



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:48 pm GMT

PDB ID : 4BGA
Title : Nucleotide-bound open form of a putative sugar kinase MK0840 from
Methanopyrus kandleri
Authors : Schacherl, M.; Baumann, U.
Deposited on : 2013-03-24
Resolution : 2.60 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

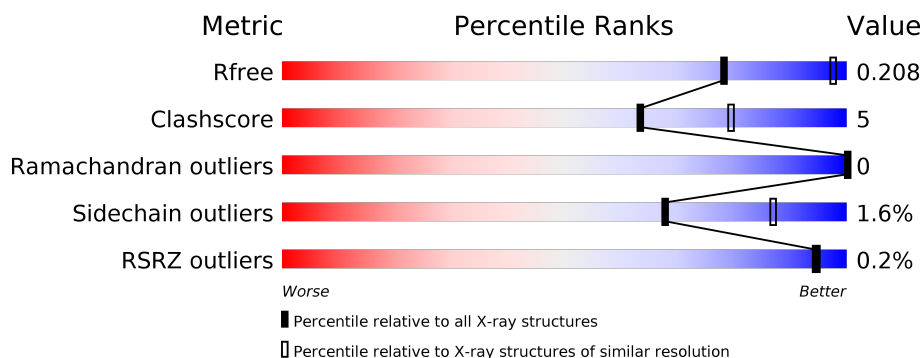
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	A	325	
1	B	325	
1	C	325	
1	D	325	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SUC	D	1354	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10064 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 PREDICTED MOLECULAR CHAPERONE DISTANTLY RELATED TO HSP70-F OLD METALLOPROTEASES.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2390	1500	416	464	10			
1	B	314	Total	C	N	O	S	0	1	0
			2396	1503	417	465	11			
1	C	322	Total	C	N	O	S	0	1	0
			2447	1531	429	476	11			
1	D	314	Total	C	N	O	S	0	1	0
			2396	1503	417	465	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	EXPRESSION TAG	UNP Q8TX37
A	35	SER	-	EXPRESSION TAG	UNP Q8TX37
A	36	HIS	-	EXPRESSION TAG	UNP Q8TX37
B	34	GLY	-	EXPRESSION TAG	UNP Q8TX37
B	35	SER	-	EXPRESSION TAG	UNP Q8TX37
B	36	HIS	-	EXPRESSION TAG	UNP Q8TX37
C	34	GLY	-	EXPRESSION TAG	UNP Q8TX37
C	35	SER	-	EXPRESSION TAG	UNP Q8TX37
C	36	HIS	-	EXPRESSION TAG	UNP Q8TX37
D	34	GLY	-	EXPRESSION TAG	UNP Q8TX37
D	35	SER	-	EXPRESSION TAG	UNP Q8TX37
D	36	HIS	-	EXPRESSION TAG	UNP Q8TX37

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

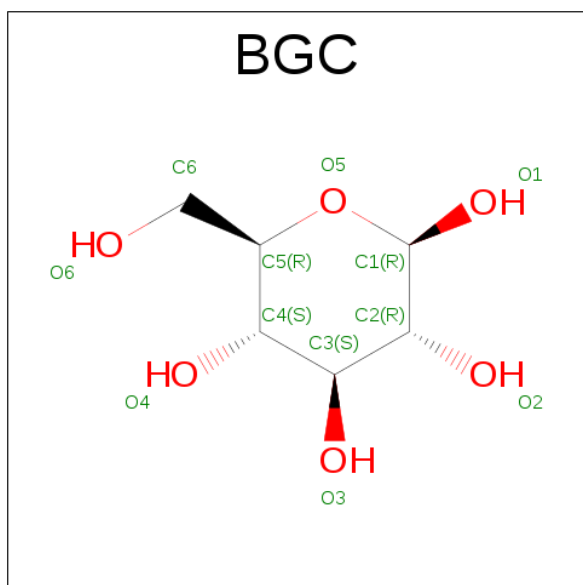
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	K	0	0
			2	2		
2	A	2	Total	K	0	0
			2	2		

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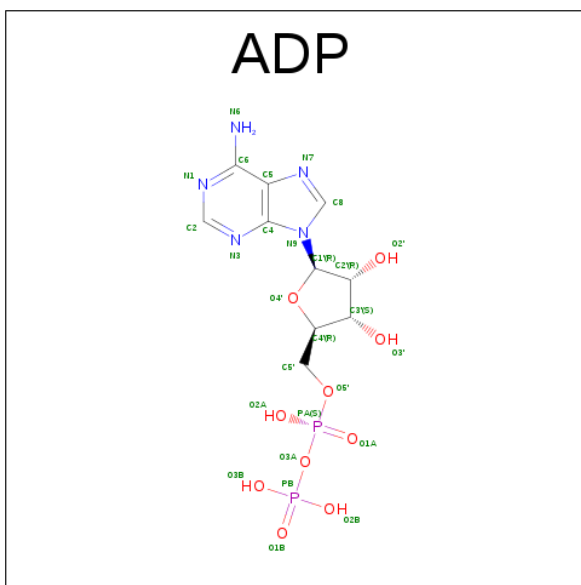
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	K	0	0
			2	2		
2	C	2	Total	K	0	0
			2	2		

- Molecule 3 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

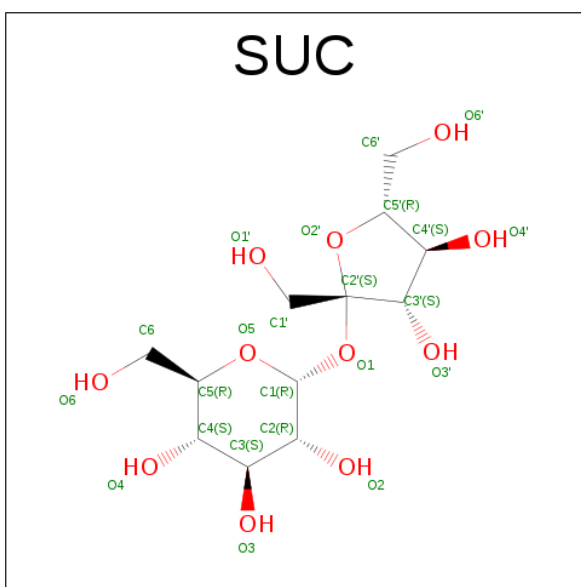


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

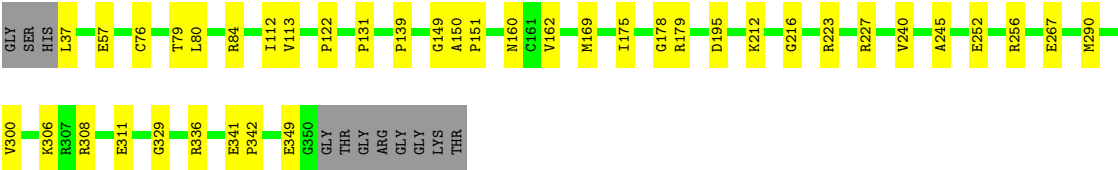
- Molecule 6 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: C₁₂H₂₂O₁₁).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	72	Total	O	0	0
			72	72		
7	B	61	Total	O	0	0
			61	61		
7	C	51	Total	O	0	0
			51	51		
7	D	38	Total	O	0	0
			38	38		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.57Å 111.67Å 87.88Å 90.00° 89.55° 90.00°	Depositor
Resolution (Å)	73.57 – 2.60 73.57 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (73.57-2.60) 99.0 (73.57-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.154 , 0.208 0.145 , 0.208	Depositor DCC
R_{free} test set	2187 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10064	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, BGC, SUC, K, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/2431	0.56	0/3304
1	B	0.32	0/2437	0.54	0/3312
1	C	0.32	0/2488	0.59	0/3377
1	D	0.33	0/2437	0.56	0/3312
All	All	0.32	0/9793	0.56	0/13305

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	A	2390	0	2375	23	0
1	B	2396	0	2379	24	0
1	C	2447	0	2431	31	0
1	D	2396	0	2379	26	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	12	1	0
3	C	12	0	12	2	0
3	D	12	0	12	0	0
4	A	27	0	12	1	0
4	B	27	0	12	0	0
4	C	27	0	12	1	0
4	D	27	0	12	1	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	C	23	0	22	2	0
6	D	23	0	22	1	0
7	A	72	0	0	0	0
7	B	61	0	0	0	0
7	C	51	0	0	1	0
7	D	38	0	0	0	0
All	All	10064	0	9704	96	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 5.

All (96) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLU:OE2	1:C:101:ARG:NH1	2.12	0.82
1:A:179:ARG:NH2	1:A:341:GLU:OE1	2.15	0.80
1:B:70:VAL:HA	1:B:73:LYS:HE2	1.65	0.78
1:C:257:ASP:OD1	1:C:260:ARG:NH2	2.22	0.73
1:C:351:GLY:H	1:C:358:THR:HG21	1.55	0.70
1:B:233:GLY:HA3	1:C:202:LEU:HA	1.76	0.66
1:D:308:ARG:NH1	1:D:311:GLU:OE1	2.29	0.65
1:C:239:ARG:O	1:C:241:ARG:NH1	2.29	0.62
1:C:63:ILE:HG13	1:C:324:GLU:HG3	1.82	0.61
1:A:62:GLU:HB2	6:C:1362:SUC:H5'	1.82	0.61
1:B:250:GLU:HG2	1:B:253:ARG:HH21	1.66	0.61
1:B:231:VAL:HG11	1:B:250:GLU:HB3	1.84	0.60
1:C:85:ARG:NH1	7:C:2011:HOH:O	2.35	0.60
1:C:204:LYS:HD3	1:C:204:LYS:N	2.17	0.60
1:C:208:GLU:O	1:C:211:LYS:HG2	2.02	0.59
1:C:169:MET:HG3	3:C:1361:BGC:H6C1	1.85	0.59
1:B:174:PRO:HG3	1:B:184:ASP:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ILE:HG13	1:B:324:GLU:HG3	1.87	0.56
1:C:204:LYS:H	1:C:204:LYS:HD3	1.71	0.55
1:D:223:ARG:O	1:D:227:ARG:HG2	2.08	0.54
1:A:54:VAL:HG23	1:A:64:VAL:HG11	1.88	0.54
1:C:68:GLU:HG2	6:C:1362:SUC:O6	2.07	0.54
1:C:231:VAL:HG11	1:C:250:GLU:HB3	1.89	0.54
1:B:252:GLU:OE2	1:B:256:ARG:NH2	2.42	0.53
1:C:202:LEU:HD11	1:C:212:LYS:HE3	1.90	0.53
1:A:252:GLU:O	1:A:256:ARG:HB2	2.08	0.53
1:D:80:LEU:O	1:D:84:ARG:HB2	2.08	0.53
1:D:112:ILE:HG13	1:D:113:VAL:HG23	1.91	0.53
1:C:149:GLY:O	1:C:329:GLY:HA3	2.09	0.52
1:B:37:LEU:HA	1:B:57:GLU:OE2	2.09	0.52
1:C:252:GLU:O	1:C:256:ARG:HB2	2.09	0.52
1:A:197:ALA:HA	1:A:259:ILE:HG21	1.92	0.52
1:D:300:VAL:HG13	1:D:306:LYS:HG3	1.92	0.51
1:A:195:ASP:OD2	4:A:1354:ADP:O3'	2.27	0.51
1:B:76:CYS:SG	1:D:84:ARG:NH1	2.83	0.51
1:D:149:GLY:O	1:D:329:GLY:HA3	2.11	0.51
1:A:149:GLY:O	1:A:329:GLY:HA3	2.10	0.51
1:A:212:LYS:HE2	1:A:267:GLU:HB3	1.93	0.51
1:C:162:VAL:HG23	1:C:290:MET:HB2	1.92	0.50
1:B:112:ILE:HG13	1:B:113:VAL:HG23	1.93	0.50
1:B:149:GLY:O	1:B:329:GLY:HA3	2.11	0.50
1:D:195:ASP:OD2	4:D:1356:ADP:O3'	2.24	0.50
1:C:169:MET:CG	3:C:1361:BGC:H6C1	2.41	0.50
1:A:179:ARG:NH2	1:A:336:ARG:HH11	2.10	0.50
1:D:240:VAL:HG22	1:D:245:ALA:HB2	1.94	0.49
1:D:252:GLU:HG2	1:D:256:ARG:HD3	1.95	0.48
1:C:63:ILE:CG1	1:C:324:GLU:HG3	2.43	0.48
1:D:212:LYS:HE3	1:D:267:GLU:HB3	1.96	0.48
1:C:195:ASP:OD2	4:C:1364:ADP:O3'	2.30	0.48
1:D:37:LEU:HA	1:D:57:GLU:OE2	2.14	0.47
1:D:178:GLY:O	1:D:336:ARG:NH2	2.47	0.47
1:B:63:ILE:CG1	1:B:324:GLU:HG3	2.44	0.47
1:A:310:SER:HA	1:A:317:VAL:HG21	1.96	0.47
1:A:174:PRO:HG2	1:A:181:ASP:HB3	1.96	0.47
1:C:221:ASN:HD22	1:C:224:ARG:NH2	2.13	0.47
1:D:160:ASN:HA	1:D:175:ILE:O	2.15	0.47
1:A:37:LEU:HA	1:A:57:GLU:OE2	2.15	0.46
1:B:123:MET:HG3	1:D:139:PRO:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:LEU:HA	1:C:57:GLU:OE2	2.15	0.46
1:D:341:GLU:HG2	1:D:342:PRO:HD2	1.98	0.46
1:A:194:LEU:HD23	1:A:273:LEU:HB3	1.97	0.46
1:C:351:GLY:H	1:C:358:THR:CG2	2.26	0.46
1:C:50:THR:OG1	1:C:94:ARG:NH2	2.50	0.45
1:B:233:GLY:CA	1:C:202:LEU:HA	2.46	0.45
1:A:152:TYR:OH	1:A:179:ARG:NH1	2.49	0.45
1:C:178:GLY:O	1:C:336:ARG:NH2	2.46	0.45
1:D:252:GLU:O	1:D:256:ARG:HB2	2.17	0.44
1:D:131:PRO:HB3	1:D:349:GLU:HG2	1.98	0.44
1:A:87:LEU:HD11	1:A:120:LEU:HG	1.99	0.44
1:B:80:LEU:HD23	1:D:113:VAL:HG11	1.99	0.44
1:B:74:ILE:HB	1:B:116:LEU:HD13	2.00	0.44
1:A:112:ILE:HG13	1:A:113:VAL:HG23	2.00	0.43
1:A:44:GLN:O	1:A:50:THR:HA	2.19	0.42
6:D:1354:SUC:H1'1	6:D:1354:SUC:H1	1.88	0.42
1:C:282:VAL:HG21	1:C:312:LEU:HB2	2.01	0.42
1:A:131:PRO:HB3	1:A:349:GLU:HG2	2.02	0.42
1:D:216:GLY:HA3	1:D:267:GLU:O	2.20	0.42
1:A:234:LYS:HA	1:A:235:PRO:HD3	1.89	0.41
1:B:346:LEU:HD21	1:D:122:PRO:HG3	2.02	0.41
1:A:314:GLU:H	1:A:314:GLU:HG3	1.67	0.41
1:C:148:VAL:HA	1:C:182:PHE:CZ	2.55	0.41
1:D:150:ALA:HB3	1:D:151:PRO:HD3	2.02	0.41
1:A:198:ALA:O	1:A:202:LEU:HB2	2.20	0.41
1:C:307:ARG:HG2	1:C:311:GLU:OE2	2.20	0.41
1:D:179:ARG:HB3	1:D:179:ARG:HE	1.58	0.41
1:B:187:VAL:HG11	3:B:1353:BGC:H6C2	2.02	0.41
1:B:80:LEU:HB3	1:D:76:CYS:HA	2.03	0.41
1:B:79:THR:HA	1:D:79:THR:HA	2.02	0.41
1:B:44:GLN:O	1:B:50:THR:HA	2.21	0.41
1:C:250:GLU:HG2	1:C:253:ARG:NH2	2.36	0.41
1:D:162:VAL:HG23	1:D:290:MET:HB2	2.03	0.41
1:A:122:PRO:O	1:A:126:GLU:HB2	2.21	0.40
1:C:265:PRO:HB2	1:C:267:GLU:OE1	2.21	0.40
1:B:209:GLY:HA3	1:B:211:LYS:NZ	2.36	0.40
1:B:154:VAL:HG21	1:B:163:HIS:CD2	2.56	0.40
1:B:174:PRO:HG2	1:B:181:ASP:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/325 (96%)	309 (99%)	3 (1%)	0	100	100
1	B	313/325 (96%)	309 (99%)	4 (1%)	0	100	100
1	C	321/325 (99%)	315 (98%)	6 (2%)	0	100	100
1	D	313/325 (96%)	307 (98%)	6 (2%)	0	100	100
All	All	1259/1300 (97%)	1240 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	253/259 (98%)	245 (97%)	8 (3%)	44	72
1	B	254/259 (98%)	251 (99%)	3 (1%)	75	91
1	C	258/259 (100%)	254 (98%)	4 (2%)	68	87
1	D	254/259 (98%)	253 (100%)	1 (0%)	93	98
All	All	1019/1036 (98%)	1003 (98%)	16 (2%)	68	87

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	VAL
1	A	202	LEU

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Mol	Chain	Res	Type
1	A	223	ARG
1	A	231	VAL
1	A	232	ASP
1	A	234	LYS
1	A	300	VAL
1	A	314	GLU
1	B	153	CYS
1	B	179	ARG
1	B	184	ASP
1	C	62	GLU
1	C	202	LEU
1	C	204	LYS
1	C	320	PHE
1	D	169	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	221	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 21 ligands modelled in this entry, 11 are monoatomic - leaving 10 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
3	BGC	A	1353	-	12,12,12	1.55	2 (16%)	17,17,17	1.31	3 (17%)
4	ADP	A	1354	-	25,29,29	0.96	1 (4%)	24,45,45	1.60	2 (8%)
3	BGC	B	1353	-	12,12,12	1.60	3 (25%)	17,17,17	1.42	4 (23%)
4	ADP	B	1355	5	25,29,29	0.93	1 (4%)	24,45,45	1.66	3 (12%)
3	BGC	C	1361	-	12,12,12	1.59	2 (16%)	17,17,17	1.25	1 (5%)
6	SUC	C	1362	-	24,24,24	0.43	0	36,36,36	0.71	0
4	ADP	C	1364	5	25,29,29	0.97	1 (4%)	24,45,45	1.62	2 (8%)
3	BGC	D	1353	-	12,12,12	1.60	2 (16%)	17,17,17	1.48	2 (11%)
6	SUC	D	1354	-	24,24,24	0.45	0	36,36,36	0.70	0
4	ADP	D	1356	5	25,29,29	1.01	1 (4%)	24,45,45	1.64	2 (8%)

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
3	BGC	A	1353	-	-	0/2/22/22	0/1/1/1
4	ADP	A	1354	-	-	0/12/32/32	0/3/3/3
3	BGC	B	1353	-	-	0/2/22/22	0/1/1/1
4	ADP	B	1355	5	-	0/12/32/32	0/3/3/3
3	BGC	C	1361	-	-	0/2/22/22	0/1/1/1
6	SUC	C	1362	-	-	0/12/51/51	0/2/2/2
4	ADP	C	1364	5	-	0/12/32/32	0/3/3/3
3	BGC	D	1353	-	-	0/2/22/22	0/1/1/1
6	SUC	D	1354	-	-	0/12/51/51	0/2/2/2
4	ADP	D	1356	5	-	0/12/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1361	BGC	C4-C3	-4.01	1.42	1.52
3	D	1353	BGC	C4-C3	-4.00	1.42	1.52
3	B	1353	BGC	C4-C3	-3.92	1.42	1.52
3	A	1353	BGC	C4-C3	-3.79	1.42	1.52
3	B	1353	BGC	C3-C2	-2.25	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1353	BGC	C3-C2	-2.01	1.47	1.52
3	C	1361	BGC	C3-C2	-2.01	1.47	1.52
3	D	1353	BGC	O5-C5	2.05	1.49	1.44
3	B	1353	BGC	O5-C5	2.12	1.49	1.44
4	B	1355	ADP	C5-C4	2.95	1.47	1.40
4	A	1354	ADP	C5-C4	3.00	1.47	1.40
4	C	1364	ADP	C5-C4	3.04	1.47	1.40
4	D	1356	ADP	C5-C4	3.14	1.47	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1354	ADP	N3-C2-N1	-6.21	123.45	128.86
4	B	1355	ADP	N3-C2-N1	-6.06	123.58	128.86
4	C	1364	ADP	N3-C2-N1	-5.94	123.68	128.86
4	D	1356	ADP	N3-C2-N1	-5.84	123.77	128.86
4	C	1364	ADP	C4-C5-N7	-3.08	106.43	109.41
4	D	1356	ADP	C4-C5-N7	-2.98	106.53	109.41
4	B	1355	ADP	C4-C5-N7	-2.78	106.73	109.41
4	A	1354	ADP	C4-C5-N7	-2.43	107.06	109.41
4	B	1355	ADP	O3B-PB-O2B	2.00	115.70	107.61
3	A	1353	BGC	O6-C6-C5	2.01	118.11	111.34
3	B	1353	BGC	O5-C5-C4	2.01	113.37	109.66
3	D	1353	BGC	O5-C5-C6	2.26	111.81	106.41
3	A	1353	BGC	O5-C1-C2	2.46	114.11	110.04
3	B	1353	BGC	O5-C5-C6	2.49	112.38	106.41
3	A	1353	BGC	O5-C5-C6	2.53	112.48	106.41
3	B	1353	BGC	O6-C6-C5	2.57	120.00	111.34
3	B	1353	BGC	O5-C1-C2	2.64	114.41	110.04
3	C	1361	BGC	O5-C1-C2	2.64	114.43	110.04
3	D	1353	BGC	O5-C1-C2	3.54	115.91	110.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1354	ADP	1	0
3	B	1353	BGC	1	0
3	C	1361	BGC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1362	SUC	2	0
4	C	1364	ADP	1	0
6	D	1354	SUC	1	0
4	D	1356	ADP	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	314/325 (96%)	-0.40	0 100 100	16, 27, 50, 58	0
1	B	314/325 (96%)	-0.44	0 100 100	17, 27, 51, 63	0
1	C	322/325 (99%)	-0.25	2 (0%) 89 88	17, 32, 65, 82	0
1	D	314/325 (96%)	-0.38	0 100 100	16, 30, 55, 71	0
All	All	1264/1300 (97%)	-0.37	2 (0%) 94 95	16, 29, 56, 82	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	203	GLY	2.6
1	C	221	ASN	2.3

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	SUC	D	1354	23/23	0.93	0.22	3.58	36,49,56,60	0
6	SUC	C	1362	23/23	0.89	0.21	1.49	36,49,56,66	0
3	BGC	A	1353	12/12	0.85	0.16	1.14	36,46,53,53	0
3	BGC	D	1353	12/12	0.80	0.16	0.89	46,55,70,77	0
3	BGC	C	1361	12/12	0.82	0.16	0.88	41,61,68,70	0
3	BGC	B	1353	12/12	0.84	0.17	0.78	42,50,59,60	0
4	ADP	D	1356	27/27	0.92	0.18	0.67	30,43,75,90	0
4	ADP	C	1364	27/27	0.89	0.15	0.15	32,45,98,109	0
4	ADP	B	1355	27/27	0.95	0.14	0.06	22,28,72,99	0
2	K	B	1351	1/1	0.99	0.13	-0.47	33,33,33,33	0
4	ADP	A	1354	27/27	0.94	0.14	-0.65	20,30,83,85	0
2	K	B	1352	1/1	0.97	0.11	-0.88	28,28,28,28	0
2	K	D	1352	1/1	0.93	0.10	-1.62	46,46,46,46	0
2	K	A	1351	1/1	0.97	0.11	-2.01	48,48,48,48	0
2	K	C	1360	1/1	0.99	0.10	-2.10	28,28,28,28	0
2	K	D	1351	1/1	0.99	0.10	-2.38	29,29,29,29	0
2	K	C	1359	1/1	0.96	0.10	-2.54	47,47,47,47	0
2	K	A	1352	1/1	0.99	0.10	-2.56	27,27,27,27	0
5	MG	B	1354	1/1	0.94	0.14	-	50,50,50,50	0
5	MG	D	1355	1/1	0.92	0.19	-	52,52,52,52	0
5	MG	C	1363	1/1	0.78	0.21	-	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.