



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 07:06 AM GMT

PDB ID : 2QYO  
Title : Crystal structure of isoflavone O-methyltransferase homolog in complex with biochanin A and SAH  
Authors : Wang, C.; Yu, X.-H.; Liu, C.-J.  
Deposited on : 2007-08-15  
Resolution : 1.95 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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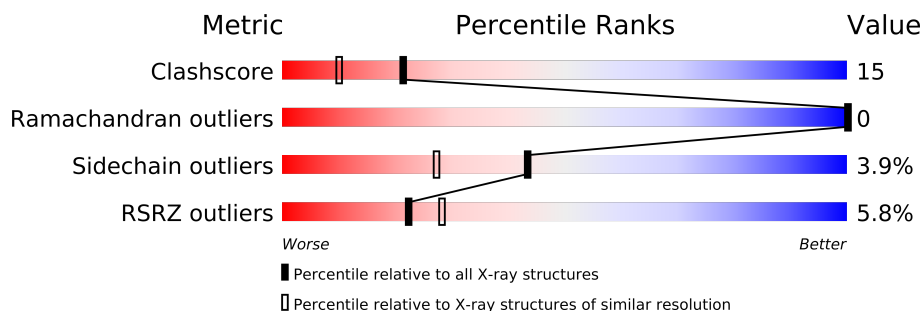
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.95 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))
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	357	
1	B	357	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	K	A	361	-	X
2	K	A	363	-	X
2	K	B	359	-	X
2	K	B	362	-	X
4	QSO	A	701	-	X
4	QSO	B	701	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5869 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

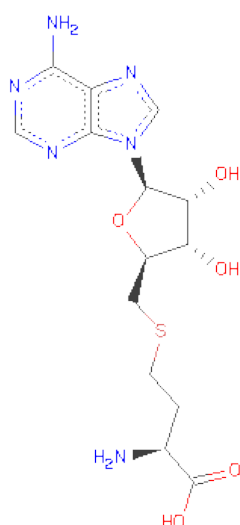
- Molecule 1 is a protein called O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	0
			2792	1788	452	531	21			
1	B	352	Total	C	N	O	S	0	0	0
			2784	1782	451	530	21			

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

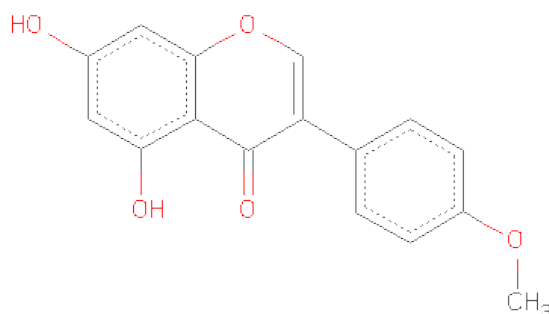
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	K	0	0
			5	5		
2	A	8	Total	K	0	0
			8	8		

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is 5,7-DIHYDROXY-3-(4-METHOXYPHENYL)-4H-CHROMEN-4-ONE (three-letter code: QSO) (formula: C<sub>16</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	16	5		
4	B	1	Total	C	O	0	0
			21	16	5		

- Molecule 5 is water.

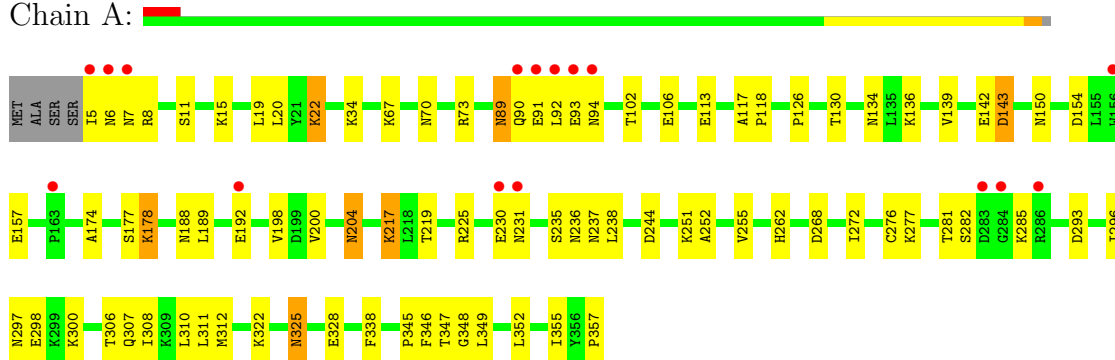
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	94	Total	O	0	0
			94	94		
5	B	92	Total	O	0	0
			92	92		

### 3 Residue-property plots

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.

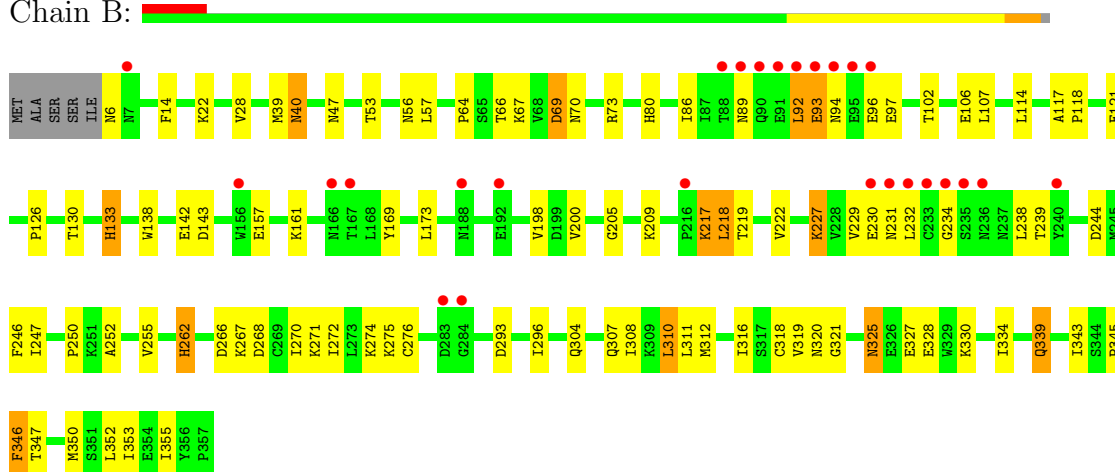
#### • Molecule 1: O-methyltransferase

Chain A:



#### • Molecule 1: O-methyltransferase

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.54Å 82.05Å 101.03Å 90.00° 101.94° 90.00°	Depositor
Resolution (Å)	31.57 – 1.95 31.57 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.5 (31.57-1.95) 95.1 (31.57-1.95)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.214 , 0.245 0.227 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 40.5	EDS
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 51789 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5869	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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: K, SAH, QSO

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	0.40	0/2842	0.75	6/3845 (0.2%)
1	B	0.40	1/2834 (0.0%)	0.75	5/3834 (0.1%)
All	All	0.40	1/5676 (0.0%)	0.75	11/7679 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	93	GLU	C-N	-5.51	1.21	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	PRO	CA-N-CD	-19.11	84.74	111.50
1	A	345	PRO	CA-N-CD	-18.45	85.66	111.50
1	B	93	GLU	CB-CA-C	-14.00	82.40	110.40
1	A	6	ASN	CA-C-N	10.06	139.33	117.20
1	B	346	PHE	CB-CG-CD1	-7.45	115.59	120.80
1	A	6	ASN	O-C-N	-7.33	110.97	122.70
1	A	143	ASP	CB-CA-C	-7.06	96.27	110.40
1	A	6	ASN	C-N-CA	-6.61	105.17	121.70
1	B	92	LEU	C-N-CA	-5.79	107.22	121.70
1	B	93	GLU	C-N-CA	-5.46	108.05	121.70
1	A	7	ASN	N-CA-C	-5.21	96.93	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2792	0	2829	80	0
1	B	2784	0	2818	114	0
2	A	8	0	0	0	0
2	B	5	0	0	0	0
3	A	26	0	19	0	0
3	B	26	0	19	0	0
4	A	21	0	11	0	0
4	B	21	0	11	1	0
5	A	94	0	0	2	0
5	B	92	0	0	5	0
All	All	5869	0	5707	174	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (174) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:89:ASN:OD1	1:B:96:GLU:HB3	1.28	1.28
1:B:89:ASN:HD21	1:B:96:GLU:N	1.29	1.27
1:B:89:ASN:ND2	1:B:96:GLU:H	1.32	1.24
1:B:93:GLU:O	1:B:94:ASN:ND2	1.78	1.14
1:A:236:ASN:O	1:A:237:ASN:HB2	1.32	1.10
1:B:92:LEU:O	1:B:93:GLU:CB	1.95	1.08
1:B:92:LEU:CD1	1:B:93:GLU:CG	2.38	1.00
1:B:92:LEU:HD12	1:B:93:GLU:CG	1.94	0.96
1:B:92:LEU:HD13	1:B:93:GLU:HG2	1.48	0.96
1:A:236:ASN:O	1:A:237:ASN:CB	2.11	0.95
1:B:92:LEU:O	1:B:93:GLU:HB2	1.17	0.95
1:B:92:LEU:CD1	1:B:93:GLU:HG2	1.97	0.94
1:B:53:THR:HB	1:B:96:GLU:OE1	1.67	0.94
1:B:89:ASN:ND2	1:B:96:GLU:N	2.00	0.92
1:A:134:ASN:HD22	1:A:150:ASN:ND2	1.68	0.91
1:B:92:LEU:CD1	1:B:93:GLU:HG3	2.02	0.89
1:B:47:ASN:ND2	5:B:784:HOH:O	2.06	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:217:LYS:HD3	1:A:217:LYS:H	1.36	0.88
1:B:89:ASN:HD21	1:B:96:GLU:CA	1.86	0.87
1:B:89:ASN:CG	1:B:96:GLU:HB3	1.99	0.82
1:A:251:LYS:HE3	1:A:282:SER:OG	1.83	0.79
1:B:89:ASN:OD1	1:B:96:GLU:CB	2.22	0.78
1:A:134:ASN:HD22	1:A:150:ASN:HD21	1.32	0.76
1:B:346:PHE:CD2	1:B:347:THR:HG23	2.23	0.73
1:B:67:LYS:HA	1:B:70:ASN:HD22	1.52	0.73
1:B:92:LEU:HD12	1:B:93:GLU:HG3	1.63	0.73
1:A:93:GLU:HG2	1:A:94:ASN:H	1.53	0.72
1:A:325:ASN:ND2	1:A:328:GLU:H	1.86	0.72
1:A:325:ASN:HD22	1:A:325:ASN:C	1.92	0.72
1:B:311:LEU:HD22	1:B:312:MET:CE	2.20	0.71
1:A:90:GLN:O	1:A:91:GLU:HB2	1.88	0.71
1:A:5:ILE:HD11	1:B:107:LEU:HG	1.73	0.71
1:A:113:GLU:HB3	1:A:178:LYS:HG2	1.70	0.71
1:B:89:ASN:HD21	1:B:96:GLU:H	0.73	0.68
1:B:222:VAL:HG23	1:B:238:LEU:HD21	1.76	0.68
1:B:198:VAL:HG11	1:B:250:PRO:HG2	1.75	0.68
1:B:89:ASN:HD21	1:B:96:GLU:C	1.97	0.68
1:A:102:THR:O	1:A:106:GLU:HG3	1.94	0.67
1:A:67:LYS:HA	1:A:70:ASN:HD22	1.60	0.66
1:B:346:PHE:HB3	1:B:350:MET:O	1.95	0.66
1:B:89:ASN:ND2	1:B:96:GLU:O	2.28	0.66
1:B:312:MET:O	1:B:316:ILE:HG12	1.96	0.66
1:A:93:GLU:HG2	1:A:94:ASN:N	2.11	0.65
1:B:325:ASN:ND2	1:B:328:GLU:HG3	2.12	0.65
1:A:217:LYS:CD	1:A:217:LYS:H	2.09	0.65
1:A:5:ILE:HG23	1:B:114:LEU:HD12	1.79	0.65
1:B:246:PHE:O	1:B:275:LYS:HE3	1.97	0.64
1:B:311:LEU:HD22	1:B:312:MET:HE1	1.79	0.64
1:A:297:ASN:ND2	1:A:300:LYS:HD2	2.13	0.64
1:A:5:ILE:HG21	5:B:729:HOH:O	1.98	0.63
1:B:126:PRO:O	1:B:130:THR:HG23	1.99	0.63
1:B:205:GLY:O	1:B:209:LYS:HG3	1.98	0.63
1:A:22:LYS:HA	1:B:308:ILE:HD13	1.81	0.63
1:A:142:GLU:O	1:A:143:ASP:HB2	1.98	0.62
1:A:126:PRO:O	1:A:130:THR:HG23	1.99	0.62
1:B:67:LYS:HA	1:B:70:ASN:ND2	2.14	0.62
1:A:174:ALA:O	1:A:178:LYS:HD3	1.99	0.62
1:A:298:GLU:HG2	1:A:306:THR:HG21	1.82	0.62
1:B:89:ASN:CG	1:B:96:GLU:O	2.39	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:316:ILE:HG22	1:B:321:GLY:HA3	1.82	0.61
1:B:325:ASN:HD21	1:B:328:GLU:HG3	1.66	0.61
1:A:91:GLU:O	1:A:92:LEU:HD12	2.01	0.60
1:B:92:LEU:HD12	1:B:92:LEU:O	2.01	0.60
1:A:89:ASN:OD1	1:A:92:LEU:HD22	2.03	0.59
1:B:102:THR:O	1:B:106:GLU:HG3	2.03	0.59
1:B:169:TYR:CE2	1:B:173:LEU:HD11	2.38	0.58
1:B:89:ASN:OD1	1:B:96:GLU:O	2.22	0.58
1:A:89:ASN:C	1:A:89:ASN:HD22	2.08	0.57
1:B:270:ILE:HG22	1:B:274:LYS:HE2	1.85	0.57
1:B:69:ASP:O	1:B:73:ARG:HG3	2.04	0.57
1:A:5:ILE:N	1:A:8:ARG:HD2	2.20	0.56
1:B:93:GLU:O	1:B:94:ASN:CG	2.43	0.55
1:A:325:ASN:HD21	1:A:328:GLU:H	1.56	0.54
1:A:308:ILE:HD13	1:B:22:LYS:HA	1.90	0.54
1:B:92:LEU:HD12	1:B:93:GLU:CB	2.36	0.53
1:B:142:GLU:O	1:B:143:ASP:HB2	2.08	0.53
1:A:34:LYS:NZ	1:B:133:HIS:HD2	2.07	0.52
1:A:5:ILE:HG12	1:B:106:GLU:CB	2.40	0.52
1:B:325:ASN:ND2	1:B:328:GLU:H	2.08	0.52
1:A:255:VAL:HG11	1:A:276:CYS:SG	2.50	0.52
1:A:230:GLU:HG3	1:A:231:ASN:OD1	2.09	0.51
1:B:198:VAL:HG23	1:B:252:ALA:CB	2.41	0.51
1:A:142:GLU:OE2	1:B:66:THR:HG23	2.11	0.51
1:B:217:LYS:HE3	5:B:768:HOH:O	2.10	0.51
1:A:298:GLU:HG2	1:A:306:THR:CG2	2.40	0.51
1:A:322:LYS:HA	1:B:73:ARG:HH12	1.76	0.51
1:B:234:GLY:HA3	1:B:238:LEU:HD12	1.93	0.51
1:B:330:LYS:O	1:B:334:ILE:HG12	2.11	0.50
1:B:157:GLU:HG2	1:B:161:LYS:HE2	1.91	0.50
1:B:89:ASN:ND2	1:B:96:GLU:C	2.65	0.50
1:A:142:GLU:O	1:A:143:ASP:CB	2.58	0.50
1:B:218:LEU:HD23	1:B:219:THR:H	1.76	0.50
1:B:327:GLU:HA	1:B:330:LYS:HZ3	1.77	0.50
1:A:5:ILE:HG12	1:B:106:GLU:HB3	1.94	0.49
1:B:198:VAL:HG23	1:B:252:ALA:HB2	1.94	0.49
1:A:67:LYS:HA	1:A:70:ASN:ND2	2.26	0.49
1:B:267:LYS:NZ	1:B:271:LYS:HE3	2.27	0.49
1:B:230:GLU:C	1:B:231:ASN:HD22	2.16	0.49
1:A:322:LYS:HB2	1:B:73:ARG:HH22	1.77	0.49
1:A:19:LEU:HD23	1:A:19:LEU:C	2.34	0.48
1:A:281:THR:HA	1:A:285:LYS:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:325:ASN:C	1:A:325:ASN:ND2	2.64	0.47
1:B:353:ILE:HG22	1:B:355:ILE:HD13	1.96	0.47
1:B:266:ASP:O	1:B:270:ILE:HG12	2.14	0.47
1:B:92:LEU:HD12	1:B:92:LEU:C	2.34	0.47
1:A:154:ASP:OD2	1:A:157:GLU:HG3	2.14	0.47
1:A:136:LYS:HG3	1:B:39:MET:SD	2.55	0.47
1:B:238:LEU:HD13	1:B:239:THR:N	2.30	0.47
1:B:227:LYS:HG3	5:B:740:HOH:O	2.15	0.46
1:A:277:LYS:HG3	1:A:357:PRO:HB3	1.98	0.46
1:B:319:VAL:O	1:B:320:ASN:HB2	2.16	0.46
1:A:225:ARG:HH12	1:A:244:ASP:HB2	1.79	0.46
1:A:117:ALA:N	1:A:118:PRO:CD	2.79	0.46
1:A:322:LYS:HA	1:B:73:ARG:NH1	2.32	0.45
1:A:189:LEU:HB2	5:A:715:HOH:O	2.16	0.45
1:B:138:TRP:CZ2	1:B:318:CYS:HA	2.51	0.45
1:A:198:VAL:HG23	1:A:252:ALA:HB2	1.98	0.45
1:A:117:ALA:HB3	1:A:118:PRO:HD3	1.98	0.45
1:A:322:LYS:HG3	1:B:73:ARG:NH2	2.32	0.45
1:A:73:ARG:HH11	1:A:73:ARG:HG3	1.81	0.45
1:A:188:ASN:O	1:A:192:GLU:HB3	2.17	0.45
1:A:5:ILE:N	1:B:106:GLU:OE1	2.49	0.45
1:B:238:LEU:C	1:B:238:LEU:HD13	2.37	0.44
1:A:297:ASN:ND2	1:A:300:LYS:CD	2.79	0.44
1:A:219:THR:HG23	5:A:755:HOH:O	2.17	0.44
1:A:11:SER:O	1:A:15:LYS:HG3	2.17	0.44
1:B:262:HIS:HE1	4:B:701:QSO:HM1	1.82	0.44
1:B:268:ASP:O	1:B:272:ILE:HG13	2.18	0.44
1:A:91:GLU:C	1:A:92:LEU:HD12	2.37	0.44
1:A:238:LEU:HD23	1:A:238:LEU:C	2.38	0.44
1:B:353:ILE:HG22	1:B:355:ILE:CD1	2.47	0.44
1:A:198:VAL:HG23	1:A:252:ALA:CB	2.48	0.44
1:B:339:GLN:HE21	1:B:339:GLN:HB2	1.49	0.44
1:A:352:LEU:HD23	1:A:352:LEU:C	2.38	0.44
1:A:296:ILE:O	1:A:325:ASN:HA	2.17	0.44
1:A:67:LYS:HD3	1:A:70:ASN:ND2	2.33	0.44
1:B:229:VAL:HA	1:B:232:LEU:HD12	2.00	0.44
1:B:117:ALA:HB3	1:B:118:PRO:HD3	1.99	0.44
1:B:255:VAL:HG11	1:B:276:CYS:SG	2.58	0.43
1:B:222:VAL:CG2	1:B:238:LEU:HD21	2.45	0.43
1:B:325:ASN:C	1:B:325:ASN:HD22	2.21	0.43
1:B:343:ILE:HG12	1:B:353:ILE:HG12	2.00	0.43
1:B:86:ILE:HG23	1:B:97:GLU:HB2	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:311:LEU:HD11	1:B:28:VAL:HB	2.01	0.43
1:B:352:LEU:C	1:B:352:LEU:HD23	2.39	0.43
1:B:117:ALA:O	1:B:121:GLU:HG3	2.18	0.43
1:A:348:GLY:N	1:B:14:PHE:HB3	2.33	0.43
1:A:204:ASN:C	1:A:204:ASN:HD22	2.22	0.43
1:B:53:THR:CB	1:B:96:GLU:OE1	2.53	0.43
1:B:40:ASN:HD22	1:B:40:ASN:N	2.17	0.42
1:B:70:ASN:ND2	5:B:783:HOH:O	2.49	0.42
1:B:230:GLU:HG2	1:B:231:ASN:ND2	2.33	0.42
1:A:312:MET:HE3	1:A:349:LEU:HD13	2.01	0.42
1:A:346:PHE:CD2	1:A:347:THR:HG23	2.54	0.42
1:A:338:PHE:CD1	1:A:355:ILE:HG22	2.54	0.42
1:B:117:ALA:N	1:B:118:PRO:CD	2.83	0.42
1:B:89:ASN:ND2	1:B:96:GLU:HB3	2.35	0.42
1:B:346:PHE:HB3	1:B:347:THR:H	1.65	0.42
1:A:5:ILE:HD11	1:B:107:LEU:CG	2.47	0.42
1:B:304:GLN:O	1:B:307:GLN:HB3	2.20	0.42
1:A:174:ALA:O	1:A:177:SER:HB3	2.19	0.41
1:B:200:VAL:HG23	1:B:255:VAL:HG13	2.03	0.41
1:A:139:VAL:O	1:B:64:PRO:HD2	2.20	0.41
1:A:268:ASP:O	1:A:272:ILE:HG13	2.20	0.41
1:B:296:ILE:O	1:B:325:ASN:HA	2.21	0.41
1:B:330:LYS:HB3	1:B:330:LYS:HZ3	1.86	0.41
1:A:307:GLN:HB2	1:B:80:HIS:CE1	2.55	0.41
1:B:244:ASP:HB3	1:B:247:ILE:HG12	2.03	0.41
1:A:34:LYS:HZ3	1:B:133:HIS:HD2	1.69	0.41
1:B:310:LEU:HD12	1:B:310:LEU:HA	1.93	0.41
1:B:92:LEU:HD12	1:B:93:GLU:HB2	2.02	0.40
1:A:89:ASN:ND2	1:A:92:LEU:HD13	2.36	0.40
1:B:270:ILE:CG2	1:B:274:LYS:HE2	2.49	0.40
1:A:200:VAL:HG23	1:A:255:VAL:HG13	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	351/357 (98%)	335 (95%)	16 (5%)	0	100	100
1	B	350/357 (98%)	341 (97%)	9 (3%)	0	100	100
All	All	701/714 (98%)	676 (96%)	25 (4%)	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	318/321 (99%)	307 (96%)	11 (4%)	48	32
1	B	317/321 (99%)	303 (96%)	14 (4%)	39	22
All	All	635/642 (99%)	610 (96%)	25 (4%)	43	27

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

Mol	Chain	Res	Type
1	A	20	LEU
1	A	22	LYS
1	A	89	ASN
1	A	178	LYS
1	A	204	ASN
1	A	217	LYS
1	A	235	SER
1	A	262	HIS
1	A	293	ASP
1	A	310	LEU
1	A	325	ASN
1	B	6	ASN
1	B	40	ASN
1	B	56	ASN
1	B	57	LEU
1	B	69	ASP
1	B	133	HIS
1	B	217	LYS
1	B	218	LEU

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Mol	Chain	Res	Type
1	B	227	LYS
1	B	262	HIS
1	B	293	ASP
1	B	310	LEU
1	B	325	ASN
1	B	339	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	48	HIS
1	A	70	ASN
1	A	72	GLN
1	A	80	HIS
1	A	89	ASN
1	A	150	ASN
1	A	204	ASN
1	A	320	ASN
1	A	325	ASN
1	B	40	ASN
1	B	48	HIS
1	B	56	ASN
1	B	62	GLN
1	B	70	ASN
1	B	72	GLN
1	B	89	ASN
1	B	133	HIS
1	B	231	ASN
1	B	320	ASN
1	B	325	ASN
1	B	339	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 17 ligands modelled in this entry, 13 are monoatomic - leaving 4 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	SAH	A	601	-	28,28,28	2.15	9 (32%)	40,40,40	2.25	12 (30%)
4	QSO	A	701	-	23,23,23	2.50	12 (52%)	31,33,33	2.01	10 (32%)
3	SAH	B	602	-	28,28,28	2.13	9 (32%)	40,40,40	2.21	10 (25%)
4	QSO	B	701	-	23,23,23	2.47	10 (43%)	31,33,33	2.03	10 (32%)

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	SAH	A	601	-	-	0/15/31/31	0/1/3/3
4	QSO	A	701	-	-	0/6/6/6	0/1/3/3
3	SAH	B	602	-	-	0/15/31/31	0/1/3/3
4	QSO	B	701	-	-	0/6/6/6	0/1/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	QSO	C4-C4A	7.74	1.52	1.40
4	B	701	QSO	C4-C4A	7.46	1.51	1.40
3	B	602	SAH	CB-CA	-5.15	1.39	1.54
3	A	601	SAH	CB-CA	-4.97	1.40	1.54
3	B	602	SAH	C1'-N9	-4.67	1.34	1.48
3	A	601	SAH	C1'-N9	-4.54	1.34	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	QSO	C4-C3	4.22	1.52	1.39
4	B	701	QSO	C4-C3	4.15	1.52	1.39
3	A	601	SAH	C4-N9	3.69	1.43	1.37
3	A	601	SAH	C5'-SD	-3.39	1.74	1.81
3	B	602	SAH	O4'-C1'	3.35	1.46	1.41
3	B	602	SAH	C4-N9	3.26	1.42	1.37
3	A	601	SAH	CB-CG	-3.21	1.38	1.51
3	B	602	SAH	CB-CG	-3.19	1.38	1.51
3	A	601	SAH	O4'-C1'	3.16	1.46	1.41
3	B	602	SAH	C2-N3	3.11	1.38	1.32
4	B	701	QSO	C4A-C8A	3.10	1.45	1.41
4	A	701	QSO	C4A-C8A	3.03	1.45	1.41
3	A	601	SAH	C2-N3	2.96	1.38	1.32
3	B	602	SAH	C5'-C4'	2.92	1.60	1.52
3	A	601	SAH	C5'-C4'	2.80	1.60	1.52
3	B	602	SAH	C5'-SD	-2.75	1.75	1.81
4	A	701	QSO	C3'-C4'	2.67	1.44	1.38
4	B	701	QSO	C3'-C4'	2.54	1.44	1.38
4	B	701	QSO	C5'-C4'	2.51	1.43	1.38
4	B	701	QSO	C8-C7	2.50	1.42	1.37
4	A	701	QSO	C8-C7	2.49	1.42	1.37
3	B	602	SAH	C8-N7	-2.43	1.29	1.34
4	A	701	QSO	C8-C8A	2.41	1.43	1.37
4	B	701	QSO	C6-C7	2.34	1.42	1.39
4	B	701	QSO	C8-C8A	2.33	1.42	1.37
4	B	701	QSO	O1-C2	2.30	1.39	1.34
4	B	701	QSO	C3'-C2'	2.29	1.43	1.38
4	A	701	QSO	C5'-C4'	2.28	1.43	1.38
3	A	601	SAH	C8-N7	-2.26	1.30	1.34
4	A	701	QSO	C6'-C1'	2.25	1.44	1.39
4	A	701	QSO	O1-C2	2.22	1.39	1.34
4	A	701	QSO	C5'-C6'	2.15	1.42	1.38
4	A	701	QSO	C3'-C2'	2.10	1.42	1.38
4	A	701	QSO	C6-C7	2.08	1.42	1.39

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	SAH	O4'-C1'-C2'	-7.72	94.93	106.77
3	B	602	SAH	O4'-C1'-C2'	-7.48	95.30	106.77
3	A	601	SAH	N3-C2-N1	-6.37	123.39	128.71
3	B	602	SAH	N3-C2-N1	-6.17	123.55	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	QSO	C8-C8A-C4A	-4.47	117.64	123.10
4	A	701	QSO	C8-C8A-C4A	-4.41	117.72	123.10
4	A	701	QSO	C8-C7-C6	-4.12	117.33	120.91
4	B	701	QSO	C8-C7-C6	-4.10	117.34	120.91
4	A	701	QSO	C5-C6-C7	3.79	123.22	119.66
3	A	601	SAH	C8-N9-C1'	3.75	133.76	126.38
3	B	602	SAH	C8-N9-C1'	3.70	133.67	126.38
3	A	601	SAH	CB-CA-N	3.68	119.12	110.14
4	B	701	QSO	C5-C6-C7	3.65	123.08	119.66
3	B	602	SAH	CB-CA-N	3.62	118.99	110.14
3	B	602	SAH	CB-CG-SD	-3.53	106.77	113.57
3	A	601	SAH	C8-N9-C4	-3.45	104.27	106.90
3	B	602	SAH	C4'-O4'-C1'	-3.42	106.04	109.75
4	A	701	QSO	O1-C2-C3	3.40	126.42	123.25
3	B	602	SAH	C8-N9-C4	-3.32	104.36	106.90
4	B	701	QSO	O1-C2-C3	3.24	126.27	123.25
4	B	701	QSO	C7-C8-C8A	3.07	123.17	120.31
4	A	701	QSO	C7-C8-C8A	2.99	123.09	120.31
3	A	601	SAH	C4'-O4'-C1'	-2.79	106.72	109.75
4	B	701	QSO	C5-C4A-C8A	2.75	121.17	117.77
3	A	601	SAH	CB-CG-SD	-2.73	108.30	113.57
4	B	701	QSO	C3-C4-C4A	-2.71	116.89	121.04
3	B	602	SAH	C1'-N9-C4	-2.70	121.96	126.64
3	A	601	SAH	C1'-N9-C4	-2.70	121.97	126.64
4	A	701	QSO	C3-C4-C4A	-2.68	116.93	121.04
3	A	601	SAH	C2-N1-C6	2.65	123.55	118.77
4	A	701	QSO	C5-C4A-C8A	2.59	120.98	117.77
4	B	701	QSO	O1-C8A-C4A	2.55	123.91	121.29
4	A	701	QSO	O1-C8A-C4A	2.51	123.86	121.29
4	B	701	QSO	C6-C5-C4A	-2.45	117.60	120.62
3	B	602	SAH	C2-N1-C6	2.42	123.14	118.77
4	A	701	QSO	C6-C5-C4A	-2.39	117.68	120.62
3	B	602	SAH	CG-CB-CA	2.29	117.05	113.22
3	A	601	SAH	C5'-SD-CG	-2.28	95.62	102.42
3	A	601	SAH	CG-CB-CA	2.14	116.81	113.22
3	A	601	SAH	O4'-C4'-C5'	-2.13	103.23	108.91
4	B	701	QSO	C3'-C4'-C5'	-2.11	116.59	120.21
4	A	701	QSO	C3'-C4'-C5'	-2.07	116.66	120.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	353/357 (98%)	0.29	16 (4%) 32 37	12, 24, 47, 64	0
1	B	352/357 (98%)	0.51	26 (7%) 14 19	13, 26, 57, 89	0
All	All	705/714 (98%)	0.40	42 (5%) 22 27	12, 25, 50, 89	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	91	GLU	10.4
1	B	92	LEU	9.3
1	B	94	ASN	8.2
1	B	90	GLN	7.8
1	A	156	TRP	7.8
1	B	93	GLU	7.2
1	B	89	ASN	6.5
1	B	233	CYS	5.3
1	B	95	GLU	5.3
1	B	88	THR	5.2
1	A	5	ILE	5.0
1	B	166	ASN	4.5
1	A	92	LEU	4.3
1	B	284	GLY	4.2
1	B	96	GLU	4.0
1	A	91	GLU	3.8
1	B	236	ASN	3.7
1	A	94	ASN	3.7
1	A	90	GLN	3.7
1	B	231	ASN	3.6
1	B	235	SER	3.2
1	B	216	PRO	3.2
1	B	234	GLY	3.0
1	B	192	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	6	ASN	2.9
1	A	283	ASP	2.8
1	B	156	TRP	2.8
1	B	283	ASP	2.7
1	A	192	GLU	2.7
1	B	167	THR	2.7
1	A	93	GLU	2.7
1	B	7	ASN	2.7
1	A	284	GLY	2.7
1	A	286	ARG	2.5
1	A	230	GLU	2.5
1	A	163	PRO	2.5
1	B	188	ASN	2.4
1	A	7	ASN	2.2
1	A	231	ASN	2.2
1	B	232	LEU	2.1
1	B	230	GLU	2.0
1	B	240	TYR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	K	A	363	1/1	0.25	13.45	7,7,7,7	0
4	QSO	B	701	21/21	0.33	5.52	67,71,73,74	0
4	QSO	A	701	21/21	0.29	4.98	63,67,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	K	B	362	1/1	0.21	4.50	56,56,56,56	0
2	K	A	361	1/1	0.17	3.28	14,14,14,14	0
2	K	B	359	1/1	0.21	2.93	15,15,15,15	0
3	SAH	A	601	26/26	0.15	1.39	23,29,35,36	0
2	K	A	362	1/1	0.18	1.17	14,14,14,14	0
3	SAH	B	602	26/26	0.13	0.41	26,30,34,35	0
2	K	B	360	1/1	0.15	0.33	25,25,25,25	0
2	K	A	364	1/1	0.16	0.29	16,16,16,16	0
2	K	A	360	1/1	0.10	0.16	23,23,23,23	0
2	K	A	359	1/1	0.15	-0.74	23,23,23,23	0
2	K	A	358	1/1	0.13	-0.78	28,28,28,28	0
2	K	A	365	1/1	0.07	-1.11	45,45,45,45	0
2	K	B	358	1/1	0.07	-3.49	27,27,27,27	0
2	K	B	361	1/1	0.05	-6.81	39,39,39,39	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.