



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:52 PM UTC

PDB ID : 5SV1 / pdb_00005sv1
Title : Structure of the ExbB/ExbD complex from E. coli at pH 4.5
Authors : Celia, H.; Botos, I.; Lloubes, R.; Buchanan, S.K.; Noinaj, N.
Deposited on : 2016-08-04
Resolution : 3.50 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

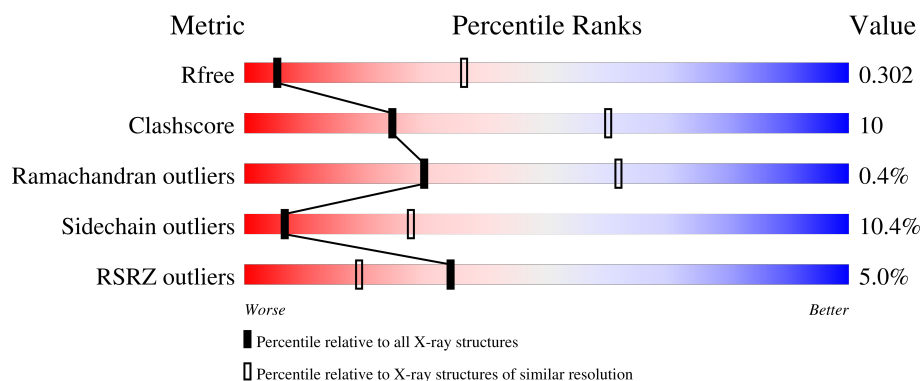
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	244	4% 67% 20% 5% 8%
1	B	244	% 65% 24% • 8%
1	C	244	2% 69% 20% • 8%
1	D	244	5% 63% 22% • 12%
1	E	244	3% 73% 15% • 9%

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Mol	Chain	Length	Quality of chain
1	F	244	3%68%21%7%
1	G	244	%67%21%8%
1	H	244	3%66%23%9%
1	I	244	6%63%23%11%
1	J	244	4%66%18%5%10%
2	Y	58	33%22%14%60%
2	Z	58	26%10%21%7%62%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16946 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 Biopolymer transport protein ExbB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1678	1071	294	307	6			
1	B	225	Total	C	N	O	S	0	0	0
			1692	1080	295	311	6			
1	C	224	Total	C	N	O	S	0	0	0
			1665	1064	288	307	6			
1	D	215	Total	C	N	O	S	0	0	0
			1599	1018	278	298	5			
1	E	223	Total	C	N	O	S	0	0	0
			1653	1050	290	308	5			
1	F	226	Total	C	N	O	S	0	0	0
			1694	1079	297	312	6			
1	G	225	Total	C	N	O	S	0	0	0
			1694	1081	298	309	6			
1	H	222	Total	C	N	O	S	0	0	0
			1668	1062	291	309	6			
1	I	216	Total	C	N	O	S	0	0	0
			1626	1034	286	301	5			
1	J	219	Total	C	N	O	S	0	0	0
			1630	1039	286	300	5			

- Molecule 2 is a protein called Biopolymer transport protein ExbD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	23	Total	C	N	O	S	0	0	0
			171	120	23	26	2			
2	Z	22	Total	C	N	O	S	0	0	0
			166	117	22	25	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	31	GLY	-	expression tag	UNP P0ABV4

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	32	GLY	-	expression tag	UNP P0ABV4
Y	33	GLY	-	expression tag	UNP P0ABV4
Y	34	GLU	-	expression tag	UNP P0ABV4
Y	35	ASN	-	expression tag	UNP P0ABV4
Y	36	LEU	-	expression tag	UNP P0ABV4
Y	37	TYR	-	expression tag	UNP P0ABV4
Y	38	PHE	-	expression tag	UNP P0ABV4
Y	39	GLN	-	expression tag	UNP P0ABV4
Z	31	GLY	-	expression tag	UNP P0ABV4
Z	32	GLY	-	expression tag	UNP P0ABV4
Z	33	GLY	-	expression tag	UNP P0ABV4
Z	34	GLU	-	expression tag	UNP P0ABV4
Z	35	ASN	-	expression tag	UNP P0ABV4
Z	36	LEU	-	expression tag	UNP P0ABV4
Z	37	TYR	-	expression tag	UNP P0ABV4
Z	38	PHE	-	expression tag	UNP P0ABV4
Z	39	GLN	-	expression tag	UNP P0ABV4

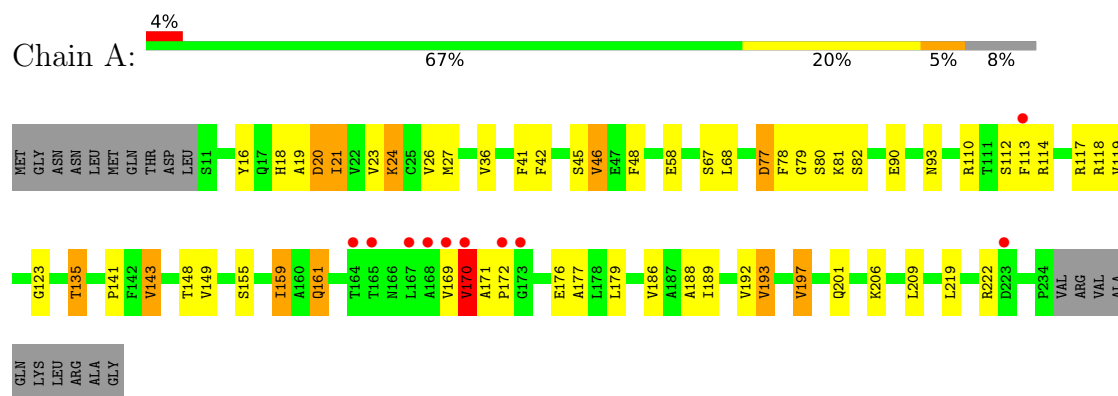
- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Hg 1 1	0	0
3	B	1	Total Hg 1 1	0	0
3	C	1	Total Hg 1 1	0	0
3	D	1	Total Hg 1 1	0	0
3	E	1	Total Hg 1 1	0	0
3	F	1	Total Hg 1 1	0	0
3	G	1	Total Hg 1 1	0	0
3	H	1	Total Hg 1 1	0	0
3	I	1	Total Hg 1 1	0	0
3	J	1	Total Hg 1 1	0	0

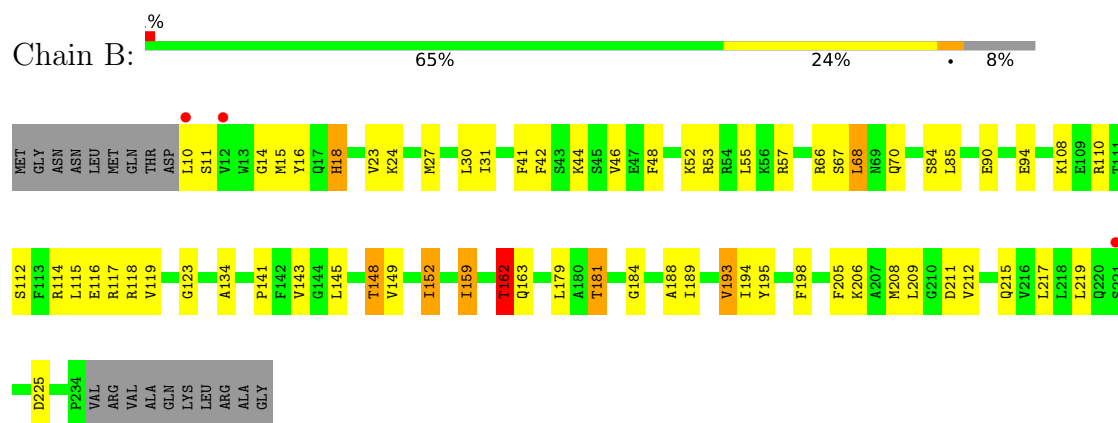
3 Residue-property plots [i](#)

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.

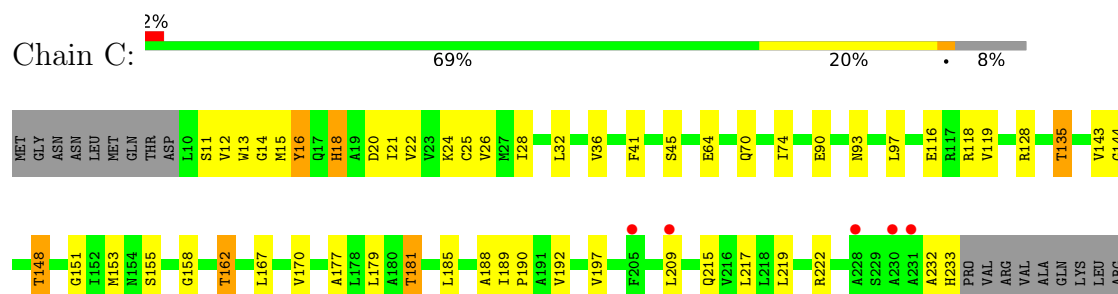
• Molecule 1: Biopolymer transport protein ExbB



• Molecule 1: Biopolymer transport protein ExbB

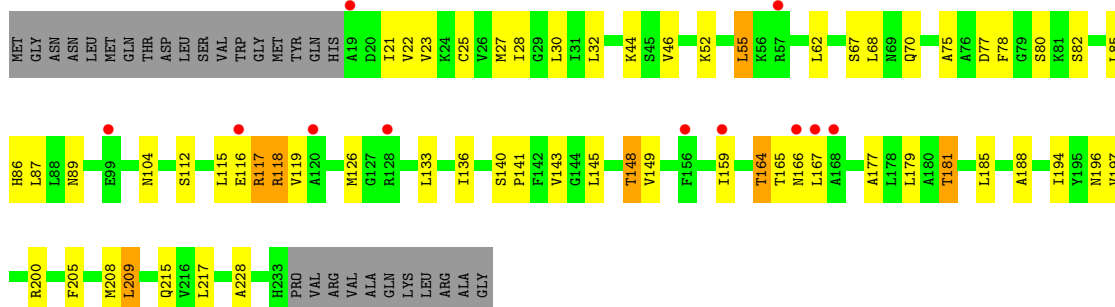


• Molecule 1: Biopolymer transport protein ExbB

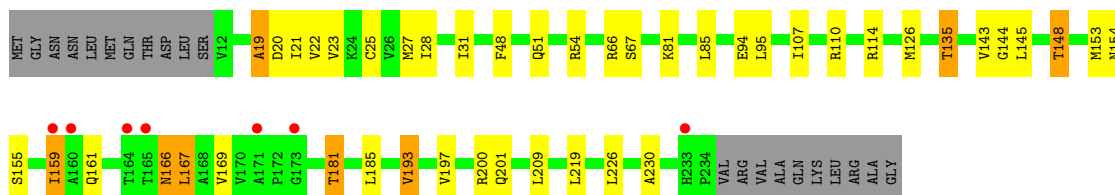


ALA
GLY

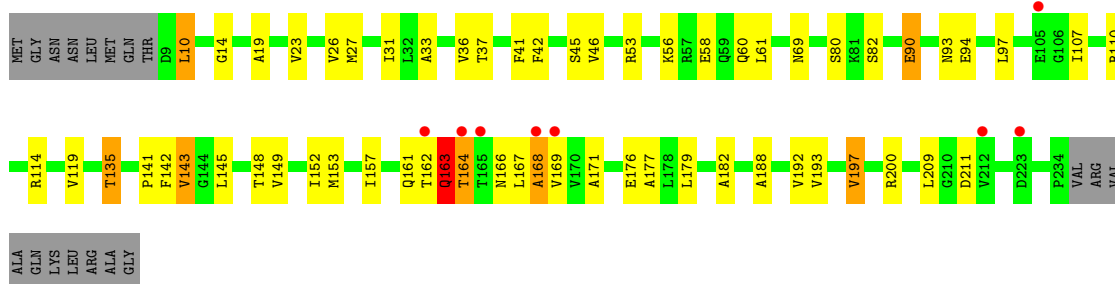
• Molecule 1: Biopolymer transport protein ExbB

Chain D: 

• Molecule 1: Biopolymer transport protein ExbB

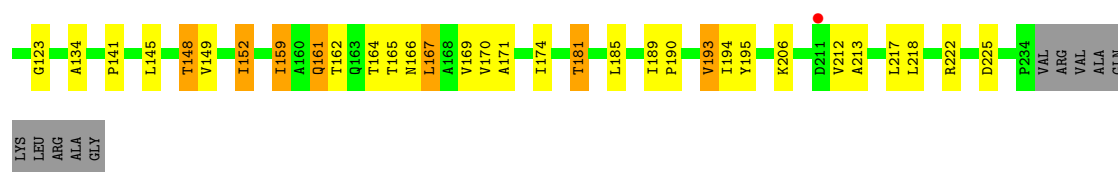
Chain E: 

• Molecule 1: Biopolymer transport protein ExbB

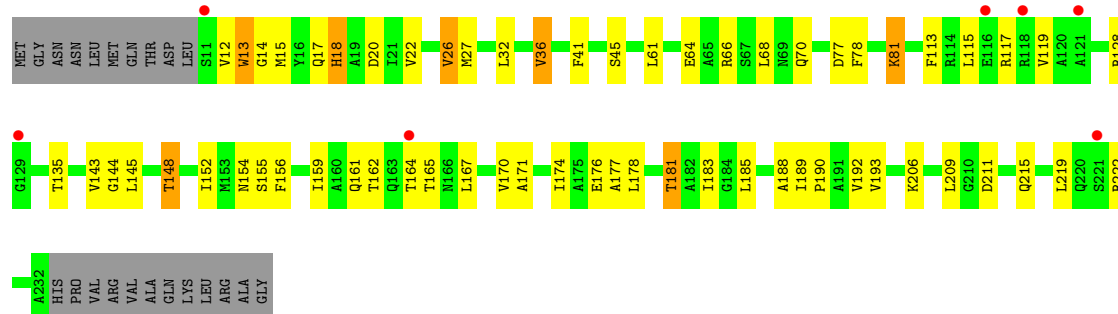
Chain F: 

• Molecule 1: Biopolymer transport protein ExbB

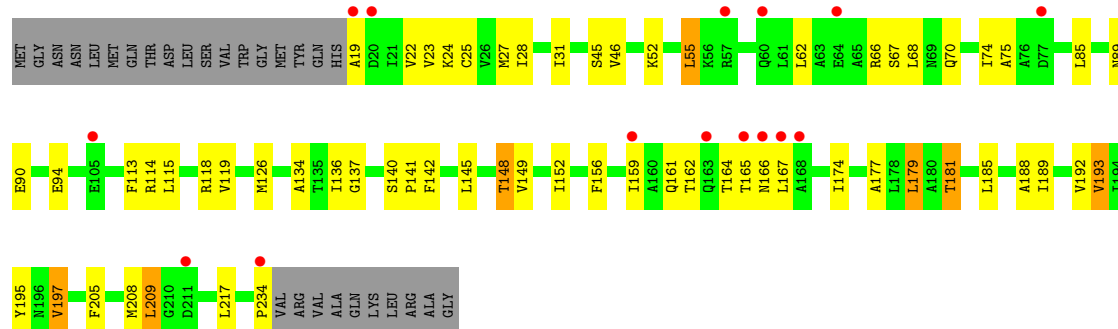
Chain G: 



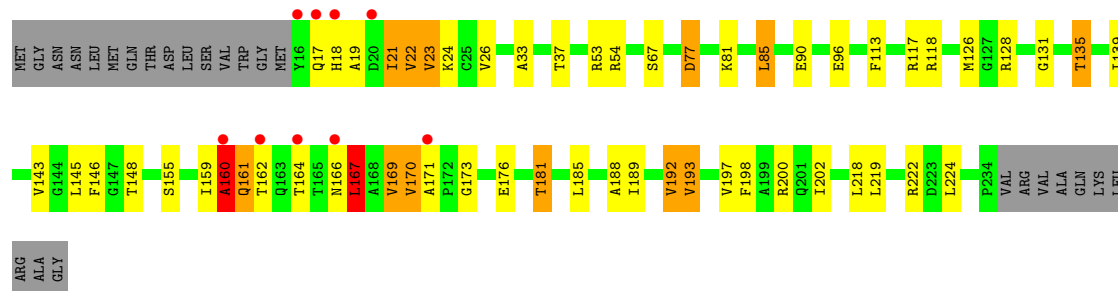
• Molecule 1: Biopolymer transport protein ExbB



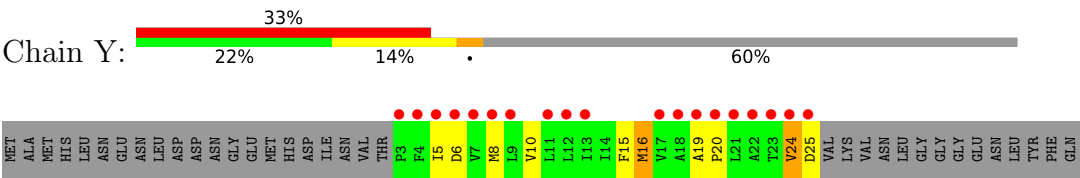
• Molecule 1: Biopolymer transport protein ExbB



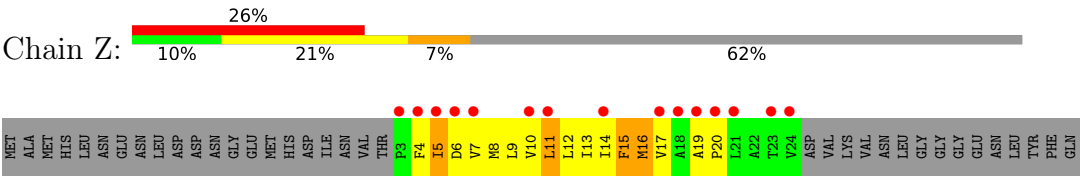
• Molecule 1: Biopolymer transport protein ExbB



• Molecule 2: Biopolymer transport protein ExbD



• Molecule 2: Biopolymer transport protein ExbD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.94Å 196.75Å 210.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 3.50 49.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.00-3.50) 94.8 (49.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.24	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.48Å)	Xtrriage
Refinement program	PHENIX (1.10_2142: ???)	Depositor
R, R_{free}	0.255 , 0.300 0.257 , 0.302	Depositor DCC
R_{free} test set	2000 reflections (3.56%)	wwPDB-VP
Wilson B-factor (Å ²)	78.1	Xtrriage
Anisotropy	0.433	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16946	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.64 % 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 1.2835e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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

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	0.33	0/1693	0.57	0/2294
1	B	0.36	0/1707	0.64	1/2315 (0.0%)
1	C	0.34	0/1678	0.54	0/2275
1	D	0.39	0/1609	0.57	0/2182
1	E	0.29	0/1663	0.55	0/2254
1	F	0.32	0/1709	0.56	0/2316
1	G	0.36	0/1709	0.66	1/2317 (0.0%)
1	H	0.36	0/1680	0.55	0/2275
1	I	0.41	0/1636	0.61	1/2214 (0.0%)
1	J	0.38	0/1640	0.67	4/2221 (0.2%)
2	Y	0.33	0/174	0.67	0/238
2	Z	0.25	0/169	0.53	0/231
All	All	0.35	0/17067	0.59	7/23132 (0.0%)

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	1
1	E	0	2
1	G	0	3
1	H	0	1
1	J	0	1
All	All	0	8

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	161	GLN	N-CA-C	-11.45	89.17	108.75
1	J	160	ALA	N-CA-C	7.61	121.05	111.24
1	J	167	LEU	N-CA-C	6.79	118.68	111.28
1	B	162	THR	N-CA-C	5.72	118.73	111.69
1	I	234	PRO	N-CA-CB	5.63	109.20	103.00
1	J	160	ALA	CA-C-N	5.39	131.41	121.70
1	J	160	ALA	C-N-CA	5.39	131.41	121.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	VAL	Peptide
1	E	166	ASN	Peptide
1	E	19	ALA	Peptide
1	G	161	GLN	Peptide
1	G	162	THR	Peptide
1	G	66	ARG	Peptide
1	H	128	ARG	Peptide
1	J	160	ALA	Peptide

5.2 Too-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 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	1678	0	1690	42	0
1	B	1692	0	1713	37	0
1	C	1665	0	1675	31	0
1	D	1599	0	1616	36	0
1	E	1653	0	1667	27	0
1	F	1694	0	1696	40	0
1	G	1694	0	1720	40	0
1	H	1668	0	1696	38	0
1	I	1626	0	1662	43	0
1	J	1630	0	1658	35	0
2	Y	171	0	191	7	0
2	Z	166	0	189	12	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
All	All	16946	0	17173	339	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 10.

All (339) 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:F:19:ALA:HB2	1:F:176:GLU:HG2	1.37	1.05
1:F:10:LEU:HG	1:F:14:GLY:HA3	1.52	0.91
1:A:21:ILE:HD11	1:I:45:SER:HB2	1.61	0.83
1:A:19:ALA:HB2	1:A:176:GLU:HG2	1.61	0.83
1:B:10:LEU:HD23	1:B:14:GLY:HA3	1.64	0.79
1:H:148:THR:HA	1:H:177:ALA:HA	1.65	0.77
1:F:141:PRO:HD3	1:F:188:ALA:HB2	1.70	0.74
1:J:21:ILE:HG23	1:J:22:VAL:H	1.53	0.73
1:F:211:ASP:OD1	1:J:117:ARG:NH1	2.23	0.72
1:G:67:SER:HB3	1:G:70:GLN:HB2	1.72	0.71
1:I:136:ILE:O	1:I:140:SER:HB2	1.91	0.70
1:D:145:LEU:HD12	1:E:185:LEU:HD11	1.73	0.70
1:A:117:ARG:NH1	1:B:211:ASP:OD1	2.25	0.70
1:A:148:THR:HA	1:A:177:ALA:HB1	1.74	0.69
1:E:20:ASP:HB3	1:E:23:VAL:HG12	1.73	0.69
1:F:27:MET:O	1:F:31:ILE:HG13	1.92	0.69
1:C:119:VAL:HG22	1:C:209:LEU:HD22	1.75	0.69
1:H:119:VAL:HG22	1:H:209:LEU:HD22	1.75	0.69
1:D:119:VAL:HG22	1:D:209:LEU:HD13	1.75	0.68
1:G:152:ILE:HG23	1:G:174:ILE:HG13	1.75	0.68
1:H:159:ILE:HA	1:H:162:THR:HG22	1.76	0.68
1:F:119:VAL:HG22	1:F:209:LEU:HD22	1.77	0.67
1:I:145:LEU:HD12	1:J:185:LEU:HD11	1.78	0.65
1:F:142:PHE:HE2	1:G:141:PRO:HG3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:ARG:NH2	1:G:225:ASP:OD2	2.30	0.65
1:A:77:ASP:HA	1:A:78:PHE:HB2	1.79	0.64
1:E:20:ASP:OD1	1:E:21:ILE:N	2.30	0.64
1:J:160:ALA:HB3	1:J:161:GLN:HB2	1.78	0.64
1:D:141:PRO:HB3	1:D:185:LEU:HD23	1.79	0.64
1:I:119:VAL:HG22	1:I:209:LEU:HD13	1.80	0.64
1:I:141:PRO:HB3	1:I:185:LEU:HD23	1.80	0.64
1:A:119:VAL:HG22	1:A:209:LEU:HD22	1.78	0.64
1:C:41:PHE:O	1:C:45:SER:HB3	1.97	0.64
1:B:119:VAL:HG22	1:B:209:LEU:HD22	1.79	0.63
1:G:20:ASP:OD1	1:G:20:ASP:N	2.26	0.63
1:H:178:LEU:HD11	2:Z:15:PHE:CZ	2.33	0.63
1:F:41:PHE:O	1:F:45:SER:HB2	1.99	0.62
1:I:140:SER:HB3	1:I:188:ALA:HB2	1.81	0.62
1:B:67:SER:HB3	1:B:70:GLN:HB2	1.82	0.62
1:G:94:GLU:OE2	1:H:222:ARG:NH1	2.33	0.62
1:F:90:GLU:O	1:F:114:ARG:NH2	2.33	0.61
1:F:26:VAL:HG13	1:F:143:VAL:HG13	1.80	0.61
1:A:193:VAL:HG13	1:E:135:THR:HG21	1.82	0.61
1:G:159:ILE:HD11	1:H:171:ALA:HB2	1.82	0.60
1:F:145:LEU:HD23	1:G:185:LEU:HD11	1.83	0.60
1:H:41:PHE:O	1:H:45:SER:HB3	2.00	0.60
1:F:41:PHE:O	1:F:45:SER:CB	2.49	0.60
1:G:117:ARG:NH1	1:H:211:ASP:OD1	2.35	0.60
1:A:77:ASP:HB2	1:A:79:GLY:H	1.67	0.60
1:F:23:VAL:HG12	1:F:27:MET:HE2	1.82	0.60
1:F:193:VAL:O	1:F:197:VAL:HG23	2.01	0.60
1:B:10:LEU:HG	1:B:11:SER:H	1.66	0.59
1:I:27:MET:O	1:I:31:ILE:HG13	2.01	0.59
1:F:152:ILE:HD13	2:Z:16:MET:HE2	1.84	0.59
1:D:75:ALA:O	1:D:85:LEU:HD13	2.03	0.59
1:G:27:MET:O	1:G:31:ILE:HG13	2.03	0.59
1:C:158:GLY:O	1:C:162:THR:OG1	2.21	0.59
1:A:222:ARG:NH1	1:E:94:GLU:OE2	2.36	0.58
1:I:148:THR:HB	1:I:177:ALA:O	2.02	0.58
1:B:27:MET:O	1:B:31:ILE:HG13	2.02	0.58
1:D:104:ASN:ND2	1:D:228:ALA:HB2	2.18	0.58
1:G:110:ARG:O	1:G:114:ARG:HG3	2.02	0.58
1:G:167:LEU:O	1:G:171:ALA:N	2.33	0.58
1:H:155:SER:HB3	1:H:170:VAL:HG13	1.85	0.58
1:A:20:ASP:OD2	1:A:21:ILE:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:LEU:O	1:D:215:GLN:NE2	2.34	0.57
1:G:159:ILE:HD13	1:H:167:LEU:HB3	1.85	0.57
1:I:94:GLU:OE2	1:J:222:ARG:NH1	2.37	0.57
1:F:163:GLN:NE2	1:F:164:THR:O	2.38	0.56
1:C:20:ASP:OD1	1:C:21:ILE:N	2.34	0.56
1:G:98:SER:OG	1:G:110:ARG:NH1	2.39	0.56
2:Z:19:ALA:HB3	2:Z:20:PRO:HD3	1.87	0.56
1:B:145:LEU:HD12	1:C:185:LEU:HD11	1.88	0.56
1:D:52:LYS:HG3	1:D:208:MET:HE1	1.87	0.56
1:J:113:PHE:CE1	1:J:117:ARG:HD2	2.40	0.56
1:I:159:ILE:HG23	1:J:167:LEU:HD11	1.87	0.56
1:A:20:ASP:O	1:A:24:LYS:HD3	2.06	0.56
1:C:22:VAL:O	1:C:26:VAL:HG23	2.06	0.56
1:I:75:ALA:O	1:I:85:LEU:HD13	2.06	0.56
1:G:123:GLY:HA3	1:G:206:LYS:HD3	1.89	0.55
1:F:33:ALA:O	1:F:37:THR:HG23	2.06	0.55
1:A:77:ASP:OD1	1:A:77:ASP:N	2.38	0.55
1:H:14:GLY:O	1:H:18:HIS:HB2	2.06	0.55
1:D:148:THR:HB	1:D:177:ALA:O	2.05	0.55
1:B:149:VAL:HG11	1:C:181:THR:HG22	1.88	0.55
1:E:23:VAL:O	1:E:27:MET:HG2	2.07	0.55
1:D:136:ILE:O	1:D:140:SER:HB2	2.08	0.54
1:J:17:GLN:C	1:J:19:ALA:HB3	2.31	0.54
1:H:12:VAL:HA	1:H:15:MET:HE2	1.89	0.54
1:B:110:ARG:O	1:B:114:ARG:HG3	2.07	0.54
1:C:14:GLY:O	1:C:18:HIS:HB2	2.06	0.54
1:G:166:ASN:O	1:G:169:VAL:HG22	2.08	0.54
1:J:173:GLY:O	1:J:176:GLU:HG2	2.07	0.54
1:A:193:VAL:O	1:A:197:VAL:HG23	2.08	0.54
1:H:66:ARG:N	1:H:70:GLN:OE1	2.40	0.54
1:A:169:VAL:HG13	1:A:170:VAL:H	1.71	0.53
2:Z:16:MET:O	2:Z:20:PRO:HD2	2.09	0.53
1:I:193:VAL:O	1:I:197:VAL:HG23	2.08	0.53
1:F:141:PRO:HD3	1:F:188:ALA:CB	2.38	0.53
1:D:149:VAL:HG21	1:E:181:THR:HG21	1.91	0.53
1:C:144:GLY:O	1:C:148:THR:HG23	2.09	0.52
1:I:165:THR:HG22	1:I:166:ASN:H	1.73	0.52
1:A:41:PHE:O	1:A:45:SER:HB2	2.10	0.52
1:C:16:TYR:CD1	1:C:16:TYR:C	2.87	0.52
1:G:62:LEU:HD21	1:G:75:ALA:HB2	1.91	0.52
1:A:41:PHE:O	1:A:45:SER:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:VAL:HG23	1:G:189:ILE:HD13	1.90	0.52
1:B:41:PHE:HB2	1:B:194:ILE:HD13	1.92	0.52
1:J:21:ILE:HG23	1:J:22:VAL:HG12	1.91	0.52
1:D:112:SER:O	1:D:116:GLU:HG2	2.09	0.52
1:D:140:SER:HB3	1:D:188:ALA:HB2	1.91	0.51
1:E:226:LEU:O	1:E:230:ALA:HB2	2.10	0.51
1:B:115:LEU:HD12	1:B:217:LEU:HG	1.91	0.51
1:E:67:SER:O	1:E:219:LEU:HD13	2.11	0.51
1:I:25:CYS:O	1:I:28:ILE:HG13	2.10	0.51
1:G:41:PHE:HB2	1:G:194:ILE:HD13	1.92	0.51
1:H:162:THR:HG23	1:H:164:THR:H	1.75	0.51
1:I:126:MET:HE2	1:I:205:PHE:CD2	2.45	0.51
1:J:131:GLY:O	1:J:135:THR:OG1	2.29	0.51
1:F:58:GLU:OE2	1:F:82:SER:OG	2.28	0.51
1:G:84:SER:OG	1:G:212:VAL:HG11	2.11	0.51
1:J:18:HIS:HA	1:J:19:ALA:C	2.36	0.51
1:A:189:ILE:O	1:A:193:VAL:HG23	2.10	0.51
1:G:145:LEU:HD12	1:H:185:LEU:HD11	1.91	0.51
1:I:23:VAL:HG12	1:I:27:MET:HE3	1.92	0.51
1:D:82:SER:O	1:D:86:HIS:ND1	2.41	0.50
1:I:156:PHE:HA	1:I:159:ILE:HG22	1.92	0.50
1:E:19:ALA:O	1:E:20:ASP:HB2	2.11	0.50
1:A:58:GLU:CD	1:A:82:SER:HG	2.19	0.50
1:D:23:VAL:HG12	1:D:27:MET:HE2	1.93	0.50
1:B:44:LYS:HB3	1:B:198:PHE:CZ	2.46	0.50
1:A:141:PRO:HD3	1:A:188:ALA:HB2	1.92	0.50
1:C:16:TYR:CE1	1:C:24:LYS:HG3	2.47	0.50
2:Y:5:ILE:O	2:Y:8:MET:N	2.45	0.50
1:I:148:THR:O	1:I:152:ILE:HG13	2.11	0.50
1:A:141:PRO:HD3	1:A:188:ALA:CB	2.42	0.50
1:G:149:VAL:HG11	1:H:181:THR:HG22	1.93	0.50
1:A:42:PHE:O	1:A:46:VAL:HG12	2.12	0.49
1:H:188:ALA:O	1:H:192:VAL:HG23	2.11	0.49
1:I:52:LYS:HG3	1:I:208:MET:HE1	1.93	0.49
1:E:110:ARG:O	1:E:114:ARG:HG3	2.13	0.49
1:G:86:HIS:HB3	1:G:118:ARG:NH2	2.27	0.49
1:H:170:VAL:HG12	1:H:174:ILE:HG13	1.94	0.49
1:C:16:TYR:C	1:C:16:TYR:HD1	2.21	0.49
1:F:42:PHE:O	1:F:46:VAL:HG12	2.13	0.49
1:B:141:PRO:HD3	1:B:188:ALA:HB2	1.94	0.49
1:D:167:LEU:HD21	1:E:167:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:LEU:HD13	1:D:208:MET:HB3	1.95	0.49
1:A:135:THR:HG21	1:B:193:VAL:HG13	1.93	0.48
1:F:148:THR:OG1	1:F:177:ALA:O	2.29	0.48
1:G:148:THR:O	1:G:152:ILE:HG13	2.13	0.48
1:J:167:LEU:HG	1:J:171:ALA:HB2	1.94	0.48
1:F:149:VAL:HG21	1:G:181:THR:HG21	1.95	0.48
1:G:23:VAL:HG12	1:G:27:MET:HE2	1.96	0.48
1:A:26:VAL:HG13	1:A:143:VAL:HG13	1.96	0.48
1:A:110:ARG:NH2	1:B:225:ASP:OD2	2.46	0.48
1:I:189:ILE:O	1:I:193:VAL:HG23	2.14	0.48
1:H:189:ILE:HB	1:H:190:PRO:HD3	1.95	0.48
1:I:161:GLN:HG3	1:I:162:THR:H	1.78	0.48
1:A:23:VAL:HG12	1:A:27:MET:HE2	1.96	0.47
1:F:188:ALA:O	1:F:192:VAL:HG23	2.14	0.47
1:D:118:ARG:HA	1:D:118:ARG:HD3	1.46	0.47
1:I:115:LEU:HD12	1:I:217:LEU:HG	1.96	0.47
1:C:148:THR:HA	1:C:177:ALA:HA	1.95	0.47
1:I:149:VAL:HG21	1:J:181:THR:HG21	1.96	0.47
1:J:193:VAL:O	1:J:197:VAL:HG23	2.14	0.47
1:B:16:TYR:CE1	1:B:24:LYS:HG2	2.48	0.47
1:B:134:ALA:HB2	1:B:195:TYR:CE2	2.50	0.47
1:H:13:TRP:HZ3	1:H:17:GLN:HB2	1.80	0.47
1:F:94:GLU:OE2	1:G:222:ARG:NH1	2.48	0.47
1:J:145:LEU:HD21	2:Z:9:LEU:HD13	1.97	0.47
1:H:156:PHE:CE2	1:I:174:ILE:HG21	2.50	0.47
1:C:135:THR:HG1	1:D:196:ASN:HD22	1.55	0.46
1:B:48:PHE:CE1	1:B:52:LYS:HD2	2.51	0.46
1:C:155:SER:HB3	1:C:170:VAL:HG13	1.96	0.46
1:D:67:SER:HG	1:D:70:GLN:H	1.57	0.46
1:J:167:LEU:O	1:J:169:VAL:N	2.48	0.46
1:J:169:VAL:HG23	1:J:170:VAL:H	1.79	0.46
1:C:148:THR:HG21	1:C:181:THR:OG1	2.15	0.46
1:E:48:PHE:CZ	1:E:201:GLN:HB3	2.51	0.46
1:I:141:PRO:HB3	1:I:185:LEU:CD2	2.45	0.46
1:B:141:PRO:HD3	1:B:188:ALA:CB	2.45	0.46
1:C:15:MET:HE3	1:C:179:LEU:HD13	1.97	0.46
1:H:20:ASP:HB2	1:H:176:GLU:OE2	2.16	0.46
1:H:32:LEU:O	1:H:36:VAL:HG12	2.16	0.46
1:E:145:LEU:HD21	2:Y:10:VAL:HG21	1.96	0.46
1:E:193:VAL:O	1:E:197:VAL:HG23	2.16	0.46
1:F:163:GLN:HE21	1:F:163:GLN:HB3	1.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:SER:O	1:A:82:SER:N	2.49	0.45
1:H:215:GLN:O	1:H:219:LEU:HG	2.16	0.45
1:I:55:LEU:CD1	1:I:208:MET:HB3	2.47	0.45
1:B:30:LEU:HD13	1:B:184:GLY:HA2	1.98	0.45
1:H:113:PHE:O	1:H:117:ARG:HB3	2.16	0.45
1:H:148:THR:HG21	1:H:181:THR:OG1	2.15	0.45
1:I:185:LEU:O	1:I:189:ILE:HG12	2.16	0.45
1:C:188:ALA:O	1:C:192:VAL:HG23	2.17	0.45
1:I:85:LEU:HG	1:I:89:ASN:ND2	2.32	0.45
1:A:155:SER:O	1:A:159:ILE:HG13	2.17	0.45
1:D:30:LEU:HD21	1:D:143:VAL:HG13	1.98	0.45
1:H:144:GLY:O	1:H:148:THR:HG23	2.16	0.45
1:B:53:ARG:HH12	1:H:161:GLN:HG3	1.82	0.45
1:B:84:SER:OG	1:B:212:VAL:HG11	2.16	0.45
1:G:170:VAL:HG13	1:G:174:ILE:HD13	1.99	0.45
1:I:114:ARG:HG2	1:J:218:LEU:HD11	1.99	0.45
1:B:15:MET:HE3	1:B:179:LEU:HD22	1.99	0.45
1:B:148:THR:O	1:B:152:ILE:HG13	2.17	0.45
1:B:215:GLN:O	1:B:219:LEU:HG	2.17	0.45
1:D:117:ARG:HD2	1:D:117:ARG:HA	1.70	0.45
1:J:54:ARG:HH12	1:J:81:LYS:HG3	1.82	0.45
1:E:144:GLY:O	1:E:148:THR:HG23	2.17	0.45
1:F:167:LEU:O	1:F:169:VAL:N	2.50	0.45
1:H:81:LYS:N	1:H:81:LYS:HD2	2.32	0.45
1:A:67:SER:O	1:A:219:LEU:HD13	2.18	0.44
1:F:166:ASN:O	1:F:168:ALA:N	2.50	0.44
1:H:61:LEU:HD23	1:H:61:LEU:HA	1.79	0.44
1:G:167:LEU:H	1:G:167:LEU:HD13	1.81	0.44
1:H:22:VAL:O	1:H:26:VAL:HG23	2.17	0.44
1:I:55:LEU:HD23	1:I:55:LEU:HA	1.75	0.44
1:J:77:ASP:OD1	1:J:77:ASP:N	2.44	0.44
1:J:85:LEU:HD23	1:J:85:LEU:HA	1.76	0.44
1:B:162:THR:N	1:B:163:GLN:HA	2.32	0.44
1:G:115:LEU:HD12	1:G:217:LEU:HG	1.98	0.44
1:I:134:ALA:HB2	1:I:195:TYR:CE1	2.53	0.44
1:J:67:SER:O	1:J:219:LEU:HD13	2.17	0.44
1:E:25:CYS:O	1:E:28:ILE:HG13	2.18	0.44
1:E:153:MET:HE2	1:E:153:MET:HB3	1.91	0.44
1:E:28:ILE:O	1:E:31:ILE:HG13	2.17	0.44
1:I:70:GLN:O	1:I:74:ILE:HG13	2.18	0.44
1:D:145:LEU:HA	1:D:181:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:THR:HG21	1:E:181:THR:OG1	2.18	0.44
1:I:137:GLY:HA3	1:I:192:VAL:HG23	1.99	0.44
1:A:159:ILE:HG13	1:A:159:ILE:H	1.66	0.43
1:E:126:MET:HE3	1:E:126:MET:HB3	1.93	0.43
1:J:224:LEU:HD23	1:J:224:LEU:HA	1.84	0.43
1:C:70:GLN:O	1:C:74:ILE:HG13	2.19	0.43
1:B:48:PHE:CE2	1:B:205:PHE:HB2	2.54	0.43
1:D:55:LEU:HA	1:D:55:LEU:HD23	1.74	0.43
1:H:27:MET:HG2	1:H:183:ILE:HD12	1.99	0.43
1:I:159:ILE:CG2	1:J:167:LEU:HD11	2.48	0.43
1:A:161:GLN:H	1:A:161:GLN:HG2	1.70	0.43
1:C:217:LEU:HD23	1:C:217:LEU:HA	1.82	0.43
1:H:14:GLY:O	1:H:18:HIS:N	2.47	0.43
2:Y:5:ILE:HA	2:Y:8:MET:SD	2.58	0.43
1:I:145:LEU:HA	1:I:181:THR:HG23	1.99	0.43
2:Z:9:LEU:O	2:Z:13:ILE:HB	2.19	0.43
1:E:209:LEU:HD12	1:E:209:LEU:HA	1.85	0.43
1:B:123:GLY:HA3	1:B:206:LYS:HE2	2.01	0.43
1:C:151:GLY:HA3	1:C:177:ALA:HB2	2.00	0.43
1:F:135:THR:HG21	1:G:193:VAL:HG13	1.99	0.43
1:G:61:LEU:HD23	1:G:61:LEU:HA	1.78	0.43
1:D:25:CYS:O	1:D:28:ILE:HG13	2.18	0.43
1:D:126:MET:HE2	1:D:205:PHE:CD2	2.53	0.43
1:I:19:ALA:N	1:I:24:LYS:HE2	2.34	0.43
1:J:23:VAL:O	1:J:26:VAL:HG22	2.18	0.43
1:C:28:ILE:O	1:C:32:LEU:HG	2.19	0.43
1:C:189:ILE:HB	1:C:190:PRO:HD3	2.00	0.43
1:A:143:VAL:HG23	1:B:189:ILE:HD13	2.00	0.42
1:B:159:ILE:HD13	1:C:167:LEU:HB3	2.01	0.42
1:E:20:ASP:OD2	1:E:154:ASN:ND2	2.52	0.42
1:F:157:ILE:O	1:F:161:GLN:HG2	2.19	0.42
2:Z:11:LEU:HD22	2:Z:11:LEU:HA	1.82	0.42
1:C:20:ASP:O	1:C:24:LYS:HB2	2.20	0.42
1:D:179:LEU:HD23	1:D:179:LEU:HA	1.73	0.42
1:E:107:ILE:HA	1:E:110:ARG:NH1	2.34	0.42
1:F:93:ASN:O	1:F:97:LEU:HG	2.19	0.42
1:G:185:LEU:HD23	1:G:185:LEU:HA	1.88	0.42
2:Y:19:ALA:HB3	2:Y:20:PRO:HD3	2.00	0.42
1:A:93:ASN:HB3	1:A:114:ARG:HH22	1.83	0.42
1:I:142:PHE:HB3	1:J:189:ILE:HD11	2.02	0.42
2:Y:24:VAL:HB	2:Y:25:ASP:CA	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:LEU:HD23	1:D:209:LEU:HA	1.91	0.42
1:F:61:LEU:HD23	1:F:61:LEU:HA	1.86	0.42
1:F:168:ALA:HA	1:F:171:ALA:HB2	2.01	0.42
1:B:208:MET:HE3	1:B:208:MET:HB2	1.79	0.42
1:B:30:LEU:HD23	1:B:30:LEU:HA	1.88	0.42
1:C:153:MET:HE2	1:C:153:MET:HB3	1.97	0.42
1:D:165:THR:HG22	1:D:166:ASN:H	1.84	0.42
1:I:118:ARG:HA	1:I:118:ARG:HD3	1.90	0.42
1:A:48:PHE:CZ	1:A:201:GLN:HB3	2.55	0.42
1:A:149:VAL:HG21	1:B:181:THR:HG21	2.00	0.42
1:D:85:LEU:HG	1:D:89:ASN:ND2	2.35	0.42
1:F:107:ILE:HA	1:F:110:ARG:NH1	2.35	0.42
1:F:168:ALA:HA	1:F:171:ALA:CB	2.50	0.42
2:Z:5:ILE:HB	2:Z:8:MET:HE2	2.02	0.42
1:A:81:LYS:HB2	1:A:81:LYS:HE3	1.56	0.42
1:C:93:ASN:O	1:C:97:LEU:HG	2.20	0.42
1:J:188:ALA:O	1:J:192:VAL:HG13	2.19	0.42
1:B:94:GLU:OE2	1:C:222:ARG:NH1	2.52	0.42
1:H:77:ASP:O	1:H:78:PHE:C	2.63	0.42
1:B:112:SER:O	1:B:116:GLU:HG2	2.20	0.41
1:G:87:LEU:HD13	1:G:213:ALA:HB2	2.02	0.41
1:C:232:ALA:HB3	1:C:233:HIS:HA	2.01	0.41
1:I:62:LEU:HA	1:I:62:LEU:HD23	1.81	0.41
1:J:17:GLN:O	1:J:19:ALA:HB3	2.20	0.41
1:B:14:GLY:O	1:B:18:HIS:N	2.53	0.41
1:B:42:PHE:CZ	1:I:31:ILE:HD13	2.55	0.41
1:F:153:MET:HE2	1:F:153:MET:HB3	1.93	0.41
1:J:33:ALA:O	1:J:37:THR:HG23	2.21	0.41
1:C:215:GLN:O	1:C:219:LEU:HG	2.21	0.41
1:H:115:LEU:HA	1:H:115:LEU:HD23	1.81	0.41
1:E:54:ARG:HH12	1:E:81:LYS:HE2	1.85	0.41
1:G:194:ILE:HD13	1:G:194:ILE:HG21	1.90	0.41
1:H:145:LEU:HD21	2:Z:7:VAL:HG13	2.02	0.41
1:J:161:GLN:O	1:J:162:THR:OG1	2.28	0.41
2:Z:5:ILE:HB	2:Z:8:MET:CE	2.50	0.41
1:A:188:ALA:O	1:A:192:VAL:HG23	2.21	0.41
1:D:115:LEU:HD12	1:D:217:LEU:HG	2.03	0.41
1:G:134:ALA:HB2	1:G:195:TYR:CE2	2.55	0.41
1:G:189:ILE:N	1:G:190:PRO:HD2	2.36	0.41
1:H:13:TRP:O	1:H:13:TRP:HE3	2.04	0.41
1:A:171:ALA:HB2	1:E:159:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:LYS:HD2	1:D:44:LYS:HA	1.91	0.41
1:E:95:LEU:HD23	1:E:95:LEU:HA	1.88	0.41
1:F:93:ASN:HB3	1:F:114:ARG:HH22	1.85	0.41
1:G:218:LEU:HA	1:G:218:LEU:HD23	1.83	0.41
1:I:126:MET:HE3	1:I:126:MET:HB3	1.99	0.41
1:I:142:PHE:HZ	2:Z:4:PHE:HE1	1.67	0.41
1:I:179:LEU:HD23	1:I:179:LEU:HA	1.79	0.41
1:D:78:PHE:HD1	1:D:78:PHE:HA	1.74	0.41
1:F:56:LYS:O	1:F:60:GLN:HG3	2.21	0.41
1:A:123:GLY:HA3	1:A:206:LYS:HE2	2.03	0.40
1:D:164:THR:HG22	1:D:165:THR:H	1.85	0.40
1:J:135:THR:O	1:J:139:ILE:HG12	2.21	0.40
1:A:112:SER:O	1:A:113:PHE:C	2.64	0.40
1:G:189:ILE:O	1:G:193:VAL:HG23	2.20	0.40
1:H:189:ILE:O	1:H:193:VAL:HG22	2.22	0.40
2:Y:24:VAL:HB	2:Y:25:ASP:C	2.46	0.40
1:A:16:TYR:CE1	1:A:24:LYS:HE3	2.57	0.40
1:J:126:MET:HE3	1:J:126:MET:HB3	2.01	0.40
2:Z:10:VAL:O	2:Z:14:ILE:HB	2.21	0.40
1:A:77:ASP:CA	1:A:78:PHE:HB2	2.49	0.40
1:F:182:ALA:HB1	1:J:146:PHE:HE1	1.86	0.40
1:G:112:SER:O	1:G:116:GLU:HG2	2.20	0.40
1:A:171:ALA:HB3	1:A:172:PRO:HD3	2.03	0.40
1:C:128:ARG:O	1:D:200:ARG:NH1	2.31	0.40
1:D:87:LEU:HD22	1:D:115:LEU:HD22	2.02	0.40
1:D:133:LEU:HD13	1:D:194:ILE:HG22	2.03	0.40
1:J:198:PHE:O	1:J:202:ILE:HB	2.21	0.40
2:Y:16:MET:O	2:Y:20:PRO:HD2	2.20	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	221/244 (91%)	209 (95%)	11 (5%)	1 (0%)	24	57
1	B	222/244 (91%)	213 (96%)	8 (4%)	1 (0%)	24	57
1	C	221/244 (91%)	212 (96%)	9 (4%)	0	100	100
1	D	212/244 (87%)	202 (95%)	10 (5%)	0	100	100
1	E	220/244 (90%)	214 (97%)	6 (3%)	0	100	100
1	F	223/244 (91%)	211 (95%)	8 (4%)	4 (2%)	6	34
1	G	222/244 (91%)	214 (96%)	8 (4%)	0	100	100
1	H	219/244 (90%)	210 (96%)	9 (4%)	0	100	100
1	I	213/244 (87%)	203 (95%)	9 (4%)	1 (0%)	24	57
1	J	216/244 (88%)	208 (96%)	6 (3%)	2 (1%)	14	47
2	Y	21/58 (36%)	19 (90%)	2 (10%)	0	100	100
2	Z	20/58 (34%)	17 (85%)	3 (15%)	0	100	100
All	All	2230/2556 (87%)	2132 (96%)	89 (4%)	9 (0%)	30	62

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	162	THR
1	I	67	SER
1	J	21	ILE
1	F	163	GLN
1	F	168	ALA
1	A	20	ASP
1	B	68	LEU
1	F	164	THR
1	J	166	ASN

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	167/189 (88%)	149 (89%)	18 (11%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	171/189 (90%)	153 (90%)	18 (10%)	6	27
1	C	165/189 (87%)	148 (90%)	17 (10%)	7	28
1	D	160/189 (85%)	144 (90%)	16 (10%)	7	28
1	E	164/189 (87%)	148 (90%)	16 (10%)	7	30
1	F	168/189 (89%)	156 (93%)	12 (7%)	13	38
1	G	171/189 (90%)	156 (91%)	15 (9%)	9	32
1	H	169/189 (89%)	154 (91%)	15 (9%)	9	32
1	I	165/189 (87%)	150 (91%)	15 (9%)	9	32
1	J	162/189 (86%)	138 (85%)	24 (15%)	3	17
2	Y	19/50 (38%)	15 (79%)	4 (21%)	1	6
2	Z	19/50 (38%)	12 (63%)	7 (37%)	0	1
All	All	1700/1990 (85%)	1523 (90%)	177 (10%)	7	27

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	21	ILE
1	A	24	LYS
1	A	36	VAL
1	A	46	VAL
1	A	68	LEU
1	A	77	ASP
1	A	90	GLU
1	A	118	ARG
1	A	135	THR
1	A	143	VAL
1	A	159	ILE
1	A	161	GLN
1	A	170	VAL
1	A	179	LEU
1	A	186	VAL
1	A	193	VAL
1	A	197	VAL
1	B	18	HIS
1	B	23	VAL
1	B	46	VAL
1	B	55	LEU

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Mol	Chain	Res	Type
1	B	57	ARG
1	B	66	ARG
1	B	68	LEU
1	B	85	LEU
1	B	90	GLU
1	B	117	ARG
1	B	118	ARG
1	B	143	VAL
1	B	148	THR
1	B	152	ILE
1	B	159	ILE
1	B	162	THR
1	B	181	THR
1	B	193	VAL
1	C	11	SER
1	C	12	VAL
1	C	13	TRP
1	C	16	TYR
1	C	18	HIS
1	C	25	CYS
1	C	36	VAL
1	C	64	GLU
1	C	90	GLU
1	C	116	GLU
1	C	118	ARG
1	C	135	THR
1	C	143	VAL
1	C	148	THR
1	C	162	THR
1	C	181	THR
1	C	197	VAL
1	D	21	ILE
1	D	22	VAL
1	D	32	LEU
1	D	46	VAL
1	D	55	LEU
1	D	68	LEU
1	D	77	ASP
1	D	80	SER
1	D	117	ARG
1	D	118	ARG
1	D	148	THR

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Mol	Chain	Res	Type
1	D	159	ILE
1	D	164	THR
1	D	181	THR
1	D	197	VAL
1	D	209	LEU
1	E	22	VAL
1	E	51	GLN
1	E	66	ARG
1	E	85	LEU
1	E	135	THR
1	E	143	VAL
1	E	148	THR
1	E	155	SER
1	E	159	ILE
1	E	161	GLN
1	E	166	ASN
1	E	167	LEU
1	E	169	VAL
1	E	181	THR
1	E	193	VAL
1	E	200	ARG
1	F	10	LEU
1	F	36	VAL
1	F	53	ARG
1	F	69	ASN
1	F	80	SER
1	F	90	GLU
1	F	135	THR
1	F	143	VAL
1	F	163	GLN
1	F	179	LEU
1	F	197	VAL
1	F	200	ARG
1	G	10	LEU
1	G	20	ASP
1	G	53	ARG
1	G	55	LEU
1	G	68	LEU
1	G	85	LEU
1	G	117	ARG
1	G	148	THR
1	G	152	ILE

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Mol	Chain	Res	Type
1	G	159	ILE
1	G	164	THR
1	G	165	THR
1	G	167	LEU
1	G	181	THR
1	G	193	VAL
1	H	13	TRP
1	H	18	HIS
1	H	26	VAL
1	H	36	VAL
1	H	64	GLU
1	H	68	LEU
1	H	81	LYS
1	H	135	THR
1	H	143	VAL
1	H	148	THR
1	H	152	ILE
1	H	154	ASN
1	H	165	THR
1	H	181	THR
1	H	206	LYS
1	I	22	VAL
1	I	46	VAL
1	I	55	LEU
1	I	66	ARG
1	I	68	LEU
1	I	90	GLU
1	I	113	PHE
1	I	148	THR
1	I	164	THR
1	I	167	LEU
1	I	179	LEU
1	I	181	THR
1	I	193	VAL
1	I	197	VAL
1	I	209	LEU
1	J	22	VAL
1	J	23	VAL
1	J	24	LYS
1	J	53	ARG
1	J	77	ASP
1	J	85	LEU

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Mol	Chain	Res	Type
1	J	90	GLU
1	J	96	GLU
1	J	118	ARG
1	J	128	ARG
1	J	135	THR
1	J	143	VAL
1	J	148	THR
1	J	155	SER
1	J	159	ILE
1	J	161	GLN
1	J	164	THR
1	J	167	LEU
1	J	169	VAL
1	J	170	VAL
1	J	181	THR
1	J	192	VAL
1	J	193	VAL
1	J	200	ARG
2	Y	6	ASP
2	Y	15	PHE
2	Y	16	MET
2	Y	24	VAL
2	Z	5	ILE
2	Z	6	ASP
2	Z	11	LEU
2	Z	12	LEU
2	Z	15	PHE
2	Z	16	MET
2	Z	17	VAL

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	72	ASN
1	B	166	ASN
1	E	125	GLN
1	F	72	ASN
1	F	163	GLN
1	G	86	HIS
1	G	215	GLN
1	H	154	ASN
1	I	215	GLN

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Mol	Chain	Res	Type
1	J	51	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	MLY	A	108	1	9,10,11	0.44	0	6,11,13	0.74	0
1	MLY	E	108	1	9,10,11	0.47	0	6,11,13	0.91	0
1	MLY	H	108	1	9,10,11	0.42	0	6,11,13	0.92	0
1	MLY	I	108	1	9,10,11	0.53	0	6,11,13	0.85	0
1	MLY	F	108	1	9,10,11	0.45	0	6,11,13	0.81	0
1	MLY	C	108	1	9,10,11	0.51	0	6,11,13	0.75	0
1	MLY	J	108	1	9,10,11	0.53	0	6,11,13	1.02	0
1	MLY	B	108	1	9,10,11	0.49	0	6,11,13	1.06	1 (16%)
1	MLY	D	108	1	9,10,11	0.55	0	6,11,13	0.87	0
1	MLY	G	108	1	9,10,11	0.59	0	6,11,13	1.22	1 (16%)

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
1	MLY	A	108	1	-	1/8/9/11	-
1	MLY	E	108	1	-	1/8/9/11	-
1	MLY	H	108	1	-	1/8/9/11	-
1	MLY	I	108	1	-	1/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	F	108	1	-	1/8/9/11	-
1	MLY	C	108	1	-	1/8/9/11	-
1	MLY	J	108	1	-	1/8/9/11	-
1	MLY	B	108	1	-	1/8/9/11	-
1	MLY	D	108	1	-	1/8/9/11	-
1	MLY	G	108	1	-	1/8/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	108	MLY	CH2-NZ-CH1	-2.08	104.39	109.72
1	B	108	MLY	CH2-NZ-CH1	-2.05	104.46	109.72

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	108	MLY	CD-CE-NZ-CH2
1	G	108	MLY	CD-CE-NZ-CH2
1	E	108	MLY	CD-CE-NZ-CH2
1	F	108	MLY	CD-CE-NZ-CH2
1	I	108	MLY	CD-CE-NZ-CH2
1	J	108	MLY	CD-CE-NZ-CH2
1	A	108	MLY	CD-CE-NZ-CH2
1	C	108	MLY	CD-CE-NZ-CH2
1	D	108	MLY	CD-CE-NZ-CH2
1	H	108	MLY	CD-CE-NZ-CH2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - 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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	223/244 (91%)	0.24	10 (4%)	38 20	61, 84, 137, 199	0
1	B	224/244 (91%)	0.24	3 (1%)	75 50	53, 78, 133, 169	0
1	C	223/244 (91%)	0.29	5 (2%)	62 37	50, 89, 136, 180	0
1	D	214/244 (87%)	0.19	11 (5%)	33 19	48, 74, 166, 244	0
1	E	222/244 (90%)	0.12	7 (3%)	50 29	57, 94, 157, 209	0
1	F	225/244 (92%)	0.24	8 (3%)	46 25	52, 89, 151, 183	0
1	G	224/244 (91%)	0.23	3 (1%)	75 50	62, 81, 129, 154	0
1	H	221/244 (90%)	0.11	7 (3%)	50 29	40, 77, 136, 181	0
1	I	215/244 (88%)	0.41	15 (6%)	22 14	44, 74, 162, 243	0
1	J	218/244 (89%)	0.20	9 (4%)	41 22	56, 87, 141, 168	0
2	Y	23/58 (39%)	3.27	19 (82%)	0 0	119, 141, 167, 170	0
2	Z	22/58 (37%)	2.63	15 (68%)	0 0	98, 151, 168, 180	0
All	All	2254/2556 (88%)	0.28	112 (4%)	34 19	40, 84, 151, 244	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	7	VAL	7.0
1	D	166	ASN	5.7
2	Y	3	PRO	5.5
1	A	169	VAL	5.5
2	Z	17	VAL	5.2
1	J	16	TYR	4.8
2	Z	3	PRO	4.7
2	Y	9	LEU	4.6
2	Y	21	LEU	4.6
2	Y	19	ALA	4.6
1	I	166	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	I	57	ARG	4.2
2	Z	10	VAL	4.2
1	J	17	GLN	4.2
2	Z	14	ILE	4.2
2	Y	6	ASP	4.1
2	Y	5	ILE	4.1
1	A	170	VAL	3.9
1	A	168	ALA	3.9
1	A	167	LEU	3.9
2	Y	24	VAL	3.8
1	A	164	THR	3.8
1	F	169	VAL	3.7
1	I	168	ALA	3.6
1	D	168	ALA	3.6
2	Z	19	ALA	3.6
1	H	116	GLU	3.6
2	Y	11	LEU	3.6
2	Z	11	LEU	3.5
1	A	165	THR	3.5
1	C	228	ALA	3.5
2	Y	8	MET	3.4
2	Y	22	ALA	3.3
1	F	168	ALA	3.2
2	Z	6	ASP	3.2
2	Y	18	ALA	3.2
1	I	64	GLU	3.2
1	I	19	ALA	3.2
1	J	166	ASN	3.2
1	C	205	PHE	3.2
1	D	156	PHE	3.1
1	G	211	ASP	3.1
1	I	163	GLN	3.0
1	I	77	ASP	3.0
1	D	159	ILE	2.9
1	E	164	THR	2.9
1	D	167	LEU	2.9
1	B	10	LEU	2.9
1	B	12	VAL	2.9
1	I	159	ILE	2.8
2	Z	18	ALA	2.8
1	A	172	PRO	2.8
1	I	60	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
2	Z	23	THR	2.8
2	Y	4	PHE	2.8
1	I	165	THR	2.8
1	J	18	HIS	2.7
1	A	173	GLY	2.7
1	J	162	THR	2.7
2	Y	20	PRO	2.7
1	D	120	ALA	2.7
1	H	164	THR	2.7
1	J	160	ALA	2.7
1	E	173	GLY	2.7
1	E	160	ALA	2.6
1	D	116	GLU	2.6
2	Z	21	LEU	2.6
2	Z	24	VAL	2.6
1	C	231	ALA	2.5
1	I	234	PRO	2.5
2	Z	7	VAL	2.5
1	F	164	THR	2.5
1	H	11	SER	2.5
1	I	167	LEU	2.5
2	Y	12	LEU	2.5
1	G	44	LYS	2.5
2	Y	17	VAL	2.5
1	H	221	SER	2.5
1	D	19	ALA	2.4
1	A	223	ASP	2.4
1	C	209	LEU	2.4
1	J	20	ASP	2.4
1	F	162	THR	2.3
1	D	128	ARG	2.3
1	F	165	THR	2.3
1	I	211	ASP	2.2
2	Y	25	ASP	2.2
1	B	221	SER	2.2
2	Y	13	ILE	2.2
1	A	113	PHE	2.2
1	G	59	GLN	2.2
1	I	105	GLU	2.2
1	E	165	THR	2.2
2	Z	20	PRO	2.2
1	D	57	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	164	THR	2.1
2	Y	23	THR	2.1
2	Z	5	ILE	2.1
2	Z	4	PHE	2.1
1	E	159	ILE	2.1
1	H	121	ALA	2.1
1	F	212	VAL	2.1
1	D	99	GLU	2.1
1	F	105	GLU	2.1
1	E	171	ALA	2.1
1	E	233	HIS	2.0
1	H	129	GLY	2.0
1	H	118	ARG	2.0
1	I	20	ASP	2.0
1	F	223	ASP	2.0
1	C	230	ALA	2.0
1	J	171	ALA	2.0

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

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(Å ²)	Q<0.9
1	MLY	I	108	11/12	0.83	0.17	57,63,79,97	0
1	MLY	B	108	11/12	0.86	0.25	48,49,71,80	0
1	MLY	J	108	11/12	0.88	0.14	59,59,63,94	0
1	MLY	C	108	11/12	0.89	0.19	46,49,69,84	0
1	MLY	G	108	11/12	0.89	0.19	61,62,66,75	0
1	MLY	A	108	11/12	0.90	0.17	70,72,94,108	0
1	MLY	H	108	11/12	0.91	0.14	40,41,48,49	0
1	MLY	E	108	11/12	0.93	0.14	57,60,67,104	0
1	MLY	D	108	11/12	0.94	0.10	47,48,52,109	0
1	MLY	F	108	11/12	0.94	0.11	46,51,62,70	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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. 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(Å ²)	Q<0.9
3	HG	D	301	1/1	0.38	0.13	598,598,598,598	0
3	HG	I	301	1/1	0.39	0.12	683,683,683,683	0
3	HG	H	301	1/1	0.44	0.21	563,563,563,563	0
3	HG	E	301	1/1	0.48	0.12	582,582,582,582	0
3	HG	C	301	1/1	0.51	0.15	467,467,467,467	0
3	HG	J	301	1/1	0.56	0.16	593,593,593,593	0
3	HG	B	301	1/1	0.60	0.15	514,514,514,514	0
3	HG	G	301	1/1	0.66	0.14	502,502,502,502	0
3	HG	F	301	1/1	0.78	0.22	487,487,487,487	0
3	HG	A	301	1/1	0.83	0.17	370,370,370,370	0

6.5 Other polymers

There are no such residues in this entry.