



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:11 am BST

PDB ID : 5AQR
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 : 1.91 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

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

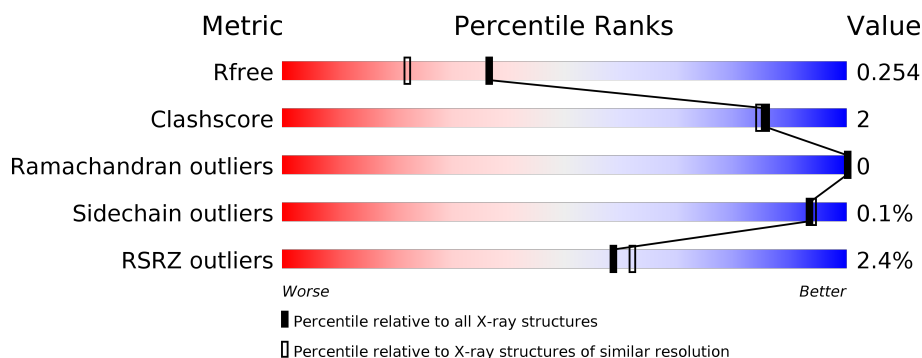
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 ≥ 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	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
1	C	386	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>.</div> <div>.</div> </div> </div>
1	E	386	<div> <div>5%</div> <div> <div></div> <div>94%</div> <div>5%</div> <div>.</div> </div> </div>
2	B	118	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>5%</div> </div> </div>
2	D	118	<div> <div>%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
2	F	118	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>.</div> <div>.</div> </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12112 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	1	0
			2915	1833	509	563	10			
1	C	381	Total	C	N	O	S	0	0	0
			2891	1813	504	565	9			
1	E	381	Total	C	N	O	S	0	0	0
			2859	1794	498	558	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	112	Total	C	N	O	S	0	0	0
			861	548	145	164	4			

Continued on next page...

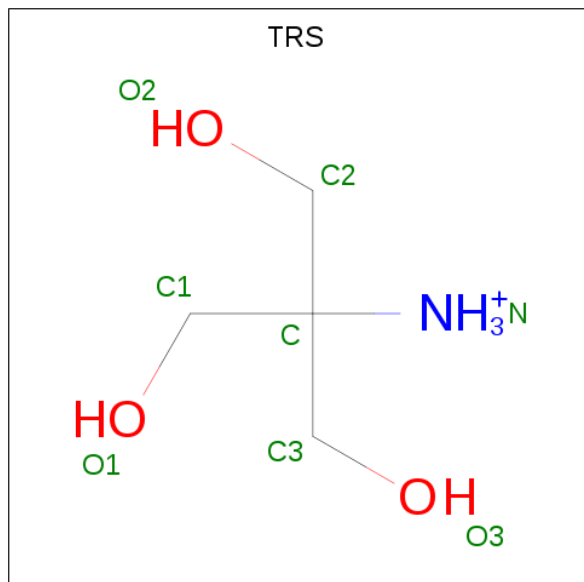
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	112	Total	C	N	O	S	0	0	0
			867	549	146	168	4			
2	F	113	Total	C	N	O	S	0	0	0
			869	546	147	172	4			

There are 15 discrepancies between the modelled and reference sequences:

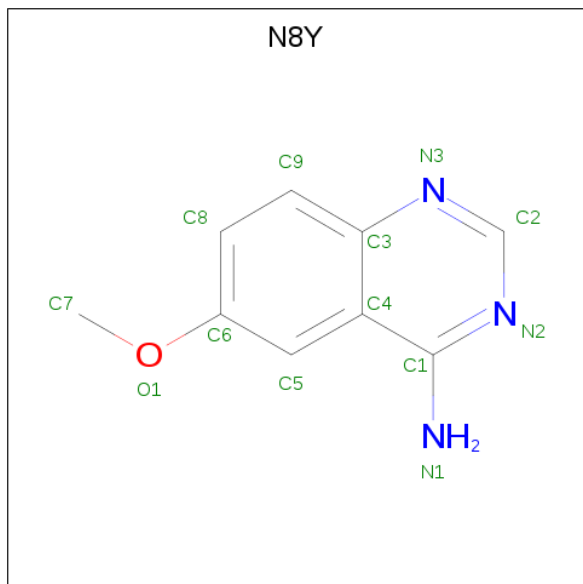
Chain	Residue	Modelled	Actual	Comment	Reference
B	146	GLY	-	expression tag	UNP Q99933
B	147	PRO	-	expression tag	UNP Q99933
B	148	LEU	-	expression tag	UNP Q99933
B	149	GLY	-	expression tag	UNP Q99933
B	150	SER	-	expression tag	UNP Q99933
D	146	GLY	-	expression tag	UNP Q99933
D	147	PRO	-	expression tag	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 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



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

- Molecule 4 is 6-methoxyquinazolin-4-amine (three-letter code: N8Y) (formula: C₉H₉N₃O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			13	9	3	1		
4	C	1	Total	C	N	O	0	0
			13	9	3	1		
4	E	1	Total	C	N	O	0	0
			13	9	3	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



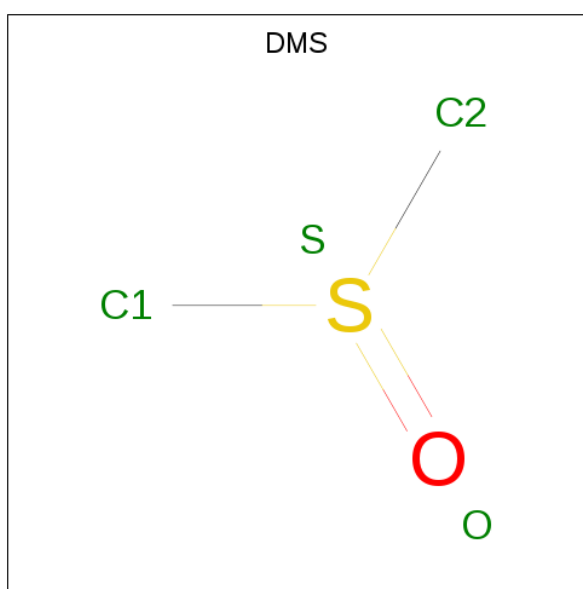
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

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

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

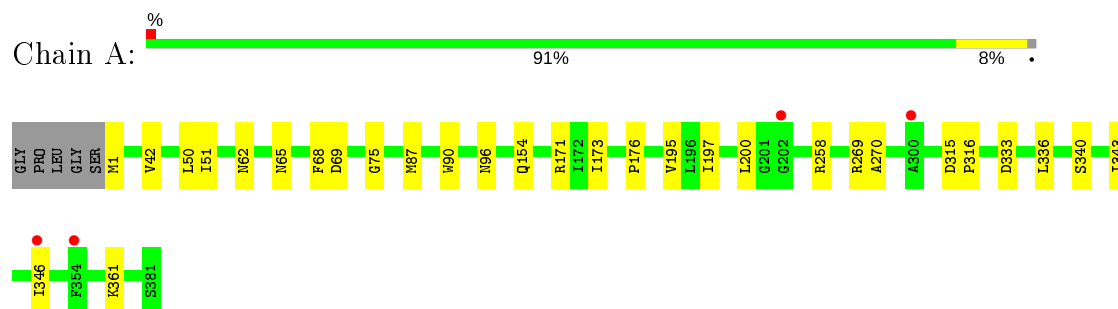
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	226	Total 226	O 226	0	0
8	B	46	Total 46	O 46	0	0
8	C	199	Total 199	O 199	0	0
8	D	42	Total 42	O 42	0	0
8	E	111	Total 111	O 111	0	0
8	F	26	Total 26	O 26	0	0

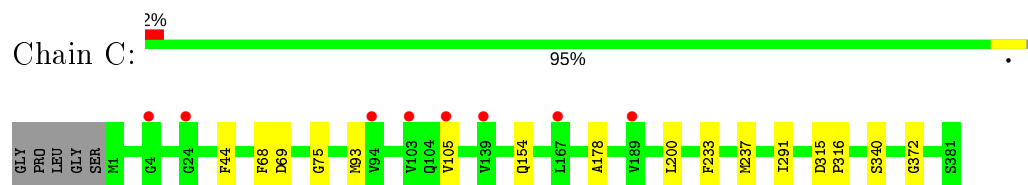
3 Residue-property plots [i](#)

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.

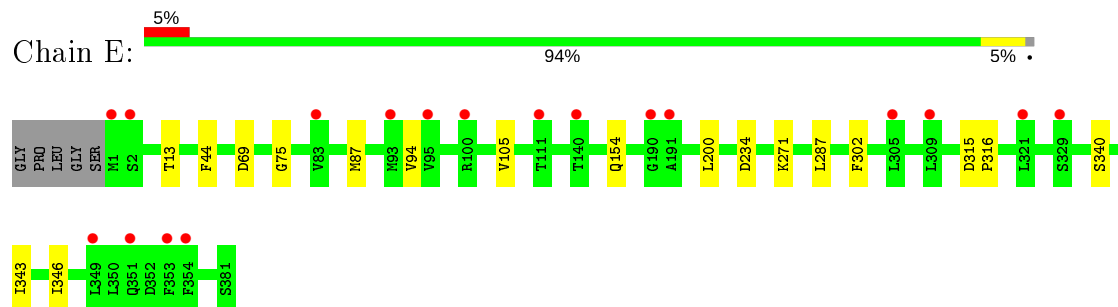
- Molecule 1: HEAT SHOCK COGNATE 71 KDA PROTEIN



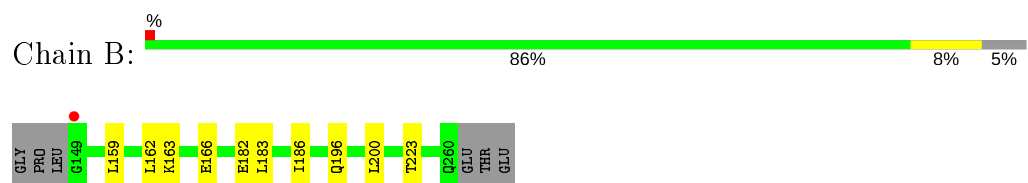
- Molecule 1: HEAT SHOCK COGNATE 71 KDA PROTEIN



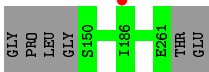
- Molecule 1: HEAT SHOCK COGNATE 71 KDA PROTEIN



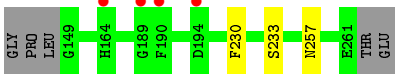
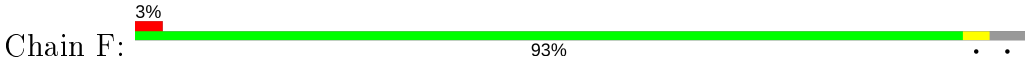
- Molecule 2: BAG FAMILY MOLECULAR CHAPERONE REGULATOR 1



- Molecule 2: BAG FAMILY MOLECULAR CHAPERONE REGULATOR 1



● Molecule 2: BAG FAMILY MOLECULAR CHAPERONE REGULATOR 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	232.60 Å 40.99 Å 207.27 Å 90.00° 122.92° 90.00°	Depositor
Resolution (Å)	47.88 – 1.91 47.87 – 1.91	Depositor EDS
% Data completeness (in resolution range)	94.2 (47.88-1.91) 94.2 (47.87-1.91)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.91 Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.208 , 0.236 0.223 , 0.254	Depositor DCC
R_{free} test set	6081 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12112	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9211e-03.*

¹Intensities estimated from amplitudes.

²Theoretical 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, TRS, DMS, N8Y, 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	0.49	0/2961	0.60	0/4005
1	C	0.48	0/2935	0.61	0/3974
1	E	0.45	0/2904	0.61	0/3939
2	B	0.54	0/868	0.58	0/1166
2	D	0.51	0/874	0.57	0/1176
2	F	0.51	0/875	0.56	0/1178
All	All	0.48	0/11417	0.60	0/15438

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	2915	0	2878	21	0
1	C	2891	0	2826	9	0
1	E	2859	0	2761	14	0
2	B	861	0	865	7	0
2	D	867	0	863	0	0
2	F	869	0	858	2	0
3	A	8	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	8	0	12	0	0
3	E	8	0	12	0	0
4	A	13	0	0	0	0
4	C	13	0	0	0	0
4	E	13	0	0	0	0
5	A	42	0	56	4	0
5	B	24	0	32	1	0
5	C	24	0	32	0	0
5	D	6	0	8	0	0
5	E	12	0	16	2	0
6	A	16	0	24	0	0
6	C	4	0	6	0	0
6	E	8	0	12	0	0
7	C	1	0	0	0	0
8	A	226	0	0	0	0
8	B	46	0	0	0	0
8	C	199	0	0	0	0
8	D	42	0	0	0	0
8	E	111	0	0	0	0
8	F	26	0	0	0	0
All	All	12112	0	11273	51	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 2.

All (51) 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:E:87:MET:HE3	1:E:94:VAL:HB	1.42	0.98
1:E:315:ASP:HB2	1:E:316:PRO:HD3	1.67	0.75
1:C:315:ASP:HB2	1:C:316:PRO:HD3	1.68	0.75
1:E:87:MET:CE	1:E:94:VAL:HB	2.19	0.71
1:A:315:ASP:HB2	1:A:316:PRO:HD3	1.74	0.69
2:B:183:LEU:HD12	2:B:200:LEU:HD22	1.80	0.63
1:E:287:LEU:O	5:E:1384:GOL:H12	2.04	0.58
2:B:186:ILE:HG22	2:B:196:GLN:HG3	1.86	0.57
1:A:42:VAL:HG22	1:A:51:ILE:HD12	1.86	0.56
1:A:176:PRO:HB2	1:A:197:ILE:HD13	1.87	0.56
1:A:50:LEU:O	1:A:51:ILE:HD13	2.07	0.55
2:B:162:LEU:O	2:B:166:GLU:HG3	2.07	0.55
1:A:171:ARG:HD2	1:A:173:ILE:CG2	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HG2	5:A:1389:GOL:H12	1.92	0.52
1:E:200:LEU:HG	1:E:340:SER:HB2	1.91	0.51
1:E:13:THR:HG22	1:E:69:ASP:OD1	2.09	0.51
1:A:269:ARG:HG2	5:A:1387:GOL:H2	1.93	0.51
1:A:96:ASN:H	5:A:1385:GOL:H11	1.76	0.51
1:A:200:LEU:HG	1:A:340:SER:HB2	1.93	0.50
2:B:159:LEU:O	2:B:163:LYS:HG3	2.11	0.50
1:A:270:ALA:HB2	5:A:1387:GOL:H32	1.91	0.50
1:A:87:MET:HA	1:A:90:TRP:CE3	2.46	0.49
1:E:315:ASP:HB2	1:E:316:PRO:CD	2.40	0.49
1:C:200:LEU:HG	1:C:340:SER:HB2	1.95	0.49
1:A:269:ARG:CZ	2:B:223:THR:HG22	2.42	0.48
1:E:271:LYS:HG3	1:E:302:PHE:CZ	2.48	0.48
1:E:287:LEU:O	5:E:1384:GOL:C1	2.62	0.47
1:C:178:ALA:O	1:C:372:GLY:HA3	2.13	0.47
2:B:183:LEU:HD12	2:B:200:LEU:CD2	2.45	0.47
1:E:315:ASP:CB	1:E:316:PRO:HD3	2.41	0.47
1:C:291:ILE:HD11	2:F:257:ASN:OD1	2.16	0.46
1:A:68:PHE:O	1:A:69:ASP:HB2	2.16	0.46
1:A:336:LEU:HD12	1:A:361:LYS:HB3	1.98	0.45
1:A:62:ASN:HD21	1:A:65:ASN:HB2	1.80	0.45
2:B:182:GLU:O	2:B:186:ILE:HG12	2.17	0.45
1:C:315:ASP:HB2	1:C:316:PRO:CD	2.43	0.43
1:A:258:ARG:HH11	5:B:1261:GOL:H31	1.82	0.43
1:C:75:GLY:HA3	1:C:154:GLN:HA	2.01	0.43
1:A:42:VAL:HG13	1:A:51:ILE:CD1	2.49	0.43
2:F:230:PHE:HB3	2:F:233:SER:HB2	2.01	0.42
1:E:234:ASP:OD1	1:E:271:LYS:HD3	2.20	0.42
1:A:171:ARG:CD	1:A:173:ILE:CG2	2.97	0.42
1:E:44:PHE:CD1	1:E:105:VAL:HG21	2.55	0.41
1:C:233:PHE:O	1:C:237:MET:HG3	2.21	0.41
1:C:68:PHE:O	1:C:69:ASP:HB2	2.19	0.41
1:A:343:ILE:HB	1:A:346:ILE:HD12	2.03	0.41
1:C:44:PHE:CD1	1:C:105:VAL:HG21	2.55	0.41
1:E:343:ILE:HB	1:E:346:ILE:HD12	2.03	0.40
1:A:75:GLY:HA3	1:A:154:GLN:HA	2.03	0.40
1:A:195:VAL:HG22	1:A:333:ASP:HB2	2.03	0.40
1:E:75:GLY:HA3	1:E:154:GLN:HA	2.03	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	380/386 (98%)	375 (99%)	5 (1%)	0	100	100
1	C	379/386 (98%)	376 (99%)	3 (1%)	0	100	100
1	E	379/386 (98%)	375 (99%)	4 (1%)	0	100	100
2	B	110/118 (93%)	110 (100%)	0	0	100	100
2	D	110/118 (93%)	109 (99%)	1 (1%)	0	100	100
2	F	111/118 (94%)	110 (99%)	1 (1%)	0	100	100
All	All	1469/1512 (97%)	1455 (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	303/319 (95%)	303 (100%)	0	100	100
1	C	298/319 (93%)	297 (100%)	1 (0%)	92	93
1	E	290/319 (91%)	290 (100%)	0	100	100
2	B	89/107 (83%)	89 (100%)	0	100	100
2	D	91/107 (85%)	91 (100%)	0	100	100
2	F	91/107 (85%)	91 (100%)	0	100	100
All	All	1162/1278 (91%)	1161 (100%)	1 (0%)	93	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	93	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 32 ligands modelled in this entry, 1 is monoatomic - leaving 31 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	$\# Z > 2$
5	GOL	C	1385	-	5,5,5	0.08	0	5,5,5	0.24	0
5	GOL	B	1264	-	5,5,5	0.03	0	5,5,5	0.20	0
5	GOL	A	1386	-	5,5,5	0.05	0	5,5,5	0.26	0
5	GOL	E	1385	-	5,5,5	0.08	0	5,5,5	0.16	0
6	DMS	E	1386	-	3,3,3	0.28	0	3,3,3	0.30	0
5	GOL	C	1387	-	5,5,5	0.06	0	5,5,5	0.18	0
5	GOL	D	1262	-	5,5,5	0.14	0	5,5,5	0.29	0
5	GOL	A	1384	-	5,5,5	0.26	0	5,5,5	0.44	0
5	GOL	B	1263	-	5,5,5	0.07	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	N8Y	E	1383	-	14,14,14	0.14	0	18,19,19	0.63	0
5	GOL	B	1261	-	5,5,5	0.06	0	5,5,5	0.22	0
3	TRS	A	1382	-	7,7,7	0.22	0	9,9,9	0.39	0
5	GOL	B	1262	-	5,5,5	0.10	0	5,5,5	0.24	0
5	GOL	A	1390	-	5,5,5	0.10	0	5,5,5	0.26	0
5	GOL	C	1384	-	5,5,5	0.17	0	5,5,5	0.61	0
6	DMS	A	1392	-	3,3,3	0.26	0	3,3,3	0.25	0
5	GOL	E	1384	-	5,5,5	0.25	0	5,5,5	0.73	0
4	N8Y	A	1383	-	14,14,14	0.16	0	18,19,19	0.62	0
5	GOL	C	1386	-	5,5,5	0.11	0	5,5,5	0.15	0
3	TRS	E	1382	-	7,7,7	0.24	0	9,9,9	0.28	0
3	TRS	C	1382	-	7,7,7	0.20	0	9,9,9	0.31	0
5	GOL	A	1387	-	5,5,5	0.11	0	5,5,5	0.30	0
6	DMS	A	1393	-	3,3,3	0.27	0	3,3,3	0.22	0
5	GOL	A	1389	-	5,5,5	0.07	0	5,5,5	0.17	0
5	GOL	A	1385	-	5,5,5	0.08	0	5,5,5	0.31	0
6	DMS	A	1396	-	3,3,3	0.26	0	3,3,3	0.28	0
6	DMS	A	1391	-	3,3,3	0.26	0	3,3,3	0.39	0
6	DMS	E	1387	-	3,3,3	0.28	0	3,3,3	0.19	0
5	GOL	A	1388	-	5,5,5	0.10	0	5,5,5	0.35	0
6	DMS	C	1388	-	3,3,3	0.17	0	3,3,3	0.16	0
4	N8Y	C	1383	-	14,14,14	0.20	0	18,19,19	0.61	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
5	GOL	C	1385	-	-	0/4/4/4	-
5	GOL	B	1264	-	-	0/4/4/4	-
5	GOL	A	1386	-	-	0/4/4/4	-
5	GOL	E	1385	-	-	0/4/4/4	-
5	GOL	C	1387	-	-	0/4/4/4	-
5	GOL	D	1262	-	-	2/4/4/4	-
5	GOL	A	1384	-	-	0/4/4/4	-
5	GOL	B	1263	-	-	0/4/4/4	-
4	N8Y	E	1383	-	-	0/2/2/2	0/2/2/2
5	GOL	B	1261	-	-	0/4/4/4	-
3	TRS	A	1382	-	-	1/9/9/9	-
5	GOL	B	1262	-	-	2/4/4/4	-
5	GOL	A	1390	-	-	1/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	1384	-	-	3/4/4/4	-
5	GOL	E	1384	-	-	0/4/4/4	-
4	N8Y	A	1383	-	-	0/2/2/2	0/2/2/2
5	GOL	C	1386	-	-	0/4/4/4	-
3	TRS	E	1382	-	-	3/9/9/9	-
3	TRS	C	1382	-	-	6/9/9/9	-
5	GOL	A	1387	-	-	0/4/4/4	-
5	GOL	A	1389	-	-	0/4/4/4	-
5	GOL	A	1385	-	-	2/4/4/4	-
5	GOL	A	1388	-	-	2/4/4/4	-
4	N8Y	C	1383	-	-	0/2/2/2	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1382	TRS	N-C-C2-O2
5	B	1262	GOL	C1-C2-C3-O3
3	E	1382	TRS	C3-C-C1-O1
3	E	1382	TRS	N-C-C1-O1
3	C	1382	TRS	C2-C-C1-O1
3	C	1382	TRS	C3-C-C1-O1
3	C	1382	TRS	N-C-C1-O1
5	A	1385	GOL	O1-C1-C2-O2
5	C	1384	GOL	O1-C1-C2-C3
5	C	1384	GOL	C1-C2-C3-O3
5	A	1385	GOL	O1-C1-C2-C3
5	B	1262	GOL	O2-C2-C3-O3
5	C	1384	GOL	O2-C2-C3-O3
5	A	1388	GOL	O2-C2-C3-O3
3	E	1382	TRS	C2-C-C1-O1
5	D	1262	GOL	C1-C2-C3-O3
3	C	1382	TRS	C1-C-C3-O3
3	C	1382	TRS	C2-C-C3-O3
5	A	1390	GOL	O1-C1-C2-C3
5	D	1262	GOL	O2-C2-C3-O3
3	C	1382	TRS	N-C-C3-O3
5	A	1388	GOL	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1261	GOL	1	0
5	E	1384	GOL	2	0
5	A	1387	GOL	2	0
5	A	1389	GOL	1	0
5	A	1385	GOL	1	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, 95th 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 ²)	Q<0.9
1	A	381/386 (98%)	0.06	4 (1%) 82 84	22, 35, 54, 73	0
1	C	381/386 (98%)	0.17	8 (2%) 63 66	21, 39, 58, 71	0
1	E	381/386 (98%)	0.39	18 (4%) 31 34	27, 49, 71, 93	0
2	B	112/118 (94%)	0.15	1 (0%) 84 85	21, 37, 56, 64	0
2	D	112/118 (94%)	0.08	1 (0%) 84 85	21, 37, 69, 113	0
2	F	113/118 (95%)	0.05	4 (3%) 44 47	24, 39, 72, 78	0
All	All	1480/1512 (97%)	0.18	36 (2%) 59 62	21, 40, 64, 113	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	SER	4.7
1	E	349	LEU	4.6
1	E	191	ALA	3.7
1	E	354	PHE	3.3
1	C	167	LEU	3.3
1	C	94	VAL	3.2
2	F	189	GLY	3.0
2	F	190	PHE	3.0
2	F	194	ASP	2.9
1	C	139	VAL	2.9
1	E	351	GLN	2.9
1	C	105	VAL	2.9
1	E	95	VAL	2.8
1	A	354	PHE	2.8
1	E	1	MET	2.8
1	E	100	ARG	2.6
1	E	353	PHE	2.6
1	E	329	SER	2.6
1	A	202	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	189	VAL	2.6
2	B	149	GLY	2.5
2	D	186	ILE	2.5
1	E	93	MET	2.5
1	E	111	THR	2.5
1	E	140	THR	2.3
1	E	190	GLY	2.3
1	A	300	ALA	2.3
1	C	4	GLY	2.2
1	E	309	LEU	2.2
1	C	103	VAL	2.2
1	A	346	ILE	2.2
1	E	83	VAL	2.2
1	E	321	LEU	2.1
1	C	24	GLY	2.1
1	E	305	LEU	2.0
2	F	164	HIS	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, 95th 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(\AA^2)	Q<0.9
5	GOL	A	1388	6/6	0.56	0.17	63,68,69,69	0
5	GOL	A	1385	6/6	0.78	0.31	54,60,62,63	0
3	TRS	E	1382	8/8	0.78	0.15	42,49,50,52	0
5	GOL	D	1262	6/6	0.79	0.27	49,51,53,56	0
5	GOL	A	1386	6/6	0.80	0.15	73,74,75,76	0
5	GOL	B	1262	6/6	0.82	0.13	38,43,47,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	B	1264	6/6	0.82	0.23	82,83,83,84	0
5	GOL	B	1261	6/6	0.84	0.24	57,59,61,63	0
5	GOL	A	1387	6/6	0.84	0.12	45,48,51,54	0
5	GOL	C	1387	6/6	0.85	0.14	69,70,72,74	0
5	GOL	A	1390	6/6	0.87	0.29	43,51,52,54	0
5	GOL	B	1263	6/6	0.88	0.15	60,66,67,67	0
6	DMS	A	1391	4/4	0.89	0.15	64,65,66,66	0
5	GOL	C	1386	6/6	0.89	0.16	60,64,64,65	0
3	TRS	C	1382	8/8	0.90	0.13	42,46,48,50	0
5	GOL	C	1385	6/6	0.90	0.15	56,57,58,59	0
5	GOL	A	1389	6/6	0.90	0.21	63,65,68,70	0
7	CL	C	1396	1/1	0.91	0.13	57,57,57,57	0
5	GOL	E	1384	6/6	0.91	0.16	34,37,42,43	0
6	DMS	A	1392	4/4	0.92	0.16	69,71,72,72	0
5	GOL	E	1385	6/6	0.92	0.15	60,61,61,61	0
4	N8Y	E	1383	13/13	0.92	0.14	32,37,46,47	0
6	DMS	A	1396	4/4	0.92	0.18	81,81,81,81	0
5	GOL	A	1384	6/6	0.92	0.12	25,35,39,45	0
5	GOL	C	1384	6/6	0.92	0.11	26,31,31,36	0
6	DMS	A	1393	4/4	0.94	0.11	36,42,45,45	0
3	TRS	A	1382	8/8	0.94	0.10	35,38,40,42	0
6	DMS	E	1386	4/4	0.95	0.17	78,79,79,79	0
6	DMS	C	1388	4/4	0.95	0.11	55,56,58,58	0
4	N8Y	C	1383	13/13	0.95	0.13	26,28,37,37	0
4	N8Y	A	1383	13/13	0.96	0.09	20,24,33,34	0
6	DMS	E	1387	4/4	0.97	0.12	54,57,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.