



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2024 – 02:39 AM EDT

PDB ID : 6L9J  
Title : Structure of yeast Snf5 and Swi3 subcomplex  
Authors : Long, J.; Zhou, H.  
Deposited on : 2019-11-10  
Resolution : 2.64 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
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) : 2.37.1

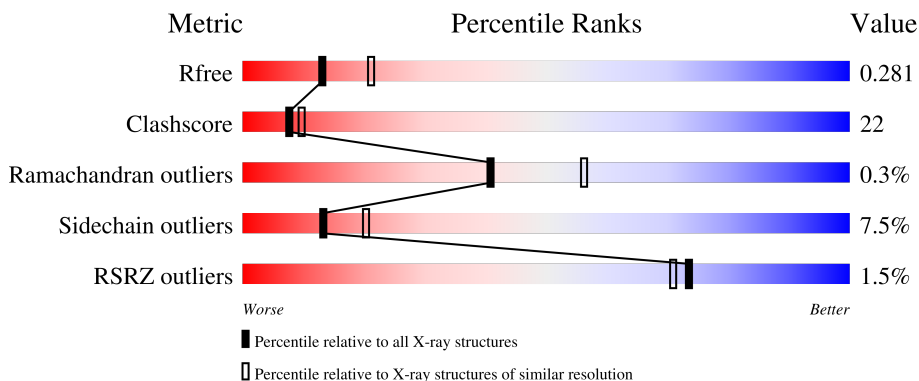
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 of 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	227	
1	D	227	
1	G	227	
1	J	227	
2	B	187	

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Mol	Chain	Length	Quality of chain
2	C	187	 26% 22% 48%
2	E	187	 % 33% 19% 47%
2	F	187	 25% 25% 49%
2	H	187	 % 36% 15% 48%
2	I	187	 % 29% 21% 49%
2	K	187	 % 35% 13% 50%
2	L	187	 35% 15% 49%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13745 atoms, of which 72 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 SWI/SNF chromatin-remodeling complex subunit SNF5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	209	Total 1722	C 1078	N 293	O 344	S 7	0	0	0
1	D	213	Total 1760	C 1102	N 300	O 351	S 7	0	0	0
1	G	210	Total 1739	C 1090	N 297	O 345	S 7	0	0	0
1	J	207	Total 1706	C 1068	N 290	O 341	S 7	0	0	0

- Molecule 2 is a protein called SWI/SNF complex subunit SWI3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	94	Total 793	C 516	N 138	O 137	S 2	0	0	0
2	C	97	Total 817	C 530	N 142	O 143	S 2	0	0	0
2	E	99	Total 832	C 539	N 145	O 146	S 2	0	0	0
2	F	95	Total 801	C 520	N 139	O 140	S 2	0	0	0
2	H	97	Total 816	C 529	N 142	O 143	S 2	0	0	0
2	I	95	Total 801	C 520	N 139	O 140	S 2	0	0	0
2	K	94	Total 793	C 516	N 138	O 137	S 2	0	0	0
2	L	95	Total 801	C 520	N 139	O 140	S 2	0	0	0

- Molecule 3 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
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	F	1	Total	C	H	O	0	0
			14	3	8	3		
3	H	1	Total	C	H	O	0	0
			14	3	8	3		
3	K	1	Total	C	H	O	0	0
			14	3	8	3		
3	L	1	Total	C	H	O	0	0
			14	3	8	3		
3	L	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total	O	0	0
			27	27		
4	B	20	Total	O	0	0
			20	20		
4	C	14	Total	O	0	0
			14	14		

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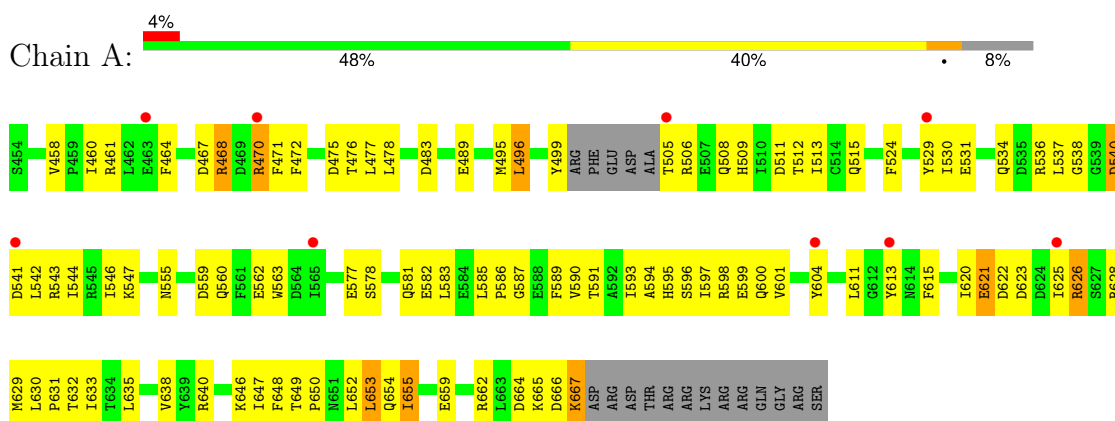
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	D	28	Total 28	O 28	0	0
4	E	14	Total 14	O 14	0	0
4	F	15	Total 15	O 15	0	0
4	G	25	Total 25	O 25	0	0
4	H	16	Total 16	O 16	0	0
4	I	13	Total 13	O 13	0	0
4	J	34	Total 34	O 34	0	0
4	K	19	Total 19	O 19	0	0
4	L	13	Total 13	O 13	0	0

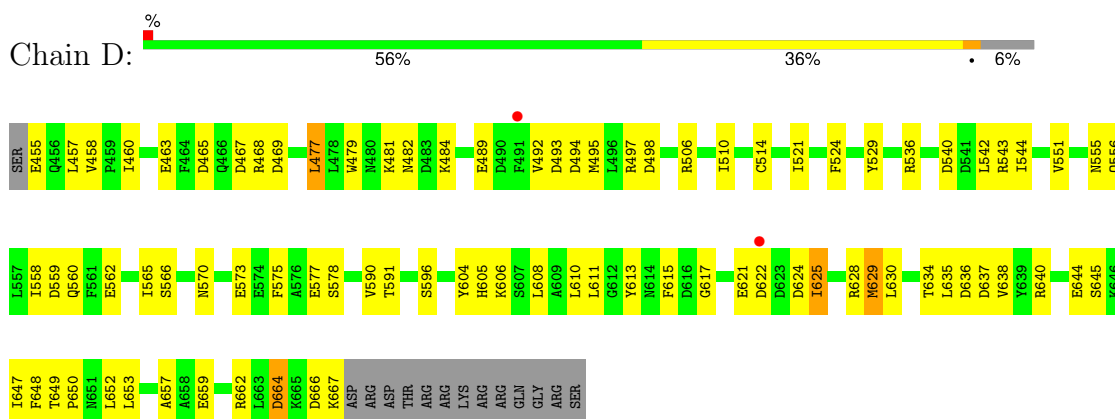
### 3 Residue-property plots i

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.

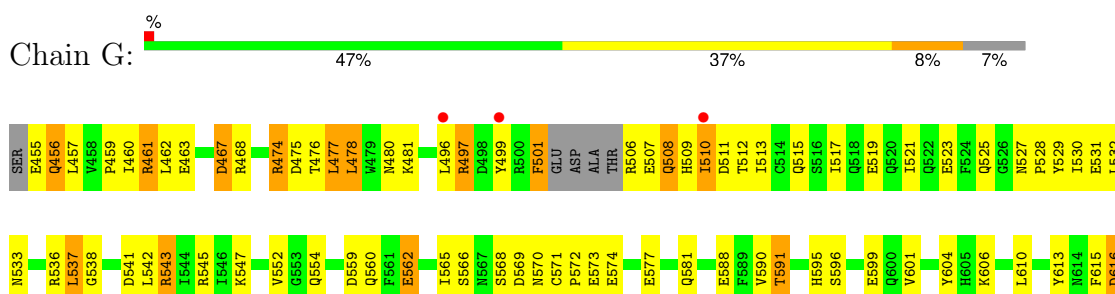
- Molecule 1: SWI/SNF chromatin-remodeling complex subunit SNF5



- Molecule 1: SWI/SNF chromatin-remodeling complex subunit SNF5

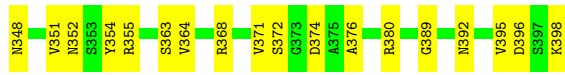
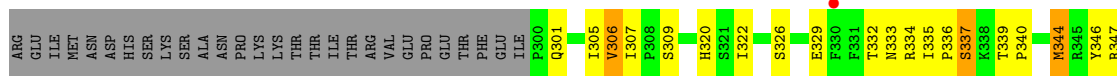


- Molecule 1: SWI/SNF chromatin-remodeling complex subunit SNF5

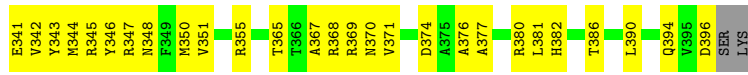
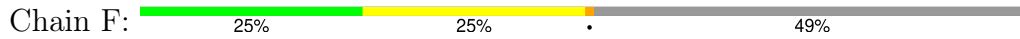




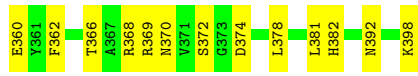
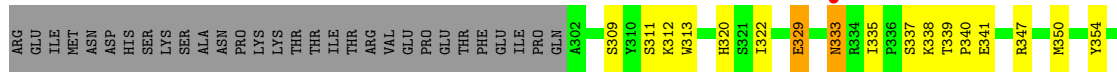
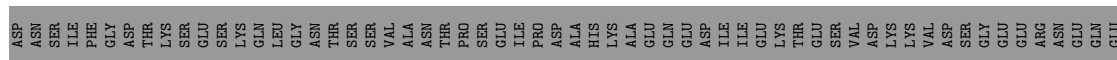
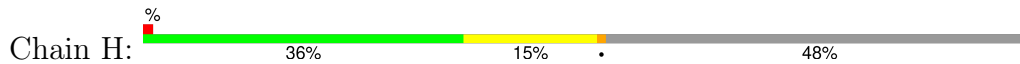




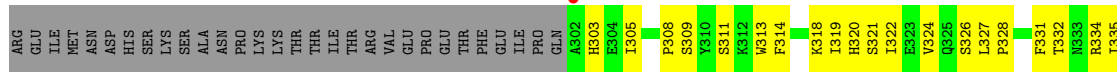
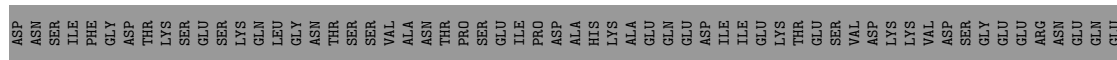
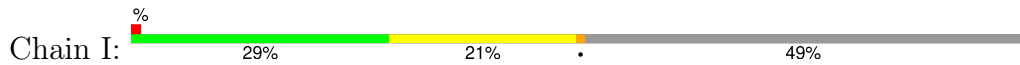
● Molecule 2: SWI/SNF complex subunit SWI3



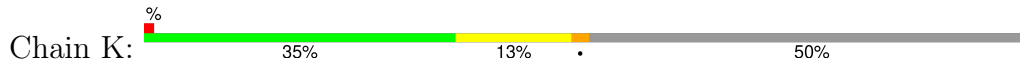
● Molecule 2: SWI/SNF complex subunit SWI3

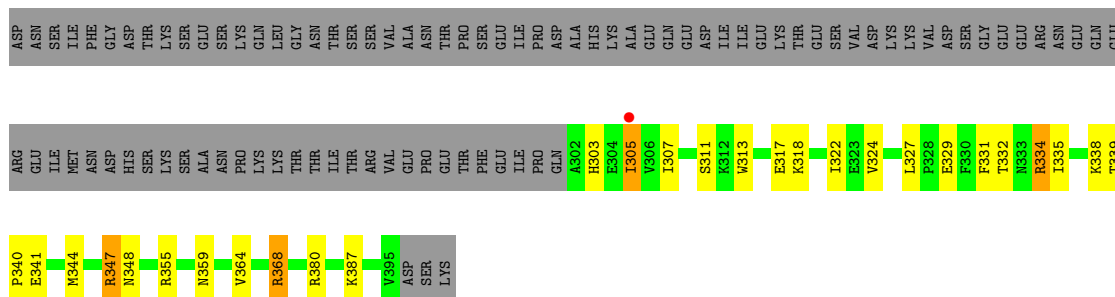


● Molecule 2: SWI/SNF complex subunit SWI3



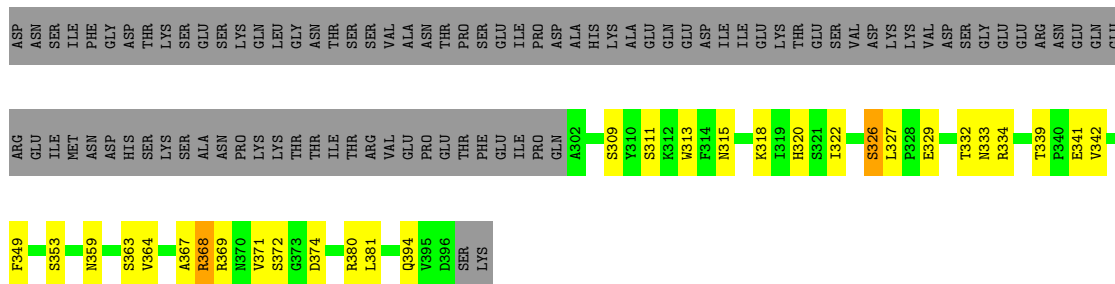
● Molecule 2: SWI/SNF complex subunit SWI3





- Molecule 2: SWI/SNF complex subunit SWI3

Chain L: 35% 15% 49%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	205.52Å 146.46Å 154.33Å 90.00° 131.20° 90.00°	Depositor
Resolution (Å)	48.62 – 2.64 48.62 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.62-2.64) 96.9 (48.62-2.64)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.65Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.229 , 0.280 0.231 , 0.281	Depositor DCC
$R_{free}$ test set	4879 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.7	Xtrriage
Anisotropy	0.802	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 16.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.096 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13745	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: 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	0.40	0/1750	0.55	0/2363
1	D	0.44	0/1790	0.54	0/2418
1	G	0.43	0/1768	0.56	0/2386
1	J	0.46	1/1734 (0.1%)	0.54	0/2342
2	B	0.51	0/817	0.55	0/1108
2	C	0.47	0/842	0.59	0/1142
2	E	0.51	0/857	0.56	0/1161
2	F	0.51	0/825	0.55	0/1119
2	H	0.52	0/840	0.53	0/1138
2	I	0.48	0/825	0.57	0/1119
2	K	0.47	0/817	0.54	0/1108
2	L	0.48	0/825	0.56	0/1119
All	All	0.46	1/13690 (0.0%)	0.55	0/18523

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	G	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	580	CYS	CB-SG	-6.31	1.71	1.82

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	616	ASP	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	1722	0	1661	89	0
1	D	1760	0	1694	82	0
1	G	1739	0	1675	118	0
1	J	1706	0	1641	81	0
2	B	793	0	782	24	2
2	C	817	0	802	46	0
2	E	832	0	820	24	2
2	F	801	0	786	50	0
2	H	816	0	804	22	1
2	I	801	0	786	47	0
2	K	793	0	782	25	1
2	L	801	0	786	33	0
3	E	24	32	32	1	0
3	F	6	8	8	0	0
3	H	6	8	8	2	0
3	K	6	8	8	2	0
3	L	12	16	16	0	0
4	A	27	0	0	1	0
4	B	20	0	0	6	0
4	C	14	0	0	1	0
4	D	28	0	0	2	0
4	E	14	0	0	2	0
4	F	15	0	0	2	0
4	G	25	0	0	2	0
4	H	16	0	0	1	0
4	I	13	0	0	1	0
4	J	34	0	0	3	0
4	K	19	0	0	4	0
4	L	13	0	0	1	0
All	All	13673	72	13091	580	3

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 22.

The worst 5 of 580 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)
2:I:369:ARG:NH1	1:J:659:GLU:OE1	1.88	1.06
1:G:541:ASP:HB2	2:I:335:ILE:HD11	1.36	1.05
1:J:570:ASN:OD1	2:L:380:ARG:NH2	1.95	1.00
1:D:460:ILE:HB	1:D:477:LEU:HD22	1.45	0.98
1:G:570:ASN:OD1	2:I:380:ARG:NH2	1.96	0.98

All (3) 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:E:398:LYS:O	2:K:380:ARG:NH1[3_445]	2.06	0.14
2:B:380:ARG:NH1	2:H:398:LYS:O[3_444]	2.16	0.04
2:B:319:ILE:O	2:E:334:ARG:NH1[4_647]	2.19	0.01

## 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	205/227 (90%)	184 (90%)	20 (10%)	1 (0%)	29	43
1	D	211/227 (93%)	195 (92%)	15 (7%)	1 (0%)	29	43
1	G	206/227 (91%)	186 (90%)	20 (10%)	0	100	100
1	J	203/227 (89%)	186 (92%)	15 (7%)	2 (1%)	15	22
2	B	92/187 (49%)	91 (99%)	1 (1%)	0	100	100
2	C	95/187 (51%)	88 (93%)	7 (7%)	0	100	100
2	E	97/187 (52%)	92 (95%)	5 (5%)	0	100	100
2	F	93/187 (50%)	83 (89%)	10 (11%)	0	100	100
2	H	95/187 (51%)	90 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	93/187 (50%)	84 (90%)	9 (10%)	0	100	100
2	K	92/187 (49%)	89 (97%)	3 (3%)	0	100	100
2	L	93/187 (50%)	86 (92%)	6 (6%)	1 (1%)	14	20
All	All	1575/2404 (66%)	1454 (92%)	116 (7%)	5 (0%)	41	56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	333	ASN
1	J	580	CYS
1	A	665	LYS
1	J	470	ARG
1	D	664	ASP

### 5.3.2 Protein sidechains [i](#)

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	193/209 (92%)	177 (92%)	16 (8%)	11	16
1	D	196/209 (94%)	187 (95%)	9 (5%)	27	41
1	G	194/209 (93%)	172 (89%)	22 (11%)	6	7
1	J	191/209 (91%)	179 (94%)	12 (6%)	18	27
2	B	87/173 (50%)	80 (92%)	7 (8%)	12	18
2	C	90/173 (52%)	78 (87%)	12 (13%)	4	4
2	E	92/173 (53%)	85 (92%)	7 (8%)	13	20
2	F	88/173 (51%)	85 (97%)	3 (3%)	37	53
2	H	90/173 (52%)	83 (92%)	7 (8%)	12	19
2	I	88/173 (51%)	83 (94%)	5 (6%)	20	31
2	K	87/173 (50%)	81 (93%)	6 (7%)	15	23
2	L	88/173 (51%)	83 (94%)	5 (6%)	20	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1484/2220 (67%)	1373 (92%)	111 (8%)	13	20

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	474	ARG
2	L	368	ARG
1	G	645	SER
2	L	359	ASN
1	J	662	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	555	ASN
1	G	525	GLN
2	H	382	HIS
1	J	456	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](#)

9 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
3	GOL	H	401	-	5,5,5	0.23	0	5,5,5	0.83	0
3	GOL	E	402	-	5,5,5	0.71	0	5,5,5	0.78	0
3	GOL	E	401	-	5,5,5	0.46	0	5,5,5	0.37	0
3	GOL	L	402	-	5,5,5	0.50	0	5,5,5	0.26	0
3	GOL	F	401	-	5,5,5	0.52	0	5,5,5	0.39	0
3	GOL	E	403	-	5,5,5	0.52	0	5,5,5	0.19	0
3	GOL	L	401	-	5,5,5	0.41	0	5,5,5	0.44	0
3	GOL	E	404	-	5,5,5	0.38	0	5,5,5	0.16	0
3	GOL	K	401	-	5,5,5	0.47	0	5,5,5	0.13	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	GOL	H	401	-	-	1/4/4/4	-
3	GOL	E	402	-	-	1/4/4/4	-
3	GOL	E	401	-	-	4/4/4/4	-
3	GOL	L	402	-	-	2/4/4/4	-
3	GOL	F	401	-	-	4/4/4/4	-
3	GOL	E	403	-	-	2/4/4/4	-
3	GOL	L	401	-	-	3/4/4/4	-
3	GOL	E	404	-	-	2/4/4/4	-
3	GOL	K	401	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	404	GOL	C1-C2-C3-O3
3	F	401	GOL	O1-C1-C2-O2
3	F	401	GOL	O1-C1-C2-C3
3	F	401	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	K	401	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	401	GOL	2	0
3	E	401	GOL	1	0
3	K	401	GOL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	209/227 (92%)	0.31	9 (4%) 35 31	29, 45, 81, 94	0
1	D	213/227 (93%)	0.14	2 (0%) 84 83	27, 46, 66, 78	0
1	G	210/227 (92%)	0.18	3 (1%) 75 73	28, 44, 74, 88	0
1	J	207/227 (91%)	0.22	4 (1%) 66 64	30, 45, 74, 94	0
2	B	94/187 (50%)	0.23	2 (2%) 63 60	26, 34, 52, 73	0
2	C	97/187 (51%)	0.14	0 100 100	33, 42, 62, 85	0
2	E	99/187 (52%)	0.25	1 (1%) 82 81	26, 34, 62, 79	0
2	F	95/187 (50%)	0.14	0 100 100	31, 41, 58, 73	0
2	H	97/187 (51%)	0.17	1 (1%) 82 81	26, 33, 50, 64	0
2	I	95/187 (50%)	0.02	1 (1%) 80 78	29, 40, 60, 79	0
2	K	94/187 (50%)	0.24	1 (1%) 80 78	30, 37, 59, 65	0
2	L	95/187 (50%)	-0.05	0 100 100	30, 41, 56, 61	0
All	All	1605/2404 (66%)	0.18	24 (1%) 73 71	26, 41, 71, 94	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	305	ILE	4.5
1	G	510	ILE	3.6
1	J	510	ILE	3.5
1	J	620	ILE	3.5
1	A	505	THR	3.4

### 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, 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(Å <sup>2</sup> )	Q<0.9
3	GOL	F	401	6/6	0.78	0.27	29,48,59,68	0
3	GOL	E	403	6/6	0.79	0.17	33,52,60,63	0
3	GOL	E	404	6/6	0.82	0.19	43,52,62,69	0
3	GOL	E	401	6/6	0.82	0.14	43,53,63,63	0
3	GOL	K	401	6/6	0.82	0.15	51,62,70,70	0
3	GOL	L	401	6/6	0.83	0.17	50,60,64,65	0
3	GOL	L	402	6/6	0.84	0.19	47,57,62,64	0
3	GOL	E	402	6/6	0.88	0.26	28,36,41,48	0
3	GOL	H	401	6/6	0.90	0.16	46,59,71,71	0

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

There are no such residues in this entry.