



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:46 AM UTC

PDB ID : 2QSD / pdb_00002qsd
Title : Crystal structure of a protein Il1583 from Idiomarina loihiensis
Authors : Patskovsky, Y.; Bonanno, J.; Sauder, J.M.; Romero, R.; Rutter, M.; Koss, J.;
Mckenzie, C.; Gheyi, T.; Bain, K.; Wasserman, S.R.; Burley, S.K.; Almo, S.C.;
New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2007-07-30
Resolution : 2.50 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

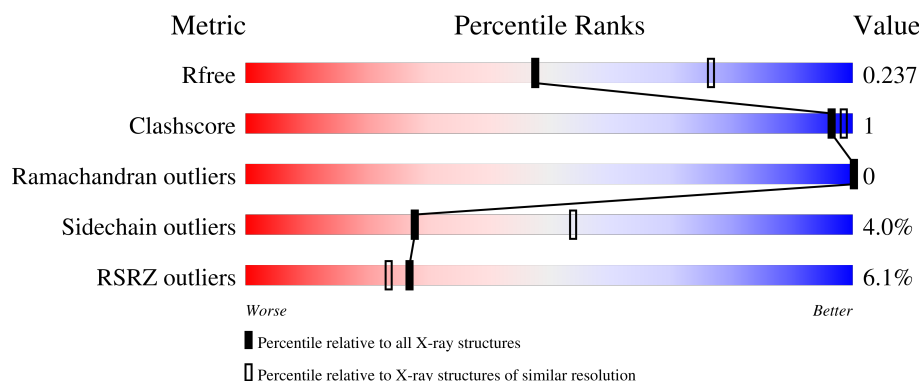
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	187	4% 75% • • 22%
1	B	187	5% 73% 5% 22%
1	C	187	5% 76% • • 21%
1	D	187	4% 75% • • 22%
1	E	187	5% 72% • • 22%

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Mol	Chain	Length	Quality of chain
1	F	187	 6% 72% 6% 22%
1	G	187	 4% 75% 6% 22%
1	H	187	 5% 72% 6% 21%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9688 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 Uncharacterized conserved protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	Se	0	0	0
			1175	756	196	220	2	1			
1	B	145	Total	C	N	O	S	Se	0	0	0
			1166	751	195	217	2	1			
1	C	147	Total	C	N	O	S	Se	0	0	0
			1179	758	197	221	2	1			
1	D	145	Total	C	N	O	S	Se	0	1	0
			1174	756	198	217	2	1			
1	E	146	Total	C	N	O	S	Se	0	0	0
			1175	756	196	220	2	1			
1	F	146	Total	C	N	O	S	Se	0	0	0
			1170	753	196	218	2	1			
1	G	146	Total	C	N	O	S	Se	0	2	0
			1185	761	200	221	2	1			
1	H	147	Total	C	N	O	S	Se	0	0	0
			1179	758	197	221	2	1			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP Q5QU98
A	0	SER	-	expression tag	UNP Q5QU98
A	1	LEU	-	expression tag	UNP Q5QU98
A	179	GLU	-	expression tag	UNP Q5QU98
A	180	GLY	-	expression tag	UNP Q5QU98
A	181	HIS	-	expression tag	UNP Q5QU98
A	182	HIS	-	expression tag	UNP Q5QU98
A	183	HIS	-	expression tag	UNP Q5QU98
A	184	HIS	-	expression tag	UNP Q5QU98
A	185	HIS	-	expression tag	UNP Q5QU98
A	186	HIS	-	expression tag	UNP Q5QU98
B	-1	MSE	-	expression tag	UNP Q5QU98
B	0	SER	-	expression tag	UNP Q5QU98

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	LEU	-	expression tag	UNP Q5QU98
B	179	GLU	-	expression tag	UNP Q5QU98
B	180	GLY	-	expression tag	UNP Q5QU98
B	181	HIS	-	expression tag	UNP Q5QU98
B	182	HIS	-	expression tag	UNP Q5QU98
B	183	HIS	-	expression tag	UNP Q5QU98
B	184	HIS	-	expression tag	UNP Q5QU98
B	185	HIS	-	expression tag	UNP Q5QU98
B	186	HIS	-	expression tag	UNP Q5QU98
C	-1	MSE	-	expression tag	UNP Q5QU98
C	0	SER	-	expression tag	UNP Q5QU98
C	1	LEU	-	expression tag	UNP Q5QU98
C	179	GLU	-	expression tag	UNP Q5QU98
C	180	GLY	-	expression tag	UNP Q5QU98
C	181	HIS	-	expression tag	UNP Q5QU98
C	182	HIS	-	expression tag	UNP Q5QU98
C	183	HIS	-	expression tag	UNP Q5QU98
C	184	HIS	-	expression tag	UNP Q5QU98
C	185	HIS	-	expression tag	UNP Q5QU98
C	186	HIS	-	expression tag	UNP Q5QU98
D	-1	MSE	-	expression tag	UNP Q5QU98
D	0	SER	-	expression tag	UNP Q5QU98
D	1	LEU	-	expression tag	UNP Q5QU98
D	179	GLU	-	expression tag	UNP Q5QU98
D	180	GLY	-	expression tag	UNP Q5QU98
D	181	HIS	-	expression tag	UNP Q5QU98
D	182	HIS	-	expression tag	UNP Q5QU98
D	183	HIS	-	expression tag	UNP Q5QU98
D	184	HIS	-	expression tag	UNP Q5QU98
D	185	HIS	-	expression tag	UNP Q5QU98
D	186	HIS	-	expression tag	UNP Q5QU98
E	-1	MSE	-	expression tag	UNP Q5QU98
E	0	SER	-	expression tag	UNP Q5QU98
E	1	LEU	-	expression tag	UNP Q5QU98
E	179	GLU	-	expression tag	UNP Q5QU98
E	180	GLY	-	expression tag	UNP Q5QU98
E	181	HIS	-	expression tag	UNP Q5QU98
E	182	HIS	-	expression tag	UNP Q5QU98
E	183	HIS	-	expression tag	UNP Q5QU98
E	184	HIS	-	expression tag	UNP Q5QU98
E	185	HIS	-	expression tag	UNP Q5QU98
E	186	HIS	-	expression tag	UNP Q5QU98

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	MSE	-	expression tag	UNP Q5QU98
F	0	SER	-	expression tag	UNP Q5QU98
F	1	LEU	-	expression tag	UNP Q5QU98
F	179	GLU	-	expression tag	UNP Q5QU98
F	180	GLY	-	expression tag	UNP Q5QU98
F	181	HIS	-	expression tag	UNP Q5QU98
F	182	HIS	-	expression tag	UNP Q5QU98
F	183	HIS	-	expression tag	UNP Q5QU98
F	184	HIS	-	expression tag	UNP Q5QU98
F	185	HIS	-	expression tag	UNP Q5QU98
F	186	HIS	-	expression tag	UNP Q5QU98
G	-1	MSE	-	expression tag	UNP Q5QU98
G	0	SER	-	expression tag	UNP Q5QU98
G	1	LEU	-	expression tag	UNP Q5QU98
G	179	GLU	-	expression tag	UNP Q5QU98
G	180	GLY	-	expression tag	UNP Q5QU98
G	181	HIS	-	expression tag	UNP Q5QU98
G	182	HIS	-	expression tag	UNP Q5QU98
G	183	HIS	-	expression tag	UNP Q5QU98
G	184	HIS	-	expression tag	UNP Q5QU98
G	185	HIS	-	expression tag	UNP Q5QU98
G	186	HIS	-	expression tag	UNP Q5QU98
H	-1	MSE	-	expression tag	UNP Q5QU98
H	0	SER	-	expression tag	UNP Q5QU98
H	1	LEU	-	expression tag	UNP Q5QU98
H	179	GLU	-	expression tag	UNP Q5QU98
H	180	GLY	-	expression tag	UNP Q5QU98
H	181	HIS	-	expression tag	UNP Q5QU98
H	182	HIS	-	expression tag	UNP Q5QU98
H	183	HIS	-	expression tag	UNP Q5QU98
H	184	HIS	-	expression tag	UNP Q5QU98
H	185	HIS	-	expression tag	UNP Q5QU98
H	186	HIS	-	expression tag	UNP Q5QU98

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

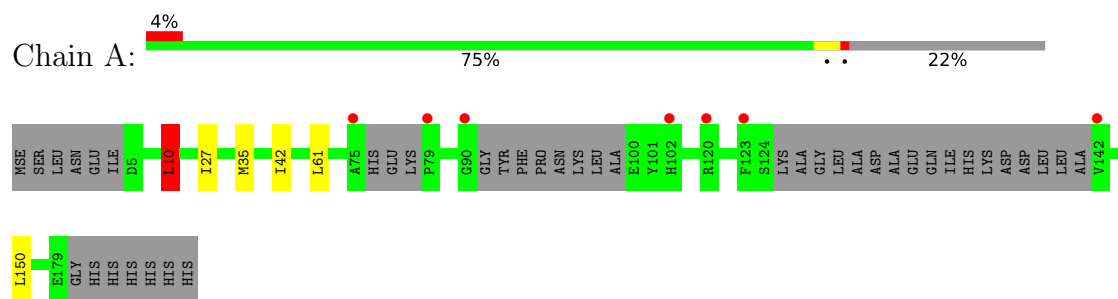
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total	O	0	0
			48	48		
3	B	39	Total	O	0	0
			39	39		
3	C	29	Total	O	0	0
			29	29		
3	D	31	Total	O	0	0
			31	31		
3	E	35	Total	O	0	0
			35	35		
3	F	39	Total	O	0	0
			39	39		
3	G	28	Total	O	0	0
			28	28		
3	H	30	Total	O	0	0
			30	30		

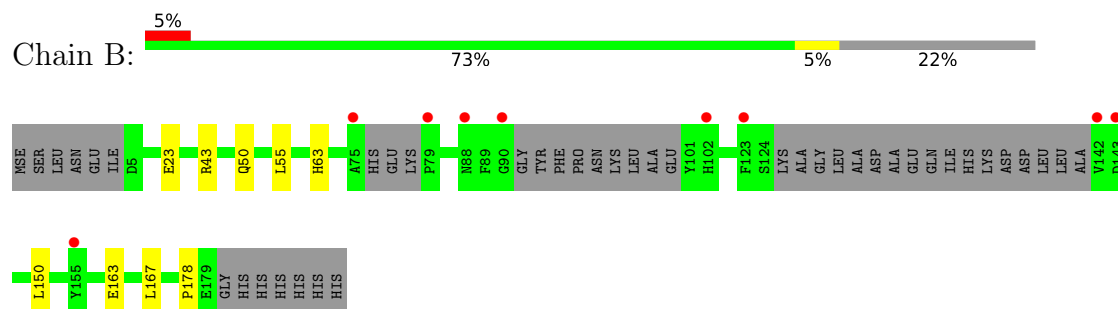
3 Residue-property plots [i](#)

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

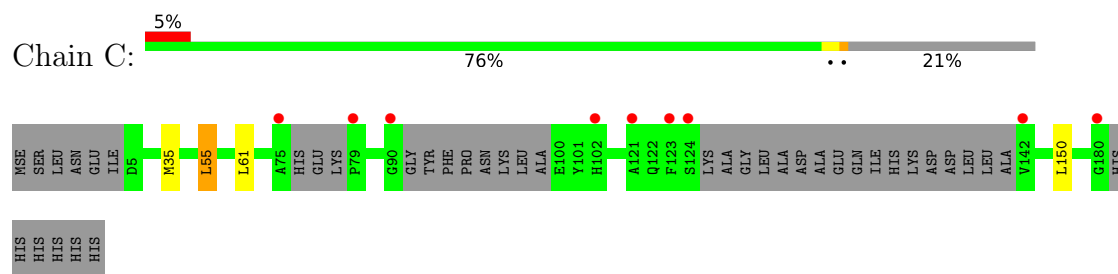
- Molecule 1: Uncharacterized conserved protein



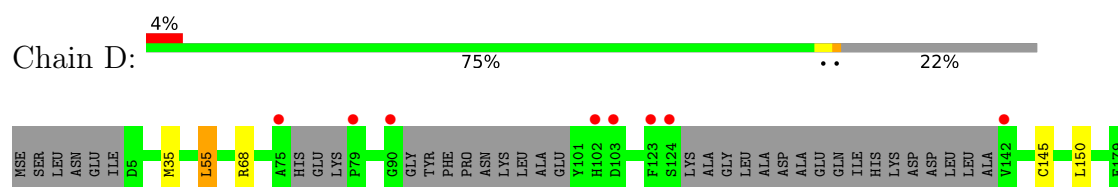
- Molecule 1: Uncharacterized conserved protein



- Molecule 1: Uncharacterized conserved protein



- Molecule 1: Uncharacterized conserved protein



GLY
HIS
HIS
HIS
HIS
HIS
HIS

- Molecule 1: Uncharacterized conserved protein

Chain E: 5% 72% 22%

MSE SER LEU ASN LEU ILE D5 L10 V11 Y12 V13 I27 M35 Q50 L55 A75 HIS GLU LYS P79 R83 F89 GLY TYR PHE PRO ASN LYS LEU ALA E100 Y101 H102 A119 R120 A121 Q122 F123 S124 LYS ALA GLY LEU ALA ASP GLU GLN ILE HIS

LYS ASP ASP LEU ALA Y142 D143 L150 L167 L177 P178 E179 G180 HIS HIS HIS HIS HIS

- Molecule 1: Uncharacterized conserved protein

Chain F: 6% 72% 6% 22%

MSE SER LEU ASN LEU ILE D5 V13 T16 I27 R43 T49 Q50 L55 A75 HIS GLU LYS P79 E80 G90 GLY TYR PHE PRO ASN LYS LEU ALA Y101 H102 D103 F104 F123 S124 LYS ALA GLY LEU ASP ALA GLU ILE HIS LYS ASP LEU

LEU ALA Y142 L150 M153 L167 L177 G180 HIS HIS HIS HIS HIS

- Molecule 1: Uncharacterized conserved protein

Chain G: 4% 75% 22%

MSE SER LEU ASN LEU ILE D5 L55 A75 HIS GLU LYS PRO E80 E81 N88 F89 G90 GLY TYR PHE PRO ASN LYS LEU ALA E100 Y101 H102 D103 F104 A121 Q122 F123 S124 LYS ALA GLY LEU ALA ASP ALA GLU ILE HIS LYS ASP ASP LEU ALA Y142 L150

M153 L167 G180 HIS HIS HIS HIS HIS

- Molecule 1: Uncharacterized conserved protein

Chain H: 5% 72% 6% 21%

MSE SER LEU ASN LEU ILE D5 L10 V11 Y12 V13 T16 I27 M35 T49 L55 A75 HIS GLU LYS P79 F89 G90 GLY TYR PHE PRO ASN LYS LEU ALA E100 Y101 H102 A121 Q122 F123 S124 LYS ALA GLY LEU ALA ASP ALA GLU ILE HIS LYS ASP

ASP LEU ALA Y142 G145 L150 L167 L177 G180 HIS HIS HIS HIS HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, α , β , γ	185.40Å 185.40Å 185.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.50) 99.6 (20.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.215 , 0.253 0.205 , 0.237	Depositor DCC
R_{free} test set	2208 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	62.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9688	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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	0.45	0/1207	0.74	1/1637 (0.1%)
1	B	0.46	0/1198	0.73	0/1625
1	C	0.45	0/1211	0.72	0/1642
1	D	0.45	0/1209	0.71	0/1639
1	E	0.46	0/1207	0.74	0/1637
1	F	0.46	0/1202	0.75	0/1630
1	G	0.46	0/1222	0.72	0/1656
1	H	0.46	0/1211	0.75	0/1642
All	All	0.46	0/9667	0.73	1/13108 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	LEU	CA-CB-CG	5.21	134.52	116.30

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	1175	0	1108	2	0
1	B	1166	0	1102	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1179	0	1111	1	0
1	D	1174	0	1115	1	0
1	E	1175	0	1108	5	0
1	F	1170	0	1105	2	0
1	G	1185	0	1122	1	0
1	H	1179	0	1111	4	0
2	E	6	0	8	1	0
3	A	48	0	0	0	0
3	B	39	0	0	0	0
3	C	29	0	0	0	0
3	D	31	0	0	0	0
3	E	35	0	0	0	0
3	F	39	0	0	0	0
3	G	28	0	0	0	0
3	H	30	0	0	0	0
All	All	9688	0	8890	19	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 1.

All (19) 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:H:35:MSE:HE2	1:H:55:LEU:HD21	1.72	0.70
1:E:50:GLN:H	2:E:187:GOL:H2	1.62	0.65
1:H:10:LEU:HD13	1:H:27:ILE:HG23	1.89	0.55
1:C:35:MSE:HE2	1:C:55:LEU:HD21	1.91	0.52
1:B:43:ARG:NH1	1:B:178:PRO:O	2.43	0.52
1:E:10:LEU:HD13	1:E:27:ILE:HG23	1.94	0.49
1:G:88[A]:ASN:HD22	1:G:104:PHE:HB3	1.79	0.47
1:F:16:THR:HG23	1:F:49:THR:HB	1.97	0.46
1:E:35:MSE:HE2	1:E:55:LEU:HD21	1.97	0.46
1:B:43:ARG:NH2	1:B:50:GLN:O	2.50	0.44
1:A:35:MSE:HE1	1:A:42:ILE:HD11	2.02	0.41
1:F:43:ARG:NH2	1:F:50:GLN:O	2.54	0.41
1:H:11:VAL:HG12	1:H:13:VAL:HG13	2.03	0.41
1:H:16:THR:HG23	1:H:49:THR:HB	2.01	0.41
1:A:10:LEU:HD13	1:A:27:ILE:HG23	2.03	0.41
1:B:63:HIS:CD2	1:B:163:GLU:HB2	2.55	0.41
1:E:11:VAL:HG12	1:E:13:VAL:HG22	2.03	0.41
1:D:35:MSE:HE2	1:D:55:LEU:HD21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:ARG:HE	1:E:83:ARG:HB2	1.63	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	138/187 (74%)	137 (99%)	1 (1%)	0	100	100
1	B	137/187 (73%)	136 (99%)	1 (1%)	0	100	100
1	C	139/187 (74%)	137 (99%)	2 (1%)	0	100	100
1	D	138/187 (74%)	135 (98%)	3 (2%)	0	100	100
1	E	138/187 (74%)	136 (99%)	2 (1%)	0	100	100
1	F	138/187 (74%)	136 (99%)	2 (1%)	0	100	100
1	G	140/187 (75%)	138 (99%)	2 (1%)	0	100	100
1	H	139/187 (74%)	136 (98%)	3 (2%)	0	100	100
All	All	1107/1496 (74%)	1091 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	127/158 (80%)	124 (98%)	3 (2%)	43	70
1	B	126/158 (80%)	122 (97%)	4 (3%)	34	62
1	C	127/158 (80%)	124 (98%)	3 (2%)	43	70
1	D	127/158 (80%)	123 (97%)	4 (3%)	35	62
1	E	127/158 (80%)	119 (94%)	8 (6%)	16	34
1	F	126/158 (80%)	119 (94%)	7 (6%)	19	39
1	G	128/158 (81%)	124 (97%)	4 (3%)	35	62
1	H	127/158 (80%)	120 (94%)	7 (6%)	19	40
All	All	1015/1264 (80%)	975 (96%)	40 (4%)	28	55

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	61	LEU
1	A	150	LEU
1	B	23	GLU
1	B	55	LEU
1	B	150	LEU
1	B	167	LEU
1	C	55	LEU
1	C	61	LEU
1	C	150	LEU
1	D	55	LEU
1	D	68	ARG
1	D	145	CYS
1	D	150	LEU
1	E	10	LEU
1	E	13	VAL
1	E	55	LEU
1	E	83	ARG
1	E	150	LEU
1	E	167	LEU
1	E	177	LEU
1	E	179	GLU
1	F	13	VAL
1	F	27	ILE
1	F	55	LEU
1	F	150	LEU
1	F	153	ASN

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Mol	Chain	Res	Type
1	F	167	LEU
1	F	177	LEU
1	G	55	LEU
1	G	81	GLU
1	G	150	LEU
1	G	167	LEU
1	H	10	LEU
1	H	55	LEU
1	H	100	GLU
1	H	145	CYS
1	H	150	LEU
1	H	167	LEU
1	H	177	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	B	60	HIS
1	C	25	HIS
1	C	60	HIS
1	D	60	HIS
1	E	60	HIS
1	F	60	HIS
1	G	25	HIS
1	G	60	HIS
1	H	60	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is 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	$\# Z > 2$
2	GOL	E	187	-	5,5,5	0.37	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
2	GOL	E	187	-	-	2/4/4/4	-

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
2	E	187	GOL	C1-C2-C3-O3
2	E	187	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	187	GOL	1	0

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	145/187 (77%)	0.02	7 (4%)	35 31	33, 53, 122, 159	0
1	B	144/187 (77%)	0.09	9 (6%)	26 23	34, 53, 123, 159	0
1	C	146/187 (78%)	0.11	9 (6%)	26 23	39, 57, 121, 160	0
1	D	144/187 (77%)	-0.03	8 (5%)	30 26	23, 55, 125, 160	1 (0%)
1	E	145/187 (77%)	0.10	10 (6%)	23 20	35, 55, 122, 159	0
1	F	145/187 (77%)	0.16	11 (7%)	20 17	36, 57, 126, 159	0
1	G	145/187 (77%)	0.15	7 (4%)	35 31	25, 57, 120, 156	2 (1%)
1	H	146/187 (78%)	0.13	10 (6%)	23 20	35, 54, 121, 160	0
All	All	1160/1496 (77%)	0.09	71 (6%)	27 23	23, 55, 125, 160	3 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	75	ALA	6.5
1	H	142	VAL	6.1
1	E	75	ALA	5.6
1	B	142	VAL	5.6
1	F	75	ALA	5.5
1	C	123	PHE	5.2
1	C	75	ALA	5.2
1	G	142	VAL	4.9
1	B	79	PRO	4.9
1	B	75	ALA	4.8
1	G	123	PHE	4.7
1	F	142	VAL	4.6
1	B	90	GLY	4.5
1	D	142	VAL	4.3
1	A	123	PHE	4.2
1	B	123	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	H	123	PHE	4.1
1	E	79	PRO	4.1
1	A	142	VAL	4.1
1	C	142	VAL	4.1
1	F	79	PRO	4.0
1	G	75	ALA	4.0
1	E	142	VAL	3.9
1	D	123	PHE	3.9
1	C	79	PRO	3.8
1	H	102	HIS	3.8
1	E	123	PHE	3.6
1	D	90	GLY	3.5
1	A	75	ALA	3.4
1	F	153	ASN	3.3
1	D	79	PRO	3.2
1	C	180	GLY	3.2
1	H	124	SER	3.1
1	G	102	HIS	3.1
1	F	123	PHE	3.1
1	B	102	HIS	3.0
1	A	79	PRO	3.0
1	H	90	GLY	3.0
1	F	102	HIS	2.9
1	B	143	ASP	2.9
1	H	180	GLY	2.9
1	D	102	HIS	2.8
1	H	89	PHE	2.8
1	D	75	ALA	2.8
1	A	102	HIS	2.7
1	H	79	PRO	2.7
1	B	155	TYR	2.6
1	E	143	ASP	2.6
1	A	90	GLY	2.5
1	E	89	PHE	2.5
1	F	124	SER	2.5
1	G	90	GLY	2.5
1	E	124	SER	2.4
1	G	153	ASN	2.4
1	C	121	ALA	2.4
1	C	102	HIS	2.3
1	C	124	SER	2.3
1	C	90	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	80	GLU	2.2
1	F	180	GLY	2.2
1	A	120	ARG	2.2
1	E	102	HIS	2.2
1	F	90	GLY	2.2
1	E	119	ALA	2.2
1	G	121	ALA	2.1
1	F	104	PHE	2.1
1	H	121	ALA	2.1
1	E	121	ALA	2.1
1	D	103	ASP	2.1
1	D	124	SER	2.1
1	B	88	ASN	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	GOL	E	187	6/6	0.91	0.11	39,56,65,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.