



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2020 – 11:47 pm BST

PDB ID : 5AQN  
Title : Fragment-based screening of HSP70 sheds light on the functional role of ATP-binding site residues  
Authors : Jones, A.M.; Westwood, I.M.; Osborne, J.D.; Matthews, T.P.; Cheeseman, M.D.; Rowlands, M.G.; Jeganathan, F.; Burke, R.; Lee, D.; Kadi, N.; Liu, M.; Richards, M.; McAndrew, C.; Yahya, N.; Dobson, S.E.; Jones, K.; Workman, P.; Collins, I.; van Montfort, R.L.M.  
Deposited on : 2015-09-22  
Resolution : 2.45 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

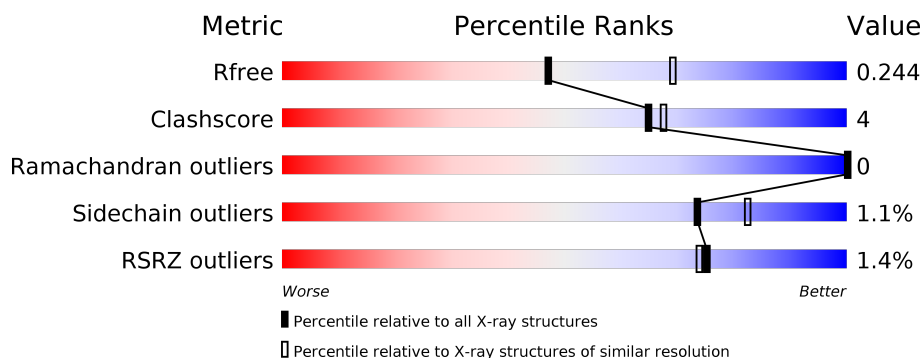
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	386	
1	C	386	
1	E	386	
2	B	118	
2	D	118	
2	F	118	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11530 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 HEAT SHOCK COGNATE 71 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2902	1826	500	567	9			
1	C	382	Total	C	N	O	S	0	0	0
			2907	1824	504	570	9			
1	E	382	Total	C	N	O	S	0	0	0
			2817	1764	487	557	9			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P11142
A	-3	PRO	-	expression tag	UNP P11142
A	-2	LEU	-	expression tag	UNP P11142
A	-1	GLY	-	expression tag	UNP P11142
A	0	SER	-	expression tag	UNP P11142
C	-4	GLY	-	expression tag	UNP P11142
C	-3	PRO	-	expression tag	UNP P11142
C	-2	LEU	-	expression tag	UNP P11142
C	-1	GLY	-	expression tag	UNP P11142
C	0	SER	-	expression tag	UNP P11142
E	-4	GLY	-	expression tag	UNP P11142
E	-3	PRO	-	expression tag	UNP P11142
E	-2	LEU	-	expression tag	UNP P11142
E	-1	GLY	-	expression tag	UNP P11142
E	0	SER	-	expression tag	UNP P11142

- Molecule 2 is a protein called BAG FAMILY MOLECULAR CHAPERONE REGULATOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	113	Total	C	N	O	S	0	0	1
			852	540	143	165	4			

*Continued on next page...*

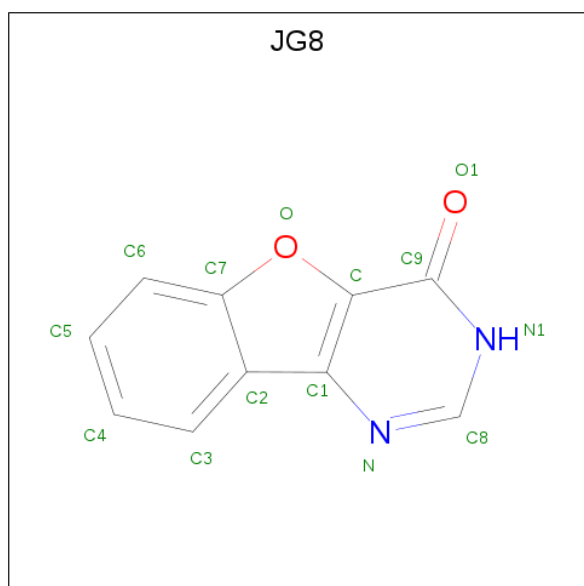
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	111	Total	C	N	O	S	0	0	0
			831	528	140	159	4			
2	F	113	Total	C	N	O	S	0	0	1
			853	540	140	169	4			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	146	GLY	-	expression tag	UNP Q99933
B	147	PRO	-	expression tag	UNP Q99933
B	148	LEU	-	expression tag	UNP Q99933
B	149	GLY	-	expression tag	UNP Q99933
B	150	SER	-	expression tag	UNP Q99933
D	146	GLY	-	expression tag	UNP Q99933
D	147	PRO	-	expression tag	UNP Q99933
D	148	LEU	-	expression tag	UNP Q99933
D	149	GLY	-	expression tag	UNP Q99933
D	150	SER	-	expression tag	UNP Q99933
F	146	GLY	-	expression tag	UNP Q99933
F	147	PRO	-	expression tag	UNP Q99933
F	148	LEU	-	expression tag	UNP Q99933
F	149	GLY	-	expression tag	UNP Q99933
F	150	SER	-	expression tag	UNP Q99933

- Molecule 3 is BENZOFURO[3,2-D]PYRIMIDIN-4(3H)-ONE (three-letter code: JG8) (formula: C<sub>10</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	10	2	2		
3	C	1	Total	C	N	O	0	0
			14	10	2	2		
3	E	1	Total	C	N	O	0	0
			14	10	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



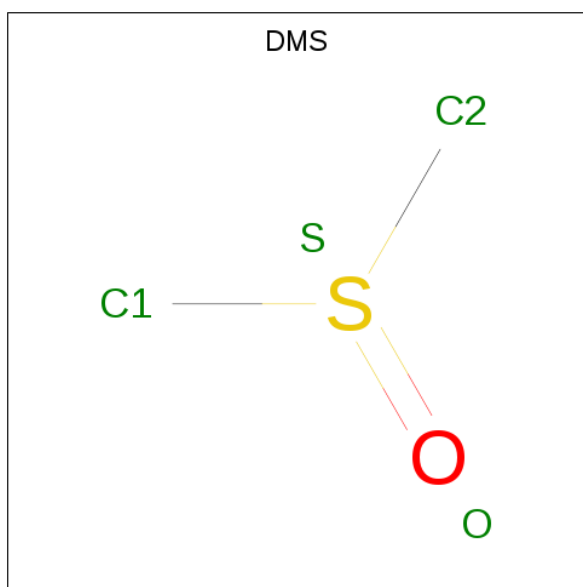
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		
5	C	1	Total	C	N	O	0	0
			8	4	1	3		
5	E	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O S 4 2 1 1	0	0
6	C	1	Total C O S 4 2 1 1	0	0
6	E	1	Total C O S 4 2 1 1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total Cl 1 1	0	0

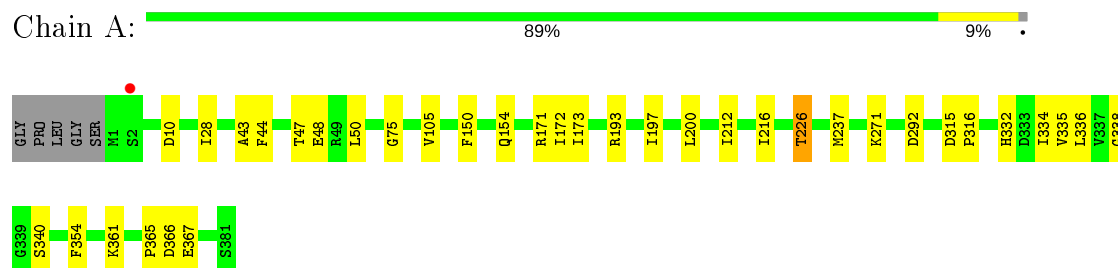
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	107	Total O 107 107	0	0
8	B	20	Total O 20 20	0	0
8	C	63	Total O 63 63	0	0
8	D	11	Total O 11 11	0	0
8	E	28	Total O 28 28	0	0
8	F	6	Total O 6 6	0	0

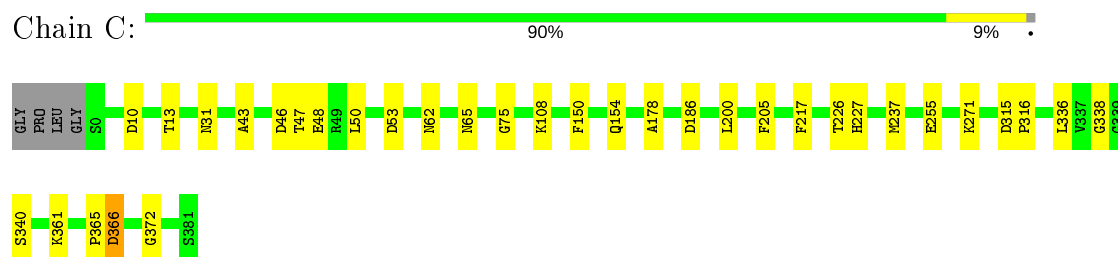
### 3 Residue-property plots [i](#)

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.

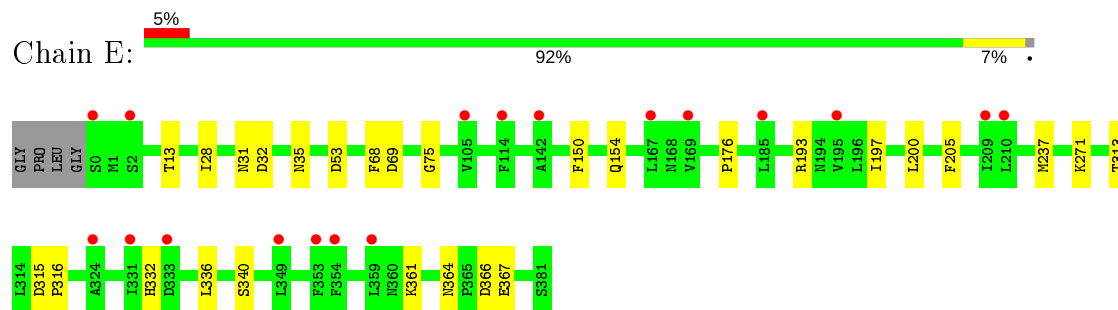
#### • Molecule 1: HEAT SHOCK COGNATE 71 KDA PROTEIN



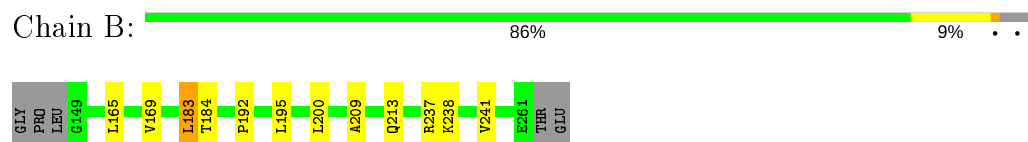
#### • Molecule 1: HEAT SHOCK COGNATE 71 KDA PROTEIN



#### • Molecule 1: HEAT SHOCK COGNATE 71 KDA PROTEIN




#### • Molecule 2: BAG FAMILY MOLECULAR CHAPERONE REGULATOR 1






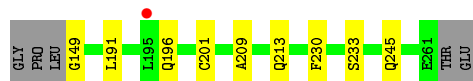
## ● Molecule 2: BAG FAMILY MOLECULAR CHAPERONE REGULATOR 1

Chain D:  %



## ● Molecule 2: BAG FAMILY MOLECULAR CHAPERONE REGULATOR 1

Chain F:  %



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	233.29 Å   41.03 Å   205.25 Å 90.00°   123.13°   90.00°	Depositor
Resolution (Å)	48.84 – 2.45 48.84 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.84-2.45) 99.9 (48.84-2.45)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.45 Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.193   ,   0.228 0.209   ,   0.244	Depositor DCC
$R_{free}$ test set	3008 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11530	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.51% 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: JG8, GOL, TRS, DMS, CL

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	0.47	0/2948	0.63	0/3991
1	C	0.45	0/2953	0.63	0/4000
1	E	0.43	0/2862	0.64	0/3892
2	B	0.53	0/859	0.63	0/1159
2	D	0.49	0/838	0.59	0/1132
2	F	0.52	0/860	0.63	0/1162
All	All	0.47	0/11320	0.63	0/15336

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	2902	0	2842	25	0
1	C	2907	0	2839	28	0
1	E	2817	0	2645	18	0
2	B	852	0	831	10	0
2	D	831	0	803	8	0
2	F	853	0	820	7	0
3	A	14	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	14	0	0	0	0
3	E	14	0	0	0	0
4	A	18	0	24	2	0
4	B	6	0	8	0	0
4	C	12	0	16	0	0
4	D	6	0	8	0	0
4	E	6	0	8	3	0
4	F	6	0	8	1	0
5	A	8	0	12	2	0
5	C	8	0	12	1	0
5	E	8	0	12	0	0
6	A	4	0	6	1	0
6	C	4	0	6	0	0
6	E	4	0	6	0	0
7	C	1	0	0	0	0
8	A	107	0	0	1	0
8	B	20	0	0	0	0
8	C	63	0	0	1	0
8	D	11	0	0	0	0
8	E	28	0	0	0	0
8	F	6	0	0	0	0
All	All	11530	0	10906	91	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 4.

All (91) 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:47:THR:HG23	2:D:205:ARG:HH12	1.36	0.89
1:A:315:ASP:HB2	1:A:316:PRO:HD3	1.55	0.88
1:C:46:ASP:O	1:C:108:LYS:HG2	1.76	0.85
2:D:209:ALA:O	2:D:213:GLN:HG3	1.77	0.84
1:C:47:THR:HG23	2:D:205:ARG:NH1	1.96	0.80
1:E:315:ASP:HB2	1:E:316:PRO:HD3	1.67	0.77
1:E:205:PHE:HE2	1:E:316:PRO:HG2	1.48	0.77
5:A:1386:TRS:H12	8:A:2007:HOH:O	1.87	0.74
1:C:75:GLY:HA3	1:C:154:GLN:HA	1.72	0.72
1:C:46:ASP:HA	1:C:108:LYS:HA	1.73	0.70
1:A:47:THR:OG1	1:A:48:GLU:OE1	2.07	0.70
1:C:47:THR:CG2	2:D:205:ARG:HH12	2.05	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:ASN:OD1	1:E:35:ASN:N	2.25	0.69
1:C:237:MET:HE1	1:C:271:LYS:HB2	1.73	0.69
1:C:315:ASP:HB2	1:C:316:PRO:HD3	1.74	0.69
1:C:10:ASP:OD2	5:C:1385:TRS:H12	1.96	0.66
2:B:209:ALA:O	2:B:213:GLN:HG3	1.97	0.64
1:C:46:ASP:OD1	1:C:47:THR:HG23	1.99	0.63
2:D:258:ILE:HG22	2:D:259:CYS:SG	2.39	0.63
1:A:10:ASP:OD2	5:A:1386:TRS:H32	2.00	0.62
1:A:237:MET:HE1	1:A:271:LYS:HB2	1.82	0.62
1:A:315:ASP:HB2	1:A:316:PRO:CD	2.31	0.60
2:F:149:GLY:N	4:F:1261:GOL:HO1	2.00	0.60
1:A:171:ARG:HD2	1:A:173:ILE:HG22	1.83	0.59
2:D:192:PRO:HD2	2:D:195:LEU:HB2	1.84	0.59
2:F:191:LEU:HD23	2:F:196:GLN:HA	1.85	0.59
2:B:183:LEU:HD13	2:B:183:LEU:C	2.23	0.58
1:E:75:GLY:HA3	1:E:154:GLN:HA	1.86	0.58
1:A:171:ARG:CD	1:A:173:ILE:HG22	2.35	0.56
1:A:75:GLY:HA3	1:A:154:GLN:HA	1.86	0.56
1:A:292:ASP:OD1	2:B:238:LYS:NZ	2.37	0.56
1:E:315:ASP:N	1:E:316:PRO:CD	2.69	0.55
1:C:336:LEU:HD12	1:C:361:LYS:HB3	1.87	0.55
2:B:183:LEU:CD2	2:B:200:LEU:HD22	2.37	0.55
4:E:1383:GOL:H12	2:F:245:GLN:NE2	2.21	0.55
1:E:237:MET:HE1	1:E:271:LYS:HB2	1.88	0.55
1:A:75:GLY:H	4:A:1385:GOL:H32	1.72	0.55
1:A:171:ARG:HD2	1:A:173:ILE:CG2	2.37	0.54
1:C:46:ASP:OD1	1:C:47:THR:N	2.40	0.54
2:B:183:LEU:HD22	2:B:200:LEU:CD2	2.39	0.52
4:E:1383:GOL:H12	2:F:245:GLN:HE21	1.73	0.52
1:C:47:THR:OG1	1:C:48:GLU:OE1	2.28	0.52
1:E:336:LEU:HD12	1:E:361:LYS:HB3	1.92	0.52
1:E:31:ASN:ND2	1:E:53:ASP:OD2	2.39	0.51
1:E:205:PHE:CE2	1:E:316:PRO:HG2	2.38	0.51
1:A:193:ARG:HA	1:A:332:HIS:ND1	2.26	0.50
1:C:47:THR:CG2	2:D:205:ARG:NH1	2.67	0.50
1:C:255:GLU:HB2	8:C:2039:HOH:O	2.11	0.50
4:E:1383:GOL:C1	2:F:245:GLN:HE21	2.24	0.50
1:E:313:THR:C	1:E:316:PRO:HD2	2.31	0.50
1:A:171:ARG:HG2	1:A:172:ILE:N	2.27	0.50
2:F:230:PHE:HB3	2:F:233:SER:HB2	1.94	0.49
1:A:336:LEU:HD12	1:A:361:LYS:HB3	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:ILE:HG13	1:E:367:GLU:OE1	2.14	0.48
1:C:46:ASP:O	1:C:108:LYS:CG	2.56	0.48
1:A:44:PHE:CD2	1:A:105:VAL:HG21	2.50	0.47
1:A:200:LEU:HG	1:A:340:SER:HB2	1.97	0.47
2:B:237:ARG:O	2:B:241:VAL:HG23	2.16	0.46
1:A:334:ILE:HD13	1:A:354:PHE:CD2	2.51	0.45
1:C:186:ASP:HB3	1:C:217:PHE:CZ	2.51	0.45
1:E:176:PRO:CB	1:E:197:ILE:HG13	2.47	0.45
1:C:62:ASN:ND2	1:C:65:ASN:HB2	2.32	0.44
2:B:183:LEU:HD23	2:B:200:LEU:HD22	1.98	0.44
1:A:338:GLY:O	1:A:365:PRO:HB2	2.18	0.44
1:C:200:LEU:HG	1:C:340:SER:HB2	2.00	0.43
1:C:338:GLY:O	1:C:365:PRO:HB2	2.18	0.43
1:A:75:GLY:HA2	4:A:1385:GOL:H11	1.99	0.43
1:C:31:ASN:ND2	1:C:53:ASP:OD2	2.44	0.43
2:B:192:PRO:HD2	2:B:195:LEU:HD12	2.01	0.43
1:C:226:THR:HG22	1:C:227:HIS:CE1	2.54	0.42
1:A:212:ILE:HA	1:A:216:ILE:O	2.19	0.42
1:E:193:ARG:HA	1:E:332:HIS:ND1	2.34	0.42
2:F:209:ALA:O	2:F:213:GLN:HG3	2.19	0.42
1:E:200:LEU:HG	1:E:340:SER:HB2	2.01	0.42
1:A:43:ALA:HB3	1:A:50:LEU:HB2	2.01	0.42
1:C:46:ASP:OD1	2:D:205:ARG:NH1	2.53	0.42
1:C:62:ASN:HD21	1:C:65:ASN:HB2	1.84	0.42
2:B:183:LEU:HD13	2:B:184:THR:N	2.34	0.42
1:C:205:PHE:HE2	1:C:316:PRO:HG2	1.85	0.42
1:E:68:PHE:O	1:E:69:ASP:HB2	2.20	0.42
2:B:165:LEU:O	2:B:169:VAL:HG23	2.20	0.42
1:E:32:ASP:OD1	1:E:32:ASP:N	2.52	0.42
1:A:197:ILE:HD13	1:A:335:VAL:HB	2.01	0.41
1:C:178:ALA:O	1:C:372:GLY:HA3	2.19	0.41
1:C:366:ASP:OD1	1:C:366:ASP:N	2.42	0.41
1:A:226:THR:HG22	6:A:1387:DMS:C1	2.50	0.41
1:E:364:ASN:HD22	1:E:367:GLU:CD	2.23	0.41
1:A:28:ILE:HG13	1:A:367:GLU:OE1	2.21	0.41
1:C:43:ALA:HB3	1:C:50:LEU:HB2	2.03	0.40
1:A:315:ASP:CB	1:A:316:PRO:HD3	2.36	0.40
1:E:315:ASP:N	1:E:316:PRO:HD2	2.36	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	379/386 (98%)	375 (99%)	4 (1%)	0	100	100
1	C	380/386 (98%)	377 (99%)	3 (1%)	0	100	100
1	E	380/386 (98%)	376 (99%)	4 (1%)	0	100	100
2	B	111/118 (94%)	110 (99%)	1 (1%)	0	100	100
2	D	109/118 (92%)	107 (98%)	2 (2%)	0	100	100
2	F	111/118 (94%)	111 (100%)	0	0	100	100
All	All	1470/1512 (97%)	1456 (99%)	14 (1%)	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	300/319 (94%)	297 (99%)	3 (1%)	76	84
1	C	302/319 (95%)	299 (99%)	3 (1%)	76	84
1	E	277/319 (87%)	274 (99%)	3 (1%)	73	82
2	B	86/107 (80%)	85 (99%)	1 (1%)	71	81
2	D	82/107 (77%)	81 (99%)	1 (1%)	71	81
2	F	86/107 (80%)	85 (99%)	1 (1%)	71	81
All	All	1133/1278 (89%)	1121 (99%)	12 (1%)	73	82

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	PHE
1	A	226	THR
1	A	366	ASP
2	B	183	LEU
1	C	13	THR
1	C	150	PHE
1	C	366	ASP
2	D	183	LEU
1	E	13	THR
1	E	150	PHE
1	E	366	ASP
2	F	201	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	151	ASN
2	F	245	GLN

### 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 ⓘ

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond



length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	A	1383	-	5,5,5	0.19	0	5,5,5	0.65	0
5	TRS	C	1385	-	7,7,7	0.22	0	9,9,9	0.24	0
4	GOL	C	1383	-	5,5,5	0.17	0	5,5,5	0.40	0
4	GOL	E	1383	-	5,5,5	0.05	0	5,5,5	0.36	0
5	TRS	E	1384	-	7,7,7	0.24	0	9,9,9	0.28	0
3	JG8	E	1382	-	13,16,16	1.25	2 (15%)	10,23,23	3.06	6 (60%)
4	GOL	C	1384	-	5,5,5	0.10	0	5,5,5	0.18	0
4	GOL	A	1384	-	5,5,5	0.17	0	5,5,5	0.60	0
3	JG8	A	1382	-	13,16,16	1.25	2 (15%)	10,23,23	3.05	6 (60%)
3	JG8	C	1382	-	13,16,16	1.23	2 (15%)	10,23,23	3.07	6 (60%)
6	DMS	A	1387	-	3,3,3	0.30	0	3,3,3	0.59	0
6	DMS	E	1385	-	3,3,3	0.30	0	3,3,3	0.43	0
4	GOL	A	1385	-	5,5,5	0.09	0	5,5,5	0.37	0
4	GOL	D	1261	-	5,5,5	0.16	0	5,5,5	0.29	0
6	DMS	C	1386	-	3,3,3	0.26	0	3,3,3	0.34	0
4	GOL	F	1261	-	5,5,5	0.16	0	5,5,5	0.63	0
5	TRS	A	1386	-	7,7,7	0.23	0	9,9,9	0.34	0
4	GOL	B	1261	-	5,5,5	0.09	0	5,5,5	0.41	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
4	GOL	A	1383	-	-	3/4/4/4	-
5	TRS	C	1385	-	-	0/9/9/9	-
4	GOL	C	1383	-	-	0/4/4/4	-
4	GOL	E	1383	-	-	0/4/4/4	-
5	TRS	E	1384	-	-	0/9/9/9	-
4	GOL	C	1384	-	-	0/4/4/4	-
4	GOL	A	1384	-	-	0/4/4/4	-
3	JG8	A	1382	-	-	-	0/3/3/3
3	JG8	C	1382	-	-	-	0/3/3/3
3	JG8	E	1382	-	-	-	0/3/3/3
4	GOL	A	1385	-	-	1/4/4/4	-
4	GOL	D	1261	-	-	0/4/4/4	-
4	GOL	F	1261	-	-	0/4/4/4	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TRS	A	1386	-	-	3/9/9/9	-
4	GOL	B	1261	-	-	0/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1382	JG8	C9-N1	2.44	1.37	1.33
3	A	1382	JG8	C9-N1	2.30	1.37	1.33
3	C	1382	JG8	C9-N1	2.27	1.37	1.33
3	C	1382	JG8	C2-C7	-2.09	1.39	1.43
3	E	1382	JG8	C2-C7	-2.08	1.39	1.43
3	A	1382	JG8	C2-C7	-2.06	1.39	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1382	JG8	C8-N1-C9	4.97	124.21	115.88
3	A	1382	JG8	C8-N1-C9	4.95	124.17	115.88
3	E	1382	JG8	C8-N1-C9	4.95	124.17	115.88
3	A	1382	JG8	C9-C-C1	-4.89	116.13	120.80
3	C	1382	JG8	C9-C-C1	-4.89	116.13	120.80
3	E	1382	JG8	C9-C-C1	-4.82	116.20	120.80
3	E	1382	JG8	C8-N-C1	-4.23	111.68	115.51
3	C	1382	JG8	C8-N-C1	-4.13	111.77	115.51
3	A	1382	JG8	C8-N-C1	-4.11	111.79	115.51
3	C	1382	JG8	C3-C2-C7	-3.40	118.23	120.38
3	E	1382	JG8	C-C1-N	3.37	128.93	124.96
3	C	1382	JG8	C-C1-N	3.34	128.89	124.96
3	A	1382	JG8	C3-C2-C7	-3.32	118.28	120.38
3	E	1382	JG8	C3-C2-C7	-3.31	118.29	120.38
3	A	1382	JG8	C-C1-N	3.30	128.85	124.96
3	C	1382	JG8	N-C8-N1	-2.30	125.09	128.68
3	E	1382	JG8	N-C8-N1	-2.28	125.11	128.68
3	A	1382	JG8	N-C8-N1	-2.27	125.13	128.68

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1383	GOL	C1-C2-C3-O3
4	A	1383	GOL	O2-C2-C3-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	A	1386	TRS	N-C-C3-O3
5	A	1386	TRS	C1-C-C3-O3
5	A	1386	TRS	C2-C-C3-O3
4	A	1383	GOL	O1-C1-C2-C3
4	A	1385	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1385	TRS	1	0
4	E	1383	GOL	3	0
6	A	1387	DMS	1	0
4	A	1385	GOL	2	0
4	F	1261	GOL	1	0
5	A	1386	TRS	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 ⓘ

### 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	381/386 (98%)	-0.18	1 (0%) 94 94	31, 48, 67, 85	0
1	C	382/386 (98%)	-0.19	0 100 100	42, 56, 76, 91	0
1	E	382/386 (98%)	0.15	18 (4%) 31 29	42, 73, 98, 124	0
2	B	113/118 (95%)	-0.34	0 100 100	34, 48, 71, 121	0
2	D	111/118 (94%)	-0.30	1 (0%) 84 85	43, 59, 94, 103	0
2	F	113/118 (95%)	-0.15	1 (0%) 84 85	41, 55, 92, 117	0
All	All	1482/1512 (98%)	-0.12	21 (1%) 75 74	31, 56, 89, 124	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	185	LEU	4.5
1	E	195	VAL	4.2
2	D	179	LEU	3.7
1	E	359	LEU	3.6
1	A	2	SER	3.2
1	E	354	PHE	3.0
1	E	2	SER	2.8
1	E	331	ILE	2.7
1	E	353	PHE	2.6
1	E	209	ILE	2.4
2	F	195	LEU	2.4
1	E	349	LEU	2.3
1	E	105	VAL	2.3
1	E	324	ALA	2.3
1	E	142	ALA	2.2
1	E	167	LEU	2.2
1	E	0	SER	2.2
1	E	333	ASP	2.1
1	E	169	VAL	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	114	PHE	2.1
1	E	210	LEU	2.1

## 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
4	GOL	A	1385	6/6	0.74	0.32	76,77,80,82	0
5	TRS	E	1384	8/8	0.82	0.28	80,82,90,92	0
4	GOL	A	1384	6/6	0.83	0.22	58,66,71,73	0
4	GOL	C	1384	6/6	0.83	0.53	85,88,89,89	0
4	GOL	D	1261	6/6	0.84	0.27	52,68,73,75	0
3	JG8	E	1382	14/14	0.85	0.20	66,74,77,78	0
6	DMS	A	1387	4/4	0.89	0.19	77,80,80,81	0
5	TRS	A	1386	8/8	0.89	0.18	52,63,65,65	0
7	CL	C	1387	1/1	0.90	0.15	64,64,64,64	0
4	GOL	F	1261	6/6	0.91	0.21	58,70,77,81	0
4	GOL	B	1261	6/6	0.91	0.18	68,72,79,83	0
4	GOL	C	1383	6/6	0.92	0.23	55,59,60,61	0
3	JG8	C	1382	14/14	0.92	0.16	51,56,58,61	0
5	TRS	C	1385	8/8	0.94	0.16	60,73,74,74	0
6	DMS	C	1386	4/4	0.95	0.23	96,97,98,98	0
6	DMS	E	1385	4/4	0.95	0.29	109,110,110,111	0
4	GOL	E	1383	6/6	0.95	0.14	56,56,61,66	0
3	JG8	A	1382	14/14	0.95	0.13	42,54,57,59	0
4	GOL	A	1383	6/6	0.96	0.15	44,48,52,52	0

## 6.5 Other polymers

There are no such residues in this entry.