



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:10 pm BST

PDB ID : 6CH2  
Title : Crystal structure of the cytoplasmic domain of FlhA and FliT-FliD complex  
Authors : Xing, Q.; Shi, K.; Kalodimos, C.G.  
Deposited on : 2018-02-21  
Resolution : 2.70 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.

---

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  
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

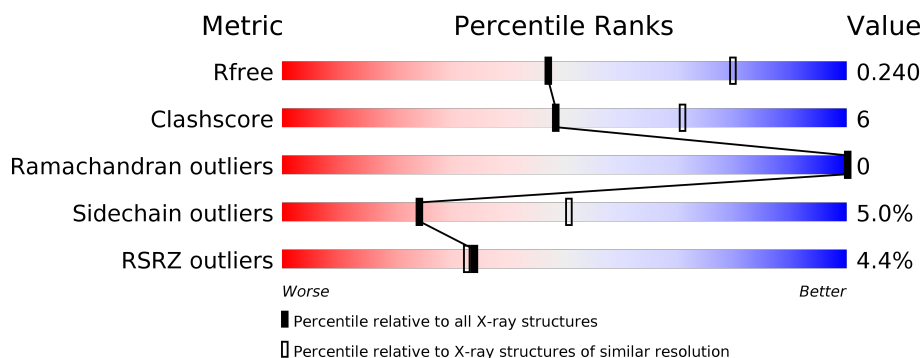
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	334	<div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	B	334	<div> <div>%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>
1	C	334	<div> <div>%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>
2	D	179	<div> <div>6%</div> <div>67%</div> <div>13%</div> <div>•</div> <div>20%</div> </div>
2	E	179	<div> <div>4%</div> <div>69%</div> <div>12%</div> <div>•</div> <div>18%</div> </div>
2	F	179	<div> <div>20%</div> <div>62%</div> <div>17%</div> <div>•</div> <div>20%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11214 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 Flagellar biosynthesis protein FlhA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2562	1621	458	474	9			
1	B	332	Total	C	N	O	S	0	0	0
			2568	1625	459	475	9			
1	C	329	Total	C	N	O	S	0	0	0
			2552	1617	455	471	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	GLY	-	expression tag	UNP P40729
B	359	GLY	-	expression tag	UNP P40729
C	359	GLY	-	expression tag	UNP P40729

- Molecule 2 is a protein called Flagellar hook-associated protein 2,Flagellar protein FliT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	144	Total	C	N	O	S	0	0	0
			1154	720	198	231	5			
2	E	147	Total	C	N	O	S	0	0	0
			1178	734	204	234	6			
2	F	143	Total	C	N	O	S	0	0	0
			1147	719	198	225	5			

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	GLY	-	expression tag	UNP P16328
D	2	ALA	-	expression tag	UNP P16328
D	3	HIS	-	expression tag	UNP P16328
D	4	MET	-	expression tag	UNP P16328
D	45	GLY	-	linker	UNP P16328

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	46	GLY	-	linker	UNP P16328
D	47	SER	-	linker	UNP P16328
D	48	GLY	-	linker	UNP P16328
D	49	GLY	-	linker	UNP P16328
D	50	SER	-	linker	UNP P16328
D	51	GLY	-	linker	UNP P16328
D	52	SER	-	linker	UNP P16328
D	53	GLY	-	linker	UNP P16328
D	54	GLY	-	linker	UNP P16328
D	55	SER	-	linker	UNP P16328
D	56	GLY	-	linker	UNP P16328
D	57	GLY	-	linker	UNP P16328
E	1	GLY	-	expression tag	UNP P16328
E	2	ALA	-	expression tag	UNP P16328
E	3	HIS	-	expression tag	UNP P16328
E	4	MET	-	expression tag	UNP P16328
E	45	GLY	-	linker	UNP P16328
E	46	GLY	-	linker	UNP P16328
E	47	SER	-	linker	UNP P16328
E	48	GLY	-	linker	UNP P16328
E	49	GLY	-	linker	UNP P16328
E	50	SER	-	linker	UNP P16328
E	51	GLY	-	linker	UNP P16328
E	52	SER	-	linker	UNP P16328
E	53	GLY	-	linker	UNP P16328
E	54	GLY	-	linker	UNP P16328
E	55	SER	-	linker	UNP P16328
E	56	GLY	-	linker	UNP P16328
E	57	GLY	-	linker	UNP P16328
F	1	GLY	-	expression tag	UNP P16328
F	2	ALA	-	expression tag	UNP P16328
F	3	HIS	-	expression tag	UNP P16328
F	4	MET	-	expression tag	UNP P16328
F	45	GLY	-	linker	UNP P16328
F	46	GLY	-	linker	UNP P16328
F	47	SER	-	linker	UNP P16328
F	48	GLY	-	linker	UNP P16328
F	49	GLY	-	linker	UNP P16328
F	50	SER	-	linker	UNP P16328
F	51	GLY	-	linker	UNP P16328
F	52	SER	-	linker	UNP P16328
F	53	GLY	-	linker	UNP P16328

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	54	GLY	-	linker	UNP P16328
F	55	SER	-	linker	UNP P16328
F	56	GLY	-	linker	UNP P16328
F	57	GLY	-	linker	UNP P16328

- 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	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	8	Total	O	0	0
			8	8		
4	C	10	Total	O	0	0
			10	10		
4	D	6	Total	O	0	0
			6	6		
4	E	5	Total	O	0	0
			5	5		

*Continued on next page...*

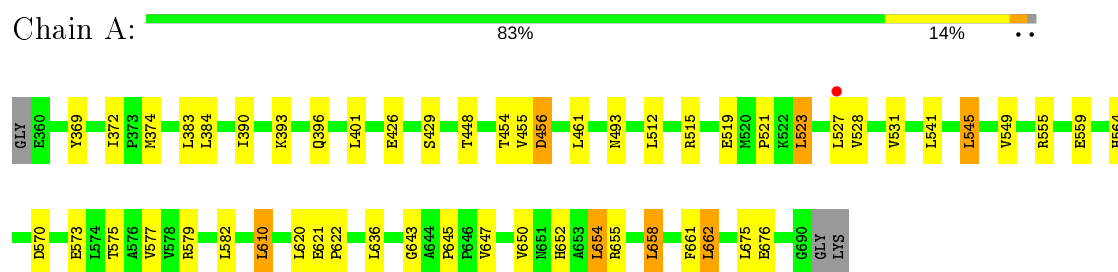
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	2	Total	O	0	0
			2	2		

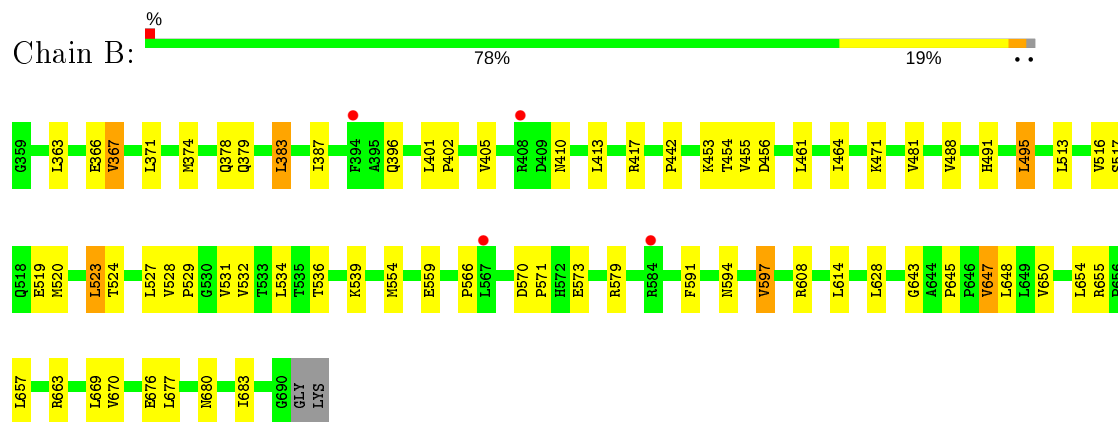
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

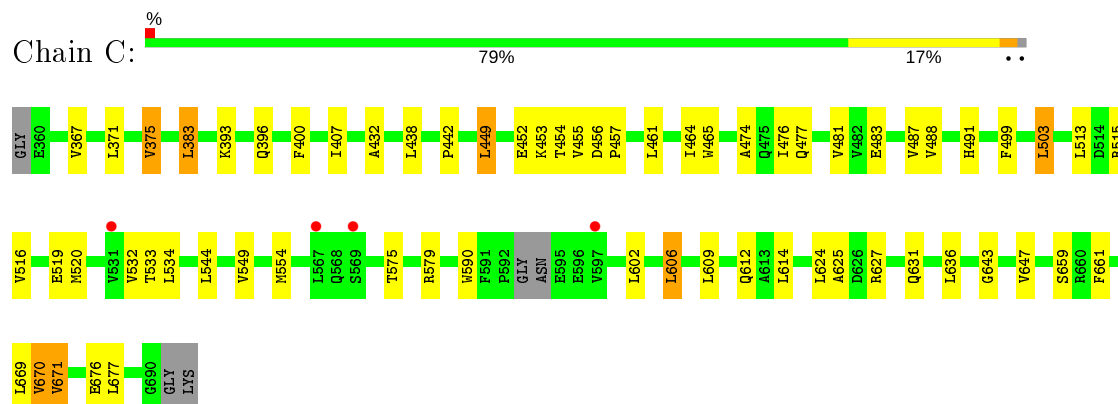
#### • Molecule 1: Flagellar biosynthesis protein FlhA



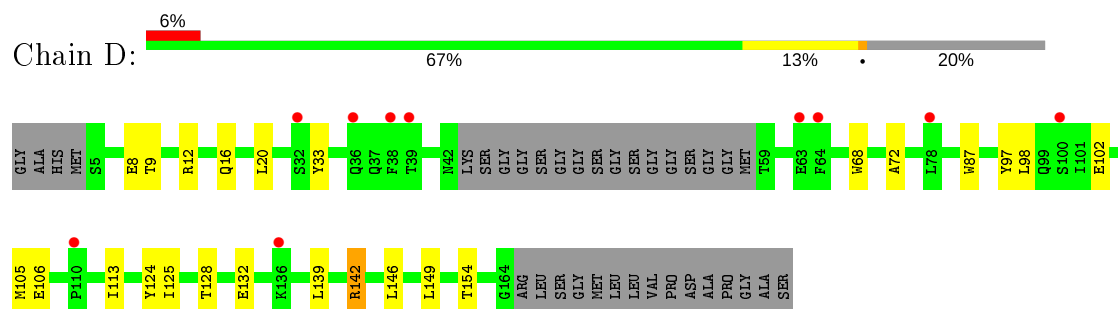
#### • Molecule 1: Flagellar biosynthesis protein FlhA



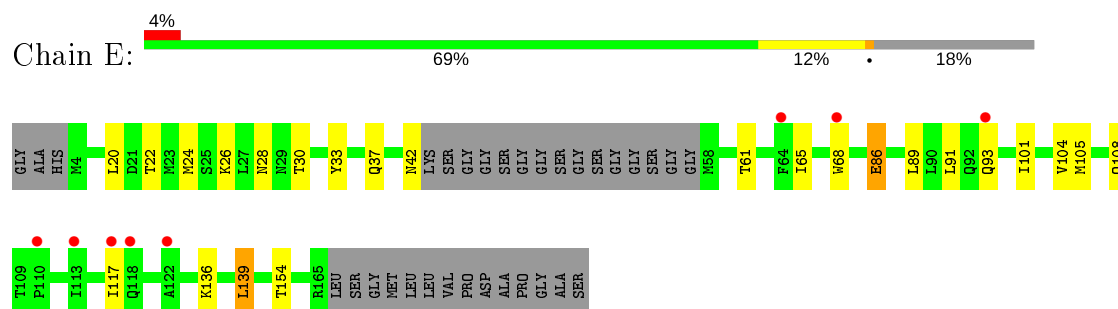
#### • Molecule 1: Flagellar biosynthesis protein FlhA



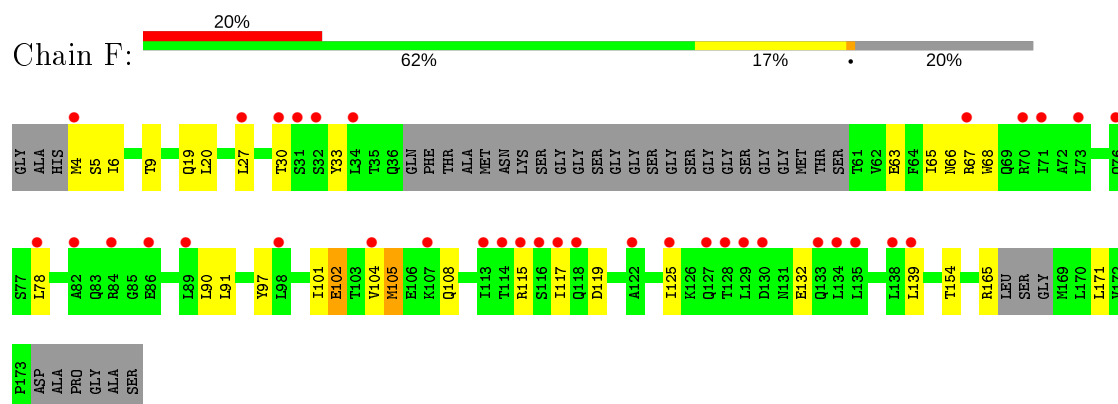
- Molecule 2: Flagellar hook-associated protein 2, Flagellar protein FliT



- Molecule 2: Flagellar hook-associated protein 2, Flagellar protein FliT



- Molecule 2: Flagellar hook-associated protein 2, Flagellar protein FliT





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.11Å 77.59Å 119.27Å 86.88° 89.00° 84.27°	Depositor
Resolution (Å)	39.70 – 2.70 77.09 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.0 (39.70-2.70) 92.2 (77.09-2.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 2.51Å)	Xtriage
Refinement program	PHENIX (dev_2747: ???)	Depositor
R, $R_{free}$	0.233 , 0.266 0.230 , 0.240	Depositor DCC
$R_{free}$ test set	2716 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.2	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 51.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11214	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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	0.25	0/2606	0.46	0/3538
1	B	0.26	0/2612	0.47	0/3546
1	C	0.25	0/2595	0.45	0/3522
2	D	0.24	0/1166	0.38	0/1573
2	E	0.24	0/1190	0.40	0/1604
2	F	0.24	0/1158	0.40	0/1561
All	All	0.25	0/11327	0.44	0/15344

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2562	0	2622	28	0
1	B	2568	0	2632	40	0
1	C	2552	0	2619	31	0
2	D	1154	0	1160	14	0
2	E	1178	0	1184	12	0
2	F	1147	0	1165	21	0
3	A	6	0	8	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	0	0
4	A	10	0	0	0	0
4	B	8	0	0	1	0
4	C	10	0	0	0	0
4	D	6	0	0	0	0
4	E	5	0	0	0	0
4	F	2	0	0	0	0
All	All	11214	0	11398	136	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 6.

All (136) 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:400:PHE:HA	1:C:515:ARG:HH12	1.54	0.72
1:A:523:LEU:HD11	1:A:559:GLU:HG3	1.72	0.72
2:D:16:GLN:OE1	2:D:142:ARG:NH1	2.23	0.71
2:F:63:GLU:OE1	2:F:66:ASN:ND2	2.28	0.67
1:B:579:ARG:NH1	1:B:676:GLU:OE2	2.29	0.66
1:A:527:LEU:HD23	1:A:528:VAL:HG23	1.77	0.65
2:E:33:TYR:CZ	2:E:105:MET:HG2	2.32	0.65
1:B:519:GLU:HA	2:F:19:GLN:HG2	1.79	0.64
1:B:643:GLY:HA2	2:E:154:THR:HG21	1.80	0.64
1:B:523:LEU:HD11	1:B:559:GLU:HG3	1.78	0.64
1:B:454:THR:OG1	1:B:455:VAL:N	2.33	0.62
1:C:476:ILE:HD12	1:C:477:GLN:HG3	1.82	0.61
2:D:98:LEU:O	2:D:102:GLU:HG2	2.01	0.61
2:F:33:TYR:CZ	2:F:105:MET:HB3	2.36	0.61
1:A:570:ASP:HB3	1:A:573:GLU:HB2	1.83	0.60
1:B:680:ASN:HD22	2:F:108:GLN:HE21	1.49	0.60
2:D:72:ALA:HA	2:D:128:THR:HG22	1.84	0.60
2:F:20:LEU:HD22	2:F:139:LEU:HD11	1.83	0.60
2:E:22:THR:HG22	2:E:26:LYS:HE2	1.83	0.59
1:B:453:LYS:HG2	1:B:464:ILE:HG12	1.84	0.59
2:D:33:TYR:CZ	2:D:105:MET:HG2	2.37	0.59
1:C:533:THR:HG23	2:D:8:GLU:HG3	1.85	0.58
1:C:643:GLY:HA2	2:F:154:THR:HG21	1.84	0.57
1:B:471:LYS:HG3	1:B:481:VAL:HG11	1.85	0.57
1:C:454:THR:OG1	1:C:455:VAL:N	2.35	0.57
1:B:570:ASP:HB3	1:B:573:GLU:HB2	1.88	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:GLY:HA2	2:D:154:THR:HG21	1.87	0.56
1:C:636:LEU:HD21	1:C:669:LEU:HD13	1.87	0.56
1:B:374:MET:HG2	1:B:383:LEU:HB2	1.87	0.55
2:E:86:GLU:HG2	2:E:89:LEU:HD12	1.88	0.55
1:B:517:SER:HA	1:B:524:THR:HG21	1.88	0.55
2:D:97:TYR:OH	2:D:132:GLU:OE2	2.20	0.55
1:B:520:MET:HG2	1:B:523:LEU:HB2	1.89	0.54
1:B:513:LEU:HD22	1:B:534:LEU:HD23	1.89	0.54
2:F:97:TYR:OH	2:F:132:GLU:OE2	2.21	0.54
2:F:4:MET:SD	2:F:4:MET:N	2.80	0.54
1:B:591:PHE:CZ	1:B:647:VAL:HG11	2.42	0.54
1:B:367:VAL:HG13	1:B:371:LEU:HB2	1.90	0.54
2:D:20:LEU:HD22	2:D:139:LEU:HD11	1.90	0.54
2:E:24:MET:HB2	2:E:139:LEU:HD12	1.89	0.53
2:F:67:ARG:HB3	2:F:104:VAL:HG22	1.90	0.53
1:A:579:ARG:NH2	1:A:676:GLU:OE2	2.41	0.53
2:E:65:ILE:HD11	2:E:117:ILE:HG23	1.89	0.53
1:B:597:VAL:HG13	1:B:683:ILE:HA	1.90	0.53
1:B:614:LEU:HD21	1:B:657:LEU:HD22	1.91	0.52
1:B:532:VAL:HG13	1:B:536:THR:HB	1.92	0.51
2:D:9:THR:HG22	2:D:12:ARG:HH21	1.76	0.51
1:C:516:VAL:HG11	1:C:554:MET:HG3	1.93	0.51
1:A:426:GLU:OE2	1:A:429:SER:OG	2.29	0.50
1:B:527:LEU:HD23	1:B:528:VAL:HG23	1.94	0.50
1:A:610:LEU:HB3	1:A:654:LEU:HD21	1.94	0.49
1:B:527:LEU:HA	1:B:531:VAL:HG22	1.93	0.49
1:C:519:GLU:N	1:C:519:GLU:OE1	2.43	0.49
1:B:645:PRO:HB2	1:B:647:VAL:HG12	1.94	0.49
1:A:521:PRO:HG3	1:B:379:GLN:NE2	2.27	0.49
1:C:393:LYS:HA	1:C:396:GLN:HG2	1.95	0.49
1:B:401:LEU:HD12	1:B:402:PRO:HD2	1.93	0.49
1:C:457:PRO:HB2	1:C:491:HIS:CG	2.48	0.48
1:A:658:LEU:HB3	1:A:662:LEU:HD22	1.96	0.48
2:F:68:TRP:CE3	2:F:125:ILE:HG12	2.49	0.48
2:E:20:LEU:HD23	2:E:91:LEU:HD21	1.96	0.48
1:A:456:ASP:OD1	1:A:461:LEU:N	2.43	0.48
2:F:65:ILE:HD11	2:F:117:ILE:HG23	1.96	0.48
1:B:680:ASN:O	2:F:108:GLN:NE2	2.46	0.47
2:E:28:ASN:HD21	2:E:136:LYS:HE3	1.79	0.47
2:F:33:TYR:CE2	2:F:105:MET:HB3	2.49	0.47
1:B:378:GLN:HE22	1:C:624:LEU:HD11	1.79	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:GLU:N	1:B:519:GLU:OE1	2.47	0.46
1:B:591:PHE:HZ	1:B:647:VAL:HG11	1.80	0.46
1:C:513:LEU:HD22	1:C:534:LEU:HD23	1.98	0.46
1:C:659:SER:HA	1:C:671:VAL:HG11	1.97	0.46
2:F:78:LEU:HD22	2:F:90:LEU:HD12	1.98	0.46
1:A:512:LEU:HD12	1:A:515:ARG:HD3	1.98	0.46
1:A:541:LEU:O	1:A:545:LEU:HD22	2.16	0.46
1:A:454:THR:OG1	1:A:455:VAL:N	2.47	0.46
1:B:491:HIS:O	1:B:495:LEU:HD22	2.16	0.46
1:A:369:TYR:HA	1:A:372:ILE:HG13	1.98	0.46
1:C:575:THR:O	1:C:579:ARG:HG3	2.16	0.46
1:C:442:PRO:HA	1:C:461:LEU:HD13	1.99	0.45
1:A:652:HIS:ND1	1:A:675:LEU:HD12	2.31	0.45
2:E:30:THR:HB	2:E:101:ILE:HD13	1.97	0.45
2:E:61:THR:O	2:E:65:ILE:HG12	2.17	0.45
1:B:366:GLU:OE2	1:B:410:ASN:ND2	2.50	0.45
1:B:516:VAL:HG11	1:B:554:MET:HG3	1.99	0.45
1:C:371:LEU:HD11	1:C:432:ALA:HB3	1.99	0.45
1:C:579:ARG:NH1	1:C:676:GLU:OE2	2.50	0.45
1:B:608:ARG:NH1	4:B:801:HOH:O	2.50	0.44
1:B:413:LEU:HD22	1:B:417:ARG:HG2	2.00	0.44
1:A:555:ARG:O	1:A:559:GLU:HB2	2.18	0.44
1:C:625:ALA:HB1	1:C:661:PHE:CZ	2.53	0.44
2:E:20:LEU:HD22	2:E:139:LEU:HD21	1.99	0.44
2:D:87:TRP:CE2	2:D:142:ARG:HG3	2.53	0.43
2:F:33:TYR:OH	2:F:105:MET:SD	2.71	0.43
1:A:374:MET:HG2	1:A:383:LEU:HB2	2.00	0.43
1:B:539:LYS:HD2	1:B:571:PRO:HB2	1.99	0.43
1:C:453:LYS:HG2	1:C:464:ILE:HG12	2.00	0.43
2:D:146:LEU:HD23	2:D:149:LEU:HD12	2.00	0.43
1:A:575:THR:O	1:A:579:ARG:HG3	2.19	0.43
1:B:387:ILE:HD13	1:B:405:VAL:HG11	2.01	0.43
1:B:663:ARG:HB3	1:B:663:ARG:HE	1.58	0.43
2:D:102:GLU:O	2:D:106:GLU:HG3	2.19	0.43
1:A:661:PHE:HD2	1:A:662:LEU:HD13	1.83	0.43
2:F:30:THR:HB	2:F:101:ILE:HD13	2.01	0.43
1:B:528:VAL:HA	1:B:529:PRO:HA	1.81	0.42
1:A:393:LYS:HA	1:A:396:GLN:HG2	2.02	0.42
1:C:627:ARG:HH21	1:C:631:GLN:HE21	1.66	0.42
2:E:68:TRP:CZ2	2:E:104:VAL:HG11	2.54	0.42
1:B:442:PRO:HA	1:B:461:LEU:HD13	1.99	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:LEU:HD22	1:B:670:VAL:N	2.34	0.42
2:F:115:ARG:O	2:F:119:ASP:HB2	2.20	0.42
1:B:531:VAL:HG11	1:B:566:PRO:HG3	2.00	0.42
1:C:383:LEU:HD11	1:C:488:VAL:HG11	2.00	0.42
1:A:621:GLU:HG3	1:A:622:PRO:HD2	2.01	0.42
1:C:499:PHE:O	1:C:503:LEU:HD22	2.19	0.42
1:B:648:LEU:HG	1:B:650:VAL:HG13	2.02	0.42
1:C:375:VAL:HG21	1:C:407:ILE:HG21	2.01	0.42
1:C:544:LEU:O	1:C:549:VAL:HG13	2.19	0.42
1:A:527:LEU:HA	1:A:531:VAL:HG22	2.02	0.42
2:F:33:TYR:OH	2:F:102:GLU:O	2.38	0.42
1:A:519:GLU:HB3	1:C:612:GLN:NE2	2.34	0.41
1:A:564:HIS:CD2	1:A:577:VAL:HG11	2.55	0.41
2:F:5:SER:O	2:F:9:THR:HG23	2.21	0.41
1:C:476:ILE:H	1:C:476:ILE:HG13	1.66	0.41
2:D:68:TRP:CE3	2:D:125:ILE:HG12	2.54	0.41
1:A:390:ILE:HD13	1:A:493:ASN:HB2	2.03	0.41
1:C:590:TRP:CZ2	1:C:670:VAL:HG11	2.56	0.41
1:A:610:LEU:HD12	1:A:610:LEU:HA	1.86	0.41
1:A:650:VAL:HG11	1:A:658:LEU:HD23	2.02	0.41
1:C:449:LEU:HD21	1:C:474:ALA:HB2	2.02	0.41
1:C:483:GLU:O	1:C:487:VAL:HG23	2.21	0.41
2:D:124:TYR:O	2:D:128:THR:HG23	2.21	0.41
2:F:20:LEU:HD23	2:F:91:LEU:HD21	2.03	0.41
1:A:645:PRO:HB2	1:A:647:VAL:HG13	2.02	0.41
2:F:33:TYR:CE2	2:F:102:GLU:HA	2.57	0.40
1:C:438:LEU:HD13	1:C:465:TRP:CE2	2.57	0.40
1:C:602:LEU:HD22	1:C:606:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

## 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	329/334 (98%)	317 (96%)	12 (4%)	0	100	100
1	B	330/334 (99%)	319 (97%)	11 (3%)	0	100	100
1	C	325/334 (97%)	314 (97%)	11 (3%)	0	100	100
2	D	140/179 (78%)	138 (99%)	2 (1%)	0	100	100
2	E	143/179 (80%)	140 (98%)	3 (2%)	0	100	100
2	F	137/179 (76%)	134 (98%)	3 (2%)	0	100	100
All	All	1404/1539 (91%)	1362 (97%)	42 (3%)	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	275/277 (99%)	260 (94%)	15 (6%)	21	46
1	B	276/277 (100%)	261 (95%)	15 (5%)	22	47
1	C	275/277 (99%)	258 (94%)	17 (6%)	18	40
2	D	131/151 (87%)	129 (98%)	2 (2%)	65	86
2	E	133/151 (88%)	127 (96%)	6 (4%)	27	55
2	F	130/151 (86%)	124 (95%)	6 (5%)	27	54
All	All	1220/1284 (95%)	1159 (95%)	61 (5%)	24	51

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	384	LEU
1	A	401	LEU
1	A	448	THR
1	A	456	ASP
1	A	523	LEU
1	A	545	LEU
1	A	549	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	582	LEU
1	A	610	LEU
1	A	620	LEU
1	A	636	LEU
1	A	654	LEU
1	A	655	ARG
1	A	658	LEU
1	A	662	LEU
1	B	363	LEU
1	B	367	VAL
1	B	383	LEU
1	B	396	GLN
1	B	456	ASP
1	B	488	VAL
1	B	495	LEU
1	B	523	LEU
1	B	594	ASN
1	B	597	VAL
1	B	628	LEU
1	B	647	VAL
1	B	654	LEU
1	B	655	ARG
1	B	677	LEU
1	C	367	VAL
1	C	375	VAL
1	C	383	LEU
1	C	449	LEU
1	C	452	GLU
1	C	456	ASP
1	C	481	VAL
1	C	503	LEU
1	C	520	MET
1	C	532	VAL
1	C	606	LEU
1	C	609	LEU
1	C	614	LEU
1	C	647	VAL
1	C	670	VAL
1	C	671	VAL
1	C	677	LEU
2	D	113	ILE
2	D	142	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	E	37	GLN
2	E	42	ASN
2	E	86	GLU
2	E	93	GLN
2	E	108	GLN
2	E	139	LEU
2	F	6	ILE
2	F	27	LEU
2	F	102	GLU
2	F	105	MET
2	F	165	ARG
2	F	171	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	379	GLN
1	B	572	HIS
2	E	99	GLN
2	E	108	GLN
2	F	66	ASN
2	F	108	GLN
2	F	156	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](#)

2 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	B	701	-	5,5,5	0.96	0	5,5,5	0.97	0
3	GOL	A	701	-	5,5,5	0.92	0	5,5,5	0.99	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	B	701	-	-	2/4/4/4	-
3	GOL	A	701	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	701	GOL	O1-C1-C2-C3
3	B	701	GOL	O1-C1-C2-O2

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	331/334 (99%)	-0.08	1 (0%) 94 95	48, 79, 117, 170	0
1	B	332/334 (99%)	-0.02	4 (1%) 79 80	42, 77, 147, 201	0
1	C	329/334 (98%)	0.11	4 (1%) 79 80	43, 86, 144, 217	0
2	D	144/179 (80%)	0.29	10 (6%) 16 15	51, 101, 159, 194	0
2	E	147/179 (82%)	0.26	8 (5%) 25 24	58, 108, 189, 252	0
2	F	143/179 (79%)	1.31	36 (25%) 0 0	73, 167, 243, 267	0
All	All	1426/1539 (92%)	0.19	63 (4%) 34 33	42, 90, 183, 267	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	135	LEU	7.6
2	F	107	LYS	6.7
2	F	134	LEU	5.8
2	F	130	ASP	5.3
2	F	27	LEU	5.2
2	F	138	LEU	5.2
2	F	30	THR	5.1
2	F	31	SER	4.6
2	E	110	PRO	4.5
2	F	34	LEU	4.3
2	E	113	ILE	4.3
2	F	78	LEU	4.3
2	E	122	ALA	4.2
2	F	128	THR	4.0
2	F	84	ARG	4.0
2	F	104	VAL	3.9
1	C	569	SER	3.8
2	F	122	ALA	3.8
2	F	86	GLU	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	F	117	ILE	3.5
2	D	136	LYS	3.4
2	F	67	ARG	3.4
2	F	133	GLN	3.3
2	D	110	PRO	3.2
2	F	32	SER	3.1
2	F	129	LEU	3.1
2	F	82	ALA	3.1
2	F	125	ILE	3.1
2	E	118	GLN	3.0
2	F	71	ILE	3.0
2	D	36	GLN	2.9
2	E	117	ILE	2.8
2	F	70	ARG	2.8
2	F	113	ILE	2.8
1	C	597	VAL	2.7
2	F	73	LEU	2.7
2	F	139	LEU	2.7
2	D	63	GLU	2.7
1	C	531	VAL	2.6
2	E	68	TRP	2.5
2	F	89	LEU	2.5
2	F	114	THR	2.4
2	E	93	GLN	2.4
2	F	98	LEU	2.4
1	B	567	LEU	2.3
2	F	4	MET	2.3
2	D	38	PHE	2.3
2	F	76	GLN	2.3
2	D	39	THR	2.2
2	D	64	PHE	2.2
2	F	118	GLN	2.2
1	B	584	ARG	2.2
2	F	116	SER	2.2
1	A	527	LEU	2.2
2	F	127	GLN	2.1
1	C	567	LEU	2.1
2	F	115	ARG	2.1
2	D	78	LEU	2.1
1	B	408	ARG	2.0
2	D	32	SER	2.0
2	D	100	SER	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	394	PHE	2.0
2	E	64	PHE	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
3	GOL	A	701	6/6	0.56	0.34	132,138,139,139	0
3	GOL	B	701	6/6	0.66	0.28	92,93,95,96	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.