



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:46 AM GMT

PDB ID : 3PUW
Title : Crystal Structure of an outward-facing MBP-Maltose transporter complex bound to ADP-AIF4
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
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

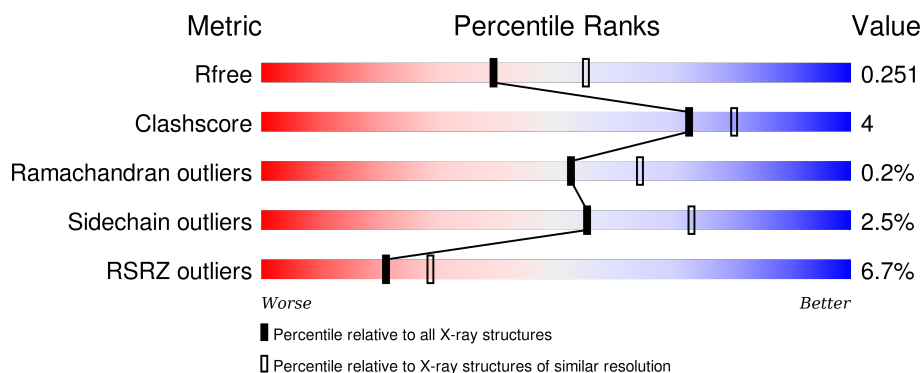
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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 ≥ 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>5%</div> <div>92%</div> <div>7%</div> </div>
2	F	514	<div> <div>9%</div> <div>83%</div> <div>12%</div> <div>5%</div> </div>
3	G	296	<div> <div>6%</div> <div>86%</div> <div>11%</div> </div>
4	A	381	<div> <div>4%</div> <div>83%</div> <div>13%</div> </div>
4	B	381	<div> <div>7%</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	4001	-	-	-	X
6	PGV	F	4010	-	-	-	X
6	PGV	G	4004	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15229 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	1877	474	558	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	2517	610	687	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	1	0
			2227	1491	355	373	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
			2909	1838	521	536	14			

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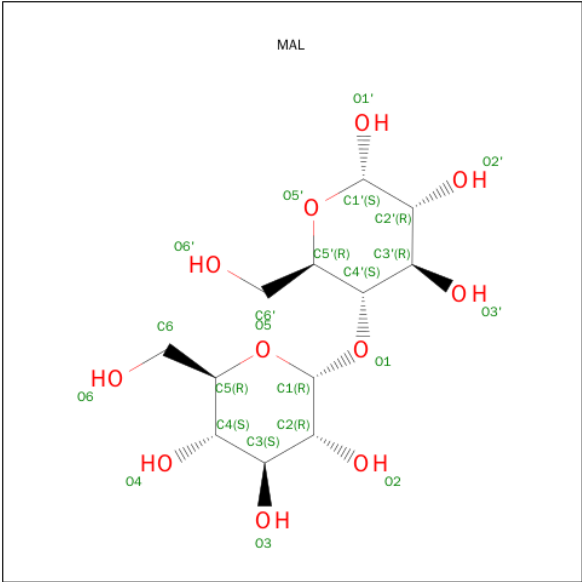
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	358	Total	C	N	O	S	0	0	0
			2787	1765	497	512	13			

There are 20 discrepancies between the modelled and reference sequences:

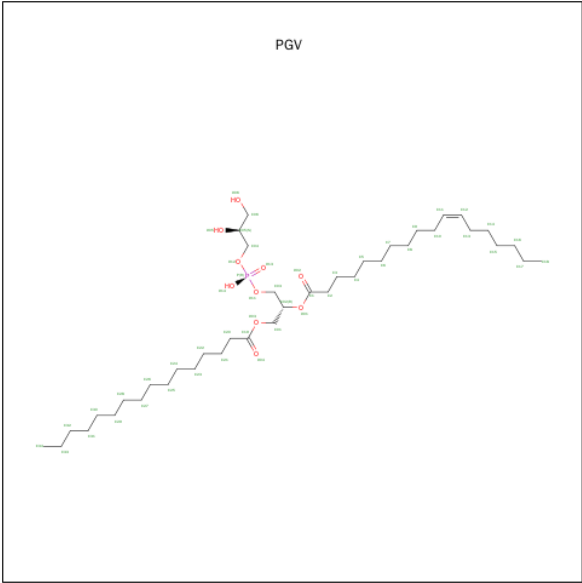
Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	EXPRESSION TAG	UNP P68187
A	373	SER	-	EXPRESSION TAG	UNP P68187
A	374	ALA	-	EXPRESSION TAG	UNP P68187
A	375	SER	-	EXPRESSION TAG	UNP P68187
A	376	HIS	-	EXPRESSION TAG	UNP P68187
A	377	HIS	-	EXPRESSION TAG	UNP P68187
A	378	HIS	-	EXPRESSION TAG	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: C₁₂H₂₂O₁₁).



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

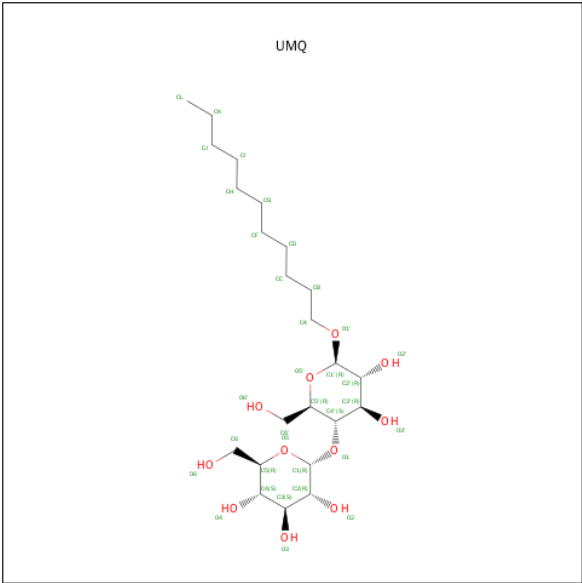
- Molecule 6 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHO RYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	C	0	0
			8	8		
6	F	1	Total	C	0	0
			17	17		
6	G	1	Total	C	0	0
			14	14		
6	G	1	Total	C	0	0
			12	12		
6	G	1	Total	C	0	0
			12	12		
6	G	1	Total	C	0	0
			15	15		
6	G	1	Total	C	0	0
			12	12		
6	G	1	Total	C	0	0
			14	14		

- Molecule 7 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: C₂₃H₄₄O₁₁).

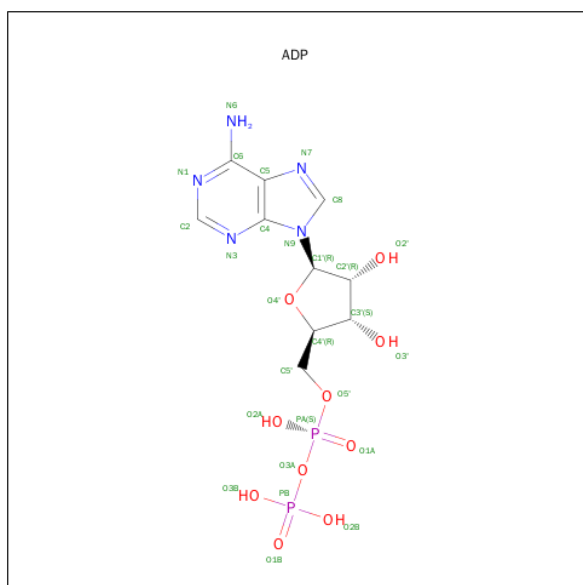


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			34	23	11		

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

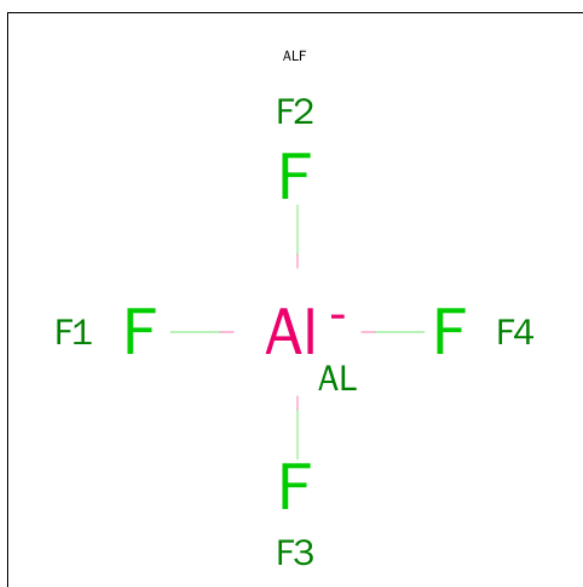
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Mg 1 1	0	0
8	A	1	Total Mg 1 1	0	0

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



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

- Molecule 10 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	Al	F	0	0
			5	1	4		
10	B	1	Total	Al	F	0	0
			5	1	4		

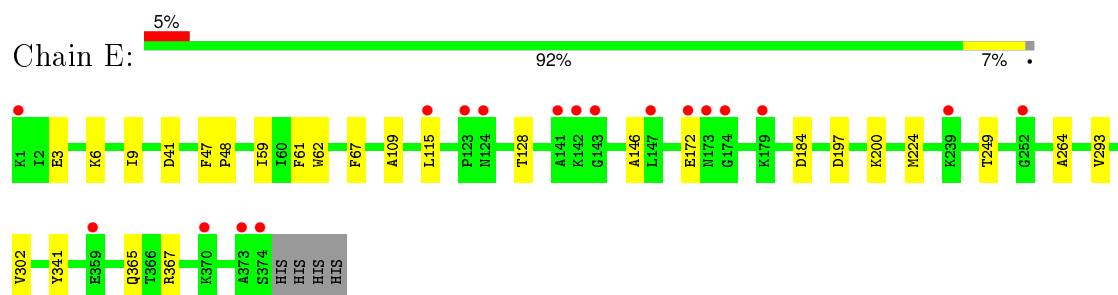
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	E	68	Total	O	0	0
			68	68		
11	F	57	Total	O	0	0
			57	57		
11	G	47	Total	O	0	0
			47	47		
11	A	47	Total	O	0	0
			47	47		
11	B	54	Total	O	0	0
			54	54		

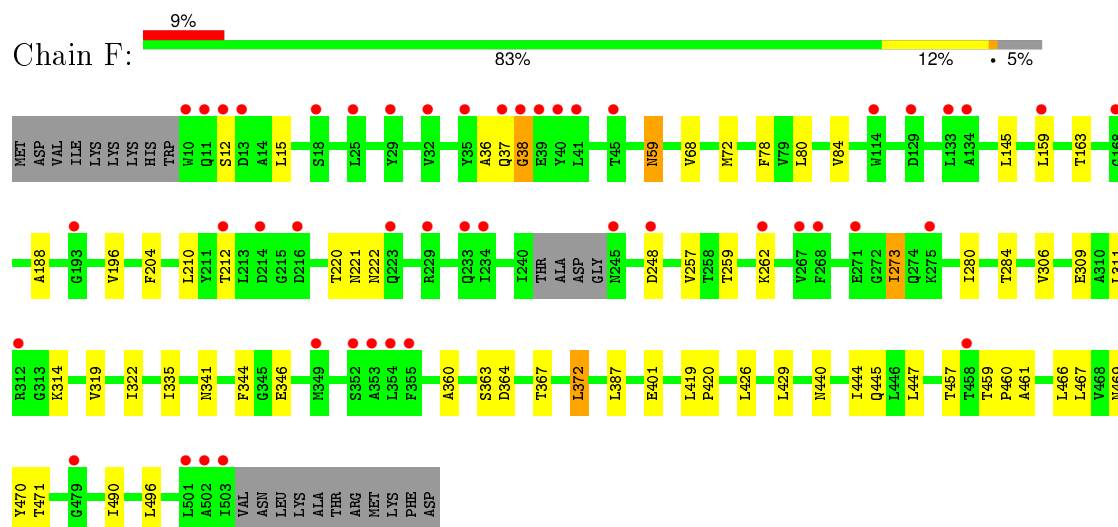
3 Residue-property plots [i](#)

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.

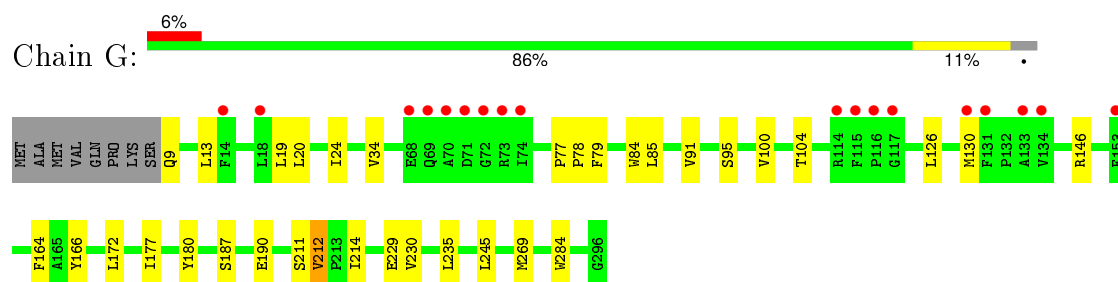
- Molecule 1: Maltose-binding periplasmic protein



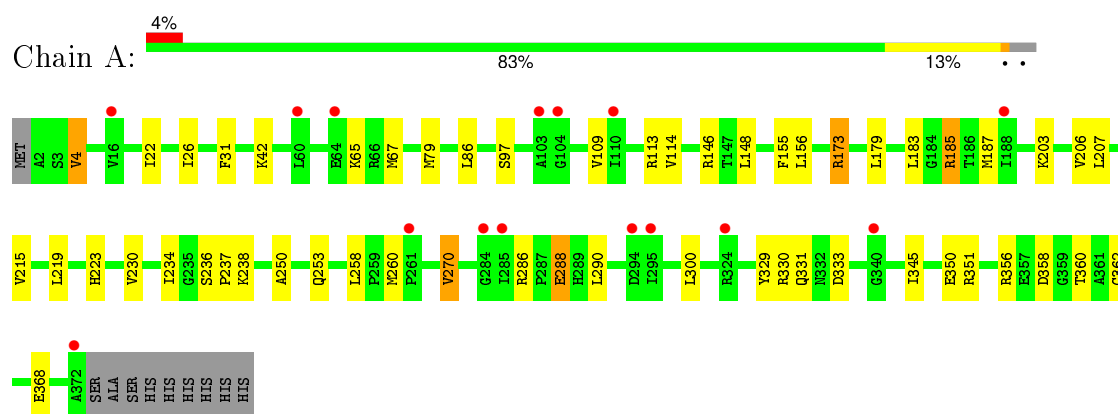
- Molecule 2: Maltose transport system permease protein malF



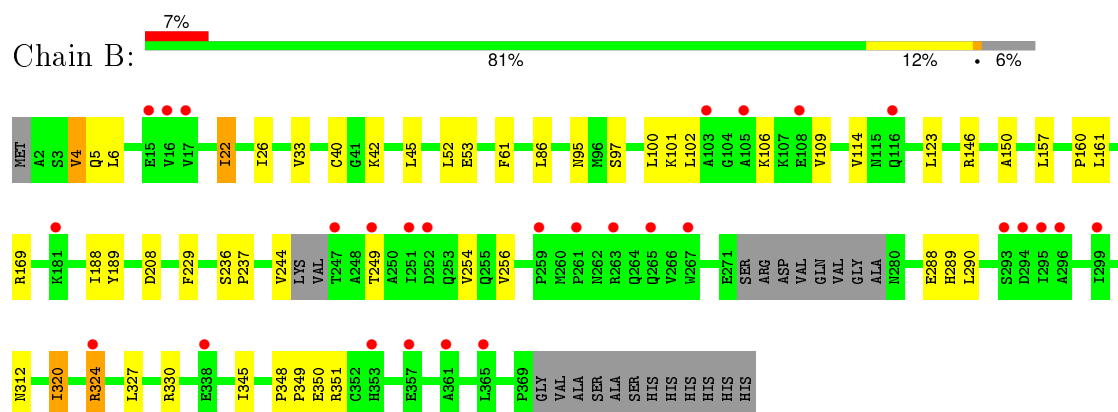
- Molecule 3: Maltose transport system permease protein malG



- 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, α , β , γ	81.88Å 97.34Å 112.34Å 85.76° 79.42° 72.45°	Depositor
Resolution (Å)	19.99 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	66.5 (19.99-2.30) 66.3 (19.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.255 0.219 , 0.251	Depositor DCC
R_{free} test set	4819 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 95877 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15229	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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, ALF, 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	0.34	0/2990	0.47	0/4059
2	F	0.36	0/3932	0.50	0/5352
3	G	0.37	0/2291	0.50	1/3131 (0.0%)
4	A	0.34	0/2962	0.53	0/4016
4	B	0.33	0/2835	0.51	0/3842
All	All	0.35	0/15010	0.50	1/20400 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	235	LEU	CA-CB-CG	5.70	128.42	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	2891	15	0
2	F	3831	0	3861	41	0
3	G	2227	0	2314	21	0
4	A	2909	0	2971	34	0
4	B	2787	0	2845	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	23	0	22	0	0
6	F	85	0	133	1	0
6	G	79	0	122	0	0
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	47	0	0	0	0
11	B	54	0	0	1	0
11	E	68	0	0	1	0
11	F	57	0	0	0	0
11	G	47	0	0	0	0
All	All	15229	0	15227	128	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 (128) 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	1.62	1.12
4:A:173[A]:ARG:HH11	4:A:173[A]:ARG:CG	1.73	1.01
4:A:173[A]:ARG:NH1	4:A:173[A]:ARG:CB	2.30	0.94
4:A:173[A]:ARG:CB	4:A:173[A]:ARG:HH11	1.82	0.92
4:A:173[A]:ARG:HH11	4:A:173[A]:ARG:HG3	1.35	0.87
4:B:6:LEU:HD22	4:B:22:ILE:HD11	1.59	0.84
1:E:115:LEU:HD21	1:E:224:MET:HE3	1.59	0.84
4:A:173[A]:ARG:HH11	4:A:173[A]:ARG:HB2	1.36	0.81
4:A:79:MET:HG3	4:A:156:LEU:HB2	1.64	0.78
4:A:223:HIS:CE1	4:A:368:GLU:HG2	2.18	0.78
3:G:91:VAL:O	3:G:95:SER:HB2	1.89	0.72
2:F:471:THR:HG21	2:F:490:ILE:HG21	1.72	0.71
2:F:444:ILE:HG13	2:F:466:LEU:HG	1.73	0.70
1:E:367:ARG:HD2	2:F:460:PRO:HG3	1.75	0.69
4:A:356:ARG:HH11	4:A:360:THR:HG23	1.58	0.68
2:F:335:ILE:HD12	3:G:34:VAL:HG22	1.75	0.67
2:F:284:THR:HG22	2:F:466:LEU:HA	1.76	0.66
4:A:86:LEU:HA	4:A:146:ARG:NH2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:4:VAL:HG13	4:B:26:ILE:HB	1.79	0.65
3:G:104:THR:HG22	3:G:177:ILE:HD13	1.80	0.63
3:G:187:SER:HA	3:G:190:GLU:HB2	1.82	0.61
2:F:471:THR:CG2	2:F:490:ILE:HG21	2.31	0.61
2:F:309:GLU:HA	2:F:314:LYS:NZ	2.16	0.60
4:B:290:LEU:HD22	4:B:345:ILE:HD13	1.84	0.59
2:F:372:LEU:HD13	2:F:447:LEU:HD23	1.85	0.58
2:F:280:ILE:O	2:F:284:THR:HG23	2.04	0.58
2:F:159:LEU:HD11	2:F:188:ALA:HB1	1.84	0.58
2:F:471:THR:HG23	2:F:490:ILE:HD13	1.85	0.58
4:B:106:LYS:HB2	4:B:109:VAL:HB	1.87	0.57
4:A:260[A]:MET:HE2	4:A:300:LEU:HD22	1.86	0.56
2:F:196:VAL:CG1	2:F:204:PHE:HB3	2.36	0.55
2:F:341:ASN:O	2:F:344:PHE:O	2.25	0.54
4:A:173[A]:ARG:CB	4:A:173[A]:ARG:CZ	2.84	0.54
2:F:59:ASN:H	2:F:59:ASN:HD22	1.56	0.54
2:F:360:ALA:HB1	2:F:363:SER:HB2	1.89	0.54
4:A:4:VAL:HG13	4:A:26:ILE:HB	1.89	0.54
4:B:157:LEU:HB3	4:B:160:PRO:HG3	1.91	0.53
2:F:471:THR:HG21	2:F:490:ILE:CG2	2.37	0.52
1:E:146:ALA:O	1:E:224:MET:HG2	2.10	0.52
4:B:288:GLU:HG3	4:B:330:ARG:HD3	1.92	0.52
4:B:249:THR:HG22	4:B:254:VAL:HG13	1.91	0.51
2:F:273:ILE:HA	2:F:470:TYR:OH	2.10	0.51
3:G:126:LEU:O	3:G:130:MET:HG2	2.09	0.51
3:G:100:VAL:O	3:G:104:THR:HG23	2.09	0.51
2:F:36:ALA:O	2:F:38:GLY:N	2.44	0.51
2:F:429:LEU:HD23	3:G:172:LEU:HD22	1.93	0.51
4:A:358:ASP:OD1	4:A:360:THR:HG22	2.11	0.50
4:A:288:GLU:HG2	4:B:312:ASN:HB2	1.92	0.50
4:B:320:ILE:HD11	4:B:327:LEU:HB2	1.94	0.50
1:E:41[B]:ASP:OD2	11:E:407:HOH:O	2.20	0.50
1:E:3:GLU:HB3	1:E:6:LYS:HE2	1.93	0.50
2:F:319:VAL:O	2:F:322:ILE:HG13	2.13	0.49
2:F:335:ILE:HD12	3:G:34:VAL:CG2	2.43	0.49
4:B:324:ARG:H	4:B:324:ARG:HD3	1.77	0.48
4:A:183:LEU:HB3	4:A:185:ARG:HG3	1.95	0.48
4:B:236:SER:HA	4:B:237:PRO:C	2.33	0.48
2:F:68:VAL:HG12	2:F:72:MET:HG3	1.96	0.48
4:B:40:CYS:SG	4:B:42:LYS:HG3	2.54	0.48
4:B:161:LEU:HB3	4:B:169:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:33:VAL:HG12	4:B:189:TYR:HB3	1.96	0.47
4:A:42:LYS:HG2	4:A:207:LEU:HD12	1.97	0.47
3:G:20:LEU:O	3:G:24:ILE:HG12	2.14	0.47
1:E:109:ALA:HA	1:E:302:VAL:HA	1.97	0.47
4:A:236:SER:HA	4:A:237:PRO:C	2.35	0.46
4:A:206:VAL:HG21	4:A:234:ILE:HD11	1.98	0.46
4:A:329:TYR:CE2	4:A:331:GLN:HG2	2.51	0.46
2:F:387:LEU:HD13	2:F:429:LEU:HD13	1.97	0.46
4:B:86:LEU:HA	4:B:146:ARG:NH2	2.31	0.46
2:F:259:THR:HB	2:F:262:LYS:HD2	1.97	0.46
2:F:419:LEU:HB3	2:F:420:PRO:HD3	1.98	0.46
2:F:309:GLU:HA	2:F:314:LYS:HZ2	1.81	0.45
4:B:100:LEU:HD13	4:B:150:ALA:HA	1.98	0.45
4:A:250:ALA:HB3	4:A:253:GLN:HG2	1.98	0.45
4:A:148:LEU:HD22	4:A:179:LEU:HD22	1.99	0.45
2:F:309:GLU:HA	2:F:314:LYS:HZ3	1.81	0.45
3:G:166:TYR:OH	3:G:229[A]:GLU:HG2	2.17	0.45
4:A:97:SER:HB3	4:A:114:VAL:HG21	1.98	0.45
4:A:351:ARG:NE	4:A:368:GLU:OE2	2.40	0.45
4:B:244:VAL:HB	4:B:256:VAL:HB	1.99	0.45
4:A:65:LYS:O	4:A:67:MET:HG2	2.17	0.45
1:E:9:ILE:HG12	1:E:59:ILE:HB	1.98	0.45
3:G:79:PHE:HB3	3:G:84:TRP:CH2	2.52	0.45
2:F:457:THR:HG21	2:F:461:ALA:HB3	1.99	0.44
1:E:61:PHE:CE2	1:E:264:ALA:HB2	2.52	0.44
4:B:208:ASP:HB2	4:B:229:PHE:CE2	2.52	0.44
4:B:97:SER:HB3	4:B:114:VAL:HG21	1.98	0.44
3:G:180:TYR:CE2	3:G:211:SER:HA	2.52	0.44
4:A:270:VAL:HG13	4:A:362:CYS:HB3	2.00	0.44
4:A:203:LYS:HD3	4:A:215:VAL:CG1	2.48	0.44
4:A:230:VAL:HG13	4:A:234:ILE:HD13	2.00	0.44
2:F:12:SER:HB2	2:F:15:LEU:HB2	1.99	0.44
1:E:184:ASP:HB2	1:E:365:GLN:CD	2.38	0.44
2:F:212:THR:HG23	2:F:222:ASN:HD21	1.83	0.44
3:G:212:VAL:HG22	3:G:284:TRP:CE3	2.53	0.43
4:A:173[A]:ARG:NH1	4:A:173[A]:ARG:HG3	2.15	0.43
6:F:4001:PGV:H82	3:G:19:LEU:HD13	2.00	0.43
1:E:197:ASP:HA	1:E:200:LYS:HB2	2.01	0.43
1:E:62:TRP:HB3	1:E:67:PHE:CE1	2.53	0.43
4:A:290:LEU:HD22	4:A:345:ILE:HD13	2.00	0.43
4:A:286:ARG:HB3	4:A:288:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:341:TYR:CE2	2:F:460:PRO:HB3	2.54	0.42
1:E:47:PHE:HB3	1:E:48:PRO:HD3	2.00	0.42
2:F:78:PHE:HZ	3:G:164:PHE:CD2	2.37	0.42
3:G:9:GLN:O	3:G:9:GLN:HG3	2.19	0.42
3:G:85:LEU:HD22	3:G:269:MET:HE3	2.00	0.42
2:F:401:GLU:HG2	4:B:52:LEU:HD22	2.02	0.42
2:F:80:LEU:O	2:F:84:VAL:HG23	2.20	0.42
2:F:364:ASP:HB3	2:F:367:THR:OG1	2.20	0.42
3:G:214:ILE:HA	3:G:214:ILE:HD12	1.93	0.42
2:F:273:ILE:HG22	2:F:459:THR:HG21	2.01	0.42
4:A:109:VAL:O	4:A:113:ARG:HG2	2.20	0.42
2:F:284:THR:HG21	2:F:467:LEU:H	1.85	0.41
4:B:146:ARG:HD2	11:B:404:HOH:O	2.21	0.41
2:F:78:PHE:HZ	3:G:164:PHE:CE2	2.37	0.41
4:B:348:PRO:HA	4:B:349:PRO:HD3	1.87	0.41
4:B:289:HIS:CG	4:B:351:ARG:HD2	2.55	0.41
4:A:288:GLU:HG3	4:A:330:ARG:HD3	2.03	0.41
4:B:4:VAL:HG11	4:B:188:ILE:HD11	2.03	0.41
1:E:62:TRP:HB3	1:E:67:PHE:HE1	1.85	0.41
1:E:128:THR:HG22	1:E:249:THR:OG1	2.20	0.41
2:F:346:GLU:H	2:F:346:GLU:CD	2.24	0.41
4:B:5:GLN:HG2	4:B:61:PHE:HB2	2.03	0.40
3:G:84:TRP:HB3	3:G:245:LEU:HA	2.03	0.40
4:A:155:PHE:HB2	4:A:187:MET:HG2	2.02	0.40
2:F:445:GLN:HG2	2:F:469:ASN:ND2	2.36	0.40
3:G:77:PRO:HA	3:G:78:PRO:HD3	1.97	0.40
4:B:95:ASN:O	4:B:146:ARG:HG3	2.20	0.40
2:F:210:LEU:HG	2:F:221:ASN:OD1	2.21	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%)	362 (96%)	12 (3%)	1 (0%)	46	57
2	F	488/514 (95%)	472 (97%)	14 (3%)	2 (0%)	39	48
3	G	287/296 (97%)	281 (98%)	5 (2%)	1 (0%)	46	57
4	A	373/381 (98%)	362 (97%)	11 (3%)	0	100	100
4	B	352/381 (92%)	338 (96%)	14 (4%)	0	100	100
All	All	1875/1950 (96%)	1815 (97%)	56 (3%)	4 (0%)	52	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	37	GLN
2	F	38	GLY
1	E	172	GLU
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	300/303 (99%)	298 (99%)	2 (1%)	88	95
2	F	404/424 (95%)	391 (97%)	13 (3%)	46	62
3	G	231/237 (98%)	228 (99%)	3 (1%)	76	87
4	A	318/323 (98%)	305 (96%)	13 (4%)	37	50
4	B	305/323 (94%)	295 (97%)	10 (3%)	45	61
All	All	1558/1610 (97%)	1517 (97%)	41 (3%)	55	71

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	293[A]	VAL
1	E	293[B]	VAL
2	F	59	ASN
2	F	145	LEU

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Mol	Chain	Res	Type
2	F	163	THR
2	F	220	THR
2	F	248	ASP
2	F	257	VAL
2	F	273	ILE
2	F	306	VAL
2	F	311	LEU
2	F	372	LEU
2	F	426	LEU
2	F	440	ASN
2	F	496	LEU
3	G	13	LEU
3	G	146	ARG
3	G	212	VAL
4	A	4	VAL
4	A	22	ILE
4	A	31	PHE
4	A	173[A]	ARG
4	A	173[B]	ARG
4	A	185	ARG
4	A	219	LEU
4	A	238	LYS
4	A	258	LEU
4	A	270	VAL
4	A	288	GLU
4	A	333	ASP
4	A	350	GLU
4	B	4	VAL
4	B	22	ILE
4	B	45	LEU
4	B	53	GLU
4	B	101	LYS
4	B	102	LEU
4	B	123	LEU
4	B	320	ILE
4	B	324	ARG
4	B	350	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	253	GLN

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Mol	Chain	Res	Type
2	F	59	ASN
2	F	98	ASN
2	F	437	ASN
2	F	440	ASN
4	A	5	GLN

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	8	22,29,29	0.75	0	27,45,45	2.27	2 (7%)
10	ALF	A	3001	-	0,4,4	0.00	-	0,6,6	0.00	-
9	ADP	B	2502	8	22,29,29	0.72	0	27,45,45	2.31	3 (11%)
10	ALF	B	3002	-	0,4,4	0.00	-	0,6,6	0.00	-
5	MAL	F	2000	-	24,24,24	0.42	0	35,35,35	0.79	1 (2%)
6	PGV	F	4001	-	50,50,50	1.07	3 (6%)	51,56,56	1.09	4 (7%)
6	PGV	F	4002	-	8,8,50	0.31	0	7,7,56	0.43	0
6	PGV	F	4008	-	7,7,50	0.30	0	6,6,56	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PGV	F	4010	-	16,16,50	0.99	1 (6%)	15,15,56	0.84	1 (6%)
7	UMQ	F	5004	-	35,35,35	0.44	0	46,46,46	0.63	0
6	PGV	G	4003	-	13,13,50	1.09	1 (7%)	11,12,56	0.92	0
6	PGV	G	4004	-	11,11,50	1.02	1 (9%)	10,10,56	0.99	1 (10%)
6	PGV	G	4005	-	11,11,50	1.02	1 (9%)	10,10,56	0.98	1 (10%)
6	PGV	G	4006	-	14,14,50	1.06	1 (7%)	12,13,56	0.89	1 (8%)
6	PGV	G	4007	-	11,11,50	1.02	1 (9%)	10,10,56	1.04	1 (10%)
6	PGV	G	4009	-	13,13,50	1.11	1 (7%)	11,12,56	0.91	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	8	-	0/12/32/32	0/3/3/3
10	ALF	A	3001	-	-	0/0/0/0	0/0/0/0
9	ADP	B	2502	8	-	0/12/32/32	0/3/3/3
10	ALF	B	3002	-	-	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	-	-	0/14/14/55	0/0/0/0
7	UMQ	F	5004	-	-	0/20/60/60	0/2/2/2
6	PGV	G	4003	-	-	0/11/11/55	0/0/0/0
6	PGV	G	4004	-	-	0/9/9/55	0/0/0/0
6	PGV	G	4005	-	-	0/9/9/55	0/0/0/0
6	PGV	G	4006	-	-	0/12/12/55	0/0/0/0
6	PGV	G	4007	-	-	0/9/9/55	0/0/0/0
6	PGV	G	4009	-	-	0/11/11/55	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	4005	PGV	C11-C12	3.15	1.53	1.29
6	G	4004	PGV	C11-C12	3.16	1.53	1.29
6	G	4007	PGV	C11-C12	3.16	1.53	1.29
6	F	4001	PGV	C12-C11	3.69	1.53	1.31
6	F	4010	PGV	C12-C11	3.71	1.53	1.31
6	G	4003	PGV	C12-C11	3.73	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	4006	PGV	C12-C11	3.75	1.53	1.31
6	G	4009	PGV	C12-C11	3.77	1.53	1.31
6	F	4001	PGV	O03-C19	4.12	1.45	1.33
6	F	4001	PGV	O01-C1	4.14	1.46	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	2502	ADP	N3-C2-N1	-10.73	120.68	128.89
9	A	2501	ADP	N3-C2-N1	-10.71	120.70	128.89
6	G	4007	PGV	C10-C11-C12	-2.37	110.70	133.31
9	B	2502	ADP	PA-O3A-PB	-2.33	124.86	132.67
6	F	4001	PGV	O03-C19-O04	-2.25	117.68	123.49
6	G	4005	PGV	C10-C11-C12	-2.24	111.98	133.31
6	G	4004	PGV	C10-C11-C12	-2.23	112.08	133.31
6	G	4006	PGV	C13-C12-C11	-2.07	110.92	125.34
6	F	4010	PGV	C13-C12-C11	-2.04	111.11	125.34
9	B	2502	ADP	C4-C5-N7	-2.04	107.60	109.48
9	A	2501	ADP	PA-O3A-PB	-2.03	125.86	132.67
6	F	4001	PGV	C10-C11-C12	-2.03	111.24	125.34
5	F	2000	MAL	C1'-O5'-C5'	2.38	117.88	113.47
6	F	4001	PGV	O03-C19-C20	3.01	121.08	111.90
6	F	4001	PGV	O01-C1-C2	4.12	120.48	111.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	4001	PGV	1	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	E	374/378 (98%)	0.11	18 (4%)	34	43	26, 54, 86, 105	1 (0%)
2	F	490/514 (95%)	0.50	47 (9%)	10	15	27, 56, 112, 162	0
3	G	288/296 (97%)	0.12	18 (6%)	23	31	24, 37, 80, 99	0
4	A	371/381 (97%)	0.17	15 (4%)	42	51	23, 52, 81, 95	1 (0%)
4	B	358/381 (93%)	0.40	28 (7%)	16	22	22, 61, 130, 160	0
All	All	1881/1950 (96%)	0.28	126 (6%)	21	29	22, 53, 101, 162	2 (0%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	37	GLN	9.5
2	F	38	GLY	8.8
4	B	16	VAL	8.7
4	B	251	ILE	8.6
4	A	295	ILE	7.6
2	F	40	TYR	6.8
3	G	70	ALA	6.5
3	G	133	ALA	6.1
4	B	295	ILE	5.9
3	G	116	PRO	5.6
2	F	355	PHE	5.5
4	B	267	TRP	5.2
2	F	349	MET	4.9
3	G	71	ASP	4.8
1	E	374	SER	4.8
3	G	73	ARG	4.7
2	F	354	LEU	4.6
2	F	503	ILE	4.5
3	G	117	GLY	4.5
2	F	245	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
3	G	114	ARG	4.5
2	F	353	ALA	4.4
2	F	29	TYR	4.2
4	B	324	ARG	4.2
4	B	105	ALA	4.2
1	E	172	GLU	4.0
4	B	357	GLU	4.0
1	E	179	LYS	4.0
4	B	249	THR	3.9
2	F	271	GLU	3.8
4	B	15	GLU	3.8
4	A	110	ILE	3.8
4	B	299	ILE	3.7
4	A	104	GLY	3.7
2	F	11	GLN	3.6
1	E	143	GLY	3.6
3	G	69	GLN	3.6
2	F	35	TYR	3.6
4	A	103	ALA	3.5
1	E	373	ALA	3.5
2	F	502	ALA	3.3
2	F	248	ASP	3.2
4	B	293	SER	3.2
1	E	1	LYS	3.2
2	F	312	ARG	3.2
2	F	214	ASP	3.1
2	F	501	LEU	3.1
2	F	12	SER	3.1
4	B	294	ASP	3.1
4	B	181	LYS	3.1
2	F	18	SER	3.1
4	B	265	GLN	3.1
3	G	68	GLU	3.1
1	E	141	ALA	3.1
2	F	229	ARG	3.0
2	F	45	THR	3.0
2	F	41	LEU	3.0
4	B	252	ASP	3.0
4	A	324	ARG	2.9
2	F	25	LEU	2.9
2	F	129	ASP	2.8
4	B	261	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
4	A	261	PRO	2.8
4	B	108	GLU	2.8
2	F	10	TRP	2.7
4	B	263	ARG	2.7
3	G	72	GLY	2.7
1	E	142	LYS	2.7
2	F	262	LYS	2.7
4	A	294	ASP	2.7
3	G	134	VAL	2.6
4	A	372	ALA	2.6
3	G	153	PHE	2.6
2	F	193	GLY	2.6
2	F	39	GLU	2.6
2	F	234	ILE	2.6
2	F	479	GLY	2.5
4	B	353	HIS	2.5
3	G	74	ILE	2.5
1	E	147	LEU	2.5
4	A	285	ILE	2.5
3	G	131	PHE	2.4
4	A	16	VAL	2.4
2	F	212	THR	2.4
2	F	458	THR	2.4
4	B	247	THR	2.4
4	B	361	ALA	2.4
1	E	252	GLY	2.3
2	F	352	SER	2.3
1	E	123	PRO	2.3
2	F	159	LEU	2.3
4	B	259	PRO	2.3
1	E	370	LYS	2.3
2	F	133	LEU	2.3
4	B	103	ALA	2.3
4	B	338	GLU	2.3
1	E	239	LYS	2.2
3	G	14	PHE	2.2
3	G	115	PHE	2.2
4	A	60	LEU	2.2
4	B	296	ALA	2.2
2	F	114	TRP	2.2
4	B	365	LEU	2.2
4	A	64	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	168	GLY	2.1
4	A	284	GLY	2.1
1	E	173	ASN	2.1
2	F	275	LYS	2.1
3	G	130	MET	2.1
2	F	267	VAL	2.1
2	F	268	PHE	2.1
2	F	134	ALA	2.1
1	E	115	LEU	2.1
3	G	18	LEU	2.1
1	E	124	ASN	2.1
1	E	174	GLY	2.1
2	F	216	ASP	2.1
4	B	116	GLN	2.1
2	F	223	GLN	2.0
2	F	233	GLN	2.0
4	A	340	GLY	2.0
4	A	188	ILE	2.0
2	F	13	ASP	2.0
2	F	32	VAL	2.0
4	B	17	VAL	2.0
1	E	359	GLU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	PGV	G	4004	12/51	0.85	0.16	4.31	50,54,58,59	0
6	PGV	F	4010	17/51	0.68	0.25	4.28	72,78,80,81	0
6	PGV	F	4001	51/51	0.83	0.23	2.13	61,67,74,76	0
6	PGV	G	4009	14/51	0.72	0.21	1.65	62,63,66,66	0
6	PGV	F	4002	9/51	0.87	0.20	1.27	38,41,45,47	0
7	UMQ	F	5004	34/34	0.93	0.17	0.90	56,66,71,72	0
6	PGV	G	4005	12/51	0.69	0.15	0.74	66,71,73,74	0
8	MG	B	1502	1/1	0.99	0.11	0.62	22,22,22,22	0
6	PGV	G	4006	15/51	0.70	0.16	0.33	63,70,78,79	0
10	ALF	B	3002	5/5	0.99	0.11	0.25	27,28,28,29	0
9	ADP	A	2501	27/27	0.97	0.11	0.11	25,37,45,46	0
9	ADP	B	2502	27/27	0.94	0.12	0.01	31,43,52,54	0
10	ALF	A	3001	5/5	0.98	0.09	-0.16	19,20,21,21	0
5	MAL	F	2000	23/23	0.94	0.10	-0.30	37,38,43,45	0
8	MG	A	1501	1/1	0.98	0.08	-0.98	26,26,26,26	0
6	PGV	G	4007	12/51	0.80	0.20	-	86,91,96,97	0
6	PGV	F	4008	8/51	0.80	0.23	-	60,64,66,67	0
6	PGV	G	4003	14/51	0.63	0.31	-	76,83,85,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.