPRESSION TAG	UNP P68187
A	377	HIS	-	EXPRESSION TAG	UNP P68187
A	378	HIS	-	EXPRESSION TAG	UNP P68187
A	379	HIS	-	EXPRESSION TAG	UNP P68187
A	380	HIS	-	EXPRESSION TAG	UNP P68187
A	381	HIS	-	EXPRESSION TAG	UNP P68187
B	372	ALA	-	EXPRESSION TAG	UNP P68187
B	373	SER	-	EXPRESSION TAG	UNP P68187
B	374	ALA	-	EXPRESSION TAG	UNP P68187
B	375	SER	-	EXPRESSION TAG	UNP P68187
B	376	HIS	-	EXPRESSION TAG	UNP P68187
B	377	HIS	-	EXPRESSION TAG	UNP P68187
B	378	HIS	-	EXPRESSION TAG	UNP P68187
B	379	HIS	-	EXPRESSION TAG	UNP P68187
B	380	HIS	-	EXPRESSION TAG	UNP P68187
B	381	HIS	-	EXPRESSION TAG	UNP P68187

- Molecule 5 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: C<sub>23</sub>H<sub>44</sub>O<sub>11</sub>).



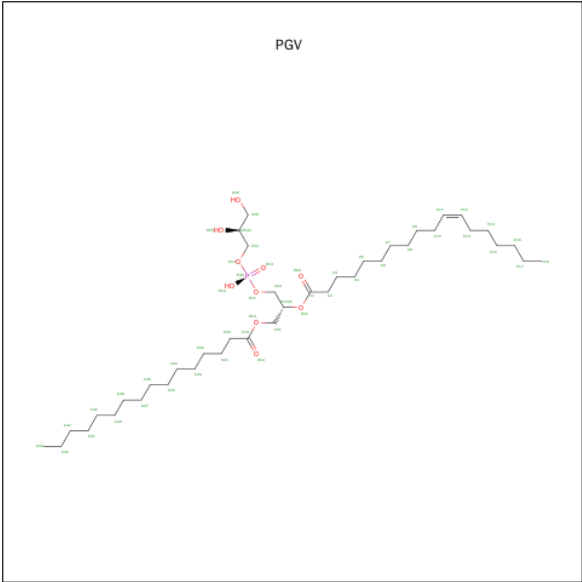
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			34	23	11		

- Molecule 6 is SUGAR (MALTOSE) (three-letter code: MAL) (formula:  $C_{12}H_{22}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	C	O	0	0
			23	12	11		

- Molecule 7 is (1R)-2-{\{[(2S)-2,3-DIHYDROXYPROPYL]OXY\}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula:  $C_{40}H_{77}O_{10}P$ ).

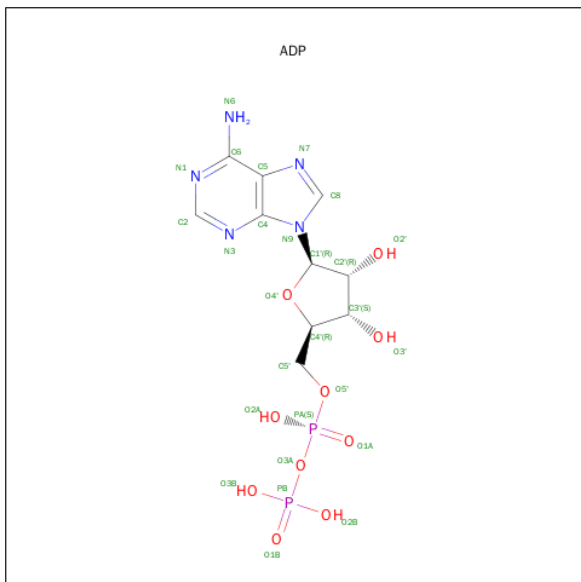


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total C O P 51 40 10 1	0	0
7	F	1	Total C 9 9	0	0
7	F	1	Total C 8 8	0	0
7	F	1	Total C 13 13	0	0
7	G	1	Total C 8 8	0	0
7	G	1	Total C 12 12	0	0
7	G	1	Total C 10 10	0	0
7	G	1	Total C 7 7	0	0
7	G	1	Total C 9 9	0	0
7	G	1	Total C 12 12	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

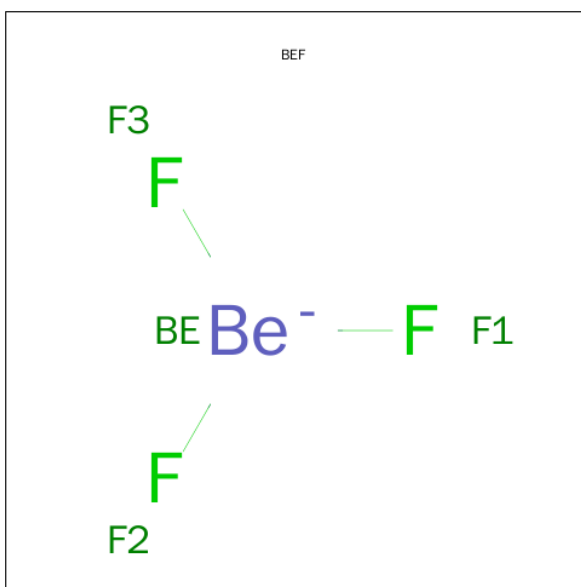
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Mg 1 1	0	0
8	A	1	Total Mg 1 1	0	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 10 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula:  $BeF_3$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total 4	Be 1	F 3	0	0
10	B	1	Total 4	Be 1	F 3	0	0

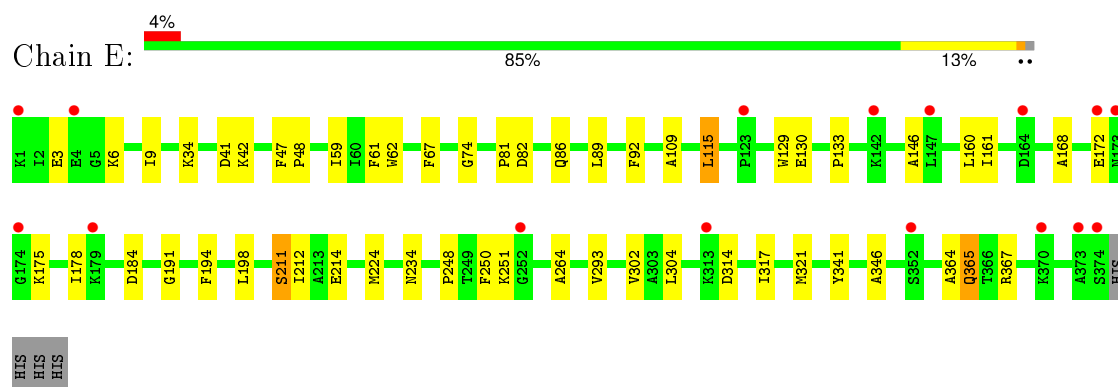
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	E	56	Total 56	O 56	0	0
11	F	44	Total 44	O 44	0	0
11	G	51	Total 51	O 51	0	0
11	A	61	Total 61	O 61	0	0
11	B	40	Total 40	O 40	0	0

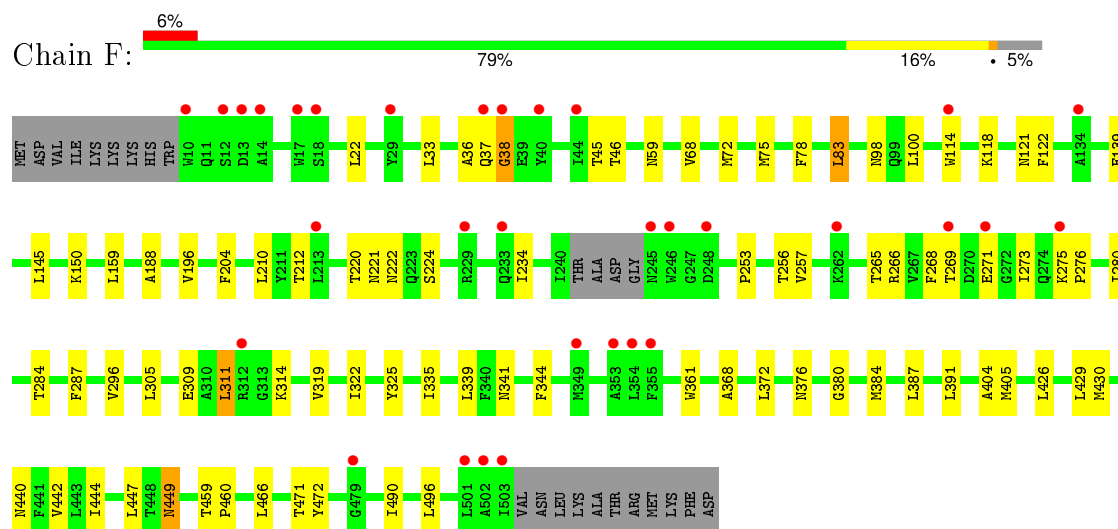
### 3 Residue-property plots

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

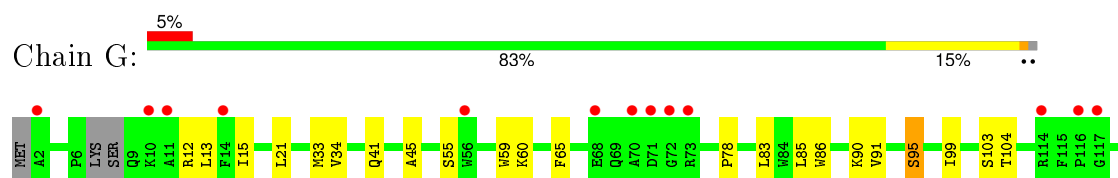
- Molecule 1: Maltose-binding periplasmic protein



- Molecule 2: Maltose transport system permease protein malF

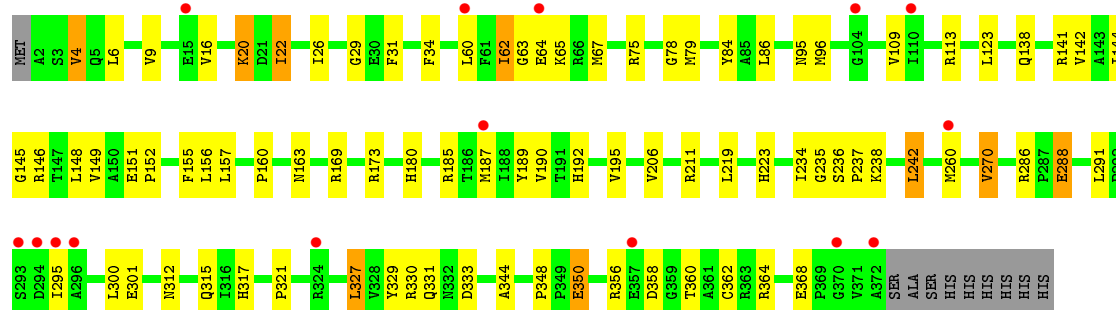
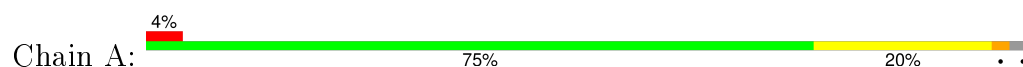


- Molecule 3: Maltose transport system permease protein malG

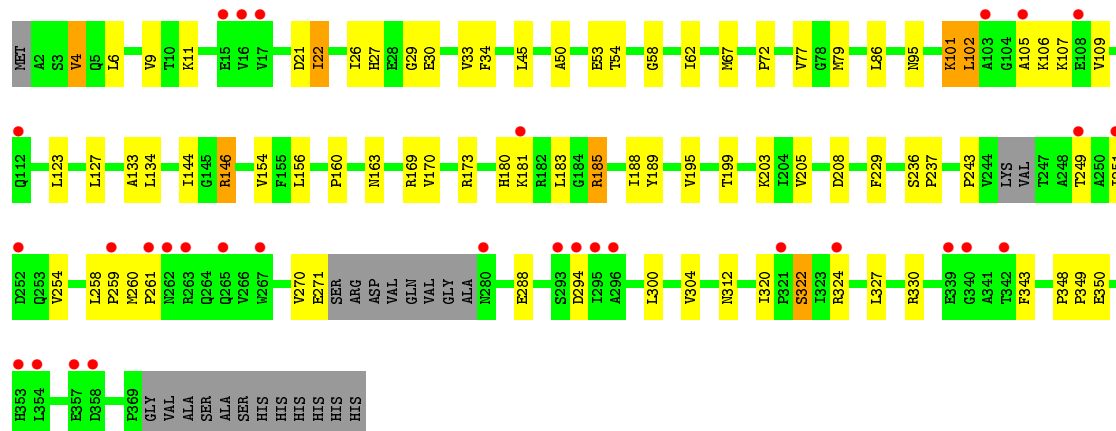
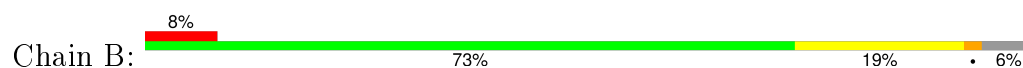




- Molecule 4: Maltose/maltodextrin import ATP-binding protein MalK



- Molecule 4: Maltose/maltodextrin import ATP-binding protein MalK



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.13Å 97.34Å 112.84Å 85.58° 78.98° 72.25°	Depositor
Resolution (Å)	19.81 – 2.30 19.81 – 2.20	Depositor EDS
% Data completeness (in resolution range)	64.8 (19.81-2.30) 57.8 (19.81-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.228 , 0.265 0.226 , 0.262	Depositor DCC
$R_{free}$ test set	4725 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.1	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 95976 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	15273	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, UMQ, ADP, BEF, PGV, MAL

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	E	0.57	2/2990 (0.1%)	0.60	0/4059
2	F	0.51	0/3932	0.62	1/5351 (0.0%)
3	G	0.58	0/2334	0.61	1/3188 (0.0%)
4	A	0.54	0/2991	0.68	1/4055 (0.0%)
4	B	0.50	0/2870	0.63	1/3889 (0.0%)
All	All	0.54	2/15117 (0.0%)	0.63	4/20542 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	251	LYS	CD-CE	7.38	1.69	1.51
1	E	250	PHE	CG-CD1	5.08	1.46	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	235	LEU	CA-CB-CG	6.78	130.89	115.30
4	B	146	ARG	NE-CZ-NH2	-6.14	117.23	120.30
2	F	33	LEU	CA-CB-CG	5.52	128.00	115.30
4	A	242	LEU	CA-CB-CG	5.43	127.78	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2915	0	2898	32	0
2	F	3831	0	3869	59	0
3	G	2270	0	2364	32	0
4	A	2929	0	3011	75	0
4	B	2816	0	2881	47	0
5	E	34	0	44	2	0
6	F	23	0	22	1	0
7	F	81	0	122	0	0
7	G	58	0	82	3	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	27	0	12	2	0
9	B	27	0	12	0	0
10	A	4	0	0	0	0
10	B	4	0	0	0	0
11	A	61	0	0	10	0
11	B	40	0	0	5	0
11	E	56	0	0	4	0
11	F	44	0	0	8	0
11	G	51	0	0	3	0
All	All	15273	0	15317	237	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.

All (237) 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)
2:F:471:THR:HG21	2:F:490:ILE:HG21	1.18	1.16
4:B:6:LEU:HD22	4:B:22:ILE:HD11	1.36	1.06
2:F:471:THR:CG2	2:F:490:ILE:HG21	1.87	1.04
4:A:62[A]:ILE:HG23	4:A:67:MET:HG3	1.38	1.02
2:F:405[B]:MET:HA	2:F:405[B]:MET:CE	1.92	0.99
4:B:134:LEU:HD23	11:B:400:HOH:O	1.66	0.93
1:E:115:LEU:HD21	1:E:224:MET:HE3	1.50	0.91
2:F:471:THR:HG21	2:F:490:ILE:CG2	2.00	0.91
4:A:187[B]:MET:CE	4:A:187[B]:MET:C	2.43	0.87
4:A:286:ARG:HB3	4:A:288:GLU:OE1	1.76	0.84
2:F:405[B]:MET:HA	2:F:405[B]:MET:HE3	1.59	0.83
2:F:339:LEU:HD21	3:G:33[B]:MET:SD	2.19	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:187[B]:MET:HE3	4:A:187[B]:MET:O	1.79	0.82
2:F:471:THR:HG23	2:F:490:ILE:HD13	1.60	0.81
4:A:356:ARG:HH11	4:A:360:THR:HG23	1.46	0.81
4:A:31:PHE:CE1	4:A:187[B]:MET:HE1	2.16	0.81
3:G:91:VAL:O	3:G:95:SER:HB2	1.79	0.81
4:A:187[B]:MET:HE3	4:A:187[B]:MET:C	2.00	0.81
4:A:235:GLY:HA2	11:A:431:HOH:O	1.81	0.79
4:A:223:HIS:CE1	4:A:368:GLU:HG2	2.19	0.78
4:A:163:ASN:OD1	11:A:425:HOH:O	2.01	0.77
4:B:188[B]:ILE:HD12	4:B:189:TYR:N	1.98	0.77
4:B:320:ILE:HD11	4:B:327:LEU:HB2	1.70	0.73
4:A:79:MET:HG3	4:A:156:LEU:HB2	1.71	0.73
4:A:187[B]:MET:CE	4:A:187[B]:MET:O	2.37	0.73
3:G:166:TYR:OH	3:G:229:GLU:HG2	1.90	0.72
2:F:284:THR:HG22	2:F:466:LEU:HA	1.72	0.72
2:F:159:LEU:HD11	2:F:188:ALA:HB1	1.72	0.71
11:A:425:HOH:O	4:B:163:ASN:OD1	2.07	0.71
4:B:169:ARG:HD3	11:B:404:HOH:O	1.91	0.70
4:A:288:GLU:HG2	4:B:312:ASN:HB2	1.72	0.70
4:A:67:MET:HE1	4:A:75:ARG:HA	1.73	0.70
1:E:62:TRP:HB3	1:E:67:PHE:HE1	1.56	0.70
2:F:372:LEU:HD12	2:F:447:LEU:HD23	1.74	0.69
4:A:329:TYR:CE2	4:A:331:GLN:HG2	2.28	0.69
2:F:280:ILE:O	2:F:284:THR:HG23	1.93	0.68
2:F:78:PHE:HZ	3:G:164:PHE:CE2	2.13	0.67
1:E:34:LYS:HD3	11:E:407:HOH:O	1.95	0.67
4:A:60[B]:LEU:HD12	4:A:67:MET:HB2	1.75	0.67
2:F:405[A]:MET:HE1	4:B:77[A]:VAL:HG12	1.78	0.66
4:B:133:ALA:O	11:B:400:HOH:O	2.13	0.65
4:A:157:LEU:CD1	4:A:187[B]:MET:SD	2.84	0.65
3:G:78:PRO:HD2	11:G:344:HOH:O	1.95	0.65
4:A:301:GLU:HG3	4:A:344:ALA:HB2	1.79	0.64
1:E:211:SER:HB2	11:E:390:HOH:O	1.98	0.64
1:E:367:ARG:HD2	2:F:460:PRO:HG3	1.82	0.61
4:B:188[B]:ILE:HD12	4:B:188[B]:ILE:C	2.21	0.60
4:A:86:LEU:HA	4:A:146:ARG:NH2	2.17	0.60
4:A:65:LYS:O	4:A:67:MET:HG2	2.02	0.58
2:F:405[B]:MET:HA	2:F:405[B]:MET:HE2	1.84	0.58
4:A:270:VAL:HG13	4:A:362:CYS:HB3	1.86	0.58
1:E:146:ALA:O	1:E:224:MET:HG2	2.03	0.58
3:G:86:TRP:CE2	3:G:90:LYS:HD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:260[B]:MET:SD	4:A:321:PRO:HG2	2.44	0.57
4:B:34:PHE:CD1	4:B:188[B]:ILE:HD11	2.40	0.57
4:A:206:VAL:HG21	4:A:234:ILE:HD11	1.87	0.56
2:F:372:LEU:HD21	2:F:444:ILE:HD12	1.87	0.56
4:A:187[B]:MET:HE1	4:A:189:TYR:HB2	1.86	0.56
4:A:6:LEU:HB3	4:A:9:VAL:CG2	2.35	0.56
4:B:101:LYS:HE2	4:B:105:ALA:HB1	1.87	0.56
4:B:156:LEU:HD23	4:B:188[B]:ILE:HG23	1.88	0.55
4:B:11:LYS:HD3	4:B:54:THR:O	2.07	0.55
3:G:166:TYR:CZ	3:G:229:GLU:HG2	2.42	0.55
4:B:195:VAL:O	4:B:199:THR:HG23	2.07	0.55
4:B:288:GLU:HG3	4:B:330:ARG:HD3	1.86	0.55
2:F:341:ASN:O	2:F:344:PHE:O	2.25	0.55
4:A:187[B]:MET:C	4:A:187[B]:MET:SD	2.85	0.54
2:F:442:VAL:HG23	11:F:530:HOH:O	2.06	0.54
4:B:208:ASP:HB2	4:B:229:PHE:CE2	2.41	0.54
4:A:60[B]:LEU:HD11	4:A:62[B]:ILE:HG13	1.90	0.54
4:B:183:LEU:HB3	4:B:185:ARG:HG3	1.89	0.54
2:F:444:ILE:HG13	2:F:466:LEU:HG	1.89	0.54
1:E:42:LYS:HD2	11:E:393:HOH:O	2.08	0.54
4:A:329:TYR:CZ	4:A:331:GLN:HG2	2.43	0.54
4:B:4:VAL:HG13	4:B:26:ILE:HB	1.89	0.54
3:G:99:ILE:HG23	3:G:170:ILE:HG22	1.90	0.53
4:A:358:ASP:OD1	4:A:360:THR:HG22	2.08	0.53
4:B:249:THR:HG22	4:B:254:VAL:HG13	1.91	0.53
2:F:121:ASN:HB3	11:F:534:HOH:O	2.08	0.53
4:A:187[B]:MET:CE	4:A:189:TYR:HB2	2.39	0.53
3:G:104:THR:HG21	3:G:208:LEU:HD21	1.91	0.53
2:F:449:ASN:ND2	11:F:547:HOH:O	2.35	0.52
2:F:265:THR:O	2:F:268:PHE:N	2.41	0.52
2:F:36:ALA:O	2:F:38:GLY:N	2.40	0.52
3:G:83:LEU:HD13	7:G:4003:PGV:H52	1.92	0.52
2:F:309:GLU:HA	2:F:314:LYS:NZ	2.24	0.52
4:A:60[B]:LEU:CD1	4:A:62[B]:ILE:HG13	2.40	0.52
2:F:391:LEU:HD13	2:F:426:LEU:HD12	1.91	0.52
4:A:173[B]:ARG:HH12	4:A:195:VAL:HG11	1.76	0.51
4:A:109:VAL:O	4:A:113:ARG:HG2	2.11	0.51
2:F:118:LYS:HE3	2:F:139:GLU:CD	2.30	0.51
4:A:364:ARG:NH2	11:A:421:HOH:O	2.44	0.51
4:A:260[A]:MET:HE2	4:A:300:LEU:HD22	1.92	0.51
2:F:212:THR:HG23	2:F:222:ASN:OD1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:387:LEU:HD13	2:F:429:LEU:HD13	1.92	0.51
3:G:212:VAL:HG22	3:G:284:TRP:CE3	2.45	0.51
1:E:133:PRO:HG3	1:E:198:LEU:HD23	1.93	0.51
4:A:291:LEU:HD11	4:A:348:PRO:HB3	1.91	0.51
4:B:27:HIS:O	4:B:30:GLU:HB2	2.11	0.51
4:B:170:VAL:HG22	4:B:173:ARG:HH21	1.75	0.51
3:G:146:ARG:O	3:G:149:GLU:HG2	2.11	0.51
4:B:144:ILE:HD11	4:B:160:PRO:O	2.11	0.50
4:A:16:VAL:HG11	11:A:393:HOH:O	2.11	0.50
4:B:95:ASN:O	4:B:146:ARG:HG3	2.12	0.50
4:A:151:GLU:O	4:A:185:ARG:NH2	2.42	0.50
4:A:6:LEU:HB3	4:A:9:VAL:HG21	1.94	0.50
4:A:173[B]:ARG:NH1	4:A:195:VAL:CG1	2.74	0.50
3:G:230:VAL:HG22	3:G:246:ALA:HB1	1.93	0.49
1:E:62:TRP:HB3	1:E:67:PHE:CE1	2.43	0.49
3:G:208:LEU:HD22	3:G:215:LEU:HD11	1.93	0.49
2:F:471:THR:HG22	2:F:472:TYR:CD1	2.48	0.49
4:A:173[B]:ARG:NH1	4:A:195:VAL:HG11	2.28	0.49
4:A:157:LEU:HD12	4:A:187[B]:MET:SD	2.52	0.49
1:E:184:ASP:HB2	1:E:365:GLN:CD	2.34	0.48
4:A:146:ARG:HD2	11:A:391:HOH:O	2.13	0.48
4:A:356:ARG:NH1	4:A:360:THR:HG23	2.23	0.48
3:G:59:TRP:CE2	7:G:4006:PGV:H152	2.49	0.48
1:E:346:ALA:HB2	1:E:364:ALA:HB2	1.96	0.48
4:A:312:ASN:HB2	4:B:288:GLU:HG2	1.94	0.48
3:G:166:TYR:OH	3:G:229:GLU:CG	2.60	0.48
3:G:41:GLN:HB3	3:G:55:SER:HB2	1.94	0.48
2:F:335[A]:ILE:HD12	3:G:34:VAL:HG22	1.94	0.48
3:G:85:LEU:HD22	3:G:269:MET:HE3	1.96	0.48
3:G:129:GLN:HB3	3:G:130:MET:CE	2.43	0.48
4:A:260[A]:MET:N	4:A:260[A]:MET:SD	2.87	0.48
4:A:236:SER:HA	4:A:237:PRO:C	2.34	0.48
4:A:169:ARG:HD3	11:A:405:HOH:O	2.13	0.47
3:G:212:VAL:HG13	3:G:284:TRP:HB3	1.95	0.47
4:A:78:GLY:HA3	4:A:152:PRO:HG3	1.97	0.47
3:G:187:SER:HA	3:G:190:GLU:HB2	1.96	0.47
1:E:109:ALA:HA	1:E:302:VAL:HA	1.96	0.47
5:E:5004:UMQ:H62	11:F:535:HOH:O	2.14	0.47
4:A:350:GLU:H	4:A:350:GLU:HG3	1.53	0.47
2:F:325:TYR:O	11:F:525:HOH:O	2.20	0.47
3:G:45:ALA:HB2	3:G:260:TRP:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:245:LEU:HG	3:G:249:MET:HE2	1.96	0.47
1:E:41:ASP:HB2	11:G:305:HOH:O	2.15	0.47
2:F:98:ASN:O	2:F:256:THR:HG22	2.15	0.47
1:E:92:PHE:HZ	1:E:321:MET:HE1	1.79	0.46
4:B:6:LEU:CD2	4:B:22:ILE:HD11	2.25	0.46
4:A:123:LEU:HD11	4:A:141:ARG:HB3	1.97	0.46
2:F:75:MET:HE1	11:G:330:HOH:O	2.15	0.46
3:G:214:ILE:HA	3:G:214:ILE:HD12	1.77	0.46
1:E:47:PHE:HB3	1:E:48:PRO:HD3	1.97	0.46
3:G:60:LYS:HB3	3:G:65:PHE:HB2	1.97	0.46
4:A:145:GLY:O	4:A:149:VAL:HG23	2.16	0.46
4:A:144:ILE:HD11	4:A:160:PRO:O	2.16	0.46
4:A:329:TYR:CE2	4:A:331:GLN:CG	2.97	0.46
4:B:77[B]:VAL:HG12	4:B:154:VAL:HB	1.97	0.45
2:F:335[A]:ILE:HD12	3:G:34:VAL:CG2	2.47	0.45
4:B:348:PRO:HA	4:B:349:PRO:HD3	1.80	0.45
7:G:4003:PGV:H92	7:G:4004:PGV:H71	1.98	0.45
1:E:130:GLU:HA	1:E:194:PHE:CZ	2.52	0.45
2:F:471:THR:HG23	2:F:490:ILE:HG21	1.91	0.45
4:A:6:LEU:HD22	4:A:22:ILE:HD11	1.98	0.45
4:B:243:PRO:O	4:B:259:PRO:HG3	2.16	0.45
4:B:304:VAL:HG23	4:B:343:PHE:HB2	1.98	0.45
2:F:296:VAL:HG21	2:F:430:MET:HG2	1.99	0.45
4:B:261:PRO:HD3	4:B:322:SER:HB2	1.97	0.45
1:E:161:ILE:HA	1:E:191:GLY:HA3	1.99	0.45
2:F:275:LYS:HB2	2:F:276:PRO:HD3	1.99	0.45
2:F:384:MET:CE	11:F:553:HOH:O	2.65	0.45
2:F:384:MET:HE3	11:F:553:HOH:O	2.17	0.45
2:F:114:TRP:HB3	2:F:210:LEU:HD13	1.99	0.45
4:A:63:GLY:O	4:A:64:GLU:HB2	2.15	0.44
2:F:68:VAL:HG12	2:F:72:MET:HG3	1.98	0.44
2:F:305:LEU:O	2:F:311:LEU:HD12	2.17	0.44
4:B:258:LEU:HA	4:B:259:PRO:HD3	1.86	0.44
2:F:100:LEU:O	2:F:256:THR:HG23	2.17	0.44
4:B:34:PHE:HD2	4:B:205:VAL:HB	1.83	0.44
4:A:96:MET:HE3	4:A:145:GLY:HA3	1.99	0.44
2:F:83:LEU:C	2:F:83:LEU:HD23	2.38	0.44
1:E:341:TYR:CE2	2:F:460:PRO:HB2	2.53	0.43
4:B:50:ALA:HB2	4:B:79:MET:HE3	2.00	0.43
2:F:309:GLU:HA	2:F:314:LYS:HZ3	1.83	0.43
2:F:391:LEU:HD13	2:F:426:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2501:ADP:H1'	11:B:384:HOH:O	2.17	0.43
4:B:259:PRO:HD2	4:B:260:MET:HE2	2.00	0.43
2:F:405[B]:MET:CE	4:B:77[B]:VAL:HG23	2.48	0.43
4:A:260[A]:MET:CE	4:A:300:LEU:HD22	2.48	0.43
4:A:173[B]:ARG:NH2	11:A:428:HOH:O	2.51	0.43
1:E:74:GLY:HA3	2:F:253:PRO:HB3	2.01	0.43
2:F:122:PHE:CD1	2:F:204:PHE:HD2	2.36	0.43
9:A:2501:ADP:N3	11:A:393:HOH:O	2.36	0.43
4:A:138:GLN:O	4:A:142:VAL:HG23	2.19	0.43
4:A:29:GLY:O	4:A:180:HIS:NE2	2.51	0.43
1:E:115:LEU:HG	1:E:248:PRO:HD3	2.01	0.43
2:F:287:PHE:CZ	2:F:376:ASN:ND2	2.87	0.43
4:B:33:VAL:HA	4:B:189:TYR:O	2.19	0.43
1:E:129:TRP:CD2	1:E:160:LEU:HD13	2.52	0.43
4:A:148:LEU:HD23	4:A:155:PHE:HE2	1.84	0.43
2:F:380:GLY:HA3	6:F:2000:MAL:H61	2.01	0.43
1:E:133:PRO:HG3	1:E:198:LEU:CD2	2.49	0.42
2:F:319:VAL:O	2:F:322:ILE:HG13	2.19	0.42
1:E:3:GLU:HB3	1:E:6:LYS:HE2	2.00	0.42
4:A:20:LYS:HB2	4:A:211:ARG:HD2	2.00	0.42
4:A:223:HIS:ND1	4:A:368:GLU:HG2	2.34	0.42
4:A:192:HIS:HA	11:A:396:HOH:O	2.20	0.42
4:A:95:ASN:O	4:A:146:ARG:HG3	2.20	0.42
2:F:221:ASN:ND2	2:F:224:SER:H	2.17	0.42
3:G:12:ARG:O	3:G:15:ILE:HG22	2.19	0.42
4:B:146:ARG:HD2	11:B:396:HOH:O	2.19	0.42
4:A:187[B]:MET:O	4:A:187[B]:MET:HE2	2.20	0.42
4:B:62:ILE:HB	4:B:67:MET:HG3	2.02	0.42
3:G:104:THR:HG22	3:G:203:PHE:CZ	2.55	0.42
1:E:130:GLU:HA	1:E:194:PHE:HZ	1.85	0.42
4:B:102:LEU:HA	4:B:102:LEU:HD12	1.91	0.42
4:B:236:SER:HA	4:B:237:PRO:C	2.41	0.42
4:A:317:HIS:HA	4:A:327:LEU:O	2.20	0.41
3:G:180:TYR:CE2	3:G:211:SER:HA	2.54	0.41
4:A:34:PHE:HB2	4:A:190:VAL:HG22	2.02	0.41
1:E:314:ASP:HB3	1:E:317:ILE:HD12	2.02	0.41
2:F:404:ALA:HB1	4:B:72:PRO:HB2	2.01	0.41
2:F:78:PHE:HZ	3:G:164:PHE:CD2	2.39	0.41
2:F:459:THR:HA	2:F:460:PRO:HD3	1.91	0.41
2:F:361:TRP:O	2:F:368:ALA:HA	2.19	0.41
2:F:391:LEU:CD1	2:F:426:LEU:HD12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:106:LYS:HB2	4:B:109:VAL:HB	2.03	0.41
1:E:82:ASP:O	1:E:86:GLN:HG3	2.21	0.41
4:A:315:GLN:HG2	4:A:330:ARG:HG2	2.01	0.41
4:A:173[B]:ARG:NH1	4:A:195:VAL:HG12	2.36	0.41
1:E:61:PHE:CE2	1:E:264:ALA:HB2	2.55	0.41
4:A:270:VAL:HG13	4:A:362:CYS:CB	2.49	0.41
1:E:214:GLU:OE1	1:E:234:ASN:ND2	2.50	0.41
4:B:9:VAL:HA	4:B:58:GLY:HA3	2.01	0.41
4:A:4:VAL:HG13	4:A:26[A]:ILE:HB	2.02	0.41
4:A:187[B]:MET:HB3	4:A:187[B]:MET:HE2	1.38	0.40
4:B:29:GLY:O	4:B:180:HIS:CE1	2.74	0.40
1:E:9:ILE:HG12	1:E:59:ILE:HB	2.02	0.40
4:B:86:LEU:HA	4:B:146:ARG:NH2	2.36	0.40
1:E:129:TRP:CE2	1:E:160:LEU:HD13	2.56	0.40
1:E:81:PRO:HA	11:E:418:HOH:O	2.20	0.40
4:A:6:LEU:HB3	4:A:9:VAL:HG23	2.03	0.40
3:G:99:ILE:O	3:G:103:SER:OG	2.34	0.40
5:E:5004:UMQ:C6	11:F:535:HOH:O	2.70	0.40
1:E:89:LEU:HD22	1:E:304:LEU:HA	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	E	375/378 (99%)	363 (97%)	10 (3%)	2 (0%)	34	41
2	F	488/514 (95%)	468 (96%)	18 (4%)	2 (0%)	39	48
3	G	291/296 (98%)	286 (98%)	4 (1%)	1 (0%)	46	57
4	A	377/381 (99%)	360 (96%)	16 (4%)	1 (0%)	46	57
4	B	356/381 (93%)	335 (94%)	19 (5%)	2 (1%)	30	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1887/1950 (97%)	1812 (96%)	67 (4%)	8 (0%)	39	48

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	37	GLN
4	B	107	LYS
1	E	172	GLU
1	E	168	ALA
3	G	230	VAL
4	A	238	LYS
2	F	38	GLY
4	B	270	VAL

### 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	E	300/303 (99%)	292 (97%)	8 (3%)	52	70
2	F	404/424 (95%)	385 (95%)	19 (5%)	32	43
3	G	236/237 (100%)	232 (98%)	4 (2%)	68	83
4	A	322/323 (100%)	308 (96%)	14 (4%)	35	47
4	B	309/323 (96%)	290 (94%)	19 (6%)	23	30
All	All	1571/1610 (98%)	1507 (96%)	64 (4%)	38	50

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	115	LEU
1	E	175	LYS
1	E	178	ILE
1	E	211	SER
1	E	212	ILE
1	E	293[A]	VAL

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Mol	Chain	Res	Type
1	E	293[B]	VAL
1	E	365	GLN
2	F	22	LEU
2	F	45	THR
2	F	46	THR
2	F	59	ASN
2	F	83	LEU
2	F	145	LEU
2	F	150	LYS
2	F	196	VAL
2	F	220	THR
2	F	234	ILE
2	F	257	VAL
2	F	266	ARG
2	F	269	THR
2	F	271	GLU
2	F	273	ILE
2	F	311	LEU
2	F	440	ASN
2	F	449	ASN
2	F	496	LEU
3	G	13	LEU
3	G	21	LEU
3	G	95	SER
3	G	212	VAL
4	A	4	VAL
4	A	20	LYS
4	A	22	ILE
4	A	62[A]	ILE
4	A	62[B]	ILE
4	A	84	TYR
4	A	219	LEU
4	A	242	LEU
4	A	270	VAL
4	A	288	GLU
4	A	295	ILE
4	A	327	LEU
4	A	333	ASP
4	A	350	GLU
4	B	4	VAL
4	B	21	ASP
4	B	22	ILE

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Mol	Chain	Res	Type
4	B	45	LEU
4	B	53	GLU
4	B	101	LYS
4	B	102	LEU
4	B	123	LEU
4	B	127	LEU
4	B	181	LYS
4	B	185	ARG
4	B	203	LYS
4	B	251	ILE
4	B	271	GLU
4	B	294	ASP
4	B	300	LEU
4	B	322	SER
4	B	324	ARG
4	B	350	GLU

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

Mol	Chain	Res	Type
1	E	282	ASN
2	F	59	ASN
2	F	437	ASN
2	F	440	ASN
4	A	5	GLN
4	A	317	HIS
4	B	180	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 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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
9	ADP	A	2501	10,8	22,29,29	0.83	0	27,45,45	2.60	3 (11%)
10	BEF	A	3001	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	B	2502	10,8	22,29,29	0.83	1 (4%)	27,45,45	2.38	3 (11%)
10	BEF	B	3002	9	0,3,3	0.00	-	0,3,3	0.00	-
5	UMQ	E	5004	-	35,35,35	0.59	0	46,46,46	1.30	5 (10%)
6	MAL	F	2000	-	24,24,24	0.53	0	35,35,35	1.31	4 (11%)
7	PGV	F	4001	-	50,50,50	1.12	3 (6%)	51,56,56	1.14	3 (5%)
7	PGV	F	4002	-	8,8,50	0.29	0	7,7,56	0.68	0
7	PGV	F	4008	-	7,7,50	0.41	0	6,6,56	0.44	0
7	PGV	F	4010	-	12,12,50	1.17	1 (8%)	11,11,56	1.29	1 (9%)
7	PGV	G	4003	-	7,7,50	0.37	0	6,6,56	0.63	0
7	PGV	G	4004	-	11,11,50	1.07	1 (9%)	10,10,56	0.89	1 (10%)
7	PGV	G	4005	-	9,9,50	1.20	1 (11%)	8,8,56	1.03	1 (12%)
7	PGV	G	4006	-	6,6,50	1.43	1 (16%)	4,5,56	1.41	1 (25%)
7	PGV	G	4007	-	8,8,50	1.17	1 (12%)	7,7,56	1.21	1 (14%)
7	PGV	G	4009	-	11,11,50	1.33	1 (9%)	9,10,56	0.85	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
9	ADP	A	2501	10,8	-	0/12/32/32	0/3/3/3
10	BEF	A	3001	9	-	0/0/0/0	0/0/0/0
9	ADP	B	2502	10,8	-	0/12/32/32	0/3/3/3
10	BEF	B	3002	9	-	0/0/0/0	0/0/0/0
5	UMQ	E	5004	-	-	0/20/60/60	0/2/2/2
6	MAL	F	2000	-	-	0/8/48/48	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PGV	F	4001	-	-	0/55/55/55	0/0/0/0
7	PGV	F	4002	-	-	0/6/6/55	0/0/0/0
7	PGV	F	4008	-	-	0/5/5/55	0/0/0/0
7	PGV	F	4010	-	-	0/10/10/55	0/0/0/0
7	PGV	G	4003	-	-	0/5/5/55	0/0/0/0
7	PGV	G	4004	-	-	0/9/9/55	0/0/0/0
7	PGV	G	4005	-	-	0/7/7/55	0/0/0/0
7	PGV	G	4006	-	-	0/4/4/55	0/0/0/0
7	PGV	G	4007	-	-	0/6/6/55	0/0/0/0
7	PGV	G	4009	-	-	0/9/9/55	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2502	ADP	O4'-C1'	2.07	1.43	1.41
7	G	4007	PGV	C11-C12	3.07	1.52	1.29
7	G	4004	PGV	C11-C12	3.20	1.53	1.29
7	G	4006	PGV	C12-C11	3.21	1.53	1.29
7	G	4005	PGV	C11-C12	3.25	1.53	1.29
7	F	4010	PGV	C12-C11	3.76	1.53	1.31
7	F	4001	PGV	C12-C11	3.79	1.53	1.31
7	F	4001	PGV	O03-C19	4.02	1.45	1.33
7	G	4009	PGV	C12-C11	4.03	1.55	1.31
7	F	4001	PGV	O01-C1	4.46	1.47	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2501	ADP	N3-C2-N1	-12.30	119.47	128.89
9	B	2502	ADP	N3-C2-N1	-11.11	120.39	128.89
7	F	4010	PGV	C13-C12-C11	-3.53	110.91	127.06
6	F	2000	MAL	C6'-C5'-C4'	-2.91	104.79	113.25
9	A	2501	ADP	PA-O3A-PB	-2.61	123.92	132.67
7	G	4006	PGV	C13-C12-C11	-2.48	109.65	133.31
5	E	5004	UMQ	C1'-O5'-C5'	-2.40	109.09	113.75
7	G	4005	PGV	C10-C11-C12	-2.32	111.19	133.31
7	G	4007	PGV	C10-C11-C12	-2.30	111.41	133.31
7	G	4004	PGV	C10-C11-C12	-2.15	112.79	133.31
7	F	4001	PGV	O03-C19-O04	-2.11	118.04	123.49
9	B	2502	ADP	PA-O3A-PB	-2.05	125.79	132.67
9	A	2501	ADP	C4'-O4'-C1'	2.01	111.93	109.72
6	F	2000	MAL	O5'-C5'-C4'	2.37	114.76	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	2000	MAL	O5'-C1'-C2'	2.38	113.59	109.80
5	E	5004	UMQ	O2'-C2'-C1'	2.59	115.70	110.02
5	E	5004	UMQ	CA-O1'-C1'	2.63	118.54	113.94
5	E	5004	UMQ	O1'-C1'-C2'	2.89	111.69	108.04
5	E	5004	UMQ	C1-O5-C5	2.97	119.51	113.75
9	B	2502	ADP	O3B-PB-O2B	3.09	119.15	107.38
7	F	4001	PGV	O03-C19-C20	3.61	122.90	111.90
6	F	2000	MAL	C1'-O5'-C5'	4.24	121.31	113.47
7	F	4001	PGV	O01-C1-C2	4.58	121.49	111.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2501	ADP	2	0
5	E	5004	UMQ	2	0
6	F	2000	MAL	1	0
7	G	4003	PGV	2	0
7	G	4004	PGV	1	0
7	G	4006	PGV	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, 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	E	374/378 (98%)	0.11	16 (4%)	39	48	21, 50, 82, 94	1 (0%)
2	F	490/514 (95%)	0.33	32 (6%)	22	30	21, 52, 98, 119	0
3	G	293/296 (98%)	-0.03	15 (5%)	32	41	15, 33, 74, 94	0
4	A	371/381 (97%)	0.08	15 (4%)	42	51	17, 44, 69, 80	1 (0%)
4	B	358/381 (93%)	0.32	31 (8%)	13	18	16, 55, 105, 122	0
All	All	1886/1950 (96%)	0.18	109 (5%)	26	35	15, 47, 88, 122	2 (0%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	267	TRP	11.7
2	F	37	GLN	8.7
4	B	16	VAL	8.3
2	F	38	GLY	7.5
3	G	70	ALA	6.8
4	B	295	ILE	6.7
4	A	295	ILE	6.3
4	A	104	GLY	5.8
4	B	259	PRO	5.7
4	B	251	ILE	5.7
2	F	354	LEU	5.7
2	F	355	PHE	5.4
2	F	245	ASN	5.2
3	G	71	ASP	4.9
2	F	29	TYR	4.6
2	F	18	SER	4.5
4	B	261	PRO	4.4
4	B	15	GLU	4.3
4	A	372	ALA	4.3
3	G	116	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
2	F	271	GLU	4.2
1	E	374	SER	4.2
1	E	172	GLU	4.2
2	F	503	ILE	4.1
2	F	349	MET	4.0
3	G	114	ARG	4.0
4	B	294	ASP	3.7
4	A	324	ARG	3.7
4	B	357	GLU	3.6
3	G	117	GLY	3.6
4	A	110	ILE	3.5
3	G	2	ALA	3.5
4	A	293	SER	3.4
1	E	252	GLY	3.4
3	G	72	GLY	3.3
3	G	133	ALA	3.3
2	F	501	LEU	3.3
2	F	40	TYR	3.2
4	B	296	ALA	3.2
2	F	10	TRP	3.2
4	B	105	ALA	3.1
1	E	142	LYS	3.1
2	F	312	ARG	3.1
4	B	181	LYS	3.1
4	A	294	ASP	3.1
2	F	17	TRP	3.1
4	B	339	GLU	3.1
2	F	262	LYS	3.1
4	B	324	ARG	3.1
2	F	44	ILE	3.0
4	B	353	HIS	3.0
2	F	12	SER	3.0
4	B	265	GLN	3.0
3	G	73	ARG	3.0
4	A	64	GLU	2.9
2	F	275	LYS	2.9
4	B	263	ARG	2.9
3	G	134	VAL	2.9
1	E	147	LEU	2.9
1	E	1	LYS	2.9
4	B	108	GLU	2.8
2	F	13	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
4	B	293	SER	2.8
2	F	479	GLY	2.7
4	B	252	ASP	2.7
1	E	370	LYS	2.7
3	G	14	PHE	2.7
4	B	103	ALA	2.7
1	E	174	GLY	2.6
4	B	262	ASN	2.6
4	B	342	THR	2.6
4	B	112	GLN	2.6
4	A	15	GLU	2.6
2	F	353	ALA	2.5
2	F	134	ALA	2.5
2	F	248	ASP	2.5
2	F	213	LEU	2.5
4	B	321	PRO	2.5
4	A	187[A]	MET	2.5
4	B	358	ASP	2.5
2	F	229	ARG	2.5
3	G	68	GLU	2.4
1	E	373	ALA	2.4
4	B	280	ASN	2.4
1	E	313	LYS	2.3
2	F	14	ALA	2.3
4	B	340	GLY	2.3
1	E	123	PRO	2.2
4	A	296	ALA	2.2
2	F	269	THR	2.2
2	F	114	TRP	2.2
4	B	17	VAL	2.2
1	E	4	GLU	2.2
1	E	164	ASP	2.2
4	A	370	GLY	2.2
1	E	179	LYS	2.2
2	F	233	GLN	2.2
2	F	502	ALA	2.2
4	B	354	LEU	2.1
1	E	352	SER	2.1
4	A	357	GLU	2.1
2	F	246	TRP	2.1
3	G	56	TRP	2.1
3	G	10	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
4	A	260[A]	MET	2.0
4	B	249	THR	2.0
1	E	173	ASN	2.0
3	G	11	ALA	2.0
4	A	60[A]	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
7	PGV	F	4010	13/51	0.83	0.24	4.60	66,68,70,70	0
7	PGV	G	4009	12/51	0.70	0.20	2.89	48,49,51,52	0
7	PGV	F	4001	51/51	0.85	0.20	2.03	50,57,69,71	0
5	UMQ	E	5004	34/34	0.93	0.18	0.99	23,28,33,34	0
8	MG	B	1502	1/1	1.00	0.10	0.66	15,15,15,15	0
7	PGV	F	4002	9/51	0.89	0.13	0.43	31,33,36,39	0
8	MG	A	1501	1/1	0.98	0.10	0.40	18,18,18,18	0
6	MAL	F	2000	23/23	0.95	0.10	0.13	30,32,33,35	0
9	ADP	B	2502	27/27	0.97	0.11	-0.22	24,40,53,54	0
9	ADP	A	2501	27/27	0.98	0.09	-0.36	17,27,38,39	0
10	BEF	B	3002	4/4	0.98	0.09	-0.36	21,21,22,26	0
10	BEF	A	3001	4/4	0.97	0.08	-0.79	17,18,19,20	0
7	PGV	G	4006	7/51	0.89	0.12	-	43,45,49,51	0
7	PGV	G	4005	10/51	0.87	0.17	-	52,56,57,57	0
7	PGV	G	4004	12/51	0.84	0.17	-	43,48,58,60	0
7	PGV	G	4007	9/51	0.86	0.23	-	46,50,55,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	PGV	G	4003	8/51	0.74	0.26	-	50,54,56,58	0
7	PGV	F	4008	8/51	0.83	0.16	-	47,49,50,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.