



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:46 AM GMT

PDB ID : 3PUV  
Title : Crystal Structure of an outward-facing MBP-Maltose transporter complex bound to ADP-VO<sub>4</sub>  
Authors : Oldham, M.L.; Chen, J.  
Deposited on : 2010-12-06  
Resolution : 2.40 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.

---

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

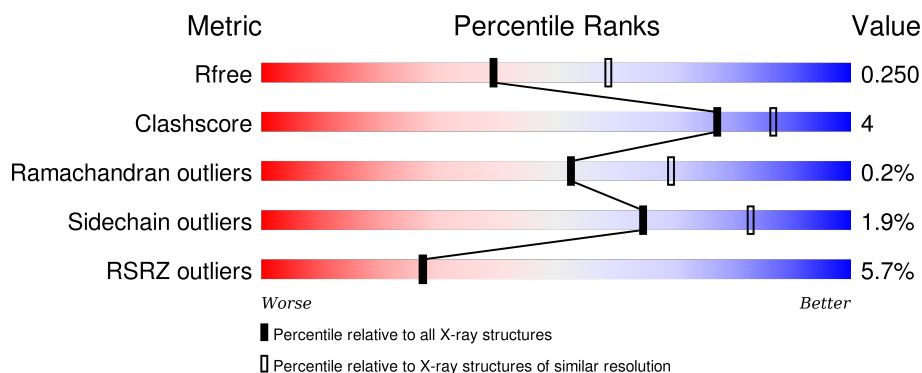
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	E	378	<div> <div>3%</div> <div>93%</div> <div>6%</div> </div>
2	F	514	<div> <div>7%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>
3	G	296	<div> <div>5%</div> <div>90%</div> <div>7%</div> </div>
4	A	381	<div> <div>3%</div> <div>85%</div> <div>11%</div> </div>
4	B	381	<div> <div>8%</div> <div>81%</div> <div>12%</div> <div>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
6	PGV	F	4010	-	-	-	X
6	PGV	G	4009	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15093 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	1	0
			2901	1869	473	553	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	0	0
			3821	2511	608	685	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	288	Total	C	N	O	S	0	0	0
			2221	1487	355	371	8			

- 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	4	0
			2910	1839	523	534	14			

*Continued on next page...*

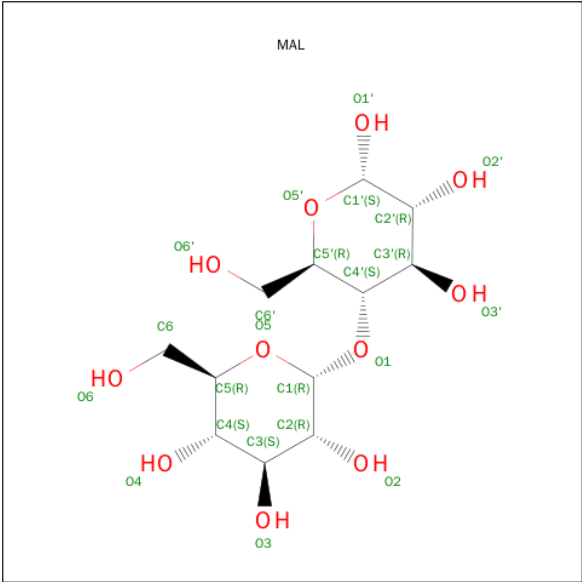
*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	358	Total	C	N	O	S	0	1	0
			2798	1771	501	513	13			

There are 20 discrepancies between the modelled and reference sequences:

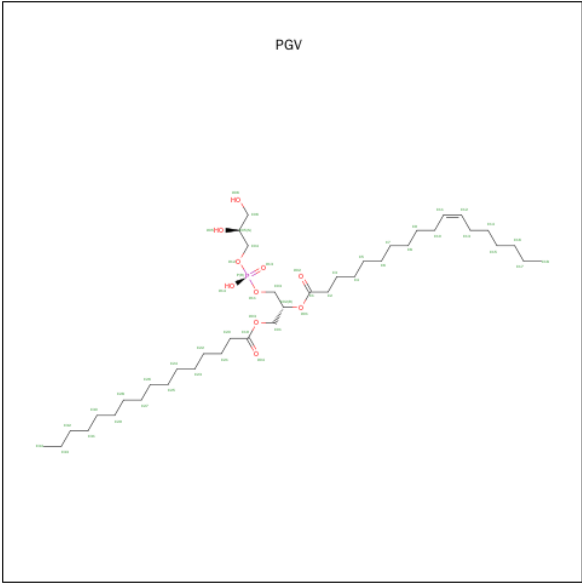
Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	EXPRESSION TAG	UNP P68187
A	373	SER	-	EXPRESSION TAG	UNP P68187
A	374	ALA	-	EXPRESSION TAG	UNP P68187
A	375	SER	-	EXPRESSION TAG	UNP P68187
A	376	HIS	-	EXPRESSION TAG	UNP P68187
A	377	HIS	-	EXPRESSION TAG	UNP P68187
A	378	HIS	-	EXPRESSION TAG	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 SUGAR (MALTOSE) (three-letter code: MAL) (formula: C<sub>12</sub>H<sub>22</sub>O<sub>11</sub>).



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

- Molecule 6 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHO RYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



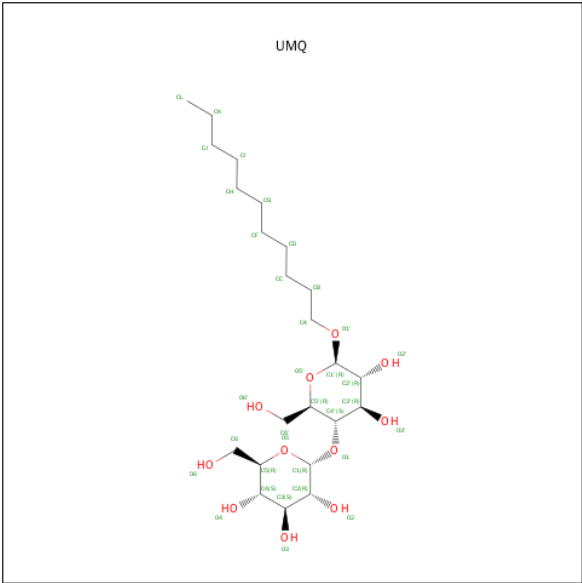
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	F	1	Total	C	O	P	0	0
			51	40	10	1		
6	F	1	Total	C			0	0
			9	9				

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	C	0	0
			8	8		
6	F	1	Total	C	0	0
			13	13		
6	G	1	Total	C	0	0
			8	8		
6	G	1	Total	C	0	0
			12	12		
6	G	1	Total	C	0	0
			10	10		
6	G	1	Total	C	0	0
			7	7		
6	G	1	Total	C	0	0
			9	9		
6	G	1	Total	C	0	0
			12	12		

- Molecule 7 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: C<sub>23</sub>H<sub>44</sub>O<sub>11</sub>).

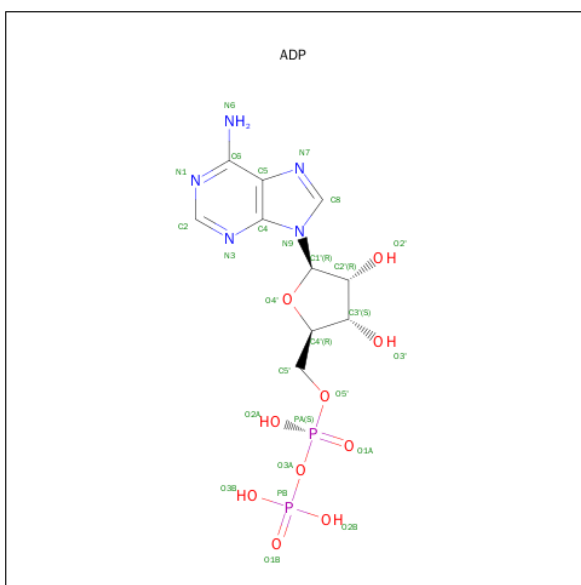


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			34	23	11		

- 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

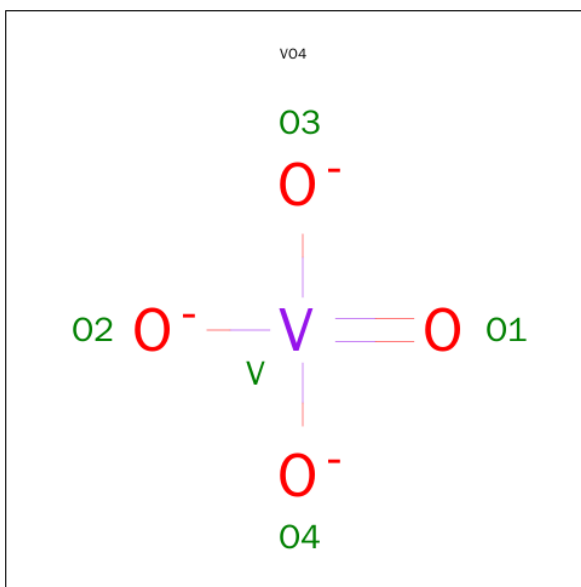
- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



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

- Molecule 10 is VANADATE ION (three-letter code: VO4) (formula:  $\text{O}_4\text{V}$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	V	0	0
			5	4	1		
10	B	1	Total	O	V	0	0
			5	4	1		

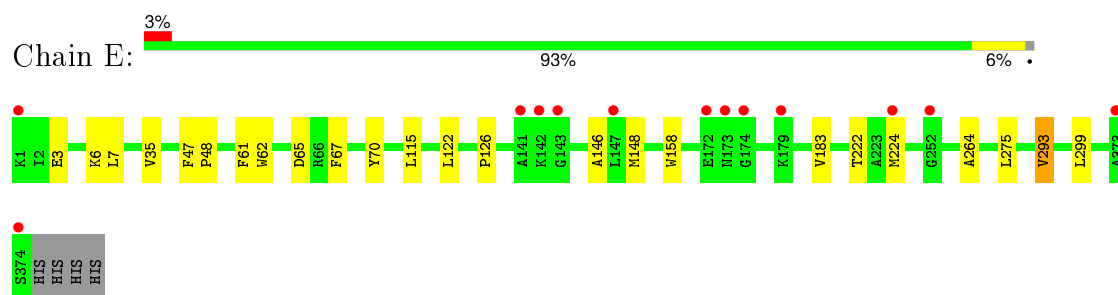
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	E	49	Total	O	0	0
			49	49		
11	F	34	Total	O	0	0
			34	34		
11	G	31	Total	O	0	0
			31	31		
11	A	38	Total	O	0	0
			38	38		
11	B	28	Total	O	0	0
			28	28		

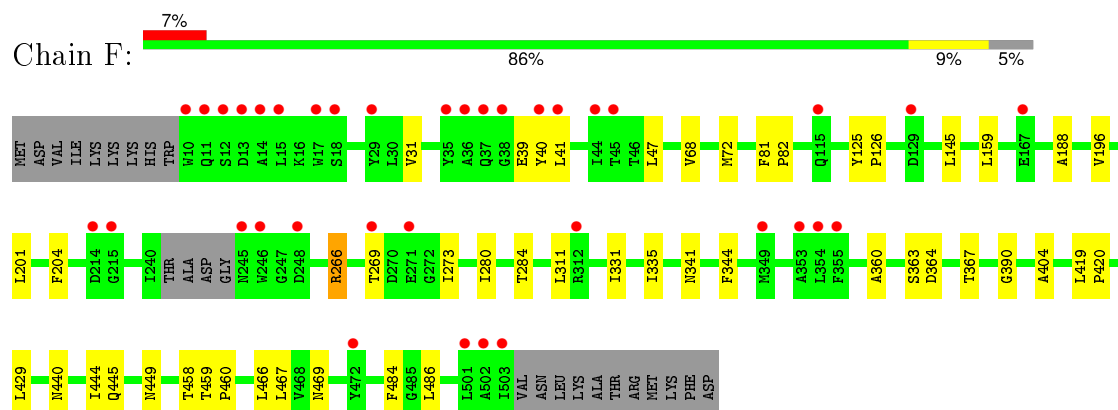
### 3 Residue-property plots [i](#)

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

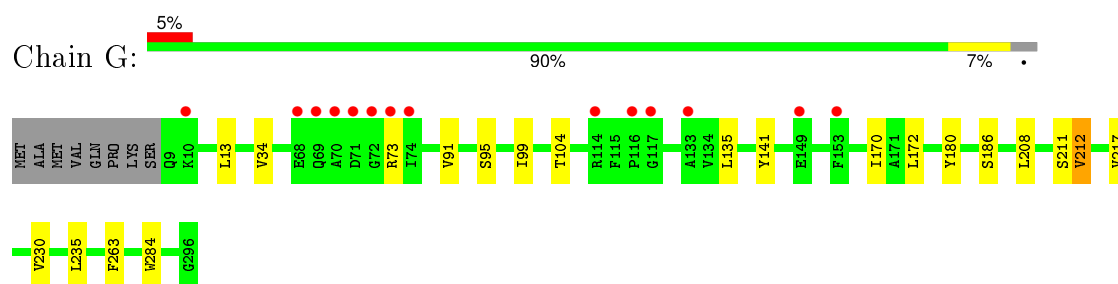
- Molecule 1: Maltose-binding periplasmic protein



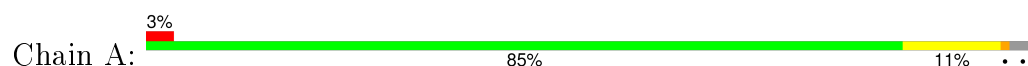
- Molecule 2: Maltose transport system permease protein malF

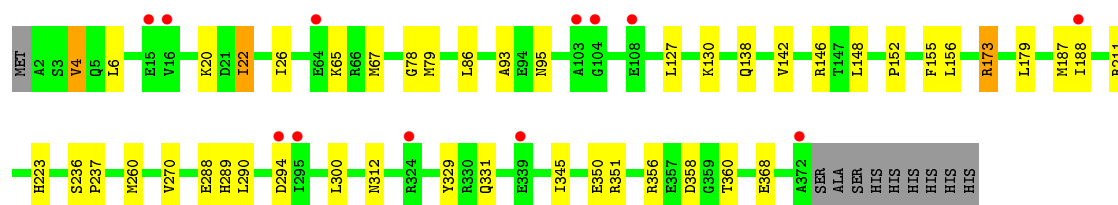


- Molecule 3: Maltose transport system permease protein malG

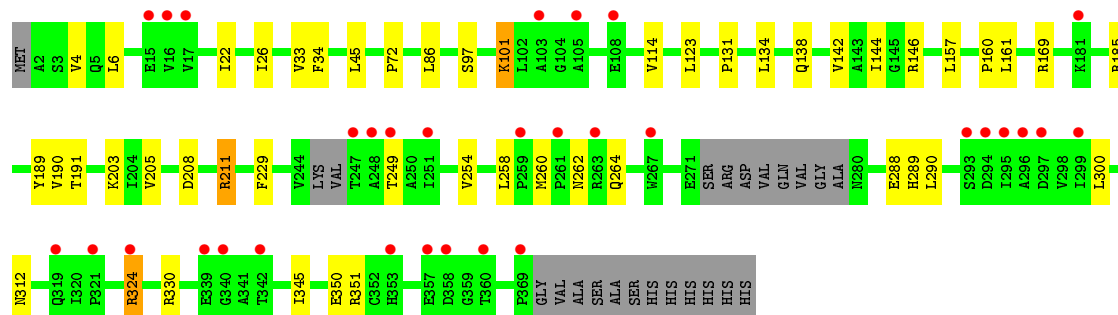
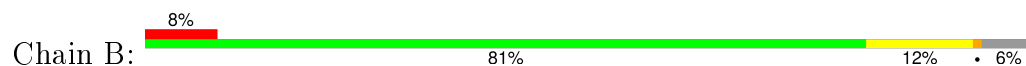


- Molecule 4: Maltose/maltodextrin import ATP-binding protein MalK





• 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, $\alpha$ , $\beta$ , $\gamma$	81.79Å 97.12Å 112.79Å 85.58° 78.71° 72.69°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	63.2 (20.00-2.40) 63.1 (20.00-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.223 , 0.253 0.221 , 0.250	Depositor DCC
$R_{free}$ test set	4002 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.9	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 30.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 80180 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	15093	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: VO4, MG, UMQ, ADP, 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	0.32	0/2973	0.45	0/4036
2	F	0.34	0/3916	0.48	0/5330
3	G	0.34	0/2282	0.45	0/3119
4	A	0.31	0/2960	0.50	0/4012
4	B	0.31	0/2846	0.48	0/3856
All	All	0.33	0/14977	0.47	0/20353

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 [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	2901	0	2882	14	0
2	F	3821	0	3849	28	0
3	G	2221	0	2308	13	0
4	A	2910	0	2978	33	0
4	B	2798	0	2856	32	0
5	F	23	0	22	0	0
6	F	81	0	122	0	0
6	G	58	0	82	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	34	0	44	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	27	0	12	0	0
9	B	27	0	12	0	0
10	A	5	0	0	0	0
10	B	5	0	0	0	0
11	A	38	0	0	0	0
11	B	28	0	0	0	0
11	E	49	0	0	0	0
11	F	34	0	0	0	0
11	G	31	0	0	0	0
All	All	15093	0	15167	110	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 4.

All (110) 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)
4:A:173[A]:ARG:NH1	4:A:173[A]:ARG:HB2	1.54	1.22
4:B:211[A]:ARG:CG	4:B:211[A]:ARG:HH11	1.67	1.07
4:A:173[A]:ARG:HH11	4:A:173[A]:ARG:CG	1.67	1.05
4:A:173[A]:ARG:CB	4:A:173[A]:ARG:HH11	1.72	1.02
4:A:173[A]:ARG:NH1	4:A:173[A]:ARG:CB	2.24	1.00
2:F:266:ARG:HG2	2:F:266:ARG:HH11	1.30	0.96
4:A:173[A]:ARG:HH11	4:A:173[A]:ARG:HG3	1.33	0.91
4:B:211[A]:ARG:HG3	4:B:211[A]:ARG:HH11	1.37	0.89
4:B:211[A]:ARG:HG2	4:B:211[A]:ARG:HH11	1.40	0.86
4:A:173[A]:ARG:HH11	4:A:173[A]:ARG:HB2	1.28	0.84
3:G:91:VAL:O	3:G:95:SER:HB2	1.87	0.74
1:E:115:LEU:HD21	1:E:224:MET:HE3	1.71	0.70
2:F:159:LEU:HD11	2:F:188:ALA:HB1	1.77	0.67
4:B:211[A]:ARG:HG2	4:B:211[A]:ARG:NH1	2.07	0.66
4:A:288:GLU:HG2	4:B:312:ASN:HB2	1.80	0.64
2:F:266:ARG:HG2	2:F:266:ARG:NH1	2.06	0.63
4:A:356:ARG:HH11	4:A:360:THR:HG23	1.65	0.61
4:A:223:HIS:CE1	4:A:368:GLU:HG2	2.36	0.60
4:A:329:TYR:CE2	4:A:331:GLN:HG2	2.37	0.60
4:B:33:VAL:HG12	4:B:189:TYR:HB3	1.84	0.60
2:F:444:ILE:HG13	2:F:466:LEU:HG	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:131:PRO:HA	4:B:134:LEU:HD12	1.86	0.57
2:F:68:VAL:HG12	2:F:72:MET:HG3	1.88	0.56
4:A:79:MET:HG3	4:A:156:LEU:HB2	1.88	0.56
4:A:173[A]:ARG:NH1	4:A:173[A]:ARG:HG3	2.10	0.55
4:B:211[A]:ARG:HG3	4:B:211[A]:ARG:NH1	2.11	0.55
4:A:6:LEU:HD22	4:A:22:ILE:HD11	1.88	0.55
4:A:155:PHE:HB2	4:A:187:MET:HG2	1.87	0.55
4:A:20:LYS:HE2	4:A:211:ARG:HD3	1.90	0.54
4:A:173[A]:ARG:CB	4:A:173[A]:ARG:CZ	2.83	0.53
1:E:3:GLU:HB3	1:E:6:LYS:HE2	1.91	0.53
4:B:288:GLU:HG3	4:B:330:ARG:HD3	1.90	0.53
3:G:99:ILE:HG23	3:G:170:ILE:HG22	1.91	0.53
4:B:97:SER:HB3	4:B:114:VAL:HG21	1.90	0.52
2:F:429:LEU:HD23	3:G:172:LEU:HD22	1.92	0.52
1:E:293[A]:VAL:HG23	1:E:299:LEU:HD11	1.92	0.51
4:B:34:PHE:HB2	4:B:190:VAL:HG22	1.90	0.51
4:A:93:ALA:HB2	4:A:127:LEU:HG	1.92	0.51
4:A:260[A]:MET:N	4:A:260[A]:MET:SD	2.83	0.51
4:B:4:VAL:HG13	4:B:26:ILE:HB	1.92	0.51
4:A:4:VAL:HG13	4:A:26:ILE:HB	1.92	0.51
2:F:419:LEU:HB3	2:F:420:PRO:HD3	1.93	0.50
4:A:4:VAL:HG11	4:A:188:ILE:HD11	1.94	0.50
1:E:146:ALA:O	1:E:224:MET:HG2	2.12	0.49
2:F:404:ALA:HB1	4:B:72:PRO:HB2	1.94	0.49
2:F:284:THR:HG22	2:F:466:LEU:HA	1.95	0.49
2:F:273:ILE:HG22	2:F:459:THR:HG21	1.95	0.48
4:B:144:ILE:HD11	4:B:160:PRO:O	2.13	0.48
1:E:122:LEU:HD21	1:E:126:PRO:HD3	1.95	0.48
3:G:180:TYR:CE2	3:G:211:SER:HA	2.48	0.48
4:B:6:LEU:HD22	4:B:22:ILE:HD11	1.96	0.47
4:B:324:ARG:H	4:B:324:ARG:HD3	1.80	0.47
4:A:312:ASN:HB2	4:B:288:GLU:HG2	1.96	0.47
4:A:358:ASP:OD1	4:A:360:THR:HG22	2.14	0.47
4:B:138:GLN:O	4:B:142:VAL:HG23	2.15	0.47
2:F:196:VAL:CG1	2:F:204:PHE:HB3	2.45	0.47
4:A:86:LEU:HA	4:A:146:ARG:HH21	1.80	0.47
4:A:236:SER:HA	4:A:237:PRO:C	2.35	0.46
2:F:484:PHE:HB3	3:G:135:LEU:HD11	1.96	0.46
2:F:364:ASP:HB3	2:F:367:THR:OG1	2.14	0.46
2:F:360:ALA:HB1	2:F:363:SER:HB2	1.96	0.46
4:A:138:GLN:O	4:A:142:VAL:HG23	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:290:LEU:HD22	4:A:345:ILE:HD13	1.98	0.46
3:G:104:THR:HG21	3:G:208:LEU:HD21	1.99	0.45
4:B:249:THR:HG22	4:B:254:VAL:HG13	1.98	0.45
2:F:39:GLU:O	2:F:41:LEU:N	2.50	0.45
4:B:86:LEU:HA	4:B:146:ARG:NH2	2.31	0.45
4:A:260[A]:MET:HE2	4:A:300:LEU:HD22	1.97	0.45
2:F:335:ILE:HD13	3:G:34:VAL:HG22	1.99	0.45
4:B:290:LEU:HD22	4:B:345:ILE:HD13	1.99	0.44
1:E:62:TRP:HB3	1:E:67:PHE:HE1	1.82	0.44
2:F:331:ILE:HD12	3:G:263:PHE:HD2	1.83	0.44
4:B:189:TYR:CE2	4:B:191:THR:HB	2.52	0.44
4:B:34:PHE:HD2	4:B:205:VAL:HB	1.83	0.44
1:E:61:PHE:CE2	1:E:264:ALA:HB2	2.52	0.44
2:F:390:GLY:HA3	3:G:217:VAL:HG21	2.00	0.43
4:B:161:LEU:HB3	4:B:169:ARG:HG2	2.01	0.43
1:E:48:PRO:HG3	1:E:70:TYR:HE1	1.83	0.43
2:F:341:ASN:O	2:F:344:PHE:O	2.37	0.43
4:B:260:MET:HG3	4:B:262:ASN:OD1	2.19	0.43
3:G:212:VAL:HG22	3:G:284:TRP:CE3	2.54	0.43
4:B:208:ASP:HB2	4:B:229:PHE:CE2	2.54	0.42
1:E:48:PRO:HG3	1:E:70:TYR:CE1	2.55	0.42
4:A:152:PRO:HD2	4:A:155:PHE:CE1	2.54	0.42
1:E:47:PHE:HB3	1:E:48:PRO:HD3	2.01	0.42
2:F:280:ILE:O	2:F:284:THR:HG23	2.20	0.42
2:F:81:PHE:HB3	2:F:82:PRO:HD3	2.02	0.42
4:B:157:LEU:HB3	4:B:160:PRO:HG3	2.01	0.42
1:E:7:LEU:HB2	1:E:35:VAL:HG22	2.01	0.42
3:G:180:TYR:HE2	3:G:211:SER:HA	1.85	0.42
4:A:148:LEU:HD22	4:A:179:LEU:HD22	2.02	0.42
2:F:284:THR:HG21	2:F:467:LEU:H	1.84	0.41
4:B:289:HIS:CG	4:B:351:ARG:HD2	2.55	0.41
2:F:266:ARG:HD3	2:F:486:LEU:HD13	2.02	0.41
2:F:445:GLN:HG2	2:F:469:ASN:ND2	2.35	0.41
4:B:211[A]:ARG:HD2	4:B:211[A]:ARG:C	2.40	0.41
1:E:275:LEU:HD23	2:F:201:LEU:HD11	2.02	0.41
4:A:78:GLY:HA3	4:A:152:PRO:HG3	2.02	0.41
3:G:141:TYR:HB2	3:G:235:LEU:HD11	2.01	0.41
4:B:211[A]:ARG:O	4:B:211[A]:ARG:HD2	2.20	0.41
2:F:335:ILE:CD1	3:G:34:VAL:HG22	2.50	0.41
2:F:125:TYR:HA	2:F:126:PRO:HD2	1.92	0.41
4:A:65:LYS:O	4:A:67:MET:HG2	2.21	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:31:VAL:HG11	2:F:47:LEU:HD13	2.02	0.41
1:E:158:TRP:HH2	1:E:183:VAL:HG12	1.84	0.41
1:E:148:MET:HB2	1:E:222:THR:HG21	2.03	0.41
4:B:258:LEU:HD23	4:B:264:GLN:HB3	2.02	0.41
4:A:95:ASN:O	4:A:146:ARG:HG3	2.22	0.40
4:A:289:HIS:CG	4:A:351:ARG:HD2	2.56	0.40
4:B:97:SER:O	4:B:101:LYS:HB2	2.22	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	373/378 (99%)	358 (96%)	15 (4%)	0	100	100
2	F	486/514 (95%)	468 (96%)	16 (3%)	2 (0%)	39	56
3	G	286/296 (97%)	282 (99%)	3 (1%)	1 (0%)	46	63
4	A	373/381 (98%)	363 (97%)	10 (3%)	0	100	100
4	B	353/381 (93%)	337 (96%)	16 (4%)	0	100	100
All	All	1871/1950 (96%)	1808 (97%)	60 (3%)	3 (0%)	52	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	40	TYR
3	G	230	VAL
2	F	460	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	E	298/303 (98%)	295 (99%)	3 (1%)	82	93
2	F	402/424 (95%)	395 (98%)	7 (2%)	68	85
3	G	230/237 (97%)	226 (98%)	4 (2%)	68	85
4	A	318/323 (98%)	310 (98%)	8 (2%)	55	76
4	B	306/323 (95%)	296 (97%)	10 (3%)	45	66
All	All	1554/1610 (96%)	1522 (98%)	32 (2%)	65	80

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	65	ASP
1	E	293[A]	VAL
1	E	293[B]	VAL
2	F	145	LEU
2	F	266	ARG
2	F	269	THR
2	F	311	LEU
2	F	440	ASN
2	F	449	ASN
2	F	458	THR
3	G	13	LEU
3	G	73	ARG
3	G	186	SER
3	G	212	VAL
4	A	4	VAL
4	A	22	ILE
4	A	130	LYS
4	A	173[A]	ARG
4	A	173[B]	ARG
4	A	270	VAL
4	A	294	ASP
4	A	350	GLU
4	B	45	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	B	101	LYS
4	B	123	LEU
4	B	185	ARG
4	B	203	LYS
4	B	211[A]	ARG
4	B	211[B]	ARG
4	B	300	LEU
4	B	324	ARG
4	B	350	GLU

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

Mol	Chain	Res	Type
2	F	437	ASN
2	F	440	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

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	0.76	0	27,45,45	2.24	2 (7%)
10	VO4	A	3001	9,8	1,4,4	1.01	0	0,6,6	0.00	-
9	ADP	B	2502	10,8	22,29,29	0.75	0	27,45,45	2.27	2 (7%)
10	VO4	B	3002	9,8	1,4,4	0.41	0	0,6,6	0.00	-
5	MAL	F	2000	-	24,24,24	0.46	0	35,35,35	0.74	1 (2%)
6	PGV	F	4001	-	50,50,50	1.05	3 (6%)	51,56,56	1.06	4 (7%)
6	PGV	F	4002	-	8,8,50	0.29	0	7,7,56	0.46	0
6	PGV	F	4008	-	7,7,50	0.29	0	6,6,56	0.43	0
6	PGV	F	4010	-	12,12,50	1.13	1 (8%)	11,11,56	1.28	1 (9%)
7	UMQ	F	5004	-	35,35,35	0.42	0	46,46,46	0.68	0
6	PGV	G	4003	-	7,7,50	0.27	0	6,6,56	0.47	0
6	PGV	G	4004	-	11,11,50	1.02	1 (9%)	10,10,56	1.03	1 (10%)
6	PGV	G	4005	-	9,9,50	1.12	1 (11%)	8,8,56	1.09	1 (12%)
6	PGV	G	4006	-	6,6,50	1.37	1 (16%)	4,5,56	1.45	1 (25%)
6	PGV	G	4007	-	8,8,50	1.19	1 (12%)	7,7,56	1.18	1 (14%)
6	PGV	G	4009	-	11,11,50	1.19	1 (9%)	9,10,56	0.96	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	VO4	A	3001	9,8	-	0/0/0/0	0/0/0/0
9	ADP	B	2502	10,8	-	0/12/32/32	0/3/3/3
10	VO4	B	3002	9,8	-	0/0/0/0	0/0/0/0
5	MAL	F	2000	-	-	0/8/48/48	0/2/2/2
6	PGV	F	4001	-	-	0/55/55/55	0/0/0/0
6	PGV	F	4002	-	-	0/6/6/55	0/0/0/0
6	PGV	F	4008	-	-	0/5/5/55	0/0/0/0
6	PGV	F	4010	-	-	0/10/10/55	0/0/0/0
7	UMQ	F	5004	-	-	0/20/60/60	0/2/2/2
6	PGV	G	4003	-	-	0/5/5/55	0/0/0/0
6	PGV	G	4004	-	-	0/9/9/55	0/0/0/0
6	PGV	G	4005	-	-	0/7/7/55	0/0/0/0
6	PGV	G	4006	-	-	0/4/4/55	0/0/0/0
6	PGV	G	4007	-	-	0/6/6/55	0/0/0/0
6	PGV	G	4009	-	-	0/9/9/55	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	4007	PGV	C11-C12	3.14	1.52	1.29
6	G	4004	PGV	C11-C12	3.15	1.52	1.29
6	G	4005	PGV	C11-C12	3.15	1.53	1.29
6	G	4006	PGV	C12-C11	3.17	1.53	1.29
6	F	4001	PGV	C12-C11	3.70	1.53	1.31
6	F	4010	PGV	C12-C11	3.73	1.53	1.31
6	G	4009	PGV	C12-C11	3.74	1.53	1.31
6	F	4001	PGV	O01-C1	4.02	1.46	1.34
6	F	4001	PGV	O03-C19	4.09	1.45	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	2502	ADP	N3-C2-N1	-10.49	120.86	128.89
9	A	2501	ADP	N3-C2-N1	-10.24	121.06	128.89
6	F	4010	PGV	C13-C12-C11	-3.34	111.78	127.06
9	B	2502	ADP	PA-O3A-PB	-2.70	123.63	132.67
9	A	2501	ADP	PA-O3A-PB	-2.56	124.07	132.67
6	G	4006	PGV	C13-C12-C11	-2.38	110.65	133.31
6	G	4007	PGV	C10-C11-C12	-2.35	110.96	133.31
6	G	4004	PGV	C10-C11-C12	-2.33	111.12	133.31
6	G	4005	PGV	C10-C11-C12	-2.29	111.49	133.31
6	F	4001	PGV	O03-C19-O04	-2.17	117.89	123.49
6	F	4001	PGV	C10-C11-C12	-2.05	111.07	125.34
5	F	2000	MAL	C1'-O5'-C5'	2.04	117.24	113.47
6	F	4001	PGV	O03-C19-C20	2.88	120.67	111.90
6	F	4001	PGV	O01-C1-C2	4.00	120.23	111.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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%)	0.01	13 (3%)	48	48	28, 60, 97, 110	1 (0%)
2	F	490/514 (95%)	0.23	36 (7%)	18	18	24, 62, 115, 163	0
3	G	288/296 (97%)	-0.13	14 (4%)	33	34	17, 39, 77, 102	0
4	A	371/381 (97%)	0.00	12 (3%)	51	51	22, 54, 89, 117	0
4	B	358/381 (93%)	0.33	32 (8%)	12	12	23, 69, 146, 171	0
All	All	1881/1950 (96%)	0.10	107 (5%)	27	27	17, 58, 109, 171	1 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	38	GLY	8.8
4	B	16	VAL	6.7
4	A	295	ILE	6.2
4	A	104	GLY	6.0
3	G	116	PRO	5.2
4	B	251	ILE	5.1
3	G	71	ASP	5.0
4	B	249	THR	5.0
2	F	354	LEU	4.9
2	F	245	ASN	4.8
3	G	70	ALA	4.7
4	B	15	GLU	4.7
2	F	271	GLU	4.6
2	F	29	TYR	4.5
4	A	372	ALA	4.5
2	F	40	TYR	4.5
4	B	295	ILE	4.4
4	B	369	PRO	4.4
4	B	263	ARG	4.3
1	E	172	GLU	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	F	214	ASP	4.0
4	B	267	TRP	4.0
2	F	10	TRP	3.8
3	G	73	ARG	3.8
2	F	355	PHE	3.7
1	E	173	ASN	3.7
3	G	133	ALA	3.6
2	F	503	ILE	3.6
4	B	103	ALA	3.6
4	B	259	PRO	3.5
2	F	14	ALA	3.5
4	B	294	ASP	3.4
4	B	261	PRO	3.3
2	F	15	LEU	3.3
4	B	296	ALA	3.3
3	G	114	ARG	3.2
2	F	18	SER	3.2
2	F	36	ALA	3.2
1	E	373	ALA	3.2
2	F	353	ALA	3.2
3	G	68	GLU	3.1
4	B	340	GLY	3.1
4	A	188	ILE	3.1
2	F	502	ALA	3.1
2	F	12	SER	3.1
2	F	129	ASP	3.1
2	F	349	MET	3.1
2	F	501	LEU	3.1
4	B	357	GLU	3.0
4	B	342	THR	3.0
4	B	247	THR	2.9
4	A	16	VAL	2.9
2	F	44	ILE	2.9
2	F	248	ASP	2.9
4	B	360	THR	2.9
1	E	374	SER	2.8
2	F	269	THR	2.8
1	E	174	GLY	2.8
2	F	41	LEU	2.8
4	B	299	ILE	2.8
2	F	13	ASP	2.8
3	G	69	GLN	2.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	B	293	SER	2.7
1	E	147	LEU	2.7
2	F	312	ARG	2.7
4	A	103	ALA	2.7
4	A	64	GLU	2.6
4	B	248	ALA	2.6
4	A	108	GLU	2.6
4	B	297	ASP	2.6
4	B	324	ARG	2.6
4	A	294	ASP	2.6
2	F	115	GLN	2.5
4	B	358	ASP	2.5
4	B	181	LYS	2.5
2	F	215	GLY	2.5
1	E	141	ALA	2.5
4	B	353	HIS	2.5
4	B	319	GLN	2.5
4	A	15	GLU	2.5
4	B	108	GLU	2.5
2	F	11	GLN	2.4
1	E	179	LYS	2.4
1	E	252	GLY	2.4
1	E	224	MET	2.4
3	G	72	GLY	2.4
2	F	37	GLN	2.4
2	F	45	THR	2.3
1	E	1	LYS	2.3
2	F	167	GLU	2.3
2	F	17	TRP	2.2
3	G	149	GLU	2.2
4	B	321	PRO	2.2
4	B	339	GLU	2.1
4	B	17	VAL	2.1
1	E	142	LYS	2.1
2	F	35	TYR	2.1
2	F	472	TYR	2.1
4	A	324	ARG	2.1
4	A	339	GLU	2.1
1	E	143	GLY	2.1
3	G	74	ILE	2.1
3	G	10	LYS	2.1
2	F	246	TRP	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	B	105	ALA	2.0
3	G	117	GLY	2.0
3	G	153	PHE	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
6	PGV	G	4009	12/51	0.77	0.24	4.10	60,61,63,63	0
6	PGV	F	4010	13/51	0.85	0.22	3.19	74,79,85,85	0
6	PGV	F	4001	51/51	0.84	0.22	1.89	64,70,77,77	0
6	PGV	F	4002	9/51	0.89	0.19	1.07	37,43,49,52	0
7	UMQ	F	5004	34/34	0.93	0.17	0.19	63,76,82,84	0
5	MAL	F	2000	23/23	0.94	0.11	0.09	38,40,42,42	0
9	ADP	A	2501	27/27	0.98	0.10	-0.44	21,32,40,43	0
8	MG	B	1502	1/1	0.99	0.10	-0.48	28,28,28,28	0
9	ADP	B	2502	27/27	0.97	0.11	-0.50	33,48,57,60	0
10	VO4	B	3002	5/5	0.99	0.10	-0.59	29,29,31,31	0
10	VO4	A	3001	5/5	0.99	0.08	-1.03	18,19,20,21	0
8	MG	A	1501	1/1	0.99	0.06	-2.56	17,17,17,17	0
6	PGV	G	4006	7/51	0.90	0.21	-	61,63,68,70	0
6	PGV	F	4008	8/51	0.84	0.18	-	53,58,61,64	0
6	PGV	G	4004	12/51	0.74	0.23	-	56,61,67,70	0
6	PGV	G	4007	9/51	0.89	0.30	-	55,62,72,72	0
6	PGV	G	4003	8/51	0.68	0.30	-	74,78,78,78	0
6	PGV	G	4005	10/51	0.80	0.21	-	58,65,70,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.