



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:56 pm BST

PDB ID : 6NR7  
Title : Rerefinement of chicken vinculin  
Authors : Stec, B.  
Deposited on : 2019-01-23  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

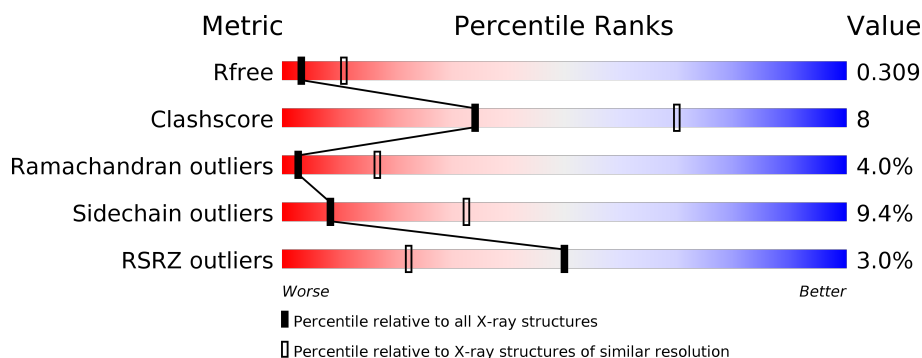
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	1086	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8443 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 Vinculin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1086	8336	5150	1516	1620	50	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

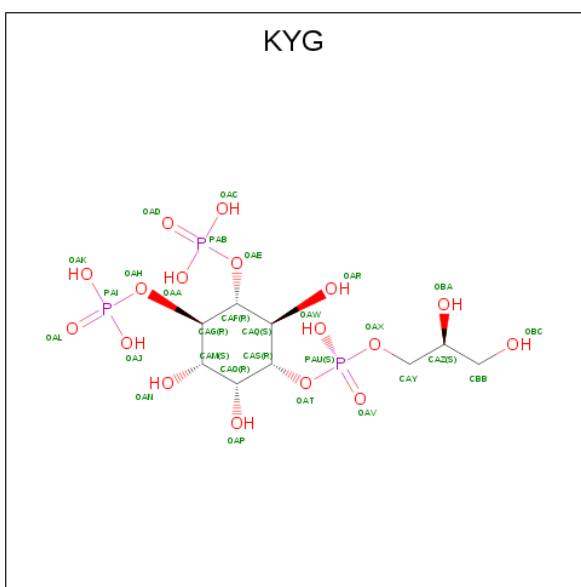
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P12003
A	-18	GLY	-	expression tag	UNP P12003
A	-17	SER	-	expression tag	UNP P12003
A	-16	SER	-	expression tag	UNP P12003
A	-15	HIS	-	expression tag	UNP P12003
A	-14	HIS	-	expression tag	UNP P12003
A	-13	HIS	-	expression tag	UNP P12003
A	-12	HIS	-	expression tag	UNP P12003
A	-11	HIS	-	expression tag	UNP P12003
A	-10	HIS	-	expression tag	UNP P12003
A	-9	SER	-	expression tag	UNP P12003
A	-8	SER	-	expression tag	UNP P12003
A	-7	GLY	-	expression tag	UNP P12003
A	-6	LEU	-	expression tag	UNP P12003
A	-5	VAL	-	expression tag	UNP P12003
A	-4	PRO	-	expression tag	UNP P12003
A	-3	ARG	-	expression tag	UNP P12003
A	-2	GLY	-	expression tag	UNP P12003
A	-1	SER	-	expression tag	UNP P12003
A	0	HIS	-	expression tag	UNP P12003

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is (1R,2R,3S,4R,5R,6S)-4-{[(S)-[(2S)-2,3-dihydroxypropoxy](hydroxy)phosphoryl]oxy}-3,5,6-trihydroxycyclohexane-1,2-diyl bis[dihydrogen (phosphate)] (three-letter code: KYG) (formula: C<sub>9</sub>H<sub>21</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			29	9	17	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		

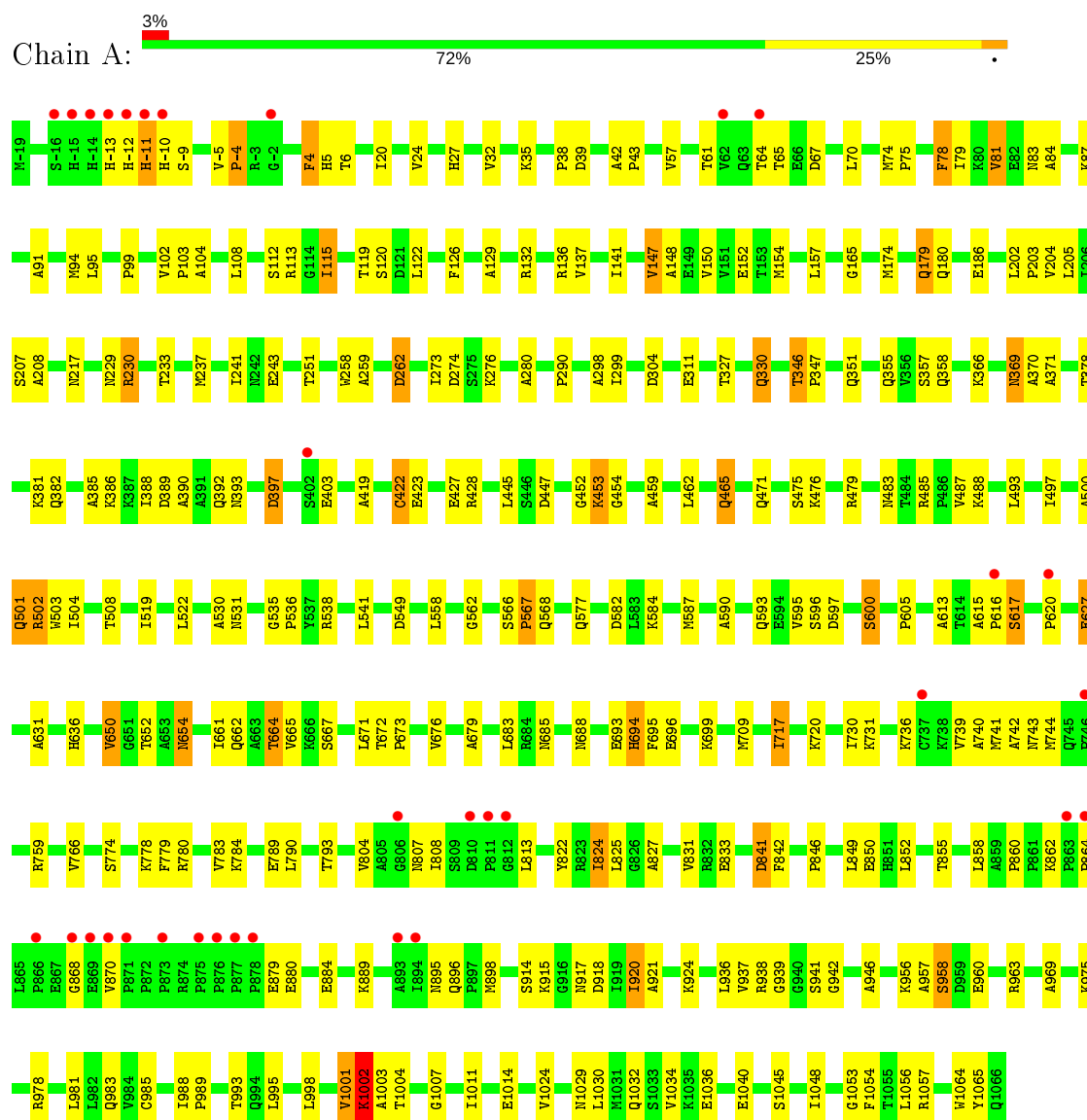
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	58	Total	O	0	0
			58	58		

### 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 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 ( $\text{RSRZ} > 2$ ). 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: Vinculin



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.02Å 126.95Å 351.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.96 – 3.00 46.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.96-3.00) 99.5 (46.96-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.219 , 0.315 0.219 , 0.309	Depositor DCC
$R_{free}$ test set	1134 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	102.6	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 87.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8443	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: PO4, KYG, SO4

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	0.72	0/8451	0.87	1/11415 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	963	ARG	NE-CZ-NH1	5.48	123.04	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	397	ASP	Peptide
1	A	652	THR	Peptide
1	A	884	GLU	Peptide

### 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	8336	0	8473	141	0
2	A	10	0	0	0	0
3	A	29	0	0	0	0
4	A	10	0	0	0	0
5	A	58	0	0	2	0
All	All	8443	0	8473	141	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 8.

All (141) 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:895:ASN:HD22	1:A:898:MET:HB2	1.50	0.77
1:A:654:ASN:HD22	1:A:654:ASN:N	1.89	0.71
1:A:627:GLU:OE1	1:A:627:GLU:HA	1.95	0.67
1:A:1001:VAL:O	1:A:1003:ALA:N	2.28	0.66
1:A:452:GLY:O	1:A:454:GLY:N	2.29	0.66
1:A:914:SER:OG	1:A:924:LYS:NZ	2.29	0.65
1:A:793:THR:HG22	1:A:824:ILE:HG12	1.77	0.65
1:A:895:ASN:HD21	1:A:1024:VAL:HG22	1.62	0.64
1:A:969:ALA:HB2	1:A:981:LEU:HD23	1.80	0.63
1:A:915:LYS:HB2	1:A:1057:ARG:NH1	2.13	0.62
1:A:462:LEU:O	1:A:465:GLN:N	2.34	0.61
1:A:42:ALA:HB3	1:A:43:PRO:HD3	1.83	0.61
1:A:27:HIS:HB2	1:A:108:LEU:HD23	1.82	0.60
1:A:1054:PHE:CZ	1:A:1056:LEU:HD21	2.37	0.59
1:A:259:ALA:HB1	1:A:378:THR:HG21	1.84	0.59
1:A:654:ASN:HD22	1:A:654:ASN:H	1.50	0.59
1:A:493:LEU:HD11	1:A:522:LEU:CD1	2.33	0.59
1:A:662:GLN:NE2	5:A:1202:HOH:O	2.35	0.59
1:A:369:ASN:O	1:A:371:ALA:N	2.36	0.58
1:A:1001:VAL:HG12	1:A:1002:LYS:N	2.18	0.58
1:A:351:GLN:O	1:A:355:GLN:NE2	2.37	0.57
1:A:613:ALA:HA	1:A:683:LEU:HD21	1.86	0.57
1:A:500:ALA:O	1:A:503:TRP:N	2.37	0.56
1:A:596:SER:O	1:A:600:SER:OG	2.23	0.56
1:A:914:SER:HG	1:A:924:LYS:NZ	2.02	0.56
1:A:685:ASN:HD22	1:A:688:ASN:HD22	1.52	0.55
1:A:530:ALA:HB2	1:A:541:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:ASN:ND2	1:A:1024:VAL:HG22	2.22	0.55
1:A:696:GLU:OE2	1:A:696:GLU:HA	2.07	0.54
1:A:74:MET:HE1	1:A:122:LEU:HD12	1.89	0.54
1:A:258:TRP:HB2	1:A:485:ARG:HH11	1.72	0.54
1:A:79:ILE:O	1:A:83:ASN:HB2	2.08	0.54
1:A:4:PHE:CZ	1:A:998:LEU:HD21	2.43	0.54
1:A:330:GLN:HA	1:A:330:GLN:HE21	1.73	0.53
1:A:280:ALA:HB1	1:A:299:ILE:HG13	1.90	0.53
1:A:20:ILE:O	1:A:24:VAL:HG23	2.09	0.53
1:A:453:LYS:O	1:A:459:ALA:HB2	2.08	0.53
1:A:137:VAL:HG21	1:A:174:MET:SD	2.50	0.52
1:A:917:ASN:HD21	1:A:920:ILE:HD13	1.74	0.52
1:A:259:ALA:CB	1:A:378:THR:HG21	2.40	0.51
1:A:147:VAL:O	1:A:147:VAL:HG12	2.10	0.51
1:A:1032:GLN:NE2	1:A:1036:GLU:HG2	2.25	0.51
1:A:804:VAL:HG21	1:A:813:LEU:HG	1.93	0.51
1:A:493:LEU:HD13	1:A:650:VAL:HA	1.94	0.50
1:A:535:GLY:N	1:A:536:PRO:HD2	2.26	0.50
1:A:390:ALA:HA	1:A:393:ASN:HD22	1.77	0.50
1:A:497:ILE:O	1:A:501:GLN:N	2.44	0.50
1:A:597:ASP:O	1:A:600:SER:OG	2.20	0.49
1:A:1001:VAL:O	1:A:1004:THR:N	2.40	0.49
1:A:672:THR:HB	1:A:673:PRO:HD3	1.94	0.49
1:A:75:PRO:HA	1:A:78:PHE:CE1	2.47	0.49
1:A:259:ALA:HB2	1:A:485:ARG:NH2	2.28	0.49
1:A:304:ASP:OD2	1:A:531:ASN:ND2	2.46	0.48
1:A:95:LEU:HD11	1:A:104:ALA:HB3	1.95	0.48
1:A:112:SER:O	1:A:115:ILE:N	2.46	0.48
1:A:208:ALA:HA	1:A:694:HIS:CE1	2.48	0.48
1:A:102:VAL:N	1:A:103:PRO:CD	2.77	0.48
1:A:157:LEU:C	1:A:157:LEU:HD23	2.34	0.48
1:A:493:LEU:HD11	1:A:522:LEU:HD11	1.94	0.48
1:A:584:LYS:NZ	5:A:1204:HOH:O	2.47	0.48
1:A:1030:LEU:O	1:A:1034:VAL:HG23	2.13	0.48
1:A:917:ASN:HD22	1:A:920:ILE:HB	1.79	0.48
1:A:1045:SER:O	1:A:1048:ILE:HG23	2.14	0.47
1:A:452:GLY:C	1:A:454:GLY:H	2.18	0.47
1:A:664:THR:HG22	1:A:665:VAL:N	2.29	0.47
1:A:595:VAL:HG11	1:A:717:ILE:HD11	1.97	0.47
1:A:20:ILE:O	1:A:20:ILE:CG2	2.62	0.47
1:A:936:LEU:HD11	1:A:946:ALA:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:VAL:O	1:A:61:THR:N	2.47	0.47
1:A:129:ALA:HA	1:A:132:ARG:NH1	2.30	0.47
1:A:731:LYS:HD3	1:A:825:LEU:HD21	1.97	0.47
1:A:91:ALA:HB1	1:A:104:ALA:HB1	1.96	0.46
1:A:627:GLU:OE1	1:A:627:GLU:CA	2.62	0.46
1:A:975:LYS:HG2	1:A:978:ARG:NH2	2.30	0.46
1:A:4:PHE:HZ	1:A:998:LEU:HD21	1.80	0.46
1:A:150:VAL:O	1:A:150:VAL:HG12	2.16	0.46
1:A:382:GLN:HA	1:A:382:GLN:OE1	2.16	0.46
1:A:957:ALA:O	1:A:960:GLU:N	2.45	0.46
1:A:780:ARG:O	1:A:784:LYS:HB2	2.16	0.46
1:A:615:ALA:O	1:A:617:SER:N	2.49	0.45
1:A:20:ILE:O	1:A:20:ILE:HG22	2.16	0.45
1:A:941:SER:OG	1:A:942:GLY:N	2.46	0.45
1:A:664:THR:HG21	1:A:709:MET:HA	1.98	0.45
1:A:988:ILE:N	1:A:989:PRO:CD	2.80	0.45
1:A:179:GLN:OE1	1:A:180:GLN:NE2	2.49	0.45
1:A:667:SER:O	1:A:671:LEU:HG	2.16	0.45
1:A:937:VAL:HG12	1:A:938:ARG:N	2.32	0.45
1:A:74:MET:HB3	1:A:75:PRO:HD3	1.98	0.44
1:A:627:GLU:O	1:A:631:ALA:N	2.48	0.44
1:A:74:MET:HE3	1:A:74:MET:HA	1.99	0.44
1:A:500:ALA:C	1:A:502:ARG:N	2.71	0.44
1:A:-5:VAL:N	1:A:-4:PRO:CD	2.81	0.44
1:A:739:VAL:HA	1:A:742:ALA:HB3	2.00	0.44
1:A:654:ASN:ND2	1:A:654:ASN:N	2.61	0.44
1:A:262:ASP:OD1	1:A:488:LYS:NZ	2.50	0.43
1:A:422:CYS:SG	1:A:423:GLU:N	2.91	0.43
1:A:661:ILE:O	1:A:664:THR:HB	2.18	0.43
1:A:202:LEU:O	1:A:204:VAL:N	2.51	0.43
1:A:280:ALA:HB2	1:A:298:ALA:HB3	1.99	0.43
1:A:419:ALA:O	1:A:428:ARG:HB2	2.18	0.43
1:A:590:ALA:O	1:A:593:GLN:N	2.50	0.43
1:A:917:ASN:ND2	1:A:920:ILE:HD13	2.32	0.43
1:A:229:ASN:HD22	1:A:229:ASN:HA	1.60	0.43
1:A:280:ALA:HB2	1:A:298:ALA:CB	2.48	0.43
1:A:273:ILE:O	1:A:276:LYS:N	2.51	0.43
1:A:207:SER:C	1:A:694:HIS:HE1	2.23	0.43
1:A:385:ALA:O	1:A:388:ILE:HG22	2.18	0.42
1:A:558:LEU:HD11	1:A:568:GLN:HG3	2.01	0.42
1:A:918:ASP:HA	1:A:921:ALA:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:SER:N	1:A:567:PRO:HD2	2.34	0.42
1:A:654:ASN:ND2	1:A:654:ASN:H	2.16	0.42
1:A:841:ASP:OD1	1:A:841:ASP:N	2.52	0.42
1:A:779:PHE:O	1:A:783:VAL:HG12	2.20	0.42
1:A:957:ALA:O	1:A:958:SER:C	2.57	0.42
1:A:-12:HIS:O	1:A:-11:HIS:ND1	2.53	0.42
1:A:504:ILE:HG12	1:A:577:GLN:HE22	1.83	0.42
1:A:84:ALA:O	1:A:87:LYS:N	2.53	0.42
1:A:148:ALA:O	1:A:230:ARG:NH2	2.53	0.42
1:A:479:ARG:O	1:A:483:ASN:ND2	2.53	0.42
1:A:67:ASP:HB3	1:A:70:LEU:HB3	2.02	0.42
1:A:78:PHE:HA	1:A:81:VAL:HG23	2.02	0.41
1:A:5:HIS:HB3	1:A:251:THR:O	2.20	0.41
1:A:243:GLU:HA	1:A:243:GLU:OE2	2.20	0.41
1:A:730:ILE:HG13	1:A:759:ARG:HG2	2.02	0.41
1:A:676:VAL:HA	1:A:679:ALA:HB3	2.02	0.41
1:A:4:PHE:N	1:A:4:PHE:CD1	2.89	0.41
1:A:741:MET:HG3	1:A:808:ILE:HG22	2.03	0.41
1:A:237:MET:O	1:A:241:ILE:HG12	2.21	0.41
1:A:695:PHE:O	1:A:699:LYS:N	2.32	0.41
1:A:789:GLU:O	1:A:827:ALA:HB1	2.21	0.41
1:A:462:LEU:O	1:A:465:GLN:HB3	2.21	0.41
1:A:605:PRO:HG2	1:A:636:HIS:CG	2.56	0.40
1:A:736:LYS:O	1:A:740:ALA:HB2	2.21	0.40
1:A:95:LEU:CD1	1:A:104:ALA:HB3	2.52	0.40
1:A:1064:TRP:CD1	1:A:1065:TYR:CD2	3.09	0.40
1:A:587:MET:HB3	1:A:650:VAL:HG21	2.04	0.40
1:A:493:LEU:HD22	1:A:650:VAL:O	2.22	0.40
1:A:205:LEU:HB2	1:A:233:THR:CG2	2.51	0.40
1:A:346:THR:HG22	1:A:347:PRO:HD2	2.03	0.40
1:A:804:VAL:HG21	1:A:813:LEU:CD2	2.51	0.40
1:A:793:THR:CG2	1:A:824:ILE:HG12	2.50	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	1084/1086 (100%)	903 (83%)	138 (13%)	43 (4%)	3	17

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	PRO
1	A	369	ASN
1	A	453	LYS
1	A	744	MET
1	A	1001	VAL
1	A	1002	LYS
1	A	186	GLU
1	A	370	ALA
1	A	397	ASP
1	A	501	GLN
1	A	562	GLY
1	A	939	GLY
1	A	1007	GLY
1	A	-4	PRO
1	A	38	PRO
1	A	136	ARG
1	A	203	PRO
1	A	389	ASP
1	A	538	ARG
1	A	790	LEU
1	A	868	GLY
1	A	879	GLU
1	A	64	THR
1	A	113	ARG
1	A	465	GLN
1	A	475	SER
1	A	487	VAL
1	A	617	SER
1	A	846	PRO
1	A	864	PRO
1	A	-11	HIS
1	A	99	PRO
1	A	147	VAL
1	A	165	GLY

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Mol	Chain	Res	Type
1	A	274	ASP
1	A	616	PRO
1	A	620	PRO
1	A	958	SER
1	A	567	PRO
1	A	860	PRO
1	A	32	VAL
1	A	1053	GLY
1	A	81	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	A	893/893 (100%)	809 (91%)	84 (9%)	8	32

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-13	HIS
1	A	-10	HIS
1	A	-9	SER
1	A	4	PHE
1	A	6	THR
1	A	35	LYS
1	A	39	ASP
1	A	65	THR
1	A	78	PHE
1	A	94	MET
1	A	115	ILE
1	A	119	THR
1	A	120	SER
1	A	126	PHE
1	A	141	ILE
1	A	152	GLU
1	A	154	MET

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Mol	Chain	Res	Type
1	A	179	GLN
1	A	217	ASN
1	A	230	ARG
1	A	262	ASP
1	A	311	GLU
1	A	327	THR
1	A	330	GLN
1	A	346	THR
1	A	357	SER
1	A	358	GLN
1	A	366	LYS
1	A	381	LYS
1	A	386	LYS
1	A	392	GLN
1	A	403	GLU
1	A	422	CYS
1	A	427	GLU
1	A	445	LEU
1	A	447	ASP
1	A	471	GLN
1	A	476	LYS
1	A	502	ARG
1	A	508	THR
1	A	519	ILE
1	A	549	ASP
1	A	582	ASP
1	A	600	SER
1	A	627	GLU
1	A	650	VAL
1	A	654	ASN
1	A	664	THR
1	A	693	GLU
1	A	694	HIS
1	A	717	ILE
1	A	720	LYS
1	A	743	ASN
1	A	766	VAL
1	A	774	SER
1	A	778	LYS
1	A	807	ASN
1	A	822	TYR
1	A	824	ILE

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Mol	Chain	Res	Type
1	A	831	VAL
1	A	833	GLU
1	A	841	ASP
1	A	842	PHE
1	A	849	LEU
1	A	850	GLU
1	A	852	LEU
1	A	855	THR
1	A	858	LEU
1	A	862	LYS
1	A	870	VAL
1	A	880	GLU
1	A	889	LYS
1	A	896	GLN
1	A	920	ILE
1	A	956	LYS
1	A	983	GLN
1	A	985	CYS
1	A	993	THR
1	A	995	LEU
1	A	1002	LYS
1	A	1011	ILE
1	A	1014	GLU
1	A	1029	ASN
1	A	1040	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	179	GLN
1	A	180	GLN
1	A	229	ASN
1	A	279	GLN
1	A	297	GLN
1	A	330	GLN
1	A	355	GLN
1	A	358	GLN
1	A	393	ASN
1	A	399	ASN
1	A	471	GLN
1	A	635	ASN

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Mol	Chain	Res	Type
1	A	654	ASN
1	A	688	ASN
1	A	694	HIS
1	A	743	ASN
1	A	747	GLN
1	A	773	ASN
1	A	836	GLN
1	A	895	ASN
1	A	949	GLN
1	A	980	ASN
1	A	1026	ASN
1	A	1029	ASN
1	A	1032	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](#)

5 ligands are modelled in this entry.

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	$\# Z  > 2$
4	PO4	A	1105	-	4,4,4	0.63	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	1102	-	4,4,4	0.37	0	6,6,6	0.07	0
4	PO4	A	1104	-	4,4,4	0.58	0	6,6,6	0.48	0
3	KYG	A	1103	-	29,29,29	0.73	0	41,45,45	1.11	4 (9%)
2	SO4	A	1101	-	4,4,4	0.38	0	6,6,6	0.05	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
3	KYG	A	1103	-	-	10/23/47/47	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1103	KYG	CAF-CAQ-CAS	4.15	117.57	108.96
3	A	1103	KYG	CAO-CAS-CAQ	2.43	114.36	110.85
3	A	1103	KYG	CAM-CAO-CAS	2.26	114.83	109.68
3	A	1103	KYG	CAQ-CAF-CAG	2.04	116.33	111.66

There are no chirality outliers.

All (10) torsion outliers are listed below:

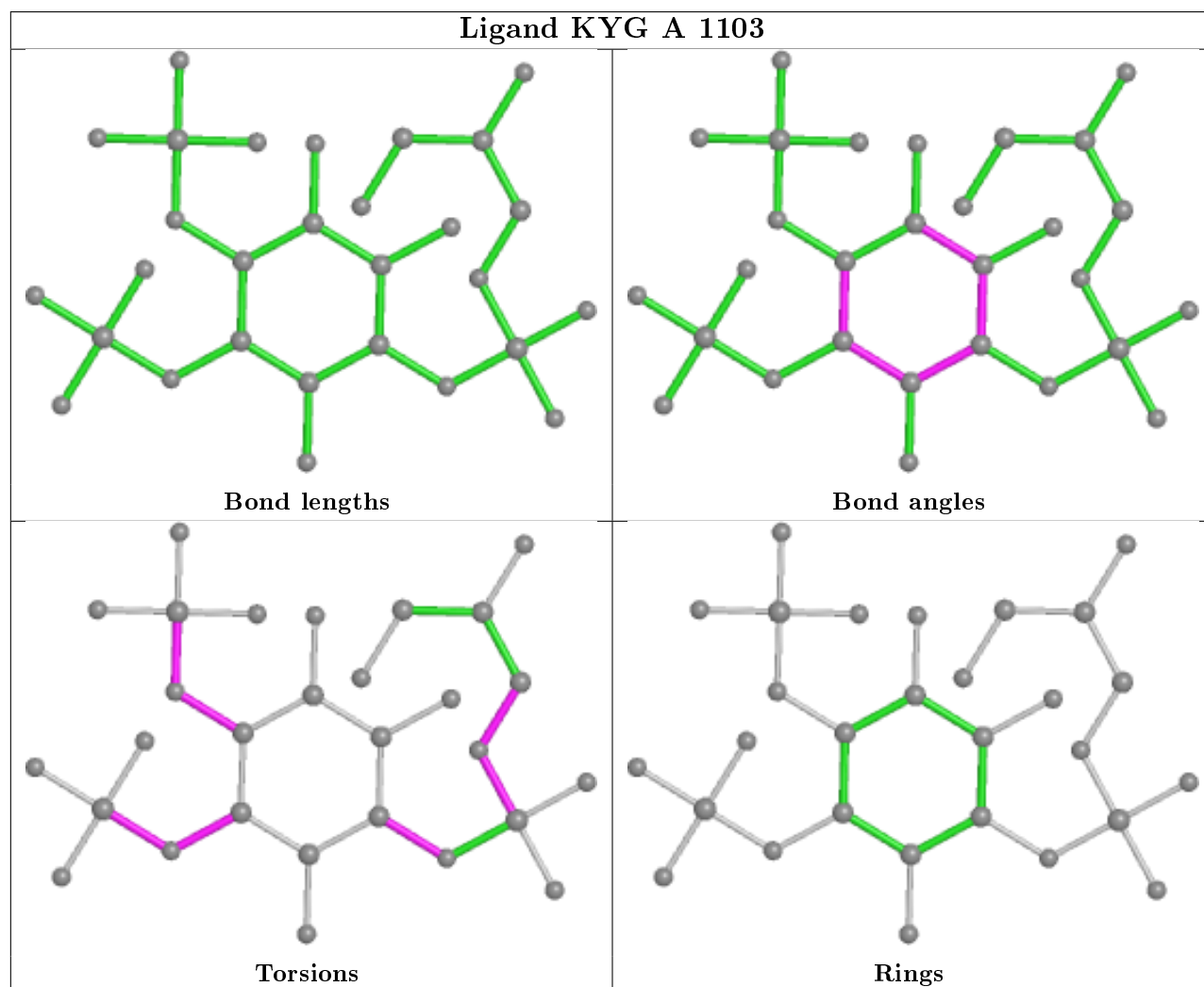
Mol	Chain	Res	Type	Atoms
3	A	1103	KYG	CAY-OAX-PAU-OAW
3	A	1103	KYG	CAQ-CAS-OAT-PAU
3	A	1103	KYG	CAO-CAS-OAT-PAU
3	A	1103	KYG	CAF-OAE-PAB-OAD
3	A	1103	KYG	CAY-OAX-PAU-OAT
3	A	1103	KYG	CAQ-CAF-OAE-PAB
3	A	1103	KYG	CAZ-CAY-OAX-PAU
3	A	1103	KYG	CAY-OAX-PAU-OAV
3	A	1103	KYG	CAG-OAH-PAI-OAL
3	A	1103	KYG	CAF-CAG-OAH-PAI

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	1086/1086 (100%)	-0.11	33 (3%)	50 22	56, 119, 187, 232	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-14	HIS	6.6
1	A	863	PRO	6.1
1	A	62	VAL	5.4
1	A	864	PRO	5.2
1	A	877	PRO	5.0
1	A	-11	HIS	5.0
1	A	620	PRO	4.8
1	A	811	PRO	4.5
1	A	875	PRO	4.4
1	A	746	PRO	3.7
1	A	-10	HIS	3.7
1	A	866	PRO	3.4
1	A	-13	HIS	3.2
1	A	812	GLY	3.2
1	A	810	ASP	3.2
1	A	-12	HIS	2.9
1	A	-16	SER	2.9
1	A	878	PRO	2.8
1	A	737	CYS	2.6
1	A	616	PRO	2.5
1	A	876	PRO	2.4
1	A	869	GLU	2.4
1	A	871	PRO	2.3
1	A	64	THR	2.3
1	A	-2	GLY	2.3
1	A	402	SER	2.2
1	A	868	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	-15	HIS	2.2
1	A	873	PRO	2.2
1	A	870	VAL	2.1
1	A	806	GLY	2.1
1	A	893	ALA	2.0
1	A	894	ILE	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](#)

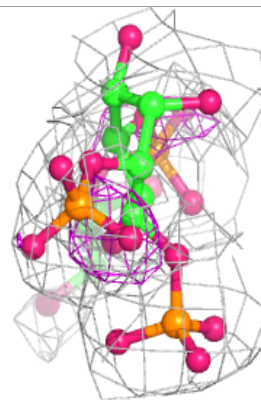
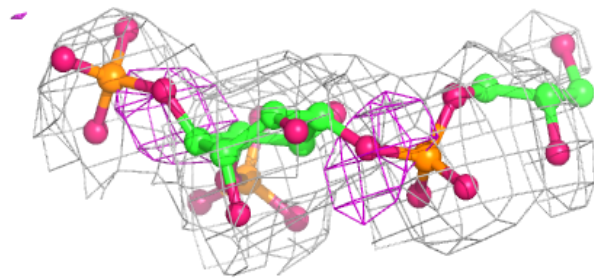
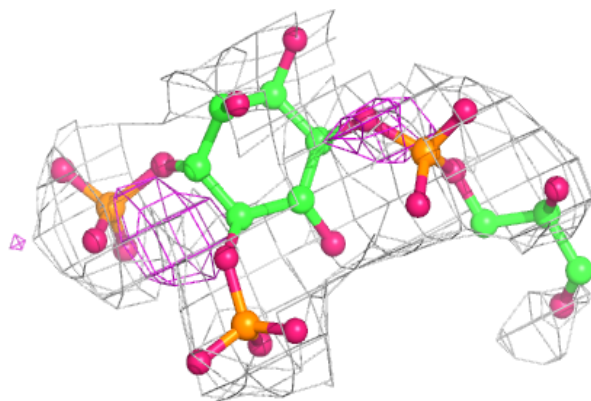
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	1101	5/5	0.74	0.29	166,168,171,172	0
3	KYG	A	1103	29/29	0.76	0.23	152,199,214,222	0
4	PO4	A	1104	5/5	0.79	0.18	166,170,183,193	0
2	SO4	A	1102	5/5	0.93	0.18	121,138,141,147	0
4	PO4	A	1105	5/5	0.93	0.16	151,161,166,170	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 KYG A 1103:**

$2mF_o-DF_c$  (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.