



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:40 PM GMT

PDB ID : 3RLF  
Title : Crystal structure of the maltose-binding protein/maltose transporter complex  
in an outward-facing conformation bound to MgAMPPNP  
Authors : Oldham, M.L.; Chen, J.  
Deposited on : 2011-04-19  
Resolution : 2.20 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

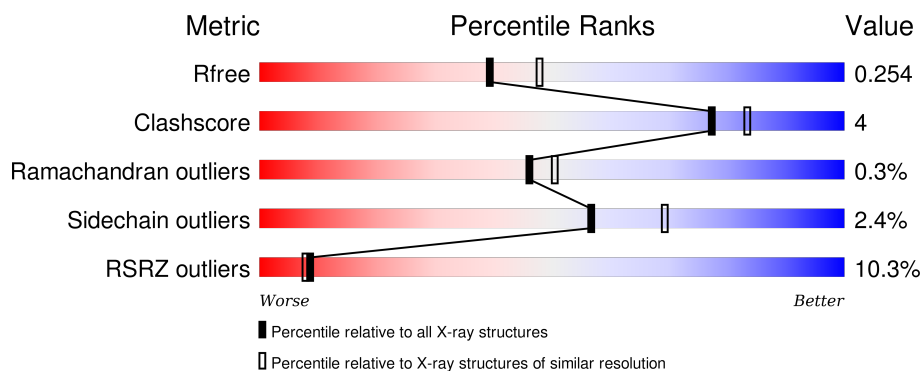
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	380	<div> <div>12%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
2	F	514	<div> <div>16%</div> <div>86%</div> <div>8%</div> <div>.</div> <div>5%</div> </div>
3	G	296	<div> <div>7%</div> <div>90%</div> <div>6%</div> <div>.</div> <div>.</div> </div>
4	A	381	<div> <div>4%</div> <div>86%</div> <div>11%</div> <div>.</div> <div>.</div> </div>
4	B	381	<div> <div>8%</div> <div>85%</div> <div>11%</div> <div>.</div> <div>.</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
5	UMQ	E	5004	-	-	-	X
7	PGV	G	4009	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 15268 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	2	0
			2914	1875	476	557	6			

There are 10 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
E	379	HIS	-	EXPRESSION TAG	UNP P0AEX9
E	380	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	1	0
			3832	2517	612	686	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	286	Total	C	N	O	S	0	2	0
			2214	1484	352	370	8			

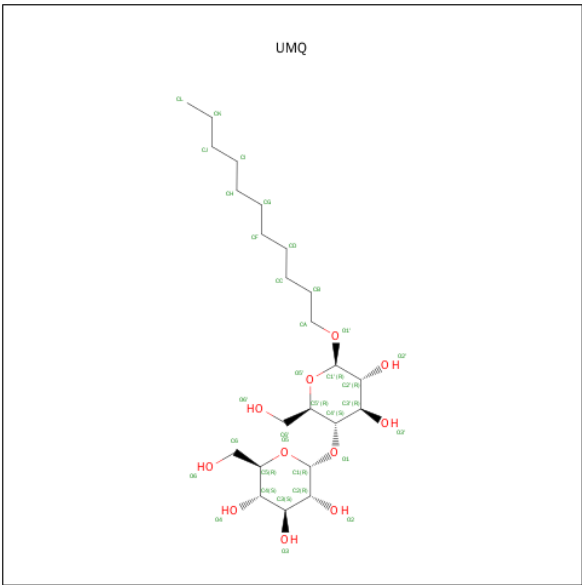
- Molecule 4 is a protein called Maltose/maltodextrin import ATP-binding protein MalK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	371	Total	C	N	O	S	0	0	0
			2876	1819	515	529	13			
4	B	371	Total	C	N	O	S	0	1	0
			2881	1822	515	531	13			

There are 20 discrepancies between the modelled and reference sequences:

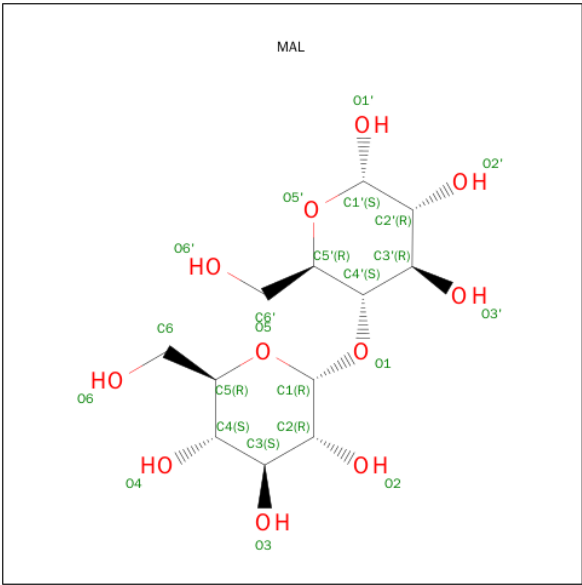
Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	EXPRESSION TAG	UNP P68187
A	373	SER	-	EXPRESSION TAG	UNP P68187
A	374	ALA	-	EXPRESSION TAG	UNP P68187
A	375	SER	-	EXPRESSION TAG	UNP P68187
A	376	HIS	-	EXPRESSION TAG	UNP P68187
A	377	HIS	-	EXPRESSION TAG	UNP P68187
A	378	HIS	-	EXPRESSION TAG	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>).



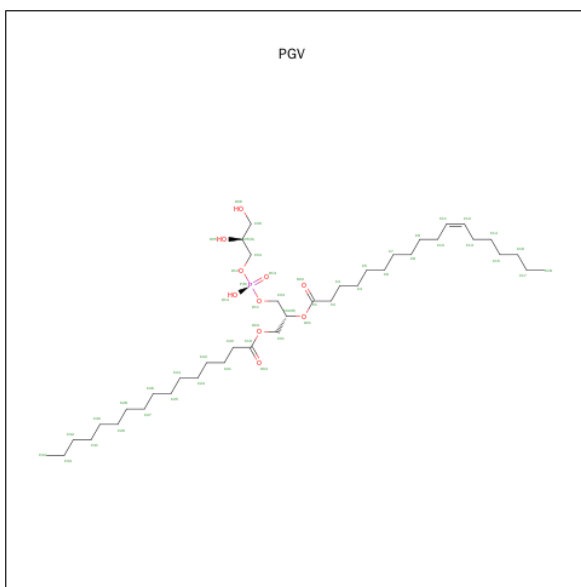
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			34	23	11		

- Molecule 6 is SUGAR (MALTOSE) (three-letter code: MAL) (formula: C<sub>12</sub>H<sub>22</sub>O<sub>11</sub>).



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<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).

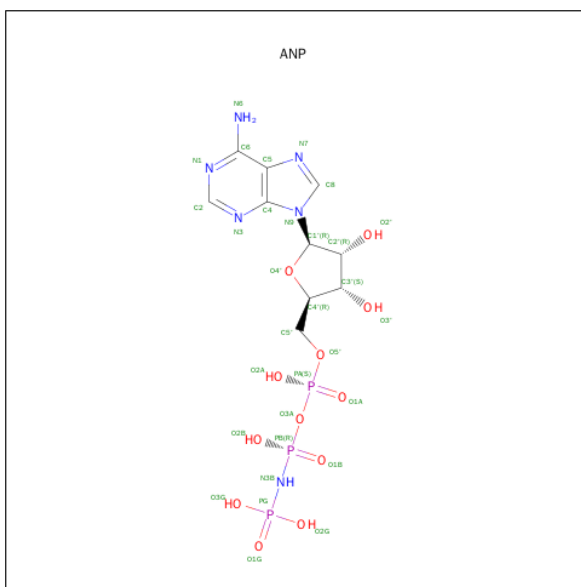


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total C O P 51 40 10 1	0	0
7	F	1	Total C 14 14	0	0
7	G	1	Total C 14 14	0	0
7	G	1	Total C 12 12	0	0

- 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 PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
9	B	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 10 is water.

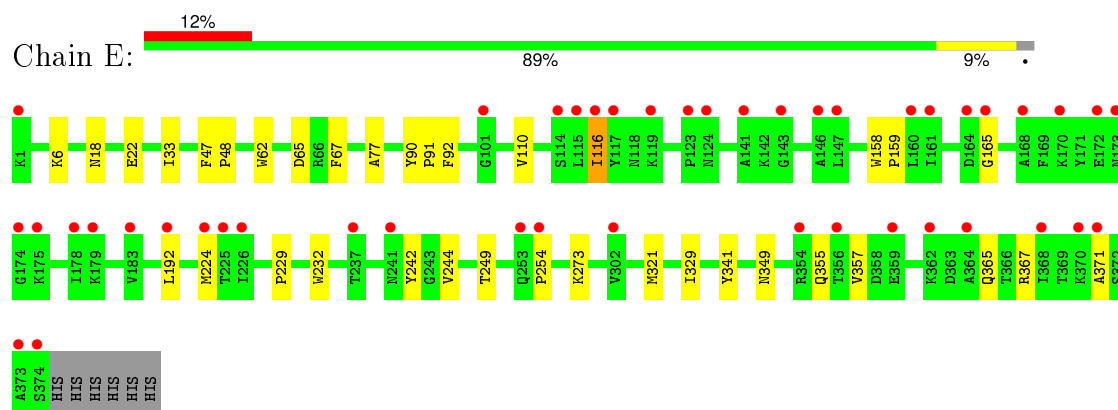
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	E	62	Total O 62 62	0	0
10	F	63	Total O 63 63	0	0
10	G	59	Total O 59 59	0	0
10	A	81	Total O 81 81	0	0
10	B	74	Total O 74 74	0	0



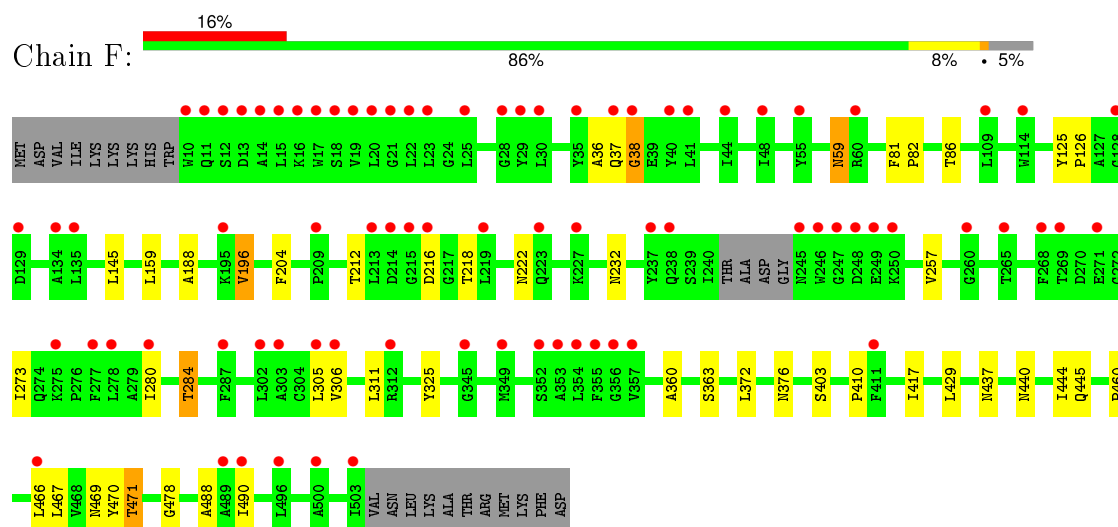
### 3 Residue-property plots [i](#)

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.

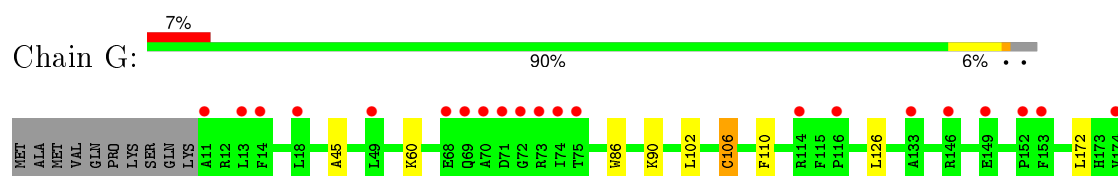
- Molecule 1: Maltose-binding periplasmic protein



- Molecule 2: Maltose transport system permease protein malF

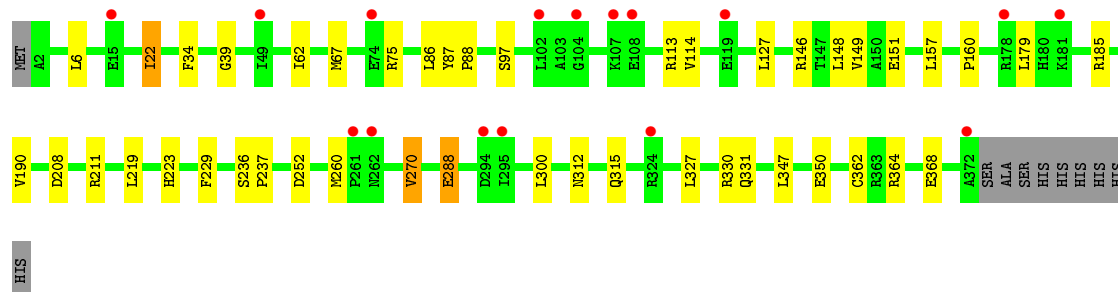
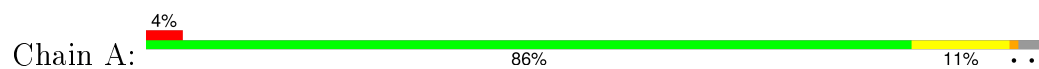


- Molecule 3: Maltose transport system permease protein malG

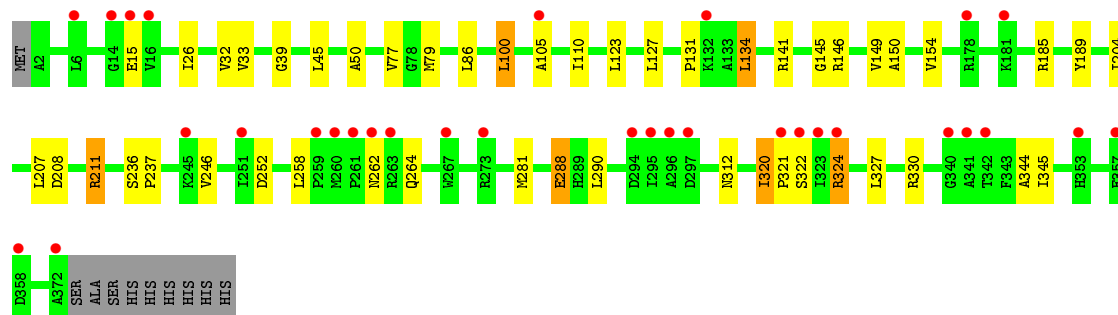
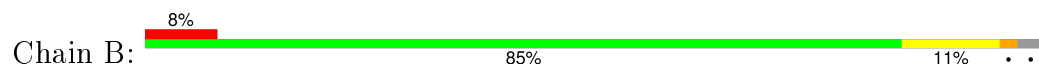




• Molecule 4: Maltose/maltodextrin import ATP-binding protein MalK



• 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, $\alpha$ , $\beta$ , $\gamma$	72.10 Å   95.81 Å   109.98 Å 86.70°   82.68°   76.40°	Depositor
Resolution (Å)	20.00 – 2.20 19.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.3 (20.00-2.20) 85.9 (19.97-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.19 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.223   ,   0.254 0.223   ,   0.254	Depositor DCC
$R_{free}$ test set	6209 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.2	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 56.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 124111 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15268	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: PGV, ANP, MG, UMQ, 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	0.34	0/2983	0.46	0/4048
2	F	0.36	0/3927	0.50	0/5344
3	G	0.37	0/2278	0.49	0/3115
4	A	0.34	0/2926	0.53	1/3968 (0.0%)
4	B	0.35	0/2932	0.53	0/3974
All	All	0.35	0/15046	0.50	1/20449 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	347	LEU	CA-CB-CG	5.08	126.98	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	2914	0	2888	19	0
2	F	3832	0	3861	32	0
3	G	2214	0	2302	11	0
4	A	2876	0	2941	26	0
4	B	2881	0	2942	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	34	0	44	0	0
6	F	23	0	22	0	0
7	F	65	0	100	2	0
7	G	26	0	44	1	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	31	0	13	2	0
9	B	31	0	13	2	0
10	A	81	0	0	1	0
10	B	74	0	0	2	0
10	E	62	0	0	0	0
10	F	63	0	0	0	0
10	G	59	0	0	0	0
All	All	15268	0	15170	111	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 (111) 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	1.42	1.01
4:A:39:GLY:H	9:A:2501:ANP:HNB1	1.16	0.94
4:B:39:GLY:H	9:B:2502:ANP:HNB1	1.18	0.88
4:A:223:HIS:CE1	4:A:368:GLU:HG2	2.12	0.85
4:B:344:ALA:CB	4:B:344:ALA:N	2.45	0.80
4:B:344:ALA:CB	4:B:344:ALA:C	2.51	0.79
4:B:141:ARG:NH1	10:B:455:HOH:O	2.05	0.78
1:E:116:ILE:HD11	1:E:242:TYR:HD2	1.51	0.76
2:F:471:THR:CG2	2:F:490:ILE:HG21	2.16	0.75
2:F:196:VAL:HG13	2:F:204:PHE:HB3	1.69	0.75
4:A:288:GLU:HG2	4:B:312:ASN:HB2	1.70	0.73
2:F:159:LEU:HD11	2:F:188:ALA:HB1	1.70	0.73
4:A:39:GLY:N	9:A:2501:ANP:HNB1	1.88	0.70
1:E:116:ILE:HD11	1:E:242:TYR:CD2	2.27	0.69
3:G:86:TRP:CE2	3:G:90:LYS:HD2	2.29	0.68
4:B:344:ALA:C	4:B:344:ALA:N	2.47	0.67
4:B:39:GLY:N	9:B:2502:ANP:HNB1	1.93	0.66
2:F:196:VAL:CG1	2:F:204:PHE:HB3	2.27	0.65
4:A:6:LEU:HD22	4:A:22:ILE:HD11	1.78	0.65
2:F:471:THR:HG21	2:F:490:ILE:CG2	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:320:ILE:HD11	4:B:327:LEU:HB2	1.80	0.63
4:A:208:ASP:O	4:A:211:ARG:HG2	2.02	0.59
1:E:367:ARG:HD2	2:F:460:PRO:HG3	1.84	0.59
2:F:280:ILE:O	2:F:284:THR:HG23	2.02	0.59
4:A:312:ASN:HB2	4:B:288:GLU:HG2	1.85	0.59
2:F:444:ILE:HG13	2:F:466:LEU:HG	1.85	0.57
4:B:324:ARG:H	4:B:324:ARG:HD3	1.70	0.57
2:F:471:THR:HG23	2:F:490:ILE:HD13	1.88	0.56
2:F:36:ALA:O	2:F:38:GLY:N	2.37	0.56
2:F:59:ASN:H	2:F:59:ASN:HD22	1.54	0.56
2:F:360:ALA:HB1	2:F:363:SER:HB2	1.90	0.54
4:A:223:HIS:ND1	4:A:368:GLU:HG2	2.22	0.54
3:G:45:ALA:HB2	3:G:260:TRP:CE2	2.43	0.54
2:F:212:THR:HG23	2:F:222:ASN:HD21	1.72	0.54
4:B:246:VAL:HG23	4:B:281:MET:HG3	1.91	0.53
4:B:288:GLU:HG3	4:B:330:ARG:HD3	1.91	0.52
4:A:97:SER:HB3	4:A:114:VAL:HG21	1.91	0.52
4:A:270:VAL:HG13	4:A:362:CYS:HB3	1.92	0.51
4:A:208:ASP:HB2	4:A:229:PHE:CE2	2.46	0.51
4:A:86:LEU:HA	4:A:146:ARG:NH2	2.25	0.50
3:G:110:PHE:HB3	3:G:178:LYS:HD2	1.93	0.50
4:B:26:ILE:HG12	4:B:32:VAL:HG21	1.93	0.50
4:A:288:GLU:HG3	4:A:330:ARG:HD3	1.94	0.50
3:G:60:LYS:HE2	7:G:4006:PGV:H201	1.94	0.50
3:G:224:ILE:HG12	3:G:274[A]:ILE:HD12	1.94	0.50
4:B:146:ARG:HD2	10:B:393:HOH:O	2.12	0.49
4:B:208:ASP:O	4:B:211:ARG:HG3	2.13	0.49
4:B:290:LEU:HD22	4:B:345:ILE:HD13	1.94	0.48
3:G:230:VAL:HB	3:G:231:PRO:HD3	1.95	0.48
1:E:116:ILE:HG12	1:E:244:VAL:HG22	1.95	0.48
2:F:445:GLN:HG2	2:F:469:ASN:HD22	1.79	0.47
1:E:62:TRP:HB3	1:E:67:PHE:HE1	1.79	0.47
2:F:403:SER:HB3	2:F:417:ILE:HD11	1.96	0.46
4:B:145:GLY:O	4:B:149:VAL:HG23	2.16	0.46
2:F:86:THR:O	2:F:488:ALA:HB1	2.14	0.46
4:A:62:ILE:HB	4:A:67:MET:HG3	1.97	0.46
2:F:376:ASN:HD21	2:F:437:ASN:ND2	2.14	0.46
2:F:273:ILE:HA	2:F:470:TYR:OH	2.15	0.46
4:A:157:LEU:HB3	4:A:160:PRO:HG3	1.96	0.46
1:E:6:LYS:HA	1:E:33:ILE:HG23	1.98	0.46
3:G:245:LEU:HG	3:G:249:MET:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:372:LEU:HD21	2:F:444:ILE:HD12	1.98	0.46
4:B:33:VAL:HG22	4:B:204:ILE:HG12	1.97	0.46
4:B:236:SER:HA	4:B:237:PRO:C	2.35	0.46
1:E:110:VAL:HG11	1:E:321:MET:HE3	1.96	0.46
4:A:260:MET:CE	4:A:300:LEU:HD22	2.46	0.45
4:B:86:LEU:HA	4:B:146:ARG:NH2	2.31	0.45
3:G:245:LEU:HG	3:G:249:MET:CE	2.47	0.45
4:B:77:VAL:HG12	4:B:154:VAL:HB	1.99	0.45
2:F:284:THR:HG21	2:F:467:LEU:H	1.80	0.45
4:B:131:PRO:HA	4:B:134:LEU:HD22	1.99	0.45
4:B:100:LEU:HB3	4:B:110:ILE:HG12	1.98	0.45
2:F:125:TYR:HA	2:F:126:PRO:HD2	1.89	0.44
4:A:86:LEU:HA	4:A:146:ARG:HH22	1.82	0.44
4:A:34:PHE:HB2	4:A:190:VAL:HG22	1.98	0.44
2:F:429:LEU:HD23	3:G:172:LEU:HD22	2.00	0.44
4:B:321:PRO:O	4:B:322:SER:HB3	2.17	0.44
1:E:18:ASN:O	1:E:22:GLU:HG2	2.18	0.44
1:E:192:LEU:HD23	1:E:357:VAL:HG13	1.98	0.44
4:B:262:ASN:ND2	4:B:264:GLN:HB2	2.33	0.44
2:F:305:LEU:O	2:F:311:LEU:HD12	2.18	0.44
2:F:216:ASP:OD1	2:F:218:THR:HG22	2.18	0.43
2:F:305:LEU:HD23	7:F:4001:PGV:H011	2.00	0.43
2:F:410:PRO:HB3	7:F:4001:PGV:H02	1.99	0.43
4:A:113:ARG:HG3	4:A:149:VAL:HG13	2.01	0.43
4:B:45:LEU:HD12	4:B:207:LEU:HD11	2.00	0.43
1:E:92:PHE:HD1	1:E:329:ILE:HD11	1.83	0.43
2:F:232:ASN:O	2:F:257:VAL:HG21	2.18	0.43
2:F:284:THR:HG22	2:F:466:LEU:HA	2.01	0.43
4:A:67:MET:HE1	4:A:75:ARG:HA	2.00	0.43
1:E:371:ALA:HB1	2:F:478:GLY:O	2.19	0.42
4:A:315:GLN:HG2	4:A:330:ARG:HG2	2.01	0.42
4:B:33:VAL:HA	4:B:189:TYR:O	2.19	0.42
1:E:349:ASN:HB3	1:E:355:GLN:HB2	2.02	0.42
1:E:77:ALA:HB2	1:E:273:LYS:HE3	2.01	0.42
1:E:229:PRO:HA	1:E:232:TRP:CE2	2.54	0.42
4:B:50:ALA:HB2	4:B:79:MET:HE3	2.01	0.42
4:A:151:GLU:O	4:A:185:ARG:NH2	2.52	0.42
4:B:100:LEU:HD13	4:B:150:ALA:HA	2.00	0.42
1:E:90:TYR:HA	1:E:91:PRO:HD3	1.95	0.42
1:E:158:TRP:N	1:E:159:PRO:CD	2.82	0.41
4:A:364:ARG:HD2	10:A:423:HOH:O	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:THR:HG22	1:E:254:PRO:HA	2.02	0.41
1:E:47:PHE:HB3	1:E:48:PRO:HD3	2.02	0.41
1:E:341:TYR:CE2	2:F:460:PRO:HB2	2.56	0.41
4:A:236:SER:HA	4:A:237:PRO:C	2.40	0.41
4:A:148:LEU:HD22	4:A:179:LEU:HD22	2.02	0.41
2:F:81:PHE:HB3	2:F:82:PRO:HD3	2.02	0.40
4:A:87:TYR:HA	4:A:88:PRO:HD3	1.87	0.40
3:G:102:LEU:O	3:G:106:CYS:HB2	2.21	0.40
3:G:177:ILE:HD11	3:G:218:VAL:HG21	2.02	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	374/380 (98%)	364 (97%)	9 (2%)	1 (0%)	46	50
2	F	487/514 (95%)	471 (97%)	14 (3%)	2 (0%)	39	42
3	G	286/296 (97%)	283 (99%)	2 (1%)	1 (0%)	46	50
4	A	369/381 (97%)	360 (98%)	9 (2%)	0	100	100
4	B	369/381 (97%)	360 (98%)	8 (2%)	1 (0%)	46	50
All	All	1885/1952 (97%)	1838 (98%)	42 (2%)	5 (0%)	46	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	37	GLN
2	F	38	GLY
1	E	165	GLY
4	B	105	ALA
3	G	230	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	299/305 (98%)	295 (99%)	4 (1%)	76	87
2	F	403/424 (95%)	395 (98%)	8 (2%)	63	76
3	G	230/237 (97%)	226 (98%)	4 (2%)	68	81
4	A	314/323 (97%)	305 (97%)	9 (3%)	50	62
4	B	315/323 (98%)	303 (96%)	12 (4%)	40	49
All	All	1561/1612 (97%)	1524 (98%)	37 (2%)	57	69

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	65	ASP
1	E	116	ILE
1	E	224	MET
1	E	365	GLN
2	F	59	ASN
2	F	145	LEU
2	F	196	VAL
2	F	284	THR
2	F	306	VAL
2	F	325	TYR
2	F	440	ASN
2	F	471	THR
3	G	106	CYS
3	G	126	LEU
3	G	212	VAL
3	G	235	LEU
4	A	22	ILE
4	A	127	LEU
4	A	219	LEU
4	A	252	ASP
4	A	270	VAL
4	A	288	GLU
4	A	327	LEU

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Mol	Chain	Res	Type
4	A	331	GLN
4	A	350	GLU
4	B	15	GLU
4	B	100	LEU
4	B	123	LEU
4	B	127	LEU
4	B	134	LEU
4	B	185	ARG
4	B	211	ARG
4	B	252	ASP
4	B	258	LEU
4	B	288	GLU
4	B	320	ILE
4	B	324	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	218	ASN
2	F	59	ASN
2	F	98	ASN
2	F	222	ASN
2	F	232	ASN
2	F	437	ASN
2	F	440	ASN
3	G	241	ASN
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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	ANP	A	2501	8	27,33,33	2.12	8 (29%)	30,52,52	2.47	7 (23%)
9	ANP	B	2502	8	27,33,33	2.07	7 (25%)	30,52,52	2.23	6 (20%)
5	UMQ	E	5004	-	35,35,35	0.43	0	46,46,46	0.85	2 (4%)
6	MAL	F	2000	-	24,24,24	0.45	0	35,35,35	0.91	2 (5%)
7	PGV	F	4001	-	50,50,50	1.06	3 (6%)	51,56,56	1.06	3 (5%)
7	PGV	F	4002	-	13,13,50	0.28	0	12,12,56	0.53	0
7	PGV	G	4006	-	13,13,50	0.27	0	12,12,56	0.54	0
7	PGV	G	4009	-	11,11,50	0.27	0	10,10,56	0.53	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	ANP	A	2501	8	-	0/12/38/38	0/3/3/3
9	ANP	B	2502	8	-	1/12/38/38	0/3/3/3
5	UMQ	E	5004	-	-	0/20/60/60	0/2/2/2
6	MAL	F	2000	-	-	0/8/48/48	0/2/2/2
7	PGV	F	4001	-	-	0/55/55/55	0/0/0/0
7	PGV	F	4002	-	-	0/11/11/55	0/0/0/0
7	PGV	G	4006	-	-	0/11/11/55	0/0/0/0
7	PGV	G	4009	-	-	0/9/9/55	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2502	ANP	PG-O3G	-2.27	1.50	1.56
9	A	2501	ANP	PG-O2G	-2.24	1.50	1.56
9	A	2501	ANP	PB-O2B	-2.12	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2502	ANP	PG-O2G	-2.01	1.51	1.56
9	A	2501	ANP	PB-O3A	2.56	1.62	1.59
9	B	2502	ANP	C5-C4	3.05	1.47	1.40
9	A	2501	ANP	C5-C4	3.16	1.47	1.40
7	F	4001	PGV	C12-C11	3.66	1.52	1.31
7	F	4001	PGV	O01-C1	4.04	1.46	1.34
9	B	2502	ANP	PG-N3B	4.11	1.74	1.63
9	B	2502	ANP	PB-N3B	4.20	1.74	1.63
7	F	4001	PGV	O03-C19	4.26	1.46	1.33
9	A	2501	ANP	PG-N3B	4.31	1.74	1.63
9	A	2501	ANP	PB-N3B	4.36	1.74	1.63
9	A	2501	ANP	PG-O1G	4.64	1.51	1.46
9	A	2501	ANP	PB-O1B	4.69	1.51	1.46
9	B	2502	ANP	PG-O1G	4.70	1.51	1.46
9	B	2502	ANP	PB-O1B	4.82	1.51	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2501	ANP	O1G-PG-N3B	-7.72	100.06	111.90
9	A	2501	ANP	N3-C2-N1	-7.43	123.21	128.89
9	B	2502	ANP	N3-C2-N1	-7.21	123.38	128.89
9	B	2502	ANP	O1G-PG-N3B	-5.75	103.07	111.90
9	A	2501	ANP	O1B-PB-N3B	-3.55	106.45	111.90
9	B	2502	ANP	O1B-PB-N3B	-3.06	107.20	111.90
9	B	2502	ANP	C4-C5-N7	-2.79	106.91	109.48
9	A	2501	ANP	C4-C5-N7	-2.74	106.96	109.48
9	A	2501	ANP	PA-O3A-PB	-2.21	125.25	132.67
7	F	4001	PGV	C10-C11-C12	-2.06	110.98	125.34
9	A	2501	ANP	O3G-PG-O2G	2.05	113.64	107.58
6	F	2000	MAL	O5'-C1'-C2'	2.24	113.37	109.80
5	E	5004	UMQ	C3'-C4'-C5'	2.34	116.14	110.84
5	E	5004	UMQ	C2'-C3'-C4'	2.36	114.77	109.60
9	B	2502	ANP	O3G-PG-O2G	2.47	114.89	107.58
7	F	4001	PGV	O03-C19-C20	2.59	119.80	111.90
6	F	2000	MAL	C1'-O5'-C5'	3.25	119.48	113.47
7	F	4001	PGV	O01-C1-C2	4.12	120.48	111.53
9	B	2502	ANP	O2B-PB-O1B	4.14	118.64	110.00
9	A	2501	ANP	O2B-PB-O1B	4.67	119.74	110.00

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	2502	ANP	O1G-PG-N3B-PB

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2501	ANP	2	0
9	B	2502	ANP	2	0
7	F	4001	PGV	2	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	374/380 (98%)	0.62	45 (12%) 6 5	30, 66, 111, 133	1 (0%)
2	F	490/514 (95%)	0.91	80 (16%) 2 2	32, 61, 127, 188	0
3	G	286/296 (96%)	0.32	21 (7%) 18 17	28, 44, 81, 108	0
4	A	371/381 (97%)	0.24	16 (4%) 39 38	27, 44, 69, 94	0
4	B	371/381 (97%)	0.31	32 (8%) 13 12	25, 46, 84, 112	0
All	All	1892/1952 (96%)	0.51	194 (10%) 9 8	25, 51, 104, 188	1 (0%)

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	10	TRP	20.1
2	F	37	GLN	11.3
2	F	38	GLY	9.2
2	F	14	ALA	7.9
2	F	29	TYR	7.6
3	G	70	ALA	7.1
2	F	355	PHE	6.9
4	B	105	ALA	6.7
3	G	72	GLY	6.6
3	G	71	ASP	6.5
1	E	172	GLU	6.4
2	F	245	ASN	6.2
3	G	74	ILE	6.1
2	F	11	GLN	6.0
2	F	269	THR	6.0
4	A	372	ALA	6.0
4	B	263	ARG	6.0
2	F	22	LEU	5.9
4	B	251	ILE	5.7
4	B	295	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
2	F	40	TYR	5.7
4	B	324	ARG	5.6
1	E	143	GLY	5.6
2	F	25	LEU	5.5
4	A	104	GLY	5.5
2	F	352	SER	5.5
2	F	357	VAL	5.5
3	G	73	ARG	5.3
2	F	503	ILE	5.3
4	B	260	MET	5.3
2	F	12	SER	5.2
1	E	173	ASN	5.1
4	A	108	GLU	5.1
1	E	373	ALA	5.0
1	E	374	SER	5.0
1	E	119	LYS	5.0
3	G	114	ARG	5.0
4	B	322	SER	4.9
2	F	248	ASP	4.9
2	F	275	LYS	4.7
4	A	294	ASP	4.6
2	F	246	TRP	4.6
2	F	271	GLU	4.4
2	F	260	GLY	4.4
2	F	15	LEU	4.3
4	B	294	ASP	4.3
3	G	69	GLN	4.3
2	F	17	TRP	4.3
2	F	354	LEU	4.3
2	F	13	ASP	4.2
2	F	278	LEU	4.2
2	F	214	ASP	4.2
2	F	216	ASP	4.2
4	A	295	ILE	4.1
4	B	296	ALA	4.1
2	F	312	ARG	4.0
2	F	411	PHE	4.0
4	B	261	PRO	3.9
1	E	178	ILE	3.9
2	F	60	ARG	3.9
2	F	353	ALA	3.9
4	A	324	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	224	MET	3.8
3	G	153	PHE	3.8
2	F	16	LYS	3.8
3	G	68	GLU	3.8
4	B	262	ASN	3.8
2	F	268	PHE	3.8
2	F	20	LEU	3.8
2	F	19	VAL	3.8
1	E	123	PRO	3.7
1	E	237	THR	3.7
4	A	261	PRO	3.6
1	E	115	LEU	3.6
2	F	18	SER	3.6
3	G	116	PRO	3.5
2	F	41	LEU	3.5
1	E	183	VAL	3.5
2	F	349	MET	3.5
1	E	147	LEU	3.5
4	B	340	GLY	3.4
4	B	323	ILE	3.4
4	B	14	GLY	3.4
1	E	170	LYS	3.3
2	F	500	ALA	3.3
4	B	15	GLU	3.3
1	E	225	THR	3.3
4	B	372	ALA	3.3
2	F	247	GLY	3.3
2	F	213	LEU	3.3
4	A	181	LYS	3.2
1	E	1	LYS	3.2
1	E	253	GLN	3.2
1	E	364	ALA	3.2
1	E	359	GLU	3.1
1	E	179	LYS	3.1
4	B	297	ASP	3.1
2	F	134	ALA	3.1
1	E	192	LEU	3.1
2	F	23	LEU	3.1
4	B	16	VAL	3.0
2	F	48	ILE	3.0
2	F	21	GLY	3.0
2	F	44	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	370	LYS	3.0
1	E	354	ARG	3.0
1	E	165	GLY	2.9
3	G	11	ALA	2.9
4	B	259	PRO	2.9
2	F	227	LYS	2.9
2	F	237	TYR	2.9
2	F	303	ALA	2.8
4	A	107	LYS	2.8
3	G	133	ALA	2.8
1	E	164	ASP	2.8
4	B	273	ARG	2.8
2	F	302	LEU	2.8
1	E	160	LEU	2.7
2	F	219	LEU	2.7
2	F	195	LYS	2.7
4	A	262	ASN	2.7
1	E	174	GLY	2.7
2	F	280	ILE	2.6
4	B	321	PRO	2.6
3	G	152	PRO	2.6
4	B	357	GLU	2.6
2	F	306	VAL	2.5
2	F	250	LYS	2.5
3	G	14	PHE	2.5
4	B	178	ARG	2.5
4	B	267	TRP	2.5
1	E	114	SER	2.5
3	G	49	LEU	2.5
1	E	116	ILE	2.5
1	E	175	LYS	2.5
1	E	117	TYR	2.5
4	B	353	HIS	2.5
1	E	368	ILE	2.5
2	F	129	ASP	2.5
1	E	146	ALA	2.4
3	G	146	ARG	2.4
1	E	226	ILE	2.4
2	F	305	LEU	2.4
4	A	49	ILE	2.4
1	E	124	ASN	2.4
4	A	74	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	490	ILE	2.4
2	F	345	GLY	2.4
1	E	168	ALA	2.4
2	F	135	LEU	2.4
3	G	18	LEU	2.4
1	E	362	LYS	2.4
2	F	128	GLY	2.3
2	F	356	GLY	2.3
2	F	209	PRO	2.3
4	B	181	LYS	2.3
2	F	238	GLN	2.3
1	E	241	ASN	2.3
4	A	15	GLU	2.3
4	B	358	ASP	2.3
2	F	215	GLY	2.3
1	E	302	VAL	2.3
1	E	356	THR	2.3
2	F	249	GLU	2.3
2	F	466	LEU	2.3
2	F	223	GLN	2.2
4	A	119	GLU	2.2
4	B	132	LYS	2.2
1	E	141	ALA	2.2
1	E	161	ILE	2.2
2	F	496	LEU	2.2
4	A	102	LEU	2.2
2	F	265	THR	2.2
4	B	341	ALA	2.2
2	F	287	PHE	2.2
2	F	109	LEU	2.2
3	G	75	THR	2.2
1	E	101	GLY	2.1
1	E	254	PRO	2.1
2	F	114	TRP	2.1
4	B	6	LEU	2.1
2	F	28	GLY	2.1
3	G	13	LEU	2.1
3	G	149	GLU	2.1
2	F	277	PHE	2.1
3	G	174	VAL	2.1
4	B	245	LYS	2.1
4	B	342	THR	2.1

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Mol	Chain	Res	Type	RSRZ
4	A	178	ARG	2.1
2	F	489	ALA	2.0
1	E	371	ALA	2.0
2	F	30	LEU	2.0
2	F	35	TYR	2.0
2	F	55	TYR	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
5	UMQ	E	5004	34/34	0.77	0.28	3.85	74,80,82,83	0
7	PGV	G	4009	12/51	0.73	0.23	2.15	70,71,74,74	0
7	PGV	F	4001	51/51	0.81	0.23	1.11	75,83,86,91	0
7	PGV	F	4002	14/51	0.72	0.25	0.92	58,60,65,66	0
7	PGV	G	4006	14/51	0.83	0.19	0.82	71,75,82,84	0
8	MG	B	1502	1/1	0.98	0.11	0.26	30,30,30,30	0
9	ANP	B	2502	31/31	0.98	0.10	-0.47	28,35,41,42	0
9	ANP	A	2501	31/31	0.98	0.09	-0.49	25,32,41,41	0
6	MAL	F	2000	23/23	0.95	0.09	-1.03	46,49,51,54	0
8	MG	A	1501	1/1	0.98	0.04	-2.65	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.