



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 12:35 AM BST

PDB ID : 3V2U
Title : Crystal structure of the yeast GAL regulon complex of the repressor, Gal80p, and the transducer, Gal3p, with galactose and ATP
Authors : Lavy, T.; Kumar, P.R.; He, H.; Joshua-Tor, L.
Deposited on : 2011-12-12
Resolution : 2.10 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

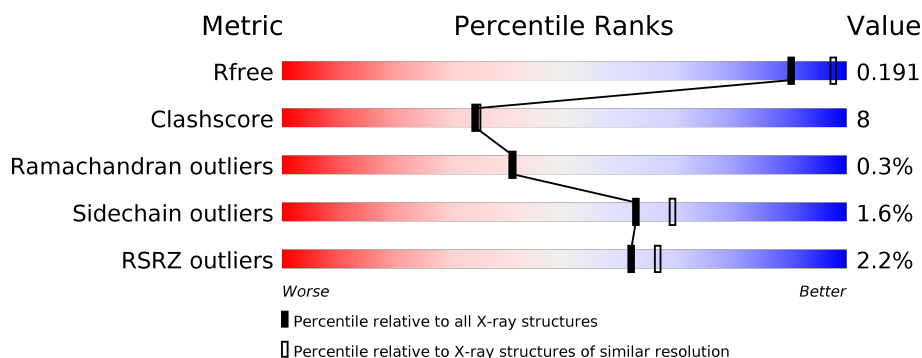
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 respectively. 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	438	<div> <div>0%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>7%</div> </div> </div>
1	B	438	<div> <div>0%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>8%</div> </div> </div>
2	C	520	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>..</div> </div> </div>
2	D	520	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>..</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15960 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 Galactose/lactose metabolism regulatory protein GAL80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	16	0
			3301	2133	544	611	13			
1	B	402	Total	C	N	O	S	0	12	0
			3230	2082	538	596	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P04387
A	-1	SER	-	expression tag	UNP P04387
A	0	HIS	-	expression tag	UNP P04387
B	-2	GLY	-	expression tag	UNP P04387
B	-1	SER	-	expression tag	UNP P04387
B	0	HIS	-	expression tag	UNP P04387

- Molecule 2 is a protein called Protein GAL3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	516	Total	C	N	O	S	0	8	0
			4103	2603	703	775	22			
2	D	514	Total	C	N	O	S	0	5	0
			4063	2578	695	768	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	SER	-	expression tag	UNP P13045
D	1	SER	-	expression tag	UNP P13045

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

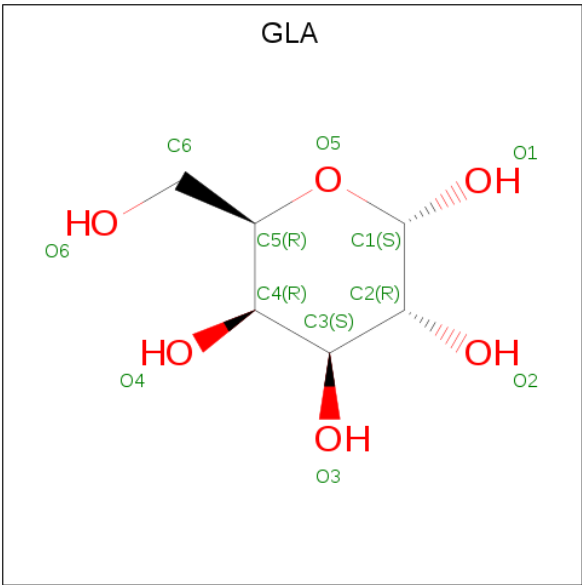


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

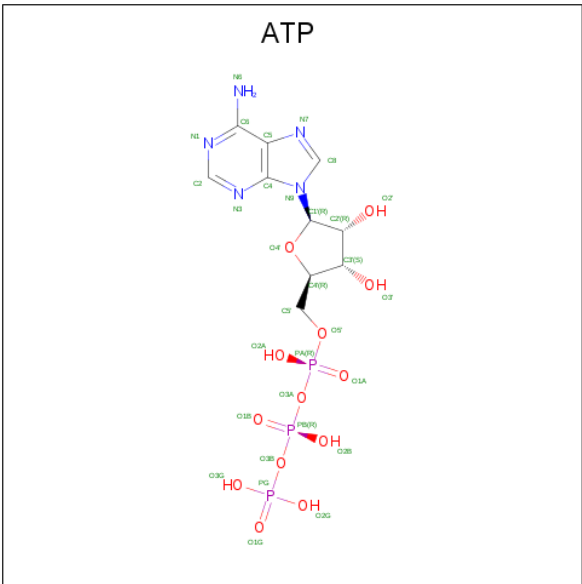
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is alpha-D-galactopyranose (three-letter code: GLA) (formula: C₆H₁₂O₆).



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

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

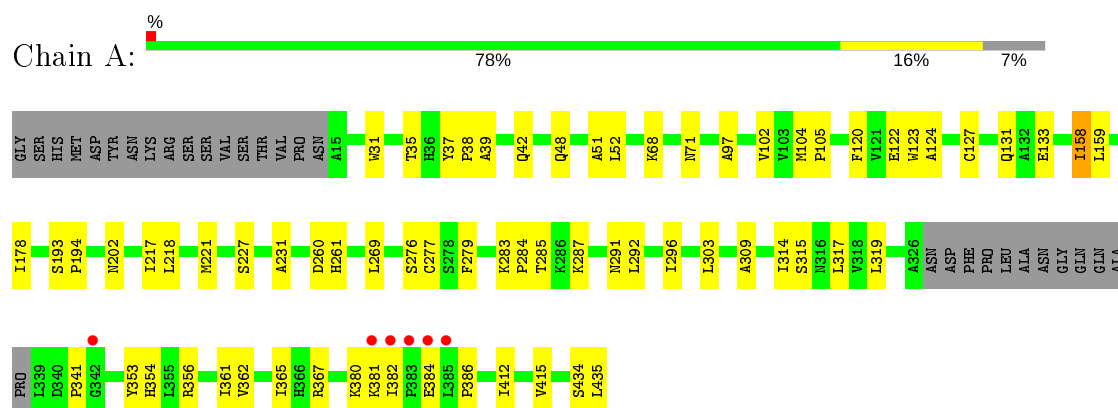
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	324	Total	O	0	0
			324	324		
7	B	304	Total	O	0	0
			304	304		
7	C	311	Total	O	0	0
			311	311		
7	D	224	Total	O	0	0
			224	224		

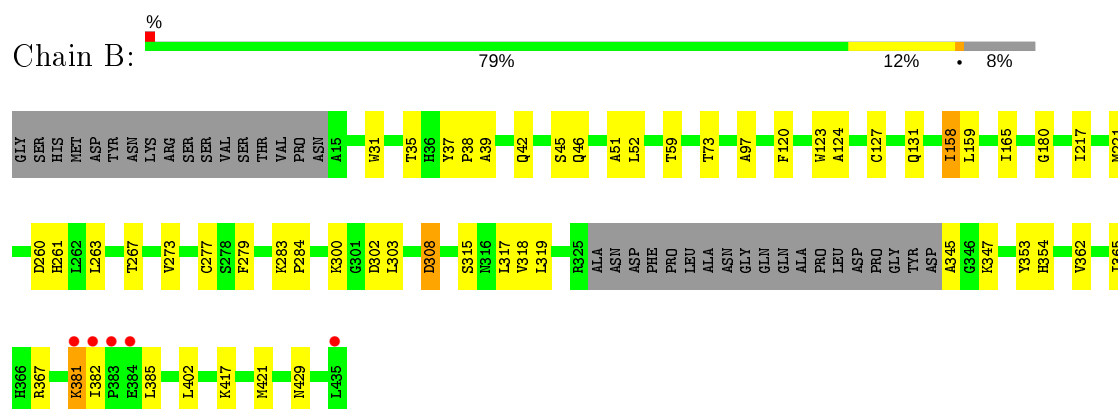
3 Residue-property plots [i](#)

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

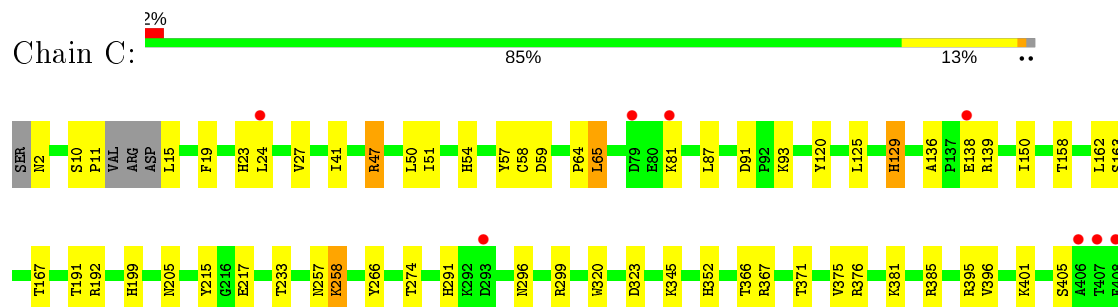
- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

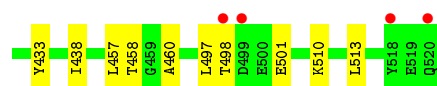


- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

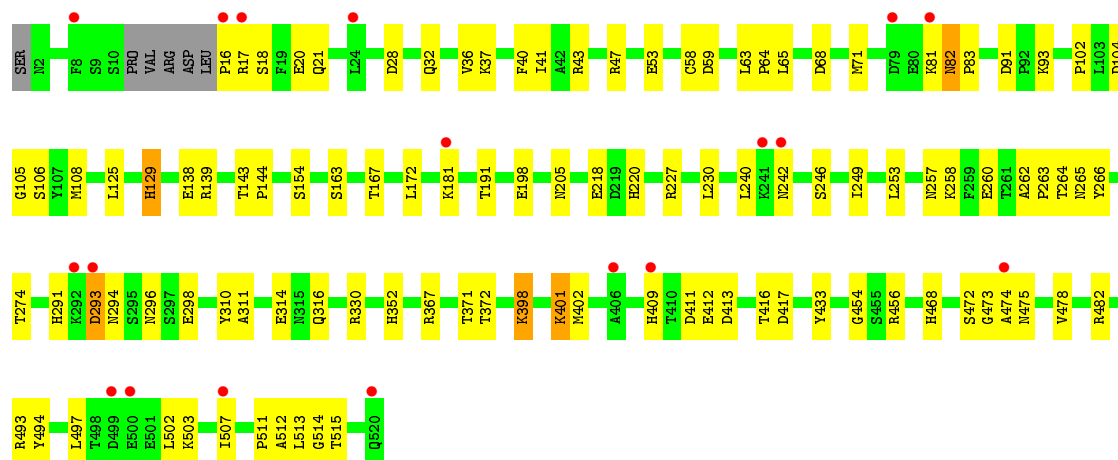
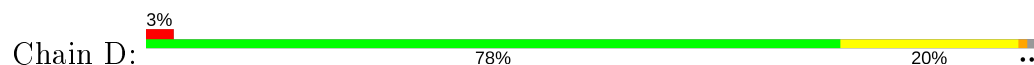


- Molecule 2: Protein GAL3





● Molecule 2: Protein GAL3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.19Å 83.22Å 92.63Å 114.04° 92.88° 90.37°	Depositor
Resolution (Å)	47.63 – 2.10 47.63 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.1 (47.63-2.10) 93.1 (47.63-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.47 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.150 , 0.197 0.145 , 0.191	Depositor DCC
R_{free} test set	1996 reflections (1.58%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.038 for -h,k,-k-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15960	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: GOL, MG, ATP, GLA

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	0.41	0/3408	0.53	0/4619
1	B	0.40	0/3318	0.52	0/4494
2	C	0.35	0/4208	0.49	0/5700
2	D	0.35	0/4167	0.48	0/5644
All	All	0.38	0/15101	0.50	0/20457

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	3301	0	3339	57	0
1	B	3230	0	3265	45	0
2	C	4103	0	4050	62	0
2	D	4063	0	4008	88	1
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	C	12	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	12	0	11	3	0
6	C	31	0	12	0	0
6	D	31	0	12	0	0
7	A	324	0	0	10	0
7	B	304	0	0	17	1
7	C	311	0	0	24	0
7	D	224	0	0	21	0
All	All	15960	0	14725	247	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (247) 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:131:GLN:NE2	7:A:1059:HOH:O	1.81	1.13
2:C:258:LYS:NZ	7:C:873:HOH:O	1.79	1.13
1:B:131:GLN:NE2	7:B:1058:HOH:O	1.82	1.12
1:A:314:ILE:HB	1:A:361:ILE:HD13	1.41	1.00
2:D:258:LYS:HE3	7:D:874:HOH:O	1.69	0.92
2:C:352:HIS:ND1	7:C:987:HOH:O	2.03	0.89
2:D:482:ARG:NH1	7:D:954:HOH:O	2.07	0.86
2:D:249:ILE:HD12	2:D:507:ILE:HD11	1.56	0.86
2:C:274:THR:OG1	7:C:984:HOH:O	1.93	0.85
2:D:43:ARG:NH1	7:D:644:HOH:O	2.10	0.84
2:D:104:ASP:HB2	2:D:106:SER:H	1.41	0.83
2:D:367[B]:ARG:NH1	7:D:1007:HOH:O	2.16	0.78
2:D:274:THR:OG1	7:D:956:HOH:O	2.01	0.78
2:D:412:GLU:OE2	2:D:416:THR:OG1	2.03	0.75
1:A:159[A]:LEU:HD12	1:A:367:ARG:HH21	1.51	0.73
2:D:260:GLU:OE2	7:D:919:HOH:O	2.07	0.73
1:B:73:THR:HG23	7:B:1091:HOH:O	1.88	0.73
1:B:429[A]:ASN:OD1	7:B:585:HOH:O	2.07	0.71
1:B:159[A]:LEU:HD12	1:B:367:ARG:HH21	1.56	0.71
1:B:46:GLN:OE1	7:B:541:HOH:O	2.09	0.70
2:D:398:LYS:O	2:D:401:LYS:HD3	1.91	0.69
2:C:233:THR:HG23	7:C:567:HOH:O	1.92	0.68
1:B:308:ASP:OD1	1:B:308:ASP:N	2.26	0.68
1:A:42:GLN:HG2	7:A:888:HOH:O	1.92	0.68
2:D:296:ASN:HB3	7:D:1109:HOH:O	1.92	0.67
2:C:266:TYR:CE1	5:C:522:GLA:H1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:274:THR:HG21	7:C:889:HOH:O	1.94	0.66
2:C:54:HIS:HE1	2:C:460:ALA:O	1.79	0.66
2:C:10:SER:HB2	2:C:11:PRO:HD2	1.77	0.65
1:A:317:LEU:O	1:A:354:HIS:HD2	1.80	0.65
7:A:754:HOH:O	2:D:367[B]:ARG:HG2	1.96	0.65
2:D:352:HIS:ND1	7:D:989:HOH:O	2.24	0.65
1:B:31:TRP:CZ2	1:B:35:THR:HG21	2.32	0.64
2:C:257:ASN:OD1	7:C:977:HOH:O	2.14	0.64
1:A:202:ASN:HB2	7:A:1080:HOH:O	1.97	0.64
2:D:242:ASN:O	2:D:475:ASN:ND2	2.31	0.64
2:C:136:ALA:HB1	2:C:139:ARG:HG2	1.80	0.63
2:D:104:ASP:CB	2:D:106:SER:H	2.11	0.63
1:B:165:ILE:HD12	1:B:221[B]:MET:HG2	1.81	0.63
1:B:39:ALA:HB2	7:B:947:HOH:O	1.99	0.63
2:C:320:TRP:O	7:C:1120:HOH:O	2.16	0.63
2:D:310:TYR:CZ	2:D:330:ARG:HG2	2.34	0.63
7:A:882:HOH:O	1:B:261:HIS:HD2	1.83	0.62
2:C:51[A]:ILE:HD11	2:C:395:ARG:HB3	1.81	0.62
1:B:123:TRP:CD2	1:B:124:ALA:HA	2.34	0.62
1:A:261:HIS:HD2	7:B:883:HOH:O	1.83	0.61
1:A:277[A]:CYS:SG	1:A:279:PHE:CE2	2.93	0.61
1:B:317:LEU:O	1:B:354:HIS:HD2	1.83	0.61
2:D:294:ASN:HB3	7:D:963:HOH:O	2.00	0.61
1:A:123:TRP:CD2	1:A:124:ALA:HA	2.36	0.60
2:C:257:ASN:HA	7:C:928:HOH:O	2.01	0.60
2:D:81:LYS:HG2	2:D:83:PRO:HD3	1.82	0.60
2:C:91:ASP:OD2	2:C:93:LYS:HE2	2.01	0.60
2:D:191:THR:CG2	2:D:230:LEU:HD21	2.32	0.60
2:C:24:LEU:HB3	7:C:1142:HOH:O	2.03	0.59
2:C:291:HIS:HE1	7:C:1145:HOH:O	1.85	0.59
2:C:296:ASN:HB3	7:C:1135:HOH:O	2.03	0.59
2:C:11:PRO:HB3	7:C:921:HOH:O	2.01	0.58
2:D:266:TYR:CE1	5:D:522:GLA:H1	2.39	0.58
1:A:362:VAL:HG13	7:A:1036:HOH:O	2.04	0.58
2:C:163:SER:O	2:C:167[B]:THR:HG23	2.03	0.58
1:B:300:LYS:NZ	7:B:548:HOH:O	2.37	0.58
1:B:303:LEU:HG	1:B:319[B]:LEU:HD11	1.85	0.58
1:B:362[B]:VAL:HG13	7:B:947:HOH:O	2.02	0.58
2:D:129:HIS:HE1	7:D:940:HOH:O	1.85	0.58
2:D:43:ARG:NH2	2:D:513:LEU:O	2.30	0.58
2:D:81:LYS:HA	2:D:83:PRO:HD3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLU:OE2	7:A:1077:HOH:O	2.17	0.57
1:A:309:ALA:O	1:A:315:SER:HB2	2.04	0.57
2:D:181:LYS:HD3	2:D:181:LYS:C	2.25	0.57
2:D:227:ARG:HD3	7:D:1111:HOH:O	2.05	0.56
1:A:48:GLN:NE2	1:A:71:ASN:HD22	2.04	0.56
1:A:277[A]:CYS:SG	1:A:279:PHE:CD2	2.99	0.55
2:D:497:LEU:HB3	2:D:502:LEU:HG	1.87	0.55
2:D:352:HIS:CD2	7:D:591:HOH:O	2.59	0.55
2:D:258:LYS:NZ	7:D:596:HOH:O	2.39	0.55
1:A:68:LYS:HE2	2:D:81:LYS:HD2	1.88	0.54
2:C:510:LYS:HB2	7:C:1154:HOH:O	2.07	0.54
2:D:472:SER:O	7:D:1114:HOH:O	2.19	0.54
2:D:40:PHE:C	2:D:41:ILE:HD12	2.27	0.54
2:D:81:LYS:HA	2:D:83:PRO:CD	2.38	0.54
2:C:299:ARG:HD2	7:C:1130:HOH:O	2.07	0.53
2:C:129:HIS:HD2	7:C:805:HOH:O	1.91	0.53
1:B:35:THR:HB	1:B:365:ILE:HG13	1.90	0.53
2:C:266:TYR:HE1	5:C:522:GLA:H1	1.71	0.53
2:D:293:ASP:OD1	2:D:293:ASP:N	2.42	0.53
1:A:31[A]:TRP:HH2	1:A:365[A]:ILE:HD11	1.72	0.53
1:B:354:HIS:HE1	7:B:918:HOH:O	1.91	0.52
2:C:192:ARG:NH1	7:C:802:HOH:O	2.41	0.52
2:D:43:ARG:NH2	2:D:514:GLY:O	2.39	0.52
1:A:277[A]:CYS:SG	1:A:279:PHE:HE2	2.32	0.52
1:B:45:SER:HB3	7:B:541:HOH:O	2.09	0.52
1:A:285:THR:HB	1:A:291:ASN:HD21	1.74	0.52
1:A:284:PRO:HB2	7:A:1085:HOH:O	2.09	0.52
1:A:35:THR:HB	1:A:365[B]:ILE:HG21	1.92	0.52
1:B:158:ILE:HG13	1:B:217:ILE:HG23	1.92	0.52
2:D:138:GLU:OE2	2:D:139:ARG:HG3	2.10	0.51
1:A:48:GLN:HE21	1:A:71:ASN:HD22	1.58	0.51
2:D:143:THR:OG1	2:D:144:PRO:HD2	2.10	0.51
2:C:438:ILE:HG13	7:C:692:HOH:O	2.10	0.51
2:C:381:LYS:O	2:C:385:ARG:HG2	2.11	0.50
1:A:39:ALA:HB2	7:A:1036:HOH:O	2.10	0.50
2:D:205:ASN:HB2	5:D:522:GLA:H2	1.92	0.50
1:B:277[A]:CYS:SG	1:B:279:PHE:CD2	3.04	0.50
2:C:191:THR:HG21	2:C:215:TYR:CE2	2.46	0.50
2:C:91:ASP:OD1	2:C:93:LYS:HG2	2.11	0.50
2:D:246:SER:OG	2:D:472:SER:HB3	2.12	0.50
2:D:104:ASP:N	2:D:105:GLY:HA2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:376:ARG:NH2	7:C:890:HOH:O	2.32	0.50
2:D:310:TYR:CE2	2:D:314:GLU:HG3	2.47	0.50
1:A:104:MET:HB2	1:A:105:PRO:HD3	1.94	0.49
2:C:158:THR:HB	7:C:675:HOH:O	2.11	0.49
2:D:58:CYS:O	2:D:59:ASP:HB2	2.12	0.49
2:D:230:LEU:HD23	7:D:925:HOH:O	2.11	0.49
2:C:401:LYS:O	2:C:405:SER:N	2.46	0.49
1:A:380:LYS:HZ3	1:A:382:ILE:HD11	1.77	0.49
2:C:199:HIS:HD2	7:C:896:HOH:O	1.96	0.49
1:A:276[A]:SER:HB3	1:B:263:LEU:HD22	1.95	0.48
1:B:37:TYR:HB3	1:B:38:PRO:HD3	1.95	0.48
2:D:71:MET:CE	2:D:154:SER:HB2	2.43	0.48
1:A:276[B]:SER:HB2	1:B:263:LEU:HD22	1.96	0.48
1:A:296:ILE:HD12	1:A:303[A]:LEU:HD22	1.95	0.48
1:A:37:TYR:HB3	1:A:38:PRO:HD3	1.95	0.48
1:B:59:THR:HG22	7:B:897:HOH:O	2.14	0.48
2:D:311:ALA:O	2:D:316:GLN:HA	2.14	0.48
2:C:162:LEU:HD23	2:C:162:LEU:C	2.34	0.48
2:D:28:ASP:O	2:D:32:GLN:HG2	2.14	0.48
2:C:217:GLU:HA	2:C:513:LEU:HA	1.94	0.48
2:D:409:HIS:HB2	2:D:413:ASP:OD2	2.14	0.48
2:C:497:LEU:HA	2:C:501:GLU:OE1	2.14	0.48
2:C:498:THR:N	2:C:501:GLU:OE1	2.42	0.48
2:D:253:LEU:CD2	2:D:497:LEU:HD21	2.44	0.48
1:A:303[A]:LEU:HG	1:A:319:LEU:HD11	1.96	0.47
1:B:345:ALA:HB1	1:B:347:LYS:NZ	2.29	0.47
2:C:54:HIS:HD2	2:C:57:TYR:OH	1.96	0.47
1:B:421[A]:MET:HE2	7:B:975:HOH:O	2.14	0.47
2:D:36:VAL:HG12	2:D:37:LYS:N	2.28	0.47
2:D:91:ASP:OD2	2:D:93:LYS:HG2	2.15	0.47
1:A:356:ARG:HD2	2:D:372:THR:HA	1.96	0.47
2:D:493:ARG:HG2	7:D:955:HOH:O	2.14	0.47
2:D:191:THR:HG21	2:D:230:LEU:HD21	1.96	0.47
2:D:310:TYR:CD2	2:D:314:GLU:HG3	2.49	0.47
2:C:199:HIS:HE1	2:C:205:ASN:O	1.98	0.46
2:D:16:PRO:O	2:D:18:SER:N	2.48	0.46
2:D:163:SER:O	2:D:167:THR:HG23	2.15	0.46
2:D:82:ASN:OD1	2:D:82:ASN:N	2.49	0.46
1:A:227:SER:HB2	1:A:269:LEU:HD23	1.98	0.46
1:A:314:ILE:HB	1:A:361:ILE:CD1	2.30	0.46
1:A:283:LYS:HA	1:A:284:PRO:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:291:HIS:O	2:D:298:GLU:HA	2.16	0.46
1:B:51:ALA:C	1:B:52:LEU:HD12	2.36	0.46
2:C:51[B]:ILE:HG22	2:C:396:VAL:HG22	1.97	0.46
2:D:125:LEU:C	2:D:125:LEU:HD23	2.36	0.46
2:D:41:ILE:N	2:D:41:ILE:HD12	2.31	0.46
1:A:31[A]:TRP:CZ3	1:A:122:GLU:OE2	2.69	0.46
1:B:381:LYS:O	1:B:381:LYS:HG3	2.16	0.45
2:D:191:THR:HG22	2:D:230:LEU:HD21	1.96	0.45
1:A:287:LYS:HG3	1:B:302:ASP:HB2	1.98	0.45
2:D:291:HIS:HE1	7:D:980:HOH:O	1.98	0.45
1:A:434:SER:OG	1:A:435:LEU:N	2.49	0.45
2:D:262:ALA:N	2:D:263:PRO:CD	2.80	0.45
1:A:31[B]:TRP:NE1	1:A:35:THR:HG21	2.32	0.45
2:D:472:SER:HA	2:D:478:VAL:HG23	1.98	0.45
2:D:494:TYR:HB3	2:D:497:LEU:HD13	1.98	0.45
1:B:277[A]:CYS:SG	1:B:279:PHE:CE2	3.10	0.45
2:C:2:ASN:HB3	7:C:1021:HOH:O	2.16	0.45
2:D:503:LYS:HA	7:D:954:HOH:O	2.16	0.45
1:A:102:VAL:O	1:A:105:PRO:HD2	2.17	0.44
1:A:384:GLU:O	1:A:386:PRO:HD3	2.17	0.44
2:C:125:LEU:C	2:C:125:LEU:HD23	2.37	0.44
2:D:266:TYR:HE1	5:D:522:GLA:H1	1.82	0.44
1:A:277[A]:CYS:HG	1:A:279:PHE:HE2	1.63	0.44
1:B:308:ASP:HA	7:B:708:HOH:O	2.17	0.44
1:B:319[A]:LEU:C	1:B:319[A]:LEU:HD23	2.37	0.44
2:C:457:LEU:C	2:C:457:LEU:HD12	2.37	0.44
2:D:21:GLN:O	2:D:21:GLN:NE2	2.50	0.44
2:D:220:HIS:O	2:D:511:PRO:HB3	2.16	0.44
1:B:345:ALA:HB3	1:B:347:LYS:HG2	1.99	0.44
2:D:454:GLY:O	2:D:468:HIS:HA	2.18	0.44
1:A:283:LYS:HB3	1:A:284:PRO:HA	2.00	0.43
2:D:274:THR:HG21	7:D:905:HOH:O	2.17	0.43
1:B:97:ALA:HA	1:B:127:CYS:SG	2.58	0.43
2:D:102:PRO:C	2:D:104:ASP:H	2.21	0.43
2:D:81:LYS:HA	2:D:83:PRO:N	2.33	0.43
1:B:42:GLN:NE2	7:B:957:HOH:O	2.51	0.43
2:C:50:LEU:HD21	2:C:65:LEU:HD21	2.00	0.43
2:D:473:GLY:O	2:D:475:ASN:N	2.51	0.43
1:B:362[A]:VAL:HG22	7:B:947:HOH:O	2.17	0.43
7:B:690:HOH:O	2:C:367[A]:ARG:HG2	2.18	0.43
2:D:264:THR:C	2:D:265:ASN:HD22	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277[A]:CYS:SG	1:B:279:PHE:HD2	2.42	0.43
1:A:158:ILE:HG13	1:A:217:ILE:HG23	1.99	0.42
1:B:267:THR:HA	1:B:273:VAL:O	2.19	0.42
1:B:319[B]:LEU:HB3	1:B:353:TYR:HB3	2.01	0.42
2:C:458:THR:O	7:C:881:HOH:O	2.21	0.42
1:B:180:GLY:HA3	1:B:279:PHE:CE1	2.54	0.42
1:A:193:SER:HA	1:A:194:PRO:HD3	1.80	0.42
2:D:163:SER:OG	2:D:198:GLU:OE1	2.36	0.42
1:B:417:LYS:HG2	1:B:421[A]:MET:SD	2.60	0.42
2:C:366:THR:O	2:C:371[B]:THR:HG23	2.19	0.42
2:C:81:LYS:HA	2:C:81:LYS:HD3	1.75	0.42
1:A:218:LEU:HA	1:A:221[B]:MET:HE3	2.01	0.42
2:D:91:ASP:OD1	2:D:93:LYS:HE2	2.19	0.42
1:B:283:LYS:HA	1:B:284:PRO:C	2.40	0.42
2:D:218:GLU:OE2	2:D:512:ALA:HA	2.20	0.42
2:C:136:ALA:HB1	2:C:139:ARG:CG	2.47	0.42
2:C:120:TYR:CE1	2:C:163:SER:HB2	2.55	0.42
2:C:375:VAL:HG22	2:C:376:ARG:N	2.35	0.42
2:C:87:LEU:HD23	2:C:150:ILE:HB	2.01	0.42
1:A:178:ILE:HD11	1:A:218:LEU:HD22	2.00	0.41
1:A:123:TRP:HZ2	1:A:412[B]:ILE:CD1	2.32	0.41
2:D:402:MET:HE1	2:D:417:ASP:HB3	2.01	0.41
2:C:23:HIS:O	2:C:27:VAL:HG23	2.20	0.41
1:B:31:TRP:CE2	1:B:35:THR:HG21	2.54	0.41
2:D:257:ASN:HA	7:D:919:HOH:O	2.20	0.41
2:D:240:LEU:HB3	2:D:411:ASP:OD1	2.19	0.41
1:B:318:VAL:HG22	1:B:354:HIS:CD2	2.55	0.41
7:B:497:HOH:O	2:C:371[B]:THR:HG21	2.20	0.41
1:A:303[B]:LEU:CD1	1:A:319:LEU:HD11	2.50	0.41
1:A:303[B]:LEU:HD11	1:A:319:LEU:HD11	2.02	0.41
2:C:352:HIS:HD2	7:C:988:HOH:O	2.03	0.41
2:C:58:CYS:O	2:C:59:ASP:HB2	2.21	0.41
1:A:51:ALA:C	1:A:52:LEU:HD12	2.41	0.41
2:C:54:HIS:CD2	2:C:57:TYR:OH	2.74	0.41
2:D:108:MET:SD	7:D:1112:HOH:O	2.62	0.41
2:D:81:LYS:CG	2:D:83:PRO:HD3	2.49	0.41
1:A:319:LEU:HB3	1:A:353:TYR:HB3	2.03	0.41
1:A:381:LYS:HD2	1:A:381:LYS:HA	1.85	0.41
2:D:172:LEU:HD22	2:D:515:THR:CG2	2.51	0.41
1:A:123:TRP:HZ2	1:A:412[B]:ILE:HD11	1.85	0.40
1:A:277[A]:CYS:SG	1:A:279:PHE:HD2	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:ILE:HD12	1:B:385:LEU:HD13	2.02	0.40
2:C:23:HIS:ND1	2:C:41:ILE:HD12	2.36	0.40
2:D:81:LYS:HG2	2:D:83:PRO:CD	2.49	0.40
2:C:345:LYS:HE3	2:C:345:LYS:HB3	1.95	0.40
2:D:82:ASN:HA	2:D:83:PRO:HD3	1.96	0.40
1:A:97:ALA:HA	1:A:127:CYS:SG	2.61	0.40
1:A:231:ALA:CB	1:A:415:VAL:HG13	2.51	0.40
2:C:352:HIS:CD2	7:C:988:HOH:O	2.75	0.40
2:C:47:ARG:HD2	2:C:47:ARG:C	2.42	0.40
2:D:172:LEU:HD22	2:D:515:THR:HG22	2.03	0.40
2:D:53:GLU:HB2	2:D:456:ARG:NH2	2.36	0.40
1:A:361:ILE:HG12	7:A:917:HOH:O	2.22	0.40
2:C:15:LEU:HB3	2:C:19:PHE:CD2	2.56	0.40
2:C:320:TRP:NE1	2:C:323:ASP:O	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:GLU:OE2	7:B:1092:HOH:O[1_666]	2.00	0.20

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	A	421/438 (96%)	411 (98%)	9 (2%)	1 (0%)	47	49
1	B	410/438 (94%)	398 (97%)	11 (3%)	1 (0%)	47	49
2	C	520/520 (100%)	507 (98%)	12 (2%)	1 (0%)	47	49
2	D	515/520 (99%)	496 (96%)	16 (3%)	3 (1%)	25	21
All	All	1866/1916 (97%)	1812 (97%)	48 (3%)	6 (0%)	41	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	17	ARG
2	D	474	ALA
1	B	381	LYS
2	D	64	PRO
2	C	64	PRO
1	A	341	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	A	366/375 (98%)	363 (99%)	3 (1%)	81	86
1	B	357/375 (95%)	351 (98%)	6 (2%)	60	67
2	C	451/447 (101%)	445 (99%)	6 (1%)	69	75
2	D	446/447 (100%)	436 (98%)	10 (2%)	52	57
All	All	1620/1644 (98%)	1595 (98%)	25 (2%)	62	71

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	PHE
1	A	158	ILE
1	A	260	ASP
1	B	120	PHE
1	B	158	ILE
1	B	260	ASP
1	B	308	ASP
1	B	315	SER
1	B	402	LEU
2	C	47	ARG
2	C	65	LEU
2	C	129	HIS
2	C	138	GLU
2	C	258	LYS

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Mol	Chain	Res	Type
2	C	433	TYR
2	D	47	ARG
2	D	63	LEU
2	D	65	LEU
2	D	68	ASP
2	D	82	ASN
2	D	129	HIS
2	D	293	ASP
2	D	398	LYS
2	D	401	LYS
2	D	433	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	131	GLN
1	A	174	ASN
1	A	230	ASN
1	A	261	HIS
1	A	265	GLN
1	A	354	HIS
1	B	131	GLN
1	B	230	ASN
1	B	261	HIS
1	B	265	GLN
1	B	354	HIS
2	C	23	HIS
2	C	54	HIS
2	C	82	ASN
2	C	199	HIS
2	C	291	HIS
2	C	336	GLN
2	D	21	GLN
2	D	96	GLN
2	D	129	HIS
2	D	265	ASN
2	D	520	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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$
5	GLA	D	522	-	12,12,12	1.79	2 (16%)	17,17,17	2.01	5 (29%)
6	ATP	C	523	4	26,33,33	1.63	6 (23%)	31,52,52	1.36	3 (9%)
5	GLA	C	522	-	12,12,12	1.79	2 (16%)	17,17,17	1.99	6 (35%)
6	ATP	D	523	4	26,33,33	1.63	5 (19%)	31,52,52	1.29	3 (9%)
3	GOL	B	524	-	5,5,5	0.30	0	5,5,5	0.54	0
3	GOL	A	524	-	5,5,5	0.31	0	5,5,5	0.49	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
5	GLA	D	522	-	-	2/2/22/22	0/1/1/1
6	ATP	C	523	4	-	4/18/38/38	0/3/3/3
5	GLA	C	522	-	-	2/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	D	523	4	-	3/18/38/38	0/3/3/3
3	GOL	B	524	-	-	0/4/4/4	-
3	GOL	A	524	-	-	2/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	522	GLA	C4-C3	-4.37	1.41	1.52
5	C	522	GLA	C4-C3	-4.34	1.41	1.52
6	D	523	ATP	C2'-C3'	-3.91	1.42	1.53
6	C	523	ATP	C2'-C3'	-3.87	1.42	1.53
6	C	523	ATP	C6-N6	3.53	1.46	1.34
6	D	523	ATP	C6-N6	3.29	1.46	1.34
6	D	523	ATP	C2'-C1'	-3.05	1.49	1.53
6	C	523	ATP	C2'-C1'	-2.94	1.49	1.53
6	C	523	ATP	O4'-C4'	-2.63	1.39	1.45
6	D	523	ATP	O4'-C4'	-2.62	1.39	1.45
5	C	522	GLA	O3-C3	2.59	1.49	1.43
5	D	522	GLA	O3-C3	2.55	1.49	1.43
6	D	523	ATP	C5'-C4'	-2.18	1.44	1.51
6	C	523	ATP	C5'-C4'	-2.16	1.44	1.51
6	C	523	ATP	O4'-C1'	2.09	1.44	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	522	GLA	O5-C1-C2	5.46	120.03	110.28
5	D	522	GLA	O5-C1-C2	5.23	119.62	110.28
6	C	523	ATP	N3-C2-N1	-4.84	121.12	128.68
6	D	523	ATP	N3-C2-N1	-4.70	121.33	128.68
5	D	522	GLA	C1-O5-C5	3.27	119.83	113.66
5	C	522	GLA	C1-O5-C5	3.07	119.47	113.66
5	D	522	GLA	C1-C2-C3	2.90	116.34	110.31
6	C	523	ATP	PA-O3A-PB	-2.72	123.49	132.83
6	C	523	ATP	O2G-PG-O3B	2.71	113.71	104.64
6	D	523	ATP	PA-O3A-PB	-2.70	123.58	132.83
5	C	522	GLA	C1-C2-C3	2.55	115.60	110.31
5	D	522	GLA	O5-C5-C4	2.45	114.14	109.69
6	D	523	ATP	C3'-C2'-C1'	2.27	104.39	100.98
5	C	522	GLA	O6-C6-C5	2.24	118.99	111.29
5	D	522	GLA	O3-C3-C2	-2.18	105.30	110.35
5	C	522	GLA	O5-C5-C4	2.06	113.43	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	522	GLA	O3-C3-C2	-2.01	105.70	110.35

There are no chirality outliers.

All (13) torsion outliers are listed below:

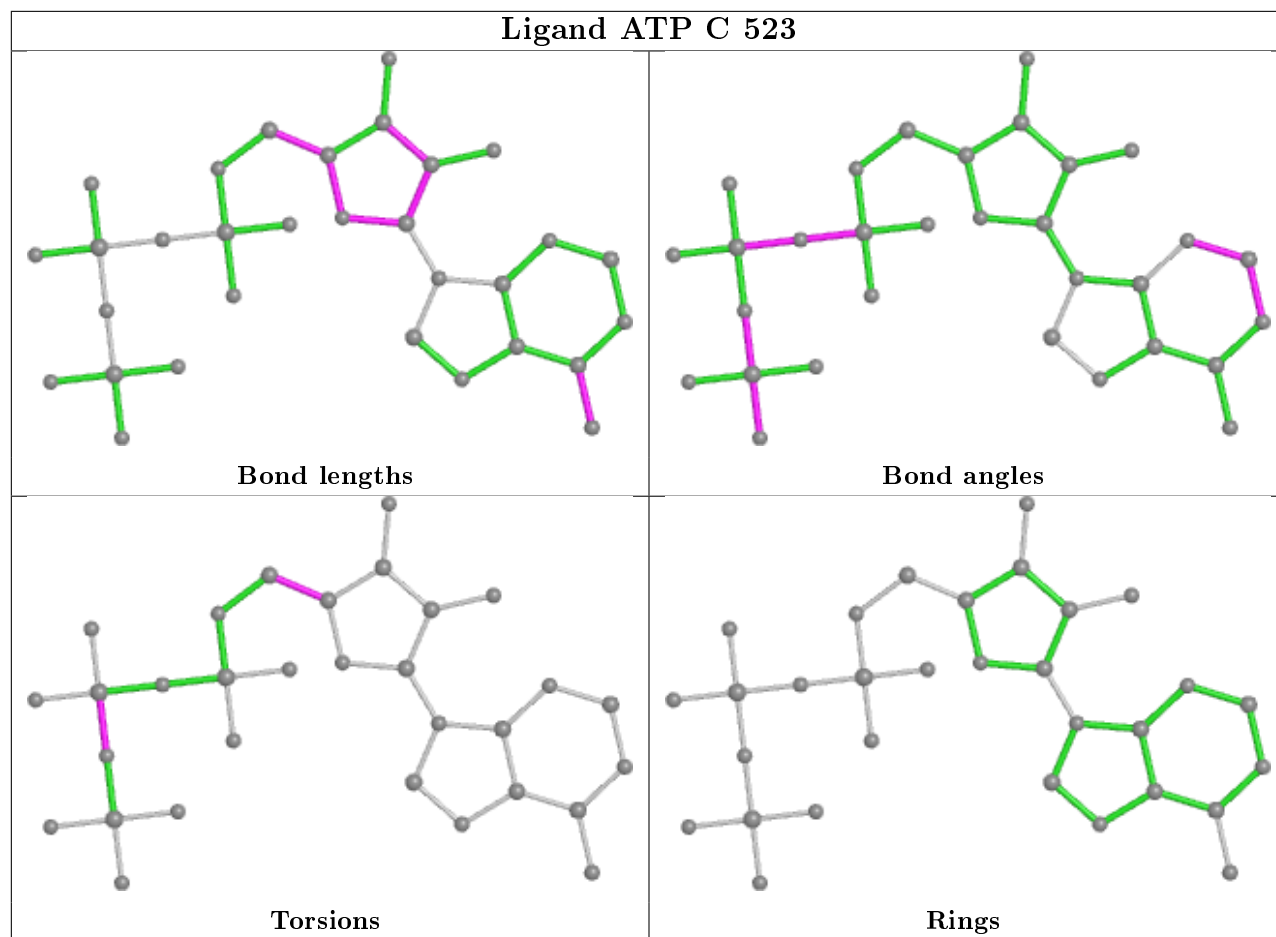
Mol	Chain	Res	Type	Atoms
5	C	522	GLA	O5-C5-C6-O6
5	D	522	GLA	O5-C5-C6-O6
3	A	524	GOL	O1-C1-C2-C3
6	C	523	ATP	C3'-C4'-C5'-O5'
3	A	524	GOL	O1-C1-C2-O2
5	C	522	GLA	C4-C5-C6-O6
6	D	523	ATP	PB-O3A-PA-O2A
6	C	523	ATP	O4'-C4'-C5'-O5'
6	C	523	ATP	PG-O3B-PB-O1B
6	C	523	ATP	PG-O3B-PB-O2B
6	D	523	ATP	PG-O3B-PB-O2B
6	D	523	ATP	C3'-C4'-C5'-O5'
5	D	522	GLA	C4-C5-C6-O6

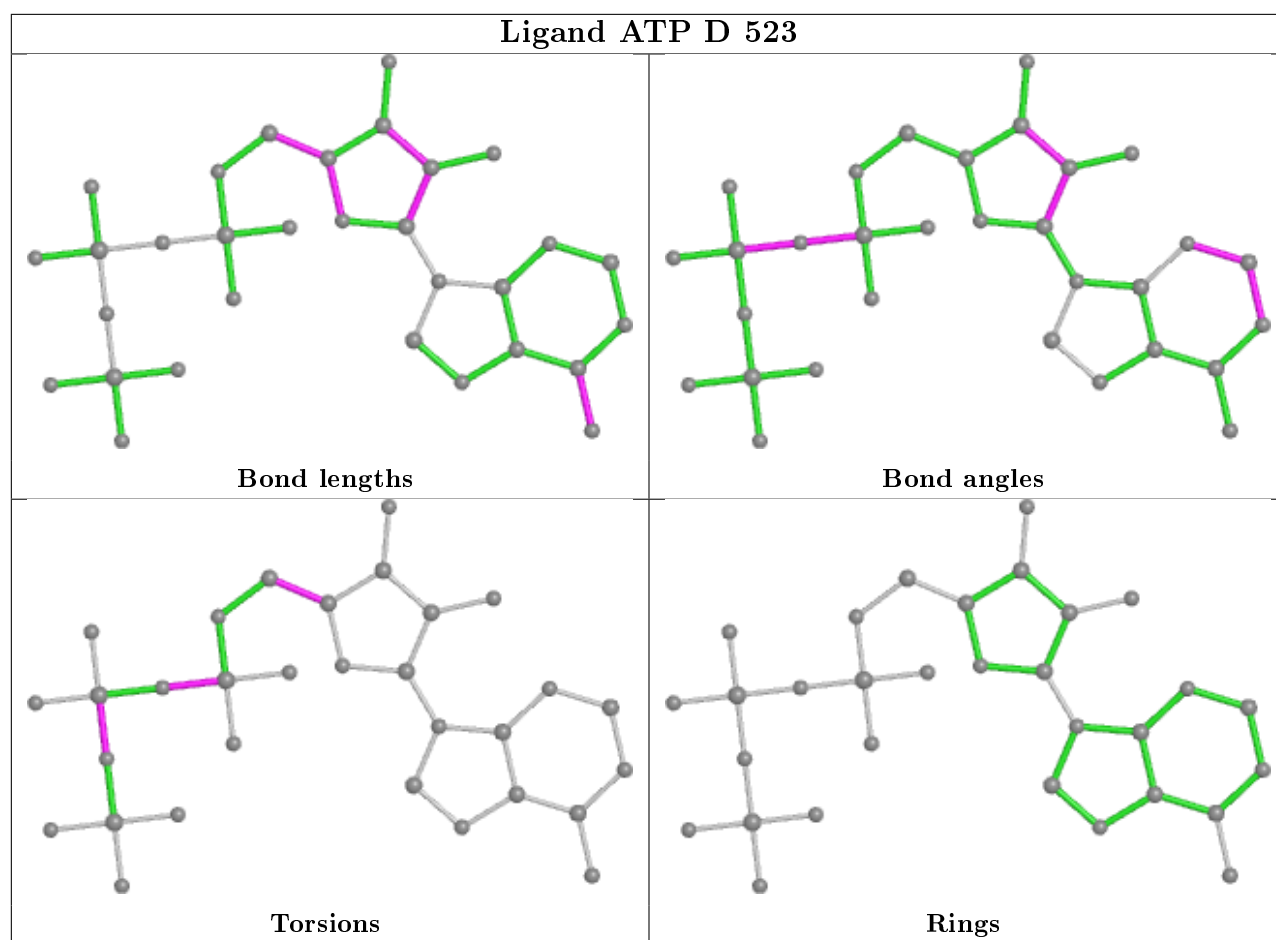
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	522	GLA	3	0
5	C	522	GLA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 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	409/438 (93%)	-0.50	6 (1%) 73 77	14, 26, 65, 103	0
1	B	402/438 (91%)	-0.58	5 (1%) 79 82	15, 28, 62, 110	0
2	C	516/520 (99%)	-0.41	12 (2%) 60 65	18, 37, 80, 112	0
2	D	514/520 (98%)	-0.17	18 (3%) 44 50	19, 45, 89, 114	0
All	All	1841/1916 (96%)	-0.40	41 (2%) 62 66	14, 34, 79, 114	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	383	PRO	4.9
1	A	383	PRO	4.3
2	C	407	THR	4.1
1	A	384	GLU	4.1
2	D	8	PHE	4.0
2	C	520	GLN	3.9
2	D	17	ARG	3.5
1	A	382	ILE	3.5
2	D	24	LEU	3.4
2	C	293	ASP	3.4
2	C	406	ALA	3.0
1	A	385	LEU	3.0
1	A	381	LYS	2.9
1	B	382	ILE	2.9
2	C	79	ASP	2.9
2	D	293	ASP	2.8
2	D	181	LYS	2.7
2	D	500	GLU	2.7
2	D	241	LYS	2.6
2	D	406	ALA	2.6
2	C	138	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	499	ASP	2.5
2	C	408	PHE	2.5
1	B	384	GLU	2.5
2	D	79	ASP	2.5
2	D	474	ALA	2.5
2	D	16	PRO	2.4
1	A	342	GLY	2.3
2	C	24	LEU	2.2
1	B	381	LYS	2.2
2	D	507	ILE	2.2
2	C	498	THR	2.2
2	D	499	ASP	2.2
2	D	292	LYS	2.2
2	C	518	TYR	2.2
1	B	435	LEU	2.1
2	D	409	HIS	2.1
2	D	520	GLN	2.0
2	C	81	LYS	2.0
2	D	81	LYS	2.0
2	D	242	ASN	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 monosaccharides 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. 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	B-factors(\AA^2)	Q<0.9
3	GOL	B	524	6/6	0.95	0.11	25,38,47,49	0
3	GOL	A	524	6/6	0.96	0.10	32,36,39,42	0
5	GLA	D	522	12/12	0.98	0.11	27,28,30,30	0

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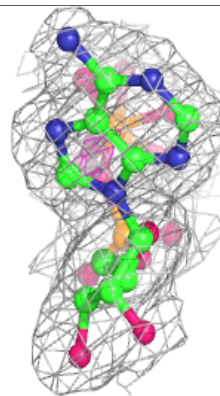
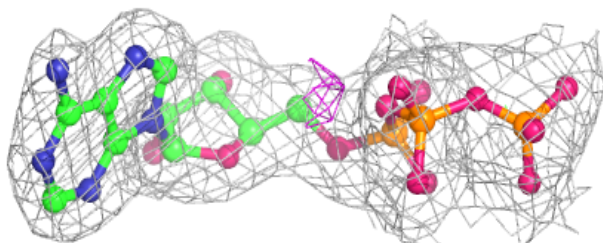
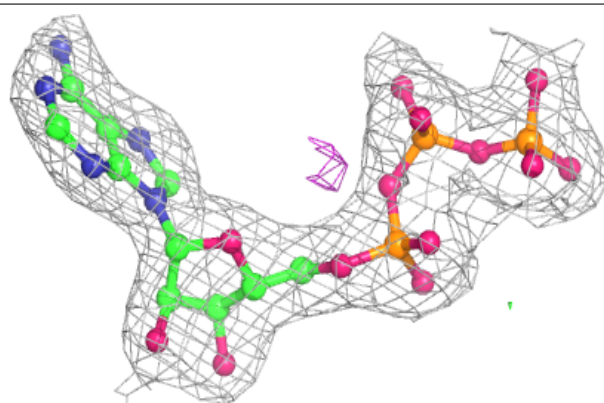
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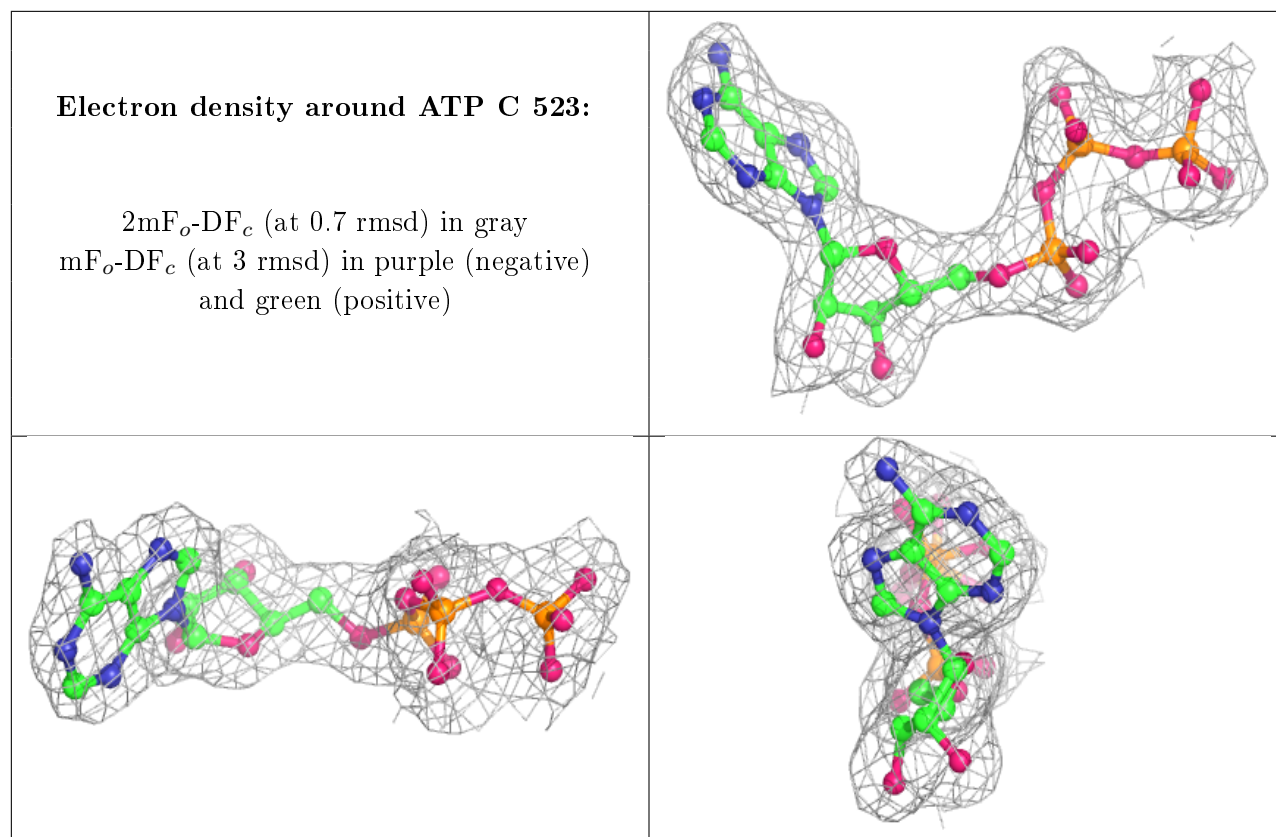
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GLA	C	522	12/12	0.98	0.11	22,24,25,25	0
4	MG	C	521	1/1	0.99	0.18	29,29,29,29	0
6	ATP	D	523	31/31	0.99	0.10	29,31,35,36	0
4	MG	D	521	1/1	0.99	0.18	31,31,31,31	0
6	ATP	C	523	31/31	0.99	0.09	23,26,29,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP D 523:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.