



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:45 PM GMT

PDB ID : 4JDL  
Title : Crystal structure of native abscisic acid receptor PYL5 at 2.65 Angstrom  
Authors : Zhang, X.; Zhang, Q.; Chen, Z.  
Deposited on : 2013-02-25  
Resolution : 2.65 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

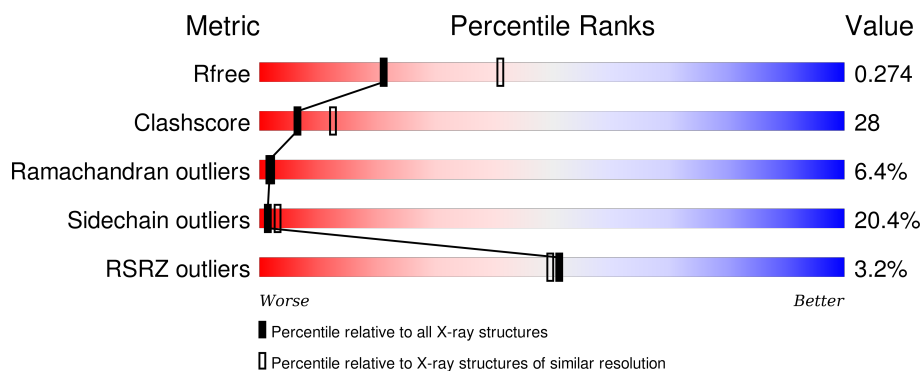
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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. 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	223	 3% 30% 30% 8% 31%
1	B	223	 2% 32% 32% • 31%
1	C	223	 % 24% 26% 6% 43%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3837 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 Absciscic acid receptor PYL5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1141	714	213	208	6			
1	B	154	Total	C	N	O	S	0	0	0
			1125	697	213	207	8			
1	C	126	Total	C	N	O	S	0	0	0
			934	577	168	184	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q9FLB1
A	-18	GLY	-	EXPRESSION TAG	UNP Q9FLB1
A	-17	SER	-	EXPRESSION TAG	UNP Q9FLB1
A	-16	SER	-	EXPRESSION TAG	UNP Q9FLB1
A	-15	HIS	-	EXPRESSION TAG	UNP Q9FLB1
A	-14	HIS	-	EXPRESSION TAG	UNP Q9FLB1
A	-13	HIS	-	EXPRESSION TAG	UNP Q9FLB1
A	-12	HIS	-	EXPRESSION TAG	UNP Q9FLB1
A	-11	HIS	-	EXPRESSION TAG	UNP Q9FLB1
A	-10	SER	-	EXPRESSION TAG	UNP Q9FLB1
A	-9	SER	-	EXPRESSION TAG	UNP Q9FLB1
A	-8	GLY	-	EXPRESSION TAG	UNP Q9FLB1
A	-7	GLU	-	EXPRESSION TAG	UNP Q9FLB1
A	-6	ASN	-	EXPRESSION TAG	UNP Q9FLB1
A	-5	LEU	-	EXPRESSION TAG	UNP Q9FLB1
A	-4	TYR	-	EXPRESSION TAG	UNP Q9FLB1
A	-3	PHE	-	EXPRESSION TAG	UNP Q9FLB1
A	-2	GLN	-	EXPRESSION TAG	UNP Q9FLB1
A	-1	GLY	-	EXPRESSION TAG	UNP Q9FLB1
A	0	HIS	-	EXPRESSION TAG	UNP Q9FLB1
B	-19	MET	-	EXPRESSION TAG	UNP Q9FLB1
B	-18	GLY	-	EXPRESSION TAG	UNP Q9FLB1
B	-17	SER	-	EXPRESSION TAG	UNP Q9FLB1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	EXPRESSION TAG	UNP Q9FLB1
B	-15	HIS	-	EXPRESSION TAG	UNP Q9FLB1
B	-14	HIS	-	EXPRESSION TAG	UNP Q9FLB1
B	-13	HIS	-	EXPRESSION TAG	UNP Q9FLB1
B	-12	HIS	-	EXPRESSION TAG	UNP Q9FLB1
B	-11	HIS	-	EXPRESSION TAG	UNP Q9FLB1
B	-10	SER	-	EXPRESSION TAG	UNP Q9FLB1
B	-9	SER	-	EXPRESSION TAG	UNP Q9FLB1
B	-8	GLY	-	EXPRESSION TAG	UNP Q9FLB1
B	-7	GLU	-	EXPRESSION TAG	UNP Q9FLB1
B	-6	ASN	-	EXPRESSION TAG	UNP Q9FLB1
B	-5	LEU	-	EXPRESSION TAG	UNP Q9FLB1
B	-4	TYR	-	EXPRESSION TAG	UNP Q9FLB1
B	-3	PHE	-	EXPRESSION TAG	UNP Q9FLB1
B	-2	GLN	-	EXPRESSION TAG	UNP Q9FLB1
B	-1	GLY	-	EXPRESSION TAG	UNP Q9FLB1
B	0	HIS	-	EXPRESSION TAG	UNP Q9FLB1
C	-19	MET	-	EXPRESSION TAG	UNP Q9FLB1
C	-18	GLY	-	EXPRESSION TAG	UNP Q9FLB1
C	-17	SER	-	EXPRESSION TAG	UNP Q9FLB1
C	-16	SER	-	EXPRESSION TAG	UNP Q9FLB1
C	-15	HIS	-	EXPRESSION TAG	UNP Q9FLB1
C	-14	HIS	-	EXPRESSION TAG	UNP Q9FLB1
C	-13	HIS	-	EXPRESSION TAG	UNP Q9FLB1
C	-12	HIS	-	EXPRESSION TAG	UNP Q9FLB1
C	-11	HIS	-	EXPRESSION TAG	UNP Q9FLB1
C	-10	SER	-	EXPRESSION TAG	UNP Q9FLB1
C	-9	SER	-	EXPRESSION TAG	UNP Q9FLB1
C	-8	GLY	-	EXPRESSION TAG	UNP Q9FLB1
C	-7	GLU	-	EXPRESSION TAG	UNP Q9FLB1
C	-6	ASN	-	EXPRESSION TAG	UNP Q9FLB1
C	-5	LEU	-	EXPRESSION TAG	UNP Q9FLB1
C	-4	TYR	-	EXPRESSION TAG	UNP Q9FLB1
C	-3	PHE	-	EXPRESSION TAG	UNP Q9FLB1
C	-2	GLN	-	EXPRESSION TAG	UNP Q9FLB1
C	-1	GLY	-	EXPRESSION TAG	UNP Q9FLB1
C	0	HIS	-	EXPRESSION TAG	UNP Q9FLB1

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

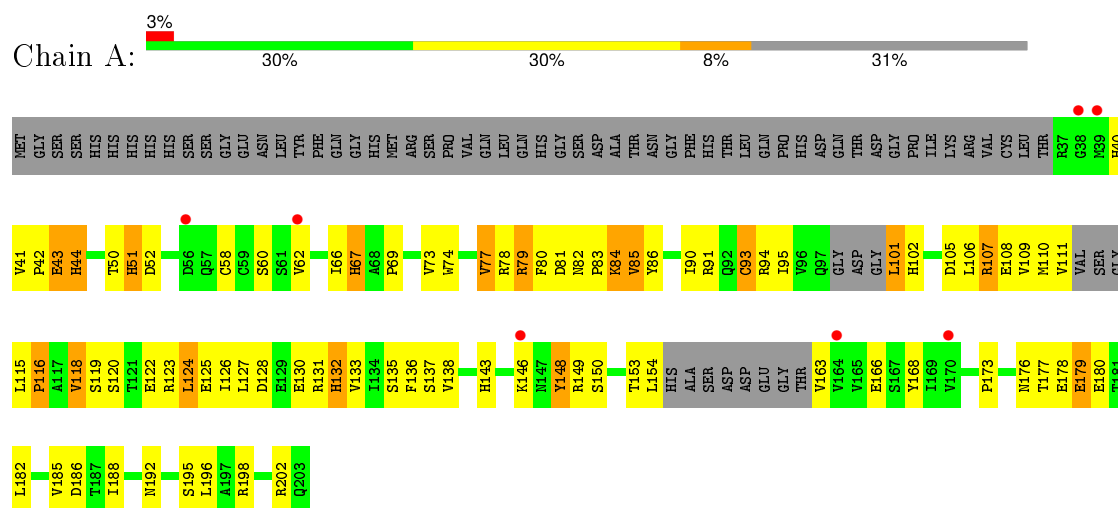
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	213	Total 213	O 213	0	0
3	B	189	Total 189	O 189	0	0
3	C	163	Total 163	O 163	0	0

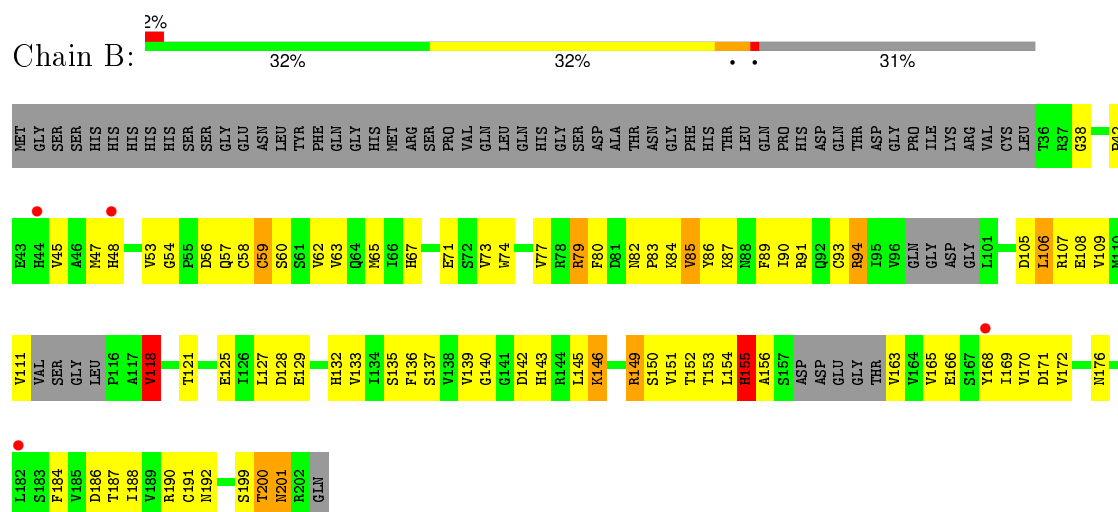
### 3 Residue-property plots

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.

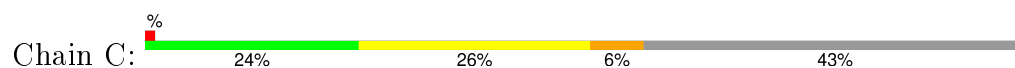
#### • Molecule 1: Absciscic acid receptor PYL5

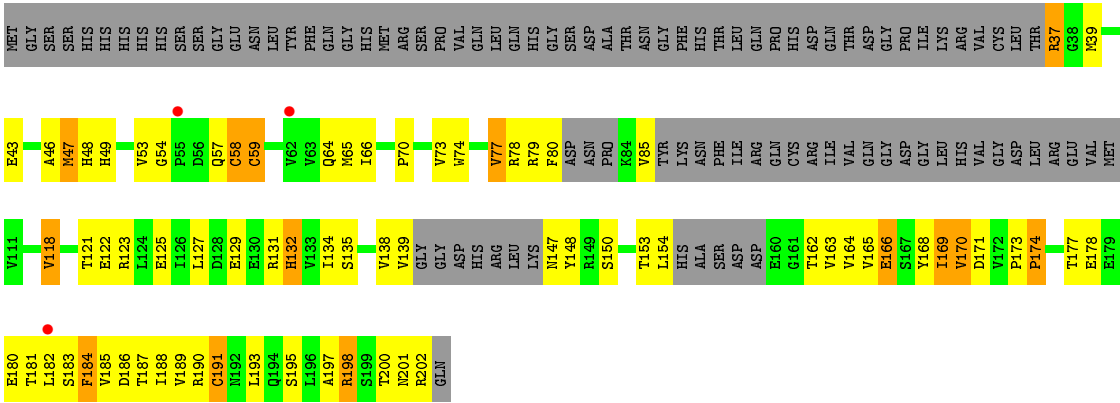


#### • Molecule 1: Absciscic acid receptor PYL5



#### • Molecule 1: Absciscic acid receptor PYL5





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.85Å 95.85Å 143.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.92 – 2.65 47.92 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.7 (47.92-2.65) 97.7 (47.92-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.27 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.253 , 0.274 0.257 , 0.274	Depositor DCC
$R_{free}$ test set	1085 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.5	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 198.3	EDS
Estimated twinning fraction	0.500 for H, K, L 0.500 for K, H, -L 0.073 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.500 for H, K, L 0.500 for K, H, -L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	4 of 21320 reflections (0.019%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3837	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.46	0/1163	0.72	0/1580
1	B	0.47	0/1145	0.73	0/1553
1	C	0.48	0/948	0.74	0/1289
All	All	0.47	0/3256	0.73	0/4422

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	200	THR	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	1141	0	1045	59	0
1	B	1125	0	1015	65	0
1	C	934	0	858	51	0
2	A	42	0	56	0	0
2	B	24	0	32	0	0
2	C	6	0	8	0	0
3	A	213	0	0	5	0
3	B	189	0	0	4	0
3	C	163	0	0	2	0
All	All	3837	0	3014	173	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 28.

All (173) 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:C:182:LEU:O	1:C:186:ASP:HB2	1.68	0.94
1:A:123:ARG:O	1:A:136:PHE:HB2	1.73	0.87
1:B:82:ASN:O	1:B:85:VAL:HG13	1.74	0.86
1:C:58:CYS:O	1:C:169:ILE:HD13	1.79	0.82
1:A:43:GLU:HG2	1:A:44:HIS:CD2	2.20	0.76
1:C:187:THR:O	1:C:191:CYS:SG	2.44	0.75
1:A:66:ILE:HG23	1:A:202:ARG:CB	2.19	0.73
1:A:101:LEU:O	1:A:102:HIS:ND1	2.22	0.71
1:B:67:HIS:O	1:B:201:ASN:ND2	2.25	0.69
1:B:187:THR:HG22	1:B:191:CYS:SG	2.32	0.69
1:B:152:THR:O	1:B:152:THR:HG22	1.96	0.66
1:B:187:THR:O	1:B:191:CYS:SG	2.55	0.64
1:B:42:PRO:HD3	1:B:155:HIS:CG	2.33	0.63
1:A:122:GLU:HA	1:A:138:VAL:HA	1.80	0.63
1:B:132:HIS:HB2	1:B:154:LEU:HB2	1.80	0.62
1:C:132:HIS:CD2	1:C:154:LEU:HD22	2.34	0.62
1:A:178:GLU:O	1:A:182:LEU:HD13	2.00	0.61
1:A:120:SER:OG	1:A:122:GLU:OE2	2.16	0.61
1:A:115:LEU:N	3:A:605:HOH:O	2.33	0.61
1:C:53:VAL:HG12	1:C:54:GLY:N	2.16	0.61
1:B:80:PHE:CE2	1:B:107:ARG:HB2	2.35	0.61
1:B:93:CYS:SG	1:B:107:ARG:HG3	2.43	0.59
1:A:67:HIS:CG	1:A:67:HIS:O	2.55	0.59
1:B:121:THR:O	1:B:139:VAL:HG12	2.02	0.59
1:B:151:VAL:HG12	1:B:153:THR:HG23	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LYS:CB	1:B:171:ASP:HB3	2.33	0.58
1:A:101:LEU:N	3:A:434:HOH:O	2.36	0.58
1:B:152:THR:N	3:B:412:HOH:O	2.28	0.58
1:A:138:VAL:HG11	1:A:143:HIS:CE1	2.39	0.58
1:A:185:VAL:O	1:A:188:ILE:N	2.37	0.58
1:A:80:PHE:CD2	1:A:124:LEU:HD12	2.39	0.58
1:B:42:PRO:HD3	1:B:155:HIS:ND1	2.19	0.57
1:A:82:ASN:ND2	3:A:476:HOH:O	2.38	0.57
1:A:123:ARG:N	1:A:137:SER:O	2.38	0.56
1:C:186:ASP:O	1:C:189:VAL:HG22	2.06	0.56
1:B:91:ARG:HD3	1:B:111:VAL:HA	1.85	0.56
1:C:73:VAL:O	1:C:77:VAL:HG23	2.06	0.55
1:B:94:ARG:NH1	1:C:183:SER:OG	2.39	0.55
1:A:40:HIS:ND1	1:A:40:HIS:O	2.40	0.55
1:C:64:GLN:O	1:C:164:VAL:HB	2.07	0.55
1:C:58:CYS:HB3	1:C:182:LEU:HD11	1.89	0.54
1:A:91:ARG:N	1:A:110:MET:O	2.41	0.54
1:B:106:LEU:HD21	1:C:37:ARG:HG3	1.90	0.54
1:C:180:GLU:O	1:C:184:PHE:HB3	2.06	0.54
1:B:121:THR:CB	1:B:140:GLY:O	2.56	0.53
1:A:101:LEU:O	1:A:102:HIS:CG	2.62	0.53
1:A:40:HIS:CG	1:A:40:HIS:O	2.61	0.53
1:A:115:LEU:HG	1:A:116:PRO:HD2	1.90	0.53
1:C:131:ARG:O	1:C:132:HIS:HB2	2.09	0.52
1:A:138:VAL:HG23	1:A:148:TYR:HB3	1.92	0.52
1:B:155:HIS:HB3	1:B:163:VAL:HB	1.91	0.52
1:C:74:TRP:CH2	1:C:134:ILE:HG23	2.45	0.51
1:C:178:GLU:CG	3:C:531:HOH:O	2.57	0.51
1:C:165:VAL:HG12	1:C:166:GLU:N	2.26	0.51
1:B:58:CYS:O	1:B:59:CYS:HB2	2.09	0.51
1:A:123:ARG:O	1:A:136:PHE:CB	2.51	0.51
1:C:58:CYS:O	1:C:169:ILE:HA	2.11	0.50
1:B:105:ASP:CB	3:B:505:HOH:O	2.60	0.50
1:C:70:PRO:CA	1:C:162:THR:OG1	2.59	0.50
1:A:42:PRO:O	1:A:43:GLU:C	2.49	0.50
1:B:57:GLN:HA	1:B:171:ASP:HA	1.93	0.50
1:A:41:VAL:N	1:A:42:PRO:CD	2.75	0.50
1:C:166:GLU:HG2	1:C:193:LEU:HD11	1.94	0.50
1:B:62:VAL:HG22	1:B:63:VAL:N	2.27	0.50
1:A:115:LEU:HG	1:A:116:PRO:CD	2.41	0.50
1:C:47:MET:SD	1:C:47:MET:N	2.85	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:VAL:HG23	1:C:118:VAL:O	2.11	0.49
1:C:85:VAL:HG22	1:C:85:VAL:O	2.13	0.49
1:B:155:HIS:CG	1:B:156:ALA:H	2.30	0.49
1:A:90:ILE:HG22	1:A:91:ARG:N	2.28	0.49
1:A:78:ARG:NH1	3:A:434:HOH:O	2.45	0.48
1:A:84:LYS:O	1:A:85:VAL:C	2.50	0.48
1:C:195:SER:O	1:C:198:ARG:HG3	2.13	0.48
1:A:195:SER:HA	1:A:198:ARG:HG2	1.95	0.48
1:A:122:GLU:HG3	1:A:138:VAL:HG22	1.96	0.48
1:B:79:ARG:NH2	1:B:82:ASN:HB3	2.28	0.48
1:B:93:CYS:HA	1:B:108:GLU:O	2.13	0.48
1:B:90:ILE:HG23	1:B:109:VAL:HG13	1.94	0.47
1:A:188:ILE:O	3:A:491:HOH:O	2.20	0.47
1:B:118:VAL:HG12	1:B:142:ASP:O	2.14	0.47
1:B:151:VAL:CG1	1:B:153:THR:HG23	2.45	0.47
1:C:181:THR:HA	1:C:184:PHE:HB3	1.96	0.47
1:C:125:GLU:HG3	1:C:135:SER:HB3	1.96	0.47
1:C:53:VAL:CG1	1:C:54:GLY:N	2.77	0.47
1:B:83:PRO:HG2	1:B:90:ILE:HG21	1.97	0.47
1:A:150:SER:OG	1:A:166:GLU:OE1	2.32	0.47
1:A:128:ASP:OD1	1:A:131:ARG:HB2	2.15	0.46
1:A:74:TRP:CE3	1:A:132:HIS:HB3	2.50	0.46
1:C:180:GLU:O	1:C:184:PHE:CB	2.63	0.46
1:C:74:TRP:HH2	1:C:134:ILE:HG23	1.78	0.46
1:B:59:CYS:SG	1:B:169:ILE:CB	3.03	0.46
1:B:152:THR:HA	1:B:166:GLU:HB2	1.96	0.46
1:B:132:HIS:CB	1:B:154:LEU:HB2	2.45	0.46
1:B:133:VAL:HG13	1:B:153:THR:HG22	1.96	0.46
1:C:188:ILE:HA	1:C:191:CYS:SG	2.56	0.46
1:C:132:HIS:HD2	1:C:154:LEU:HD22	1.77	0.46
1:B:93:CYS:SG	1:B:107:ARG:CD	3.05	0.45
1:A:120:SER:OG	1:A:122:GLU:CD	2.55	0.45
1:B:56:ASP:O	1:B:172:VAL:N	2.48	0.45
1:B:201:ASN:HB3	3:B:526:HOH:O	2.16	0.45
1:B:62:VAL:CG1	1:B:166:GLU:H	2.30	0.45
1:A:149:ARG:HG2	1:A:149:ARG:O	2.17	0.45
1:B:89:PHE:O	1:B:91:ARG:NH1	2.42	0.45
1:A:192:ASN:O	1:A:196:LEU:N	2.41	0.45
1:C:138:VAL:HG23	1:C:148:TYR:HB3	1.99	0.45
1:B:62:VAL:HG13	1:B:165:VAL:HA	1.99	0.45
1:A:69:PRO:O	1:A:73:VAL:HG23	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ARG:O	1:C:80:PHE:C	2.55	0.45
1:A:109:VAL:O	1:A:120:SER:O	2.34	0.44
1:C:138:VAL:HG12	1:C:139:VAL:N	2.32	0.44
1:B:188:ILE:O	1:B:192:ASN:N	2.51	0.44
1:A:79:ARG:HB2	1:A:85:VAL:HG21	1.98	0.44
1:A:83:PRO:CD	1:A:93:CYS:SG	3.06	0.44
1:A:153:THR:O	1:A:154:LEU:HD23	2.17	0.44
1:A:95:ILE:HA	1:A:106:LEU:O	2.18	0.44
1:B:65:MET:CG	1:B:163:VAL:HG22	2.47	0.44
1:B:125:GLU:OE2	1:B:137:SER:HB3	2.18	0.44
1:C:66:ILE:HG12	1:C:197:ALA:HA	1.99	0.44
1:C:181:THR:O	1:C:185:VAL:N	2.42	0.44
1:A:180:GLU:OE1	1:A:180:GLU:N	2.51	0.44
1:C:64:GLN:HG2	1:C:193:LEU:O	2.17	0.44
1:C:138:VAL:CG1	1:C:139:VAL:N	2.81	0.44
1:A:106:LEU:HD12	1:A:122:GLU:O	2.18	0.44
1:B:74:TRP:CE3	1:B:77:VAL:HG23	2.53	0.44
1:C:57:GLN:HA	1:C:170:VAL:O	2.18	0.43
1:B:62:VAL:HG12	1:B:166:GLU:H	1.83	0.43
1:B:135:SER:OG	1:B:150:SER:O	2.31	0.43
1:A:179:GLU:C	1:A:180:GLU:OE1	2.55	0.43
1:A:77:VAL:HG11	1:A:154:LEU:HD11	2.00	0.43
1:C:162:THR:HG22	1:C:163:VAL:N	2.33	0.43
1:C:121:THR:HG21	1:C:139:VAL:HG12	2.01	0.43
1:B:184:PHE:CG	1:B:184:PHE:O	2.72	0.43
1:B:83:PRO:HD2	1:B:93:CYS:CB	2.49	0.43
1:C:166:GLU:CG	1:C:193:LEU:HD11	2.49	0.43
1:B:128:ASP:OD1	1:B:129:GLU:N	2.53	0.42
1:A:41:VAL:HB	1:A:163:VAL:HG21	2.01	0.42
1:B:67:HIS:HB3	1:B:201:ASN:ND2	2.35	0.42
1:B:58:CYS:O	1:B:169:ILE:HA	2.19	0.42
1:C:121:THR:HB	1:C:139:VAL:O	2.20	0.42
1:A:125:GLU:O	1:A:126:ILE:HD12	2.19	0.42
1:B:187:THR:O	1:B:191:CYS:N	2.44	0.42
1:C:78:ARG:NE	1:C:129:GLU:OE2	2.53	0.42
1:B:83:PRO:HB2	1:B:87:LYS:HB2	2.02	0.41
1:A:83:PRO:HD2	1:A:93:CYS:SG	2.61	0.41
1:B:93:CYS:SG	1:B:107:ARG:HD2	2.60	0.41
1:A:82:ASN:HD22	1:A:82:ASN:HA	1.73	0.41
1:A:107:ARG:HG3	1:A:108:GLU:N	2.35	0.41
1:A:51:HIS:C	1:A:51:HIS:CD2	2.93	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:PRO:N	1:C:162:THR:OG1	2.53	0.41
1:A:133:VAL:HG13	1:A:153:THR:HG22	2.03	0.41
1:A:125:GLU:C	1:A:126:ILE:HD12	2.41	0.41
1:C:59:CYS:HB3	1:C:168:TYR:O	2.20	0.41
1:A:138:VAL:CG1	1:A:143:HIS:CE1	3.02	0.41
1:B:155:HIS:CG	1:B:156:ALA:N	2.89	0.41
1:C:201:ASN:O	1:C:202:ARG:CB	2.69	0.41
1:B:62:VAL:CG2	1:B:63:VAL:N	2.84	0.41
1:B:65:MET:HG2	1:B:163:VAL:HA	2.02	0.41
1:B:83:PRO:HD2	1:B:93:CYS:HB3	2.02	0.41
1:B:83:PRO:HD3	1:B:93:CYS:SG	2.61	0.41
1:C:165:VAL:HG12	1:C:166:GLU:H	1.86	0.41
1:A:90:ILE:HG22	1:A:91:ARG:O	2.20	0.41
1:C:122:GLU:HG3	1:C:123:ARG:H	1.85	0.41
1:C:173:PRO:O	1:C:174:PRO:C	2.58	0.41
1:A:84:LYS:O	1:A:86:TYR:N	2.53	0.41
1:C:49:HIS:NE2	1:C:153:THR:OG1	2.36	0.40
1:B:190:ARG:NH2	3:B:508:HOH:O	2.54	0.40
1:A:122:GLU:HA	1:A:137:SER:O	2.21	0.40
1:B:48:HIS:HB3	1:B:151:VAL:HG11	2.03	0.40
1:B:54:GLY:HA3	1:B:57:GLN:HB2	2.03	0.40
1:B:125:GLU:OE1	1:B:149:ARG:NE	2.55	0.40
1:C:178:GLU:HG2	3:C:531:HOH:O	2.19	0.40
1:B:65:MET:SD	1:B:163:VAL:HG22	2.61	0.40
1:B:168:TYR:CG	1:B:169:ILE:N	2.90	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	145/223 (65%)	104 (72%)	31 (21%)	10 (7%)	<b>1</b> <b>1</b>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	146/223 (66%)	106 (73%)	31 (21%)	9 (6%)	2	2
1	C	116/223 (52%)	85 (73%)	24 (21%)	7 (6%)	2	2
All	All	407/669 (61%)	295 (72%)	86 (21%)	26 (6%)	2	2

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	116	PRO
1	A	118	VAL
1	C	170	VAL
1	A	79	ARG
1	A	81	ASP
1	A	132	HIS
1	A	146	LYS
1	B	118	VAL
1	B	145	LEU
1	C	46	ALA
1	B	146	LYS
1	B	155	HIS
1	C	39	MET
1	C	132	HIS
1	C	174	PRO
1	A	50	THR
1	A	85	VAL
1	B	170	VAL
1	C	48	HIS
1	B	45	VAL
1	B	59	CYS
1	A	173	PRO
1	B	79	ARG
1	C	118	VAL
1	B	38	GLY

### 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	116/200 (58%)	89 (77%)	27 (23%)	1	2
1	B	112/200 (56%)	91 (81%)	21 (19%)	2	4
1	C	101/200 (50%)	82 (81%)	19 (19%)	2	4
All	All	329/600 (55%)	262 (80%)	67 (20%)	1	3

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	44	HIS
1	A	51	HIS
1	A	52	ASP
1	A	58	CYS
1	A	60	SER
1	A	67	HIS
1	A	77	VAL
1	A	84	LYS
1	A	93	CYS
1	A	94	ARG
1	A	101	LEU
1	A	105	ASP
1	A	107	ARG
1	A	111	VAL
1	A	118	VAL
1	A	119	SER
1	A	124	LEU
1	A	127	LEU
1	A	130	GLU
1	A	135	SER
1	A	148	TYR
1	A	168	TYR
1	A	176	ASN
1	A	177	THR
1	A	179	GLU
1	A	186	ASP
1	B	47	MET
1	B	53	VAL
1	B	60	SER
1	B	71	GLU
1	B	73	VAL
1	B	84	LYS
1	B	85	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	86	TYR
1	B	94	ARG
1	B	106	LEU
1	B	118	VAL
1	B	127	LEU
1	B	136	PHE
1	B	143	HIS
1	B	149	ARG
1	B	155	HIS
1	B	176	ASN
1	B	186	ASP
1	B	199	SER
1	B	200	THR
1	B	201	ASN
1	C	37	ARG
1	C	43	GLU
1	C	47	MET
1	C	58	CYS
1	C	59	CYS
1	C	65	MET
1	C	77	VAL
1	C	127	LEU
1	C	147	ASN
1	C	150	SER
1	C	166	GLU
1	C	169	ILE
1	C	171	ASP
1	C	177	THR
1	C	184	PHE
1	C	190	ARG
1	C	191	CYS
1	C	198	ARG
1	C	200	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	51	HIS
1	A	82	ASN
1	A	92	GLN
1	B	67	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	102	HIS
1	B	143	HIS
1	B	192	ASN
1	B	201	ASN
1	C	132	HIS
1	C	201	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

12 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	$\# Z  > 2$
2	GOL	A	301	-	5,5,5	0.29	0	5,5,5	0.49	0
2	GOL	A	302	-	5,5,5	0.44	0	5,5,5	0.67	0
2	GOL	A	303	-	5,5,5	0.51	0	5,5,5	0.47	0
2	GOL	A	304	-	5,5,5	0.35	0	5,5,5	0.36	0
2	GOL	A	305	-	5,5,5	0.31	0	5,5,5	0.36	0
2	GOL	A	306	-	5,5,5	0.46	0	5,5,5	0.51	0
2	GOL	A	307	-	5,5,5	0.36	0	5,5,5	0.61	0
2	GOL	B	301	-	5,5,5	0.21	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	B	302	-	5,5,5	0.44	0	5,5,5	0.25	0
2	GOL	B	303	-	5,5,5	0.44	0	5,5,5	0.43	0
2	GOL	B	304	-	5,5,5	0.39	0	5,5,5	0.47	0
2	GOL	C	301	-	5,5,5	0.54	0	5,5,5	0.52	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
2	GOL	A	301	-	-	0/4/4/4	0/0/0/0
2	GOL	A	302	-	-	0/4/4/4	0/0/0/0
2	GOL	A	303	-	-	0/4/4/4	0/0/0/0
2	GOL	A	304	-	-	0/4/4/4	0/0/0/0
2	GOL	A	305	-	-	0/4/4/4	0/0/0/0
2	GOL	A	306	-	-	0/4/4/4	0/0/0/0
2	GOL	A	307	-	-	0/4/4/4	0/0/0/0
2	GOL	B	301	-	-	0/4/4/4	0/0/0/0
2	GOL	B	302	-	-	0/4/4/4	0/0/0/0
2	GOL	B	303	-	-	0/4/4/4	0/0/0/0
2	GOL	B	304	-	-	0/4/4/4	0/0/0/0
2	GOL	C	301	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 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	153/223 (68%)	0.18	7 (4%) 36 34	33, 50, 68, 79	0
1	B	154/223 (69%)	0.11	4 (2%) 59 58	34, 49, 62, 76	1 (0%)
1	C	126/223 (56%)	0.07	3 (2%) 62 60	34, 49, 65, 79	0
All	All	433/669 (64%)	0.13	14 (3%) 51 50	33, 49, 65, 79	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	VAL	5.0
1	A	39	MET	3.9
1	B	182	LEU	3.7
1	A	56	ASP	3.4
1	B	44	HIS	3.1
1	A	62	VAL	3.1
1	A	38	GLY	2.7
1	C	182	LEU	2.7
1	C	62	VAL	2.4
1	A	146	LYS	2.1
1	C	55	PRO	2.1
1	B	48	HIS	2.1
1	A	170	VAL	2.0
1	B	168	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 [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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	A	301	6/6	0.95	0.12	-	15,15,16,16	0
2	GOL	B	301	6/6	0.89	0.09	-	39,39,43,43	0
2	GOL	A	305	6/6	0.92	0.14	-	30,32,33,34	0
2	GOL	B	302	6/6	0.72	0.19	-	40,46,48,48	0
2	GOL	A	303	6/6	0.81	0.26	-	30,33,34,34	0
2	GOL	A	304	6/6	0.89	0.12	-	40,41,43,43	0
2	GOL	A	307	6/6	0.84	0.15	-	37,39,42,45	0
2	GOL	B	303	6/6	0.85	0.11	-	37,40,41,41	0
2	GOL	A	302	6/6	0.84	0.11	-	28,30,32,33	0
2	GOL	B	304	6/6	0.81	0.17	-	44,45,47,47	0
2	GOL	A	306	6/6	0.85	0.12	-	42,45,47,47	0
2	GOL	C	301	6/6	0.87	0.17	-	24,24,25,26	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.