



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:20 AM GMT

PDB ID : 3KTS
Title : CRYSTAL STRUCTURE OF GLYCEROL UPTAKE OPERON ANTITERMINATOR REGULATORY PROTEIN FROM LISTERIA MONOCYTOGENES STR. 4b F2365
Authors : Patskovsky, Y.; Toro, R.; Freeman, J.; Do, J.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYS-GXRC)
Deposited on : 2009-11-25
Resolution : 2.75 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

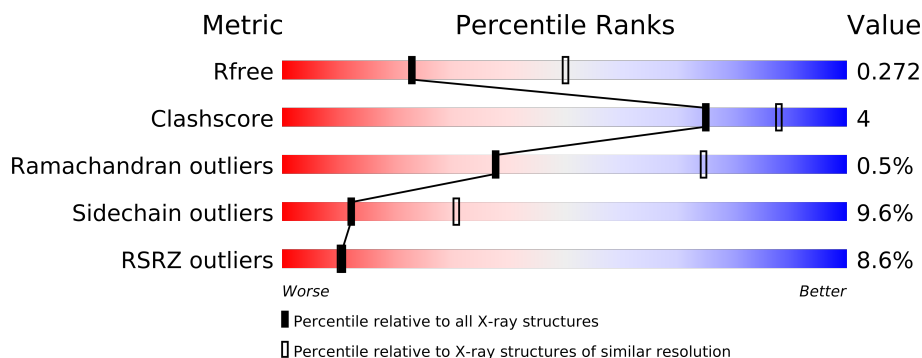
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.75 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}	66092	2406 (2.80-2.72)
Clashscore	79885	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (2.80-2.72)
RSRZ outliers	66119	2409 (2.80-2.72)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	192	
1	B	192	
1	C	192	
1	D	192	
1	E	192	
1	F	192	
1	G	192	
1	H	192	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11436 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Glycerol uptake operon antiterminator regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1425	909	242	264	10			
1	B	185	Total	C	N	O	S	0	0	0
			1425	909	242	264	10			
1	C	182	Total	C	N	O	S	0	0	0
			1403	895	237	261	10			
1	D	183	Total	C	N	O	S	0	0	0
			1411	901	238	262	10			
1	E	185	Total	C	N	O	S	0	0	0
			1425	909	242	264	10			
1	F	184	Total	C	N	O	S	0	0	0
			1415	903	239	263	10			
1	G	185	Total	C	N	O	S	0	0	0
			1425	909	242	264	10			
1	H	185	Total	C	N	O	S	0	0	0
			1425	909	242	264	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q71ZR5
A	1	LEU	-	expression tag	UNP Q71ZR5
A	183	GLU	-	expression tag	UNP Q71ZR5
A	184	GLY	-	expression tag	UNP Q71ZR5
A	185	HIS	-	expression tag	UNP Q71ZR5
A	186	HIS	-	expression tag	UNP Q71ZR5
A	187	HIS	-	expression tag	UNP Q71ZR5
A	188	HIS	-	expression tag	UNP Q71ZR5
A	189	HIS	-	expression tag	UNP Q71ZR5
A	190	HIS	-	expression tag	UNP Q71ZR5
B	0	SER	-	expression tag	UNP Q71ZR5
B	1	LEU	-	expression tag	UNP Q71ZR5
B	183	GLU	-	expression tag	UNP Q71ZR5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	184	GLY	-	expression tag	UNP Q71ZR5
B	185	HIS	-	expression tag	UNP Q71ZR5
B	186	HIS	-	expression tag	UNP Q71ZR5
B	187	HIS	-	expression tag	UNP Q71ZR5
B	188	HIS	-	expression tag	UNP Q71ZR5
B	189	HIS	-	expression tag	UNP Q71ZR5
B	190	HIS	-	expression tag	UNP Q71ZR5
C	0	SER	-	expression tag	UNP Q71ZR5
C	1	LEU	-	expression tag	UNP Q71ZR5
C	183	GLU	-	expression tag	UNP Q71ZR5
C	184	GLY	-	expression tag	UNP Q71ZR5
C	185	HIS	-	expression tag	UNP Q71ZR5
C	186	HIS	-	expression tag	UNP Q71ZR5
C	187	HIS	-	expression tag	UNP Q71ZR5
C	188	HIS	-	expression tag	UNP Q71ZR5
C	189	HIS	-	expression tag	UNP Q71ZR5
C	190	HIS	-	expression tag	UNP Q71ZR5
D	0	SER	-	expression tag	UNP Q71ZR5
D	1	LEU	-	expression tag	UNP Q71ZR5
D	183	GLU	-	expression tag	UNP Q71ZR5
D	184	GLY	-	expression tag	UNP Q71ZR5
D	185	HIS	-	expression tag	UNP Q71ZR5
D	186	HIS	-	expression tag	UNP Q71ZR5
D	187	HIS	-	expression tag	UNP Q71ZR5
D	188	HIS	-	expression tag	UNP Q71ZR5
D	189	HIS	-	expression tag	UNP Q71ZR5
D	190	HIS	-	expression tag	UNP Q71ZR5
E	0	SER	-	expression tag	UNP Q71ZR5
E	1	LEU	-	expression tag	UNP Q71ZR5
E	183	GLU	-	expression tag	UNP Q71ZR5
E	184	GLY	-	expression tag	UNP Q71ZR5
E	185	HIS	-	expression tag	UNP Q71ZR5
E	186	HIS	-	expression tag	UNP Q71ZR5
E	187	HIS	-	expression tag	UNP Q71ZR5
E	188	HIS	-	expression tag	UNP Q71ZR5
E	189	HIS	-	expression tag	UNP Q71ZR5
E	190	HIS	-	expression tag	UNP Q71ZR5
F	0	SER	-	expression tag	UNP Q71ZR5
F	1	LEU	-	expression tag	UNP Q71ZR5
F	183	GLU	-	expression tag	UNP Q71ZR5
F	184	GLY	-	expression tag	UNP Q71ZR5
F	185	HIS	-	expression tag	UNP Q71ZR5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	186	HIS	-	expression tag	UNP Q71ZR5
F	187	HIS	-	expression tag	UNP Q71ZR5
F	188	HIS	-	expression tag	UNP Q71ZR5
F	189	HIS	-	expression tag	UNP Q71ZR5
F	190	HIS	-	expression tag	UNP Q71ZR5
G	0	SER	-	expression tag	UNP Q71ZR5
G	1	LEU	-	expression tag	UNP Q71ZR5
G	183	GLU	-	expression tag	UNP Q71ZR5
G	184	GLY	-	expression tag	UNP Q71ZR5
G	185	HIS	-	expression tag	UNP Q71ZR5
G	186	HIS	-	expression tag	UNP Q71ZR5
G	187	HIS	-	expression tag	UNP Q71ZR5
G	188	HIS	-	expression tag	UNP Q71ZR5
G	189	HIS	-	expression tag	UNP Q71ZR5
G	190	HIS	-	expression tag	UNP Q71ZR5
H	0	SER	-	expression tag	UNP Q71ZR5
H	1	LEU	-	expression tag	UNP Q71ZR5
H	183	GLU	-	expression tag	UNP Q71ZR5
H	184	GLY	-	expression tag	UNP Q71ZR5
H	185	HIS	-	expression tag	UNP Q71ZR5
H	186	HIS	-	expression tag	UNP Q71ZR5
H	187	HIS	-	expression tag	UNP Q71ZR5
H	188	HIS	-	expression tag	UNP Q71ZR5
H	189	HIS	-	expression tag	UNP Q71ZR5
H	190	HIS	-	expression tag	UNP Q71ZR5

- Molecule 2 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	O	P	0	0
			10	3	6	1		
2	D	1	Total	C	O	P	0	0
			10	3	6	1		
2	E	1	Total	C	O	P	0	0
			10	3	6	1		
2	H	1	Total	C	O	P	0	0
			10	3	6	1		
2	B	1	Total	C	O	P	0	0
			10	3	6	1		
2	C	1	Total	C	O	P	0	0
			10	3	6	1		
2	A	1	Total	C	O	P	0	0
			10	3	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total	C	O	P	0	0
			10	3	6	1		

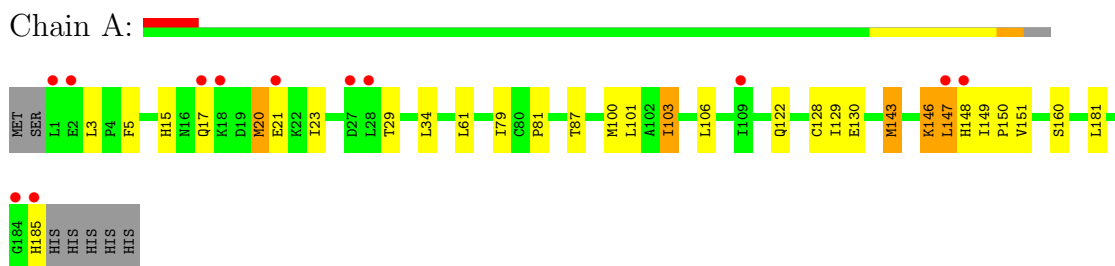
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total	O	0	0
			2	2		

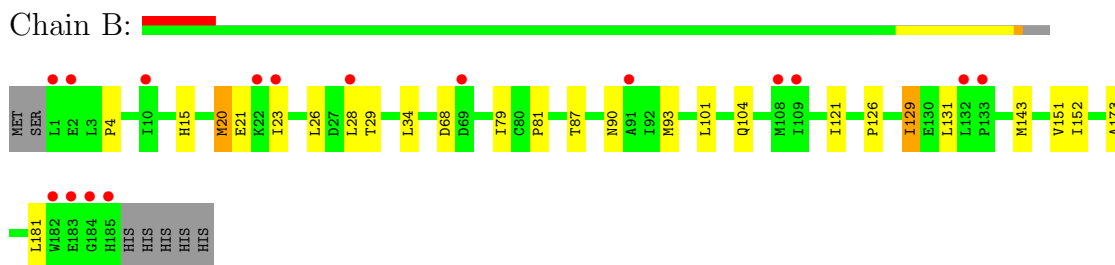
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

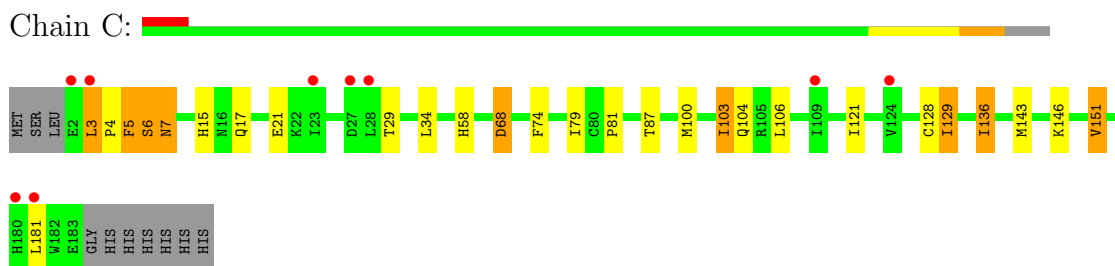
- Molecule 1: Glycerol uptake operon antiterminator regulatory protein



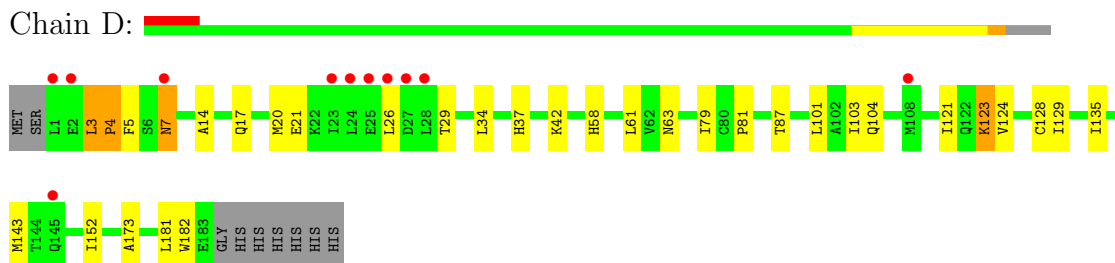
- Molecule 1: Glycerol uptake operon antiterminator regulatory protein



- Molecule 1: Glycerol uptake operon antiterminator regulatory protein

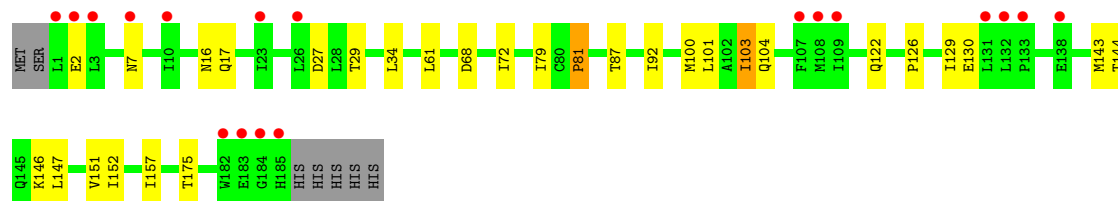


- Molecule 1: Glycerol uptake operon antiterminator regulatory protein



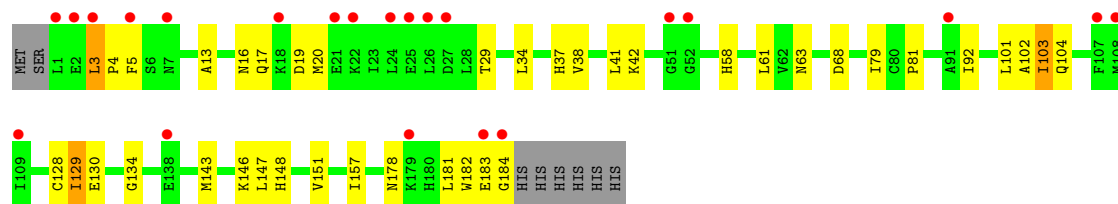
- Molecule 1: Glycerol uptake operon antiterminator regulatory protein

Chain E: 



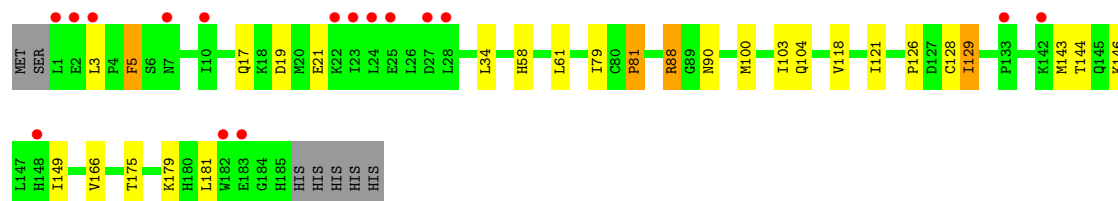
- Molecule 1: Glycerol uptake operon antiterminator regulatory protein

Chain F: 



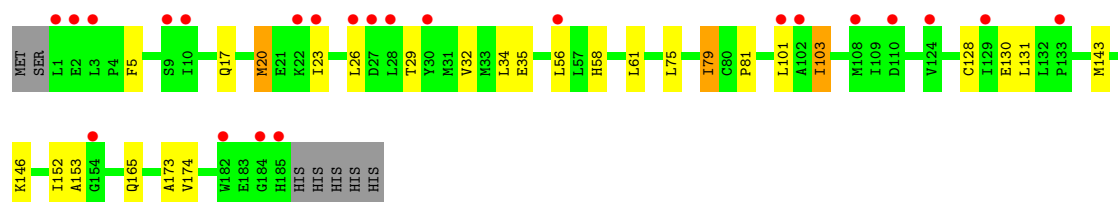
- Molecule 1: Glycerol uptake operon antiterminator regulatory protein

Chain G: 



- Molecule 1: Glycerol uptake operon antiterminator regulatory protein

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.60Å 110.60Å 130.97Å 90.00° 116.44° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75 39.09 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.75) 98.9 (39.09-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.64	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.218 , 0.272 0.224 , 0.272	Depositor DCC
R_{free} test set	1408 reflections (3.22%)	DCC
Wilson B-factor (Å ²)	92.1	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 74.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 45155 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11436	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.35	0/1447	0.57	0/1957
1	B	0.35	0/1447	0.58	0/1957
1	C	0.35	0/1424	0.57	0/1926
1	D	0.35	0/1432	0.59	0/1937
1	E	0.35	0/1447	0.58	0/1957
1	F	0.35	0/1436	0.57	0/1942
1	G	0.32	0/1447	0.53	0/1957
1	H	0.35	0/1447	0.57	0/1957
All	All	0.35	0/11527	0.57	0/15590

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	A	0	2
1	C	0	3
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	LEU	Peptide
1	A	148	HIS	Peptide
1	C	3	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	5	PHE	Peptide
1	C	7	ASN	Peptide

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1425	0	1482	12	0
1	B	1425	0	1482	9	0
1	C	1403	0	1458	9	0
1	D	1411	0	1472	12	0
1	E	1425	0	1482	8	0
1	F	1415	0	1475	19	0
1	G	1425	0	1482	14	0
1	H	1425	0	1482	11	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
2	G	10	0	0	0	0
2	H	10	0	0	0	0
3	G	2	0	0	0	0
All	All	11436	0	11815	92	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (92) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:149:ILE:HG23	1:A:150:PRO:HD2	1.27	1.09
1:G:129:ILE:HG22	1:G:149:ILE:CG2	1.83	1.09
1:G:129:ILE:HG22	1:G:149:ILE:HG22	1.39	1.05
1:A:149:ILE:CG2	1:A:150:PRO:HD2	1.94	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:181:LEU:HD12	1:F:181:LEU:O	1.67	0.93
1:G:129:ILE:HG22	1:G:149:ILE:HG21	1.63	0.80
1:A:103:ILE:HB	1:A:128:CYS:HB3	1.70	0.74
1:H:34:LEU:O	1:H:61:LEU:HB2	1.87	0.73
1:C:79:ILE:HG22	1:C:81:PRO:HD3	1.73	0.71
1:D:79:ILE:HG22	1:D:81:PRO:HD3	1.76	0.67
1:A:79:ILE:HG22	1:A:81:PRO:HD3	1.76	0.67
1:G:129:ILE:CG2	1:G:149:ILE:CG2	2.70	0.66
1:C:103:ILE:HB	1:C:128:CYS:HB3	1.78	0.65
1:D:7:ASN:O	1:D:7:ASN:ND2	2.31	0.64
1:G:3:LEU:HD13	1:G:5:PHE:CE1	2.35	0.62
1:A:149:ILE:CG2	1:A:150:PRO:CD	2.73	0.61
1:E:79:ILE:HG22	1:E:81:PRO:HD3	1.81	0.61
1:B:79:ILE:HG22	1:B:81:PRO:HD3	1.82	0.60
1:G:34:LEU:O	1:G:61:LEU:HB2	2.02	0.59
1:F:34:LEU:O	1:F:61:LEU:HB2	2.02	0.59
1:H:103:ILE:HB	1:H:128:CYS:HB3	1.86	0.57
1:D:34:LEU:O	1:D:61:LEU:HB2	2.05	0.57
1:G:3:LEU:HD13	1:G:5:PHE:HE1	1.69	0.56
1:A:103:ILE:HD11	1:A:130:GLU:HB2	1.88	0.56
1:F:181:LEU:CD1	1:F:181:LEU:O	2.50	0.55
1:C:15:HIS:CE1	1:C:34:LEU:HD13	2.40	0.55
1:G:129:ILE:CG2	1:G:149:ILE:HG21	2.34	0.55
1:A:34:LEU:O	1:A:61:LEU:HB2	2.07	0.55
1:F:103:ILE:HB	1:F:128:CYS:HB3	1.88	0.55
1:F:129:ILE:HG13	1:F:151:VAL:HG12	1.90	0.54
1:E:34:LEU:O	1:E:61:LEU:HB2	2.08	0.53
1:B:20:MET:HA	1:B:23:ILE:HG12	1.91	0.52
1:D:14:ALA:O	1:D:34:LEU:HB2	2.10	0.52
1:F:16:ASN:H	1:F:19:ASP:HB2	1.75	0.52
1:H:79:ILE:HG22	1:H:81:PRO:HD3	1.91	0.52
1:F:183:GLU:HG2	1:F:184:GLY:H	1.75	0.51
1:E:103:ILE:HD11	1:E:130:GLU:HB2	1.93	0.51
1:G:104:GLN:HE22	1:G:121:ILE:HA	1.76	0.51
1:H:103:ILE:HD11	1:H:130:GLU:HB2	1.93	0.50
1:G:79:ILE:HG22	1:G:81:PRO:HD3	1.92	0.50
1:A:122:GLN:OE1	1:A:147:LEU:HD21	2.12	0.49
1:D:104:GLN:HE22	1:D:121:ILE:HA	1.77	0.48
1:H:153:ALA:HB3	1:H:174:VAL:HG22	1.96	0.48
1:F:92:ILE:HG13	1:F:104:GLN:HG3	1.96	0.48
1:D:152:ILE:HD12	1:D:173:ALA:HB3	1.96	0.48
1:B:90:ASN:HA	1:B:93:MET:HE2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:129:ILE:HG13	1:C:151:VAL:HG12	1.95	0.48
1:F:13:ALA:HB1	1:F:34:LEU:HD11	1.97	0.47
1:B:26:LEU:HD23	1:B:28:LEU:HD12	1.97	0.47
1:G:118:VAL:HA	1:G:121:ILE:HD12	1.97	0.47
1:E:104:GLN:HB3	1:E:129:ILE:HG22	1.97	0.47
1:F:79:ILE:HG22	1:F:81:PRO:HD3	1.97	0.46
1:F:134:GLY:HA3	1:F:157:ILE:HD11	1.98	0.46
1:A:34:LEU:O	1:A:61:LEU:CB	2.64	0.46
1:H:23:ILE:HA	1:H:26:LEU:HD13	1.98	0.46
1:G:103:ILE:HG12	1:G:128:CYS:HB3	1.98	0.45
1:A:15:HIS:CE1	1:A:34:LEU:HD13	2.51	0.45
1:E:104:GLN:HE21	1:E:126:PRO:HG3	1.81	0.45
1:E:152:ILE:HG21	1:E:175:THR:HG23	1.99	0.45
1:B:152:ILE:HD12	1:B:173:ALA:HB3	1.98	0.45
1:A:143:MET:O	1:A:146:LYS:HB2	2.17	0.45
1:B:104:GLN:HE22	1:B:121:ILE:HA	1.83	0.44
1:H:20:MET:HA	1:H:23:ILE:HG12	1.99	0.44
1:D:103:ILE:HG12	1:D:128:CYS:HB3	1.99	0.44
1:B:129:ILE:HG13	1:B:151:VAL:HG12	1.99	0.43
1:E:68:ASP:O	1:E:72:ILE:HG12	2.18	0.43
1:F:3:LEU:HD11	1:F:128:CYS:HB2	1.99	0.43
1:C:6:SER:O	1:C:7:ASN:HB2	2.18	0.43
1:C:74:PHE:HB2	1:F:38:VAL:HG13	1.99	0.43
1:G:126:PRO:O	1:G:149:ILE:HD12	2.19	0.43
1:C:104:GLN:HE22	1:C:121:ILE:HA	1.84	0.43
1:F:103:ILE:HD11	1:F:130:GLU:HB2	2.01	0.42
1:D:26:LEU:HD21	1:D:182:TRP:HB3	2.00	0.42
1:D:37:HIS:HD2	1:D:63:ASN:HD22	1.66	0.42
1:B:15:HIS:CE1	1:B:34:LEU:HD13	2.55	0.42
1:H:34:LEU:O	1:H:61:LEU:CB	2.62	0.42
1:F:92:ILE:HG23	1:F:102:ALA:HB1	2.02	0.42
1:F:37:HIS:CD2	1:F:63:ASN:HD22	2.38	0.41
1:F:37:HIS:HD2	1:F:63:ASN:HD22	1.69	0.41
1:E:92:ILE:HG13	1:E:104:GLN:HG3	2.03	0.41
1:H:32:VAL:HG22	1:H:56:LEU:HB2	2.03	0.41
1:H:75:LEU:HA	1:H:79:ILE:HB	2.03	0.41
1:F:41:LEU:HD23	1:F:79:ILE:HG12	2.03	0.41
1:C:3:LEU:HA	1:C:4:PRO:HD3	1.42	0.41
1:D:123:LYS:HG2	1:D:124:VAL:HG13	2.02	0.41
1:H:152:ILE:HD12	1:H:173:ALA:HB3	2.02	0.41
1:F:178:ASN:HB3	1:F:181:LEU:CD2	2.51	0.41
1:B:104:GLN:HE21	1:B:126:PRO:HG3	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:20:MET:HA	1:A:23:ILE:HG12	2.03	0.41
1:C:136:ILE:HD13	1:D:135:ILE:HD11	2.03	0.40
1:G:88:ARG:HH21	1:G:90:ASN:HB2	1.86	0.40
1:D:3:LEU:HA	1:D:4:PRO:HD2	1.75	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	183/192 (95%)	177 (97%)	6 (3%)	0	100	100
1	B	183/192 (95%)	169 (92%)	12 (7%)	2 (1%)	21	53
1	C	180/192 (94%)	171 (95%)	8 (4%)	1 (1%)	33	70
1	D	181/192 (94%)	171 (94%)	9 (5%)	1 (1%)	33	70
1	E	183/192 (95%)	172 (94%)	10 (6%)	1 (0%)	38	74
1	F	182/192 (95%)	168 (92%)	13 (7%)	1 (0%)	38	74
1	G	183/192 (95%)	174 (95%)	8 (4%)	1 (0%)	38	74
1	H	183/192 (95%)	173 (94%)	10 (6%)	0	100	100
All	All	1458/1536 (95%)	1375 (94%)	76 (5%)	7 (0%)	38	74

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	PRO
1	B	68	ASP
1	D	4	PRO
1	G	81	PRO
1	C	68	ASP
1	E	81	PRO
1	F	4	PRO

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	157/164 (96%)	139 (88%)	18 (12%)	8	21
1	B	157/164 (96%)	148 (94%)	9 (6%)	29	61
1	C	155/164 (94%)	138 (89%)	17 (11%)	9	24
1	D	156/164 (95%)	141 (90%)	15 (10%)	12	31
1	E	157/164 (96%)	140 (89%)	17 (11%)	9	24
1	F	156/164 (95%)	140 (90%)	16 (10%)	10	27
1	G	157/164 (96%)	142 (90%)	15 (10%)	12	31
1	H	157/164 (96%)	144 (92%)	13 (8%)	16	39
All	All	1252/1312 (95%)	1132 (90%)	120 (10%)	12	31

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	5	PHE
1	A	17	GLN
1	A	20	MET
1	A	21	GLU
1	A	29	THR
1	A	87	THR
1	A	100	MET
1	A	101	LEU
1	A	103	ILE
1	A	106	LEU
1	A	129	ILE
1	A	143	MET
1	A	146	LYS
1	A	151	VAL
1	A	160	SER
1	A	181	LEU
1	A	185	HIS
1	B	20	MET
1	B	21	GLU
1	B	29	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	87	THR
1	B	101	LEU
1	B	129	ILE
1	B	131	LEU
1	B	143	MET
1	B	181	LEU
1	C	5	PHE
1	C	6	SER
1	C	17	GLN
1	C	21	GLU
1	C	29	THR
1	C	58	HIS
1	C	68	ASP
1	C	87	THR
1	C	100	MET
1	C	103	ILE
1	C	106	LEU
1	C	129	ILE
1	C	136	ILE
1	C	143	MET
1	C	146	LYS
1	C	151	VAL
1	C	181	LEU
1	D	3	LEU
1	D	5	PHE
1	D	7	ASN
1	D	17	GLN
1	D	20	MET
1	D	21	GLU
1	D	29	THR
1	D	42	LYS
1	D	58	HIS
1	D	87	THR
1	D	101	LEU
1	D	123	LYS
1	D	129	ILE
1	D	143	MET
1	D	181	LEU
1	E	2	GLU
1	E	7	ASN
1	E	16	ASN
1	E	17	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	27	ASP
1	E	29	THR
1	E	87	THR
1	E	100	MET
1	E	101	LEU
1	E	103	ILE
1	E	122	GLN
1	E	143	MET
1	E	144	THR
1	E	146	LYS
1	E	147	LEU
1	E	151	VAL
1	E	157	ILE
1	F	3	LEU
1	F	5	PHE
1	F	17	GLN
1	F	20	MET
1	F	29	THR
1	F	42	LYS
1	F	58	HIS
1	F	68	ASP
1	F	101	LEU
1	F	103	ILE
1	F	129	ILE
1	F	143	MET
1	F	146	LYS
1	F	147	LEU
1	F	148	HIS
1	F	182	TRP
1	G	5	PHE
1	G	17	GLN
1	G	19	ASP
1	G	21	GLU
1	G	58	HIS
1	G	88	ARG
1	G	100	MET
1	G	129	ILE
1	G	143	MET
1	G	144	THR
1	G	146	LYS
1	G	166	VAL
1	G	175	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	179	LYS
1	G	181	LEU
1	H	5	PHE
1	H	17	GLN
1	H	20	MET
1	H	29	THR
1	H	35	GLU
1	H	58	HIS
1	H	79	ILE
1	H	101	LEU
1	H	103	ILE
1	H	131	LEU
1	H	143	MET
1	H	146	LYS
1	H	165	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	15	HIS
1	A	58	HIS
1	A	104	GLN
1	A	165	GLN
1	B	15	HIS
1	B	104	GLN
1	C	58	HIS
1	C	104	GLN
1	C	125	GLN
1	C	178	ASN
1	D	15	HIS
1	D	63	ASN
1	D	90	ASN
1	D	104	GLN
1	D	145	GLN
1	E	7	ASN
1	E	15	HIS
1	E	17	GLN
1	E	58	HIS
1	E	104	GLN
1	E	122	GLN
1	F	15	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	17	GLN
1	F	37	HIS
1	F	58	HIS
1	F	180	HIS
1	G	58	HIS
1	G	104	GLN
1	G	165	GLN
1	H	15	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 8 ligands modelled in this entry, 8 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	185/192 (96%)	0.50	12 (6%) 18 19	69, 87, 121, 149	0
1	B	185/192 (96%)	0.65	16 (8%) 11 10	70, 94, 126, 157	0
1	C	182/192 (94%)	0.43	9 (4%) 28 30	67, 91, 124, 150	0
1	D	183/192 (95%)	0.55	11 (6%) 21 22	66, 90, 120, 150	0
1	E	185/192 (96%)	0.63	18 (9%) 8 8	64, 94, 131, 148	0
1	F	184/192 (95%)	0.71	22 (11%) 5 5	73, 100, 128, 142	0
1	G	185/192 (96%)	0.70	16 (8%) 11 10	73, 104, 140, 149	0
1	H	185/192 (96%)	0.83	23 (12%) 5 4	80, 106, 132, 153	0
All	All	1474/1536 (95%)	0.62	127 (8%) 11 10	64, 96, 131, 157	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	LEU	14.4
1	D	1	LEU	9.2
1	G	1	LEU	8.1
1	A	1	LEU	7.7
1	E	1	LEU	7.1
1	H	1	LEU	6.8
1	H	2	GLU	6.6
1	E	185	HIS	6.1
1	F	51	GLY	5.4
1	H	3	LEU	5.4
1	H	185	HIS	5.3
1	G	28	LEU	4.8
1	B	185	HIS	4.7
1	G	24	LEU	4.6
1	G	23	ILE	4.6
1	F	24	LEU	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	25	GLU	4.4
1	G	2	GLU	4.4
1	D	23	ILE	4.3
1	E	184	GLY	4.1
1	E	183	GLU	4.1
1	D	27	ASP	4.1
1	F	21	GLU	3.9
1	E	3	LEU	3.9
1	D	2	GLU	3.9
1	C	2	GLU	3.9
1	A	17	GLN	3.8
1	H	184	GLY	3.8
1	D	26	LEU	3.7
1	F	1	LEU	3.7
1	F	22	LYS	3.6
1	D	28	LEU	3.6
1	F	26	LEU	3.6
1	F	5	PHE	3.4
1	A	28	LEU	3.3
1	H	124	VAL	3.3
1	D	24	LEU	3.3
1	F	27	ASP	3.2
1	G	3	LEU	3.2
1	F	52	GLY	3.2
1	C	181	LEU	3.2
1	F	7	ASN	3.1
1	H	10	ILE	3.1
1	A	184	GLY	3.1
1	B	69	ASP	3.1
1	B	2	GLU	3.1
1	F	108	MET	3.1
1	A	21	GLU	3.0
1	E	10	ILE	2.9
1	F	183	GLU	2.9
1	C	180	HIS	2.9
1	A	148	HIS	2.9
1	F	179	LYS	2.9
1	G	182	TRP	2.9
1	B	183	GLU	2.8
1	A	147	LEU	2.8
1	H	102	ALA	2.8
1	H	182	TRP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	28	LEU	2.7
1	E	107	PHE	2.7
1	G	10	ILE	2.7
1	E	132	LEU	2.7
1	B	184	GLY	2.7
1	G	25	GLU	2.7
1	F	184	GLY	2.7
1	F	18	LYS	2.7
1	E	109	ILE	2.6
1	E	26	LEU	2.6
1	G	27	ASP	2.6
1	H	110	ASP	2.6
1	H	101	LEU	2.6
1	F	3	LEU	2.6
1	A	109	ILE	2.6
1	H	28	LEU	2.6
1	F	2	GLU	2.6
1	G	22	LYS	2.6
1	B	10	ILE	2.6
1	D	145	GLN	2.6
1	E	2	GLU	2.5
1	H	23	ILE	2.5
1	C	3	LEU	2.5
1	H	30	TYR	2.5
1	C	109	ILE	2.5
1	H	27	ASP	2.5
1	E	182	TRP	2.5
1	E	131	LEU	2.4
1	E	23	ILE	2.4
1	E	138	GLU	2.4
1	G	183	GLU	2.4
1	B	28	LEU	2.4
1	E	108	MET	2.4
1	G	7	ASN	2.3
1	H	9	SER	2.3
1	B	91	ALA	2.3
1	A	27	ASP	2.3
1	E	133	PRO	2.3
1	B	182	TRP	2.3
1	H	26	LEU	2.3
1	D	108	MET	2.3
1	F	107	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	108	MET	2.2
1	G	148	HIS	2.2
1	B	132	LEU	2.2
1	B	133	PRO	2.2
1	F	138	GLU	2.2
1	B	109	ILE	2.2
1	H	56	LEU	2.2
1	H	154	GLY	2.1
1	F	109	ILE	2.1
1	H	133	PRO	2.1
1	A	185	HIS	2.1
1	G	142	LYS	2.1
1	A	2	GLU	2.1
1	F	91	ALA	2.1
1	H	129	ILE	2.1
1	E	7	ASN	2.1
1	C	27	ASP	2.1
1	B	22	LYS	2.1
1	H	22	LYS	2.1
1	B	108	MET	2.1
1	A	18	LYS	2.0
1	B	23	ILE	2.0
1	C	124	VAL	2.0
1	G	133	PRO	2.0
1	C	23	ILE	2.0
1	D	7	ASN	2.0
1	D	25	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	UNL	D	191	10/-	0.29	1.97	78,100,105,119	0
2	UNL	F	191	10/-	0.27	1.34	100,115,125,132	0
2	UNL	B	191	10/-	0.29	1.05	68,92,96,106	0
2	UNL	G	191	10/-	0.26	0.78	106,113,120,123	0
2	UNL	A	191	10/-	0.25	0.54	77,96,105,105	0
2	UNL	C	191	10/-	0.19	-0.20	71,99,107,111	0
2	UNL	E	191	10/-	0.19	-0.60	105,123,132,137	0
2	UNL	H	191	10/-	0.18	-1.02	92,105,117,119	0

6.5 Other polymers ⓘ

There are no such residues in this entry.