



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 11:34 PM EDT

PDB ID : 1LOA / pdb_00001loa
Title : THREE-DIMENSIONAL STRUCTURES OF COMPLEXES OF LATHYRUS OCHRUS ISOLECTIN I WITH GLUCOSE AND MANNOSE: FINE SPECIFICITY OF THE MONOSACCHARIDE-BINDING SITE
Authors : Bourne, Y.; Cambillau, C.
Deposited on : 1993-01-27
Resolution : 2.20 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

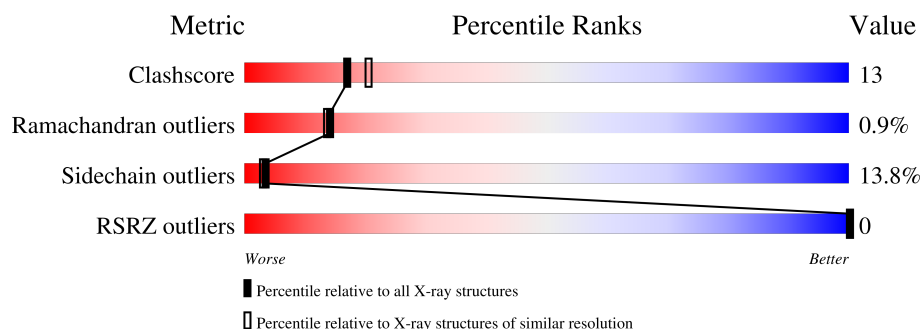
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	181	42% 45% 13% .
1	C	181	50% 37% 10% ..
1	E	181	47% 38% 10% ..
1	G	181	44% 39% 15% ..
2	B	52	58% 27% 6% 10%
2	D	52	52% 37% . 10%
2	F	52	48% 31% 10% . 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	52	 A horizontal bar chart showing the quality of chain H. The bar is divided into four segments: green (52%), yellow (29%), orange (8%), and red (10%). The segments are labeled with their respective percentages: 52%, 29%, 8%, and 10%.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7460 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 LEGUME ISOLECTIN I (ALPHA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	0	0	0
			1397	890	230	277			
1	C	180	Total	C	N	O	0	0	0
			1397	890	230	277			
1	E	180	Total	C	N	O	0	0	0
			1397	890	230	277			
1	G	180	Total	C	N	O	0	0	0
			1397	890	230	277			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ALA	LYS	conflict	UNP P04122
C	153	ALA	LYS	conflict	UNP P04122
E	153	ALA	LYS	conflict	UNP P04122
G	153	ALA	LYS	conflict	UNP P04122

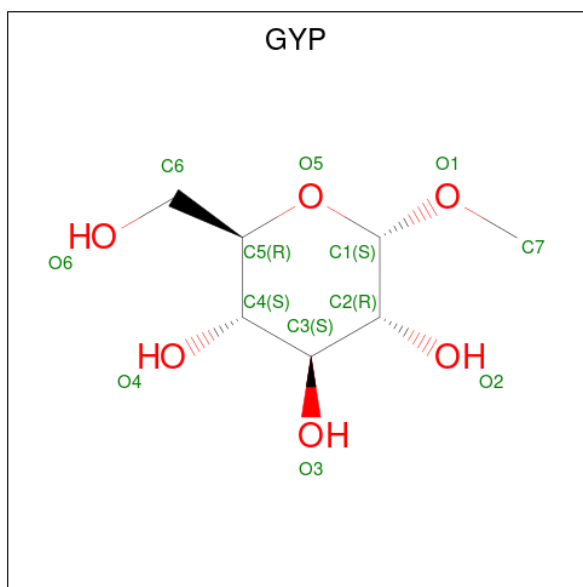
- Molecule 2 is a protein called LEGUME ISOLECTIN I (BETA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	47	Total	C	N	O	0	0	0
			381	251	58	72			
2	D	47	Total	C	N	O	0	0	0
			376	248	58	70			
2	F	47	Total	C	N	O	0	0	0
			381	251	58	72			
2	H	47	Total	C	N	O	0	0	0
			376	248	58	70			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	41	TYR	PHE	conflict	UNP P12306
D	41	TYR	PHE	conflict	UNP P12306
F	41	TYR	PHE	conflict	UNP P12306
H	41	TYR	PHE	conflict	UNP P12306

- Molecule 3 is methyl alpha-D-glucopyranoside (CCD ID: GYP) (formula: C₇H₁₄O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	7	6		
3	C	1	Total	C	O	0	0
			13	7	6		
3	E	1	Total	C	O	0	0
			13	7	6		
3	G	1	Total	C	O	0	0
			13	7	6		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	E	1	Total	Ca	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Ca 1	0	0

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mn 1	0	0
5	C	1	Total 1	Mn 1	0	0
5	F	1	Total 1	Mn 1	0	0
5	G	1	Total 1	Mn 1	0	0

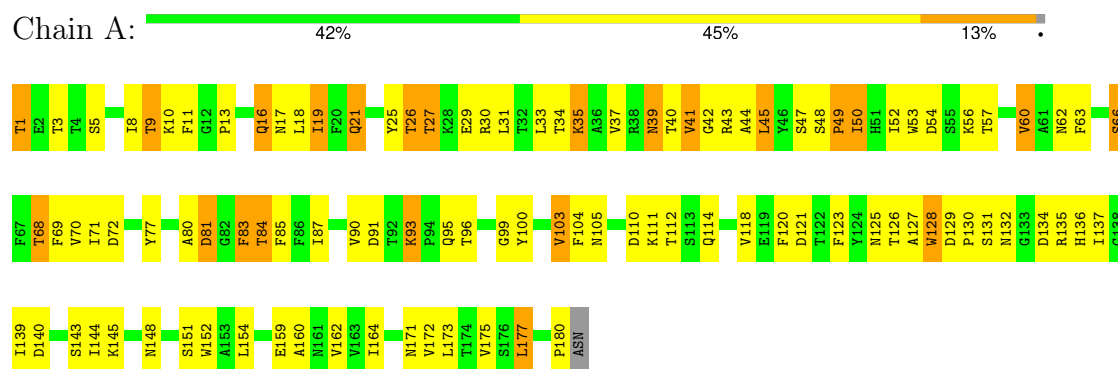
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	73	Total 73	O 73	0	0
6	B	17	Total 17	O 17	0	0
6	C	59	Total 59	O 59	0	0
6	D	8	Total 8	O 8	0	0
6	E	53	Total 53	O 53	0	0
6	F	9	Total 9	O 9	0	0
6	G	70	Total 70	O 70	0	0
6	H	9	Total 9	O 9	0	0

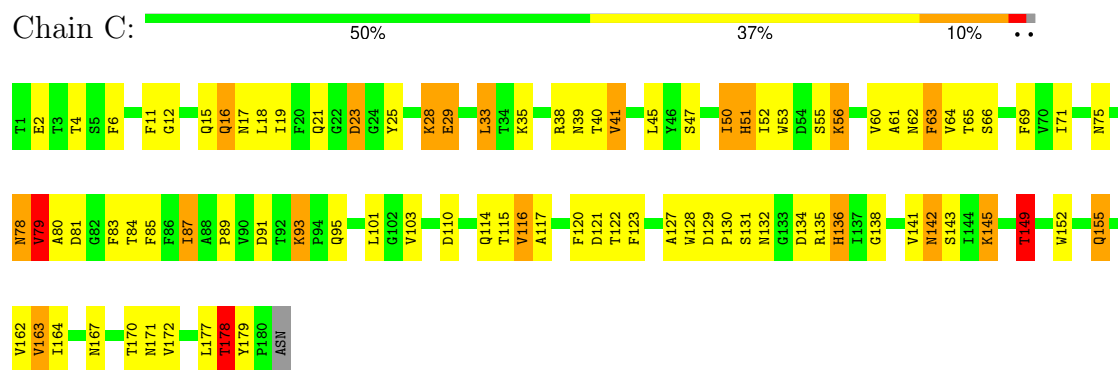
3 Residue-property plots

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.

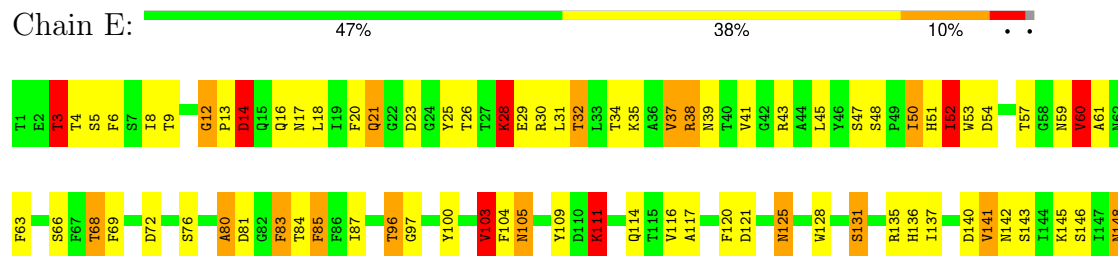
• Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)



• Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)



• Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)





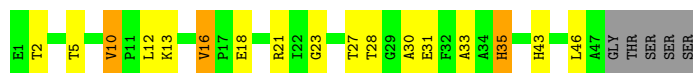
• Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)

Chain G: 44% 39% 15% ..



• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)

Chain B: 58% 27% 6% 10%



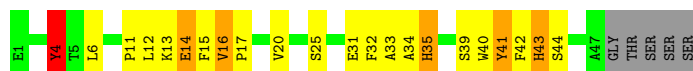
• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)

Chain D: 52% 37% 10%



• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)

Chain F: 48% 31% 10% 10%



• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)

Chain H: 52% 29% 8% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.30Å 139.80Å 62.70Å 90.00° 91.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20 8.00 – 2.21	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.20) 65.7 (8.00-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.179 , (Not available) 0.167 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 70.9	EDS
L-test for twinning ¹	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7460	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: CA, GYP, MN

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	1.37	8/1431 (0.6%)	2.21	74/1954 (3.8%)
1	C	1.24	6/1431 (0.4%)	2.19	66/1954 (3.4%)
1	E	1.31	9/1431 (0.6%)	2.27	68/1954 (3.5%)
1	G	1.25	10/1431 (0.7%)	2.11	63/1954 (3.2%)
2	B	1.41	5/394 (1.3%)	1.99	12/539 (2.2%)
2	D	1.28	3/389 (0.8%)	2.02	10/532 (1.9%)
2	F	1.39	3/394 (0.8%)	2.01	13/539 (2.4%)
2	H	1.40	3/389 (0.8%)	1.95	6/532 (1.1%)
All	All	1.31	47/7290 (0.6%)	2.15	312/9958 (3.1%)

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	E	0	1
2	D	0	1
2	F	0	1
All	All	0	3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	116	VAL	CA-CB	8.82	1.67	1.54
1	C	51	HIS	CD2-NE2	-8.65	1.28	1.37
2	H	10	VAL	CA-CB	8.02	1.62	1.53
1	E	60	VAL	CA-CB	7.94	1.67	1.55
1	A	103	VAL	CA-CB	7.47	1.64	1.54
2	F	35	HIS	CD2-NE2	-7.30	1.29	1.37
2	B	35	HIS	CD2-NE2	-7.13	1.30	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	136	HIS	CD2-NE2	-7.13	1.30	1.37
2	H	35	HIS	CD2-NE2	-6.92	1.30	1.37
1	A	172	VAL	CA-CB	6.85	1.63	1.54
1	G	51	HIS	CD2-NE2	-6.73	1.30	1.37
2	D	35	HIS	CD2-NE2	-6.47	1.30	1.37
1	A	123	PHE	C-O	6.46	1.31	1.24
1	E	51	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	50	ILE	CA-CB	6.12	1.62	1.54
2	H	43	HIS	CD2-NE2	-6.10	1.31	1.37
1	G	87	ILE	CA-CB	6.03	1.63	1.54
1	G	121	ASP	CA-CB	-5.99	1.44	1.53
1	G	162	VAL	CA-CB	5.99	1.65	1.55
1	C	116	VAL	CA-CB	5.91	1.63	1.54
1	G	23	ASP	CA-CB	-5.87	1.43	1.53
1	E	172	VAL	CA-CB	5.86	1.61	1.54
1	A	70	VAL	CA-CB	5.81	1.63	1.54
1	G	103	VAL	CA-CB	5.63	1.63	1.54
2	D	43	HIS	CD2-NE2	-5.63	1.31	1.37
1	C	178	THR	CA-CB	5.58	1.62	1.53
1	A	77	TYR	CA-CB	-5.54	1.44	1.53
1	A	60	VAL	CA-CB	5.53	1.63	1.54
2	B	43	HIS	CD2-NE2	-5.52	1.31	1.37
1	G	79	VAL	CA-CB	5.52	1.61	1.55
1	C	136	HIS	CG-ND1	-5.52	1.32	1.38
1	E	109	TYR	CA-CB	-5.46	1.46	1.52
2	B	35	HIS	CG-ND1	-5.39	1.32	1.38
1	E	158	LYS	CA-C	-5.33	1.46	1.52
2	B	43	HIS	CG-ND1	-5.29	1.32	1.38
2	F	43	HIS	CG-ND1	-5.27	1.32	1.38
1	E	32	THR	CA-CB	5.26	1.60	1.53
1	G	123	PHE	C-O	5.26	1.29	1.23
1	C	53	TRP	CA-C	-5.22	1.46	1.52
2	B	23	GLY	CA-C	-5.18	1.46	1.52
1	E	51	HIS	CG-ND1	-5.17	1.32	1.38
1	E	136	HIS	CG-ND1	-5.10	1.32	1.38
2	F	43	HIS	CD2-NE2	-5.08	1.32	1.37
2	D	35	HIS	CG-ND1	-5.05	1.32	1.38
1	G	68	THR	CA-CB	-5.02	1.45	1.53
1	A	72	ASP	CA-C	-5.01	1.46	1.52
1	C	79	VAL	CA-CB	5.00	1.62	1.54

All (312) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	14	ASP	CA-CB-CG	15.49	128.09	112.60
1	C	63	PHE	CA-CB-CG	13.28	127.08	113.80
1	G	103	VAL	CB-CA-C	9.89	120.60	110.91
1	A	140	ASP	CA-CB-CG	9.86	122.46	112.60
1	E	39	ASN	N-CA-C	9.86	125.32	111.52
1	C	17	ASN	CA-CB-CG	9.80	122.40	112.60
1	E	121	ASP	CA-CB-CG	9.71	122.31	112.60
1	C	121	ASP	CA-CB-CG	9.63	122.23	112.60
1	C	134	ASP	CA-CB-CG	9.45	122.05	112.60
1	E	30	ARG	N-CA-C	9.43	124.76	109.40
1	E	153	ALA	N-CA-C	-9.35	94.00	109.24
1	A	121	ASP	CA-CB-CG	9.34	121.94	112.60
1	C	91	ASP	CA-CB-CG	9.11	121.71	112.60
1	E	142	ASN	OD1-CG-ND2	-9.09	113.51	122.60
2	F	16	VAL	CB-CA-C	9.01	118.16	109.33
1	G	63	PHE	CA-CB-CG	8.99	122.79	113.80
1	C	83	PHE	O-C-N	-8.88	113.13	123.25
1	C	51	HIS	CB-CG-CD2	-8.85	119.70	131.20
1	C	110	ASP	CA-CB-CG	8.74	121.34	112.60
1	C	171	ASN	OD1-CG-ND2	-8.71	113.89	122.60
1	G	103	VAL	N-CA-CB	-8.62	100.08	111.90
1	C	103	VAL	CB-CA-C	8.39	118.44	111.06
2	B	16	VAL	N-CA-CB	-8.37	99.49	111.21
1	G	23	ASP	N-CA-C	8.29	123.24	113.20
1	G	142	ASN	OD1-CG-ND2	-8.27	114.33	122.60
1	E	85	PHE	N-CA-C	-8.23	95.81	109.07
1	E	63	PHE	CA-CB-CG	8.21	122.01	113.80
1	A	9	THR	N-CA-CB	-8.19	98.49	110.53
1	E	87	ILE	N-CA-C	-8.16	95.84	107.75
1	A	135	ARG	N-CA-C	-8.15	99.77	110.53
1	A	85	PHE	N-CA-C	-8.15	96.11	109.40
1	E	20	PHE	CA-CB-CG	-8.03	105.77	113.80
1	C	29	GLU	CB-CG-CD	8.01	126.21	112.60
1	A	26	THR	N-CA-CB	-7.91	97.47	110.52
1	C	69	PHE	CA-CB-CG	7.88	121.68	113.80
2	F	35	HIS	CB-CG-CD2	-7.87	120.97	131.20
1	C	51	HIS	CB-CG-ND1	7.87	134.50	122.70
1	C	53	TRP	CA-CB-CG	7.71	128.24	113.60
2	F	16	VAL	N-CA-CB	-7.67	103.43	111.64
1	A	84	THR	CA-CB-OG1	-7.66	98.11	109.60
1	A	50	ILE	CB-CG1-CD1	-7.61	97.83	113.80
1	E	4	THR	CA-CB-OG1	-7.59	98.21	109.60
1	C	80	ALA	O-C-N	-7.49	115.40	123.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	THR	CB-CA-C	7.36	121.84	109.48
1	E	141	VAL	N-CA-CB	-7.35	103.61	112.35
1	A	118	VAL	N-CA-C	-7.30	97.22	107.80
1	C	85	PHE	N-CA-C	-7.29	97.34	109.07
1	A	105	ASN	CA-CB-CG	-7.28	105.32	112.60
1	E	167	ASN	OD1-CG-ND2	-7.26	115.34	122.60
1	E	177	LEU	N-CA-C	-7.19	97.96	109.76
1	G	142	ASN	CB-CG-ND2	7.19	127.18	116.40
1	C	136	HIS	O-C-N	7.17	129.86	123.41
1	C	120	PHE	N-CA-C	-7.15	92.75	107.70
1	A	128	TRP	CG-CD2-CE3	7.13	141.03	133.90
1	G	62	ASN	CA-CB-CG	7.10	119.70	112.60
1	A	123	PHE	O-C-N	7.08	131.60	123.31
1	A	136	HIS	CA-CB-CG	7.00	120.80	113.80
1	E	80	ALA	O-C-N	-7.00	115.64	123.48
1	G	140	ASP	CA-CB-CG	6.98	119.58	112.60
1	G	85	PHE	O-C-N	-6.90	115.47	123.27
1	C	132	ASN	OD1-CG-ND2	-6.89	115.71	122.60
1	A	80	ALA	O-C-N	-6.86	116.08	123.42
1	G	87	ILE	N-CA-C	-6.86	98.24	108.46
1	A	143	SER	O-C-N	-6.85	116.68	123.46
1	E	69	PHE	CA-CB-CG	6.85	120.65	113.80
1	A	134	ASP	CA-CB-CG	6.85	119.45	112.60
1	G	71	ILE	N-CA-C	-6.81	97.81	107.75
2	H	2	THR	N-CA-CB	-6.80	99.94	111.50
1	A	137	ILE	N-CA-C	-6.78	98.58	108.89
1	A	123	PHE	CA-C-O	6.77	127.84	120.32
2	F	13	LYS	CB-CA-C	-6.72	99.26	110.68
1	E	142	ASN	CB-CG-ND2	6.71	126.47	116.40
1	A	16	GLN	N-CA-C	6.70	121.16	113.19
1	C	6	PHE	CA-C-O	-6.70	114.06	121.23
1	E	125	ASN	N-CA-C	-6.70	96.14	107.99
1	C	149	THR	N-CA-CB	-6.69	100.05	111.69
2	B	23	GLY	CA-C-O	-6.65	114.37	121.35
1	C	172	VAL	CG1-CB-CG2	-6.65	96.18	110.80
1	E	54	ASP	CA-CB-CG	6.63	119.23	112.60
1	E	48	SER	CA-C-N	6.63	126.65	119.89
1	E	48	SER	C-N-CA	6.63	126.65	119.89
1	C	23	ASP	CA-CB-CG	6.63	119.23	112.60
1	G	67	PHE	CA-CB-CG	6.62	120.42	113.80
1	E	8	ILE	N-CA-C	-6.62	95.58	109.34
1	C	95	GLN	O-C-N	-6.61	116.06	123.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ILE	N-CA-C	-6.58	98.95	108.17
1	A	91	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	112	THR	CA-CB-OG1	-6.57	99.75	109.60
1	G	81	ASP	CA-CB-CG	-6.56	106.04	112.60
2	B	2	THR	N-CA-C	-6.55	97.60	108.34
1	A	50	ILE	O-C-N	-6.53	116.48	123.14
1	G	83	PHE	N-CA-CB	-6.53	99.92	111.08
1	G	52	ILE	N-CA-CB	-6.53	100.46	111.23
1	C	55	SER	CA-C-O	-6.50	112.49	119.97
2	F	35	HIS	CB-CG-ND1	6.50	132.44	122.70
1	A	63	PHE	CA-CB-CG	6.47	120.28	113.80
1	E	125	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	C	78	ASN	CB-CA-C	-6.45	102.24	112.05
1	G	80	ALA	O-C-N	-6.45	116.33	123.04
1	C	164	ILE	N-CA-C	-6.45	98.76	108.17
1	E	3	THR	N-CA-CB	-6.43	99.57	111.52
1	C	155	GLN	CA-C-O	6.36	127.95	120.70
1	E	52	ILE	N-CA-CB	-6.36	100.74	111.23
1	A	19	ILE	N-CA-C	-6.36	98.47	107.75
1	G	51	HIS	CB-CG-CD2	-6.35	122.94	131.20
1	G	56	LYS	N-CA-C	-6.34	104.36	111.28
1	E	50	ILE	CB-CG1-CD1	-6.33	100.51	113.80
1	G	47	SER	N-CA-C	6.32	120.73	112.89
1	E	52	ILE	O-C-N	-6.32	114.67	122.57
1	G	167	ASN	CA-CB-CG	-6.32	106.28	112.60
1	E	137	ILE	N-CA-C	-6.31	99.27	108.11
1	A	177	LEU	N-CA-C	-6.30	98.63	108.90
1	E	41	VAL	CB-CA-C	-6.30	99.43	110.71
1	G	93	LYS	O-C-N	-6.27	115.77	121.66
1	G	154	LEU	CB-CA-C	-6.27	101.35	110.06
1	A	148	ASN	CB-CG-ND2	6.26	125.79	116.40
2	D	37	VAL	CA-CB-CG2	-6.26	99.77	110.40
1	C	85	PHE	O-C-N	-6.25	115.92	123.29
1	A	42	GLY	O-C-N	-6.25	118.49	123.49
1	E	68	THR	N-CA-C	-6.24	99.64	109.50
1	C	4	THR	N-CA-C	-6.22	98.48	109.06
1	E	103	VAL	N-CA-CB	-6.20	101.01	111.23
1	E	52	ILE	CB-CG1-CD1	-6.19	100.80	113.80
2	F	41	TYR	O-C-N	-6.17	116.19	123.41
1	E	37	VAL	N-CA-CB	-6.16	101.33	111.44
1	G	19	ILE	O-C-N	-6.14	116.42	122.93
1	C	103	VAL	N-CA-CB	-6.13	100.49	112.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	127	ALA	N-CA-C	6.13	118.76	111.71
1	E	135	ARG	N-CA-C	-6.11	102.42	110.43
1	C	71	ILE	N-CA-C	-6.11	99.69	108.48
1	C	6	PHE	CA-CB-CG	6.09	119.89	113.80
1	G	155	GLN	CG-CD-NE2	6.06	125.50	116.40
1	C	83	PHE	N-CA-CB	-6.06	101.54	111.66
2	D	2	THR	N-CA-CB	-6.06	101.20	111.50
1	A	84	THR	CA-CB-CG2	6.06	120.79	110.50
1	G	107	LYS	N-CA-C	-6.06	104.97	112.90
2	D	2	THR	CA-CB-OG1	-6.05	100.53	109.60
2	D	5	THR	CA-CB-OG1	-6.05	100.53	109.60
1	G	172	VAL	CG1-CB-CG2	-6.05	97.50	110.80
1	G	161	ASN	CA-CB-CG	-6.04	106.56	112.60
1	A	53	TRP	CA-CB-CG	6.02	125.04	113.60
1	G	29	GLU	N-CA-CB	-6.02	103.04	112.13
2	F	39	SER	CA-C-O	-6.01	114.84	121.33
1	G	28	LYS	N-CA-C	6.01	123.60	110.80
1	G	78	ASN	OD1-CG-ND2	-6.01	116.59	122.60
1	E	16	GLN	OE1-CD-NE2	-5.98	116.62	122.60
1	C	138	GLY	O-C-N	-5.97	118.21	123.76
1	G	85	PHE	N-CA-C	-5.95	99.54	109.24
1	E	157	GLY	O-C-N	-5.94	114.84	122.39
1	A	151	SER	CA-C-O	-5.94	115.26	121.55
1	G	179	TYR	N-CA-C	-5.93	101.36	110.32
2	D	35	HIS	CB-CG-CD2	-5.92	123.50	131.20
1	G	135	ARG	N-CA-C	-5.92	101.72	110.48
1	G	96	THR	CA-C-O	-5.91	114.54	121.16
1	G	29	GLU	CB-CG-CD	5.90	122.63	112.60
1	C	29	GLU	N-CA-CB	-5.90	103.49	112.28
1	C	50	ILE	N-CA-CB	-5.90	103.23	111.25
2	F	40	TRP	CA-CB-CG	5.89	124.79	113.60
1	A	39	ASN	N-CA-C	5.89	119.55	111.54
1	C	16	GLN	CG-CD-NE2	-5.89	107.57	116.40
1	C	171	ASN	CB-CG-ND2	5.87	125.21	116.40
1	A	48	SER	CA-C-N	5.87	125.88	119.90
1	A	48	SER	C-N-CA	5.87	125.88	119.90
1	C	25	TYR	O-C-N	-5.84	116.74	122.99
1	A	112	THR	CA-CB-CG2	5.83	120.41	110.50
1	A	145	LYS	CA-C-O	-5.83	114.34	120.58
1	E	167	ASN	N-CA-C	-5.83	97.64	108.02
1	E	175	VAL	CG1-CB-CG2	-5.82	98.01	110.80
1	G	85	PHE	CA-CB-CG	-5.80	108.00	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	9	THR	CA-CB-OG1	-5.79	100.92	109.60
2	H	47	ALA	N-CA-C	-5.79	101.72	110.28
2	H	4	TYR	N-CA-C	-5.78	98.87	108.75
1	C	35	LYS	N-CA-C	-5.77	101.65	109.95
1	G	94	PRO	CA-C-N	-5.76	116.97	123.13
1	G	94	PRO	C-N-CA	-5.76	116.97	123.13
1	E	37	VAL	CB-CA-C	5.75	119.36	110.50
1	G	155	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	A	129	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	120	PHE	N-CA-C	-5.74	95.71	107.70
1	E	160	ALA	CA-C-O	-5.73	114.51	120.70
1	A	27	THR	N-CA-C	5.72	117.82	108.55
2	D	29	GLY	N-CA-C	-5.72	101.08	111.16
1	A	21	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	C	62	ASN	N-CA-C	-5.71	101.29	110.14
2	H	5	THR	CA-C-O	-5.71	114.76	121.44
1	G	137	ILE	N-CA-C	-5.70	100.23	108.89
1	A	135	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	C	121	ASP	N-CA-CB	-5.69	101.16	110.43
1	A	145	LYS	N-CA-C	-5.68	99.26	108.41
1	E	120	PHE	CA-CB-CG	-5.64	108.16	113.80
1	G	118	VAL	N-CA-C	-5.64	98.31	107.28
1	G	163	VAL	N-CA-C	-5.64	100.36	108.48
1	G	39	ASN	N-CA-C	5.63	122.80	110.80
1	C	21	GLN	N-CA-C	-5.63	100.15	108.99
1	G	51	HIS	CA-CB-CG	-5.62	108.18	113.80
1	C	47	SER	N-CA-C	5.61	118.17	111.71
2	B	35	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	A	17	ASN	CA-CB-CG	5.59	118.19	112.60
1	G	137	ILE	O-C-N	-5.59	117.17	122.98
1	C	19	ILE	N-CA-C	-5.58	100.38	108.36
2	D	4	TYR	N-CA-C	-5.57	98.45	108.48
1	G	27	THR	CA-CB-OG1	-5.56	101.27	109.60
2	B	30	ALA	N-CA-C	-5.55	106.51	113.28
1	G	12	GLY	CA-C-N	5.55	125.90	119.47
1	G	12	GLY	C-N-CA	5.55	125.90	119.47
1	E	52	ILE	CB-CA-C	5.53	120.35	111.29
1	A	114	GLN	OE1-CD-NE2	-5.51	117.09	122.60
1	A	3	THR	O-C-N	-5.49	116.48	123.24
1	A	54	ASP	CA-CB-CG	5.48	118.08	112.60
1	C	143	SER	O-C-N	-5.47	117.57	123.42
1	C	142	ASN	OD1-CG-ND2	-5.46	117.14	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	141	VAL	CB-CA-C	5.46	117.15	111.09
1	E	143	SER	O-C-N	-5.46	117.03	123.25
2	F	4	TYR	CB-CG-CD1	-5.45	112.62	120.80
2	F	14	GLU	CB-CG-CD	5.45	121.87	112.60
1	E	47	SER	CA-C-O	-5.45	114.77	120.55
1	A	71	ILE	O-C-N	-5.45	117.46	123.18
1	C	155	GLN	CB-CG-CD	-5.44	103.35	112.60
1	E	111	LYS	CA-CB-CG	5.44	124.99	114.10
1	G	168	ALA	CA-C-O	-5.44	114.79	120.55
1	A	93	LYS	CA-C-N	5.43	125.44	119.90
1	A	93	LYS	C-N-CA	5.43	125.44	119.90
1	G	28	LYS	O-C-N	5.43	129.81	122.59
1	G	31	LEU	N-CA-C	-5.43	100.33	108.96
1	A	81	ASP	CA-CB-CG	-5.42	107.18	112.60
1	C	177	LEU	N-CA-C	-5.42	99.10	108.69
1	A	180	PRO	N-CA-C	5.41	125.64	112.10
1	A	41	VAL	N-CA-C	-5.40	100.28	108.17
1	E	131	SER	N-CA-C	5.39	117.91	111.71
1	E	121	ASP	N-CA-CB	-5.39	101.12	110.17
1	A	95	GLN	CG-CD-NE2	5.38	124.47	116.40
1	G	46	TYR	N-CA-C	-5.38	102.52	110.48
1	A	87	ILE	N-CA-C	-5.35	100.77	108.48
1	E	148	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	C	136	HIS	CA-CB-CG	-5.33	108.47	113.80
1	A	69	PHE	CA-CB-CG	5.33	119.13	113.80
1	E	59	ASN	OD1-CG-ND2	-5.32	117.28	122.60
2	F	34	ALA	CA-C-O	-5.32	115.76	121.56
1	E	160	ALA	O-C-N	-5.32	116.32	123.23
1	C	149	THR	CA-CB-OG1	-5.31	101.64	109.60
1	A	9	THR	CA-CB-OG1	-5.31	101.64	109.60
1	E	17	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	G	11	PHE	N-CA-C	-5.30	101.90	110.32
1	E	152	TRP	CG-CD2-CE3	5.29	139.19	133.90
1	A	125	ASN	N-CA-C	-5.26	98.81	108.02
1	A	45	LEU	CA-C-O	-5.26	115.16	121.11
1	A	56	LYS	O-C-N	-5.26	115.38	122.43
1	C	129	ASP	CA-C-N	5.26	126.42	119.84
1	C	129	ASP	C-N-CA	5.26	126.42	119.84
1	C	163	VAL	N-CA-C	-5.26	100.75	108.85
1	E	105	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	A	132	ASN	OD1-CG-ND2	-5.25	117.35	122.60
1	A	62	ASN	O-C-N	-5.25	117.05	123.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	62	ASN	OD1-CG-ND2	-5.25	117.36	122.60
1	G	128	TRP	CE2-CD2-CG	-5.25	100.91	107.20
1	E	167	ASN	CB-CG-ND2	5.24	124.26	116.40
1	A	31	LEU	CA-C-N	-5.24	115.77	123.00
1	A	31	LEU	C-N-CA	-5.24	115.77	123.00
2	F	13	LYS	N-CA-CB	5.24	117.92	110.06
1	E	152	TRP	CE2-CD2-CG	-5.24	100.92	107.20
1	A	49	PRO	CA-C-O	-5.24	115.44	121.36
1	C	29	GLU	N-CA-C	5.24	118.96	112.47
2	H	44	SER	O-C-N	-5.22	116.82	123.24
1	G	95	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	E	23	ASP	CA-CB-CG	-5.21	107.39	112.60
2	B	10	VAL	O-C-N	-5.21	115.16	121.10
1	E	83	PHE	O-C-N	-5.21	117.54	123.48
1	G	47	SER	CA-CB-OG	-5.21	100.68	111.10
2	B	13	LYS	CG-CD-CE	-5.20	99.34	111.30
1	A	171	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	G	9	THR	CA-CB-CG2	5.20	119.33	110.50
1	A	105	ASN	N-CA-C	5.19	120.47	113.72
1	A	8	ILE	N-CA-C	-5.17	98.59	109.34
1	G	129	ASP	CA-C-N	5.17	126.30	119.84
1	G	129	ASP	C-N-CA	5.17	126.30	119.84
2	B	18	GLU	O-C-N	5.16	127.39	122.07
1	E	12	GLY	O-C-N	-5.16	116.61	121.77
1	A	83	PHE	O-C-N	-5.16	117.37	123.25
2	B	21	ARG	N-CA-C	-5.16	101.53	109.52
1	C	39	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	C	93	LYS	CB-CG-CD	5.15	123.14	111.30
1	A	110	ASP	O-C-N	-5.15	116.45	123.14
1	E	41	VAL	N-CA-C	-5.14	100.48	108.81
1	C	78	ASN	N-CA-CB	5.13	118.04	110.49
2	D	37	VAL	CA-CB-CG1	5.13	119.13	110.40
1	E	4	THR	CA-CB-CG2	5.12	119.20	110.50
1	E	161	ASN	CA-C-O	-5.10	115.19	120.70
1	E	152	TRP	CG-CD1-NE1	-5.09	103.58	110.20
1	A	164	ILE	N-CA-C	-5.09	100.24	107.77
2	B	31	GLU	N-CA-C	-5.09	101.81	109.85
1	C	17	ASN	N-CA-C	-5.08	106.67	112.92
1	C	56	LYS	CA-CB-CG	5.08	124.26	114.10
1	A	90	VAL	O-C-N	-5.08	116.92	121.89
2	D	43	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	G	116	VAL	O-C-N	-5.08	117.67	123.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	13	LYS	CB-CG-CD	-5.07	99.63	111.30
1	E	31	LEU	CA-C-O	-5.07	115.50	120.98
1	G	78	ASN	N-CA-C	-5.06	99.17	108.02
1	C	87	ILE	N-CA-C	-5.05	101.03	108.11
2	B	35	HIS	CB-CG-ND1	5.05	130.28	122.70
2	F	40	TRP	CE2-CD2-CE3	5.05	123.85	118.80
1	E	21	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	A	33	LEU	N-CA-C	-5.04	107.25	113.41
2	H	14	GLU	CB-CG-CD	5.04	121.18	112.60
2	D	47	ALA	CA-C-O	-5.04	116.03	121.87
1	G	53	TRP	CA-CB-CG	5.04	123.17	113.60
1	E	47	SER	O-C-N	-5.03	116.79	122.12
1	E	179	TYR	N-CA-C	-5.03	102.41	110.10
1	C	16	GLN	N-CA-C	5.02	119.16	113.19
1	E	45	LEU	CD1-CG-CD2	-5.01	99.77	110.80
1	A	96	THR	N-CA-CB	-5.01	102.68	110.04
1	C	78	ASN	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	41	TYR	Sidechain
1	E	25	TYR	Sidechain
2	F	4	TYR	Sidechain

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	1397	0	1346	29	0
1	C	1397	0	1346	29	0
1	E	1397	0	1346	42	0
1	G	1397	0	1346	41	0
2	B	381	0	357	6	0
2	D	376	0	351	8	0
2	F	381	0	357	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	376	0	351	20	0
3	A	13	0	14	0	0
3	C	13	0	14	3	0
3	E	13	0	14	1	0
3	G	13	0	14	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
6	A	73	0	0	2	0
6	B	17	0	0	2	0
6	C	59	0	0	3	0
6	D	8	0	0	0	0
6	E	53	0	0	2	0
6	F	9	0	0	0	0
6	G	70	0	0	3	0
6	H	9	0	0	0	0
All	All	7460	0	6856	158	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 13.

All (158) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:PRO:HG3	1:C:149:THR:HG21	1.51	0.92
1:E:84:THR:HG21	1:E:117:ALA:HB1	1.57	0.83
1:A:21:GLN:HE22	1:A:43:ARG:HH21	1.31	0.75
1:A:10:LYS:HD2	1:A:29:GLU:HB3	1.73	0.70
1:C:122:THR:HA	1:C:135:ARG:HG2	1.75	0.69
1:A:11:PHE:O	1:A:29:GLU:HA	1.93	0.68
1:E:21:GLN:NE2	1:E:43:ARG:HE	1.93	0.67
1:A:21:GLN:HE21	1:A:43:ARG:HE	1.42	0.67
1:E:28:LYS:O	1:E:28:LYS:HE2	1.95	0.67
1:C:114:GLN:HA	1:C:142:ASN:HD21	1.64	0.63
1:G:160:ALA:HB1	1:G:177:LEU:HD13	1.82	0.62
1:G:70:VAL:HG23	2:H:38:LEU:HD11	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:PHE:CE1	2:F:42:PHE:HB3	2.35	0.62
1:E:21:GLN:HE21	1:E:43:ARG:HE	1.46	0.61
1:E:116:VAL:HG12	1:E:141:VAL:HG23	1.81	0.61
1:A:83:PHE:HB2	6:B:69:HOH:O	2.00	0.61
1:G:89:PRO:HD3	1:G:114:GLN:O	2.01	0.61
1:E:128:TRP:HB2	1:E:145:LYS:HG3	1.84	0.60
1:E:38:ARG:HD3	2:F:32:PHE:CE1	2.36	0.59
1:G:75:ASN:HD22	1:G:75:ASN:H	1.50	0.59
1:C:63:PHE:CZ	1:C:87:ILE:HD11	2.37	0.59
1:E:148:ASN:ND2	2:F:6:LEU:HD11	2.18	0.58
1:E:21:GLN:HE22	1:E:43:ARG:HH21	1.52	0.58
1:E:96:THR:OG1	1:E:105:ASN:HA	2.03	0.58
1:E:148:ASN:CG	2:F:6:LEU:HD11	2.29	0.58
1:E:97:GLY:O	1:E:100:TYR:HB2	2.04	0.57
1:E:84:THR:CG2	1:E:117:ALA:HB1	2.31	0.57
1:G:150:LYS:HB2	2:H:6:LEU:HD13	1.87	0.57
1:A:21:GLN:NE2	1:A:43:ARG:HE	2.02	0.56
2:H:38:LEU:N	2:H:38:LEU:HD12	2.20	0.56
1:G:150:LYS:HE3	2:H:5:THR:O	2.05	0.56
1:G:90:VAL:HA	2:H:21:ARG:HG3	1.88	0.56
1:E:84:THR:HG22	1:E:85:PHE:N	2.20	0.56
1:C:63:PHE:HZ	1:C:87:ILE:HD11	1.70	0.55
1:C:128:TRP:HB2	1:C:145:LYS:HG2	1.89	0.55
1:E:13:PRO:HA	1:E:26:THR:HG23	1.88	0.55
1:G:71:ILE:HG12	2:H:35:HIS:HD2	1.72	0.55
1:C:12:GLY:HA3	6:C:489:HOH:O	2.08	0.54
1:G:167:ASN:HD21	1:G:169:ALA:HB3	1.72	0.54
2:H:11:PRO:HB2	2:H:14:GLU:HG2	1.89	0.54
1:G:33:LEU:O	1:G:42:GLY:HA3	2.08	0.53
1:G:80:ALA:HB3	2:H:31:GLU:HB2	1.91	0.52
1:A:41:VAL:HG22	2:B:27:THR:HG22	1.92	0.52
1:C:75:ASN:OD1	1:C:78:ASN:HB2	2.09	0.52
1:C:78:ASN:HB3	6:C:512:HOH:O	2.09	0.52
1:G:84:THR:HG23	1:G:117:ALA:HB1	1.91	0.52
1:E:5:SER:OG	2:F:43:HIS:HD2	1.93	0.52
1:G:75:ASN:HD22	1:G:75:ASN:N	2.08	0.52
1:G:95:GLN:HB3	1:G:105:ASN:OD1	2.10	0.52
1:E:21:GLN:HE22	1:E:43:ARG:NH2	2.07	0.51
1:A:100:TYR:HB3	1:A:104:PHE:O	2.11	0.51
1:C:136:HIS:HA	1:C:152:TRP:HB3	1.93	0.51
1:E:21:GLN:NE2	1:E:43:ARG:NE	2.59	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:SER:OG	2:F:41:TYR:HD2	1.93	0.51
1:E:114:GLN:HA	2:F:15:PHE:O	2.10	0.51
2:F:11:PRO:HD2	2:F:15:PHE:CE2	2.46	0.51
1:A:25:TYR:CE2	1:A:27:THR:HB	2.46	0.51
1:C:11:PHE:O	1:C:29:GLU:HA	2.10	0.51
1:C:38:ARG:O	1:C:40:THR:HG23	2.10	0.51
1:A:1:THR:HA	2:B:46:LEU:O	2.10	0.51
1:E:114:GLN:HB3	2:F:17:PRO:HD3	1.92	0.51
2:H:38:LEU:HD12	2:H:38:LEU:H	1.74	0.51
1:G:77:TYR:CD1	1:G:77:TYR:N	2.79	0.51
1:C:60:VAL:HG12	1:C:61:ALA:H	1.75	0.50
1:A:21:GLN:HE22	1:A:43:ARG:NH2	2.06	0.50
2:F:11:PRO:HD2	2:F:15:PHE:HE2	1.76	0.50
1:A:16:GLN:HB2	2:D:19:TRP:CD2	2.47	0.50
1:A:66:SER:HA	1:A:162:VAL:O	2.13	0.49
1:A:127:ALA:HB3	1:A:128:TRP:CE3	2.48	0.49
1:G:1:THR:HA	2:H:46:LEU:O	2.13	0.49
1:A:10:LYS:HD3	6:B:64:HOH:O	2.14	0.48
1:G:21:GLN:HB2	1:G:43:ARG:HB2	1.95	0.48
1:C:2:GLU:OE1	1:C:51:HIS:HD2	1.95	0.48
1:A:13:PRO:HA	1:A:26:THR:HG23	1.96	0.48
1:E:14:ASP:HA	6:E:723:HOH:O	2.14	0.48
1:G:103:VAL:HG13	1:G:104:PHE:CD2	2.49	0.48
1:G:5:SER:HA	2:H:42:PHE:O	2.14	0.47
1:G:130:PRO:HG3	1:G:149:THR:HG21	1.97	0.47
1:C:41:VAL:HB	2:D:27:THR:HG22	1.97	0.47
1:E:83:PHE:HA	2:F:25:SER:O	2.14	0.47
1:G:75:ASN:H	1:G:75:ASN:ND2	2.12	0.47
1:A:139:ILE:HD13	1:A:173:LEU:HD23	1.96	0.47
1:E:105:ASN:HB2	6:E:697:HOH:O	2.14	0.47
1:E:103:VAL:HG12	1:E:104:PHE:CD2	2.49	0.47
1:G:41:VAL:HB	2:H:27:THR:HG22	1.96	0.47
1:C:66:SER:HB3	1:C:163:VAL:HG22	1.96	0.46
1:A:40:THR:HG22	1:A:41:VAL:N	2.29	0.46
3:C:182:GYP:H7C3	3:C:182:GYP:H5	1.96	0.46
2:F:42:PHE:HE2	2:F:44:SER:HG	1.59	0.46
1:E:61:ALA:O	1:E:168:ALA:HB2	2.15	0.46
1:E:80:ALA:CB	2:F:31:GLU:HB2	2.46	0.46
1:G:66:SER:HA	1:G:162:VAL:O	2.16	0.46
1:G:110:ASP:O	1:G:142:ASN:HB3	2.16	0.45
6:G:963:HOH:O	2:H:48:GLY:HA3	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:THR:HG22	1:A:41:VAL:H	1.81	0.45
1:A:159:GLU:HG3	6:A:285:HOH:O	2.16	0.45
6:C:509:HOH:O	2:D:21:ARG:HA	2.17	0.45
2:H:7:ASN:O	2:H:8:GLU:HG2	2.17	0.45
1:E:3:THR:HB	1:G:7:SER:OG	2.17	0.45
1:C:84:THR:CG2	1:C:117:ALA:HB1	2.47	0.45
1:G:167:ASN:HD22	1:G:170:THR:H	1.65	0.45
1:C:61:ALA:HB1	2:D:45:GLU:O	2.17	0.45
1:G:1:THR:N	6:G:920:HOH:O	2.41	0.45
1:C:15:GLN:HG3	1:C:18:LEU:HG	2.00	0.44
1:E:166:PHE:CE2	1:E:168:ALA:HA	2.52	0.44
1:A:34:THR:HG21	2:B:28:THR:HG23	2.00	0.44
1:G:113:SER:OG	1:G:115:THR:HG23	2.18	0.44
1:G:130:PRO:HG2	1:G:136:HIS:CE1	2.52	0.44
1:C:65:THR:HA	2:D:41:TYR:O	2.18	0.43
1:G:71:ILE:HG12	2:H:35:HIS:CD2	2.52	0.43
1:E:80:ALA:HB3	2:F:31:GLU:HB2	2.00	0.43
1:E:125:ASN:ND2	3:E:182:GYP:O4	2.51	0.43
1:E:21:GLN:HE21	1:E:43:ARG:NE	2.14	0.43
1:A:103:VAL:HG23	1:A:104:PHE:CD2	2.54	0.43
1:E:12:GLY:HA3	6:G:959:HOH:O	2.18	0.43
2:F:4:TYR:CD1	2:F:4:TYR:N	2.82	0.43
1:G:140:ASP:HB3	1:G:143:SER:O	2.18	0.43
1:C:28:LYS:HA	1:C:28:LYS:HD2	1.71	0.43
1:C:79:VAL:HG22	1:C:122:THR:HB	2.01	0.43
1:A:144:ILE:O	1:A:144:ILE:HG13	2.19	0.43
2:D:10:VAL:HG13	2:D:10:VAL:O	2.18	0.43
1:G:132:ASN:ND2	1:G:134:ASP:HB2	2.34	0.42
1:E:53:TRP:HA	1:E:60:VAL:HA	2.01	0.42
1:A:175:VAL:O	2:B:5:THR:HA	2.19	0.42
1:G:80:ALA:CB	2:H:31:GLU:HB2	2.49	0.42
1:C:155:GLN:HB2	1:C:179:TYR:CE1	2.55	0.42
2:H:10:VAL:HA	2:H:11:PRO:HD2	1.79	0.42
1:A:39:ASN:ND2	6:A:292:HOH:O	2.52	0.42
1:E:128:TRP:HB2	1:E:145:LYS:CG	2.50	0.42
1:G:97:GLY:HA2	2:H:27:THR:HG21	2.01	0.42
1:G:179:TYR:O	2:H:2:THR:N	2.53	0.42
1:E:84:THR:HG22	1:E:85:PHE:O	2.19	0.42
2:F:33:ALA:O	2:F:35:HIS:CD2	2.72	0.42
1:E:117:ALA:HB3	1:E:140:ASP:HB2	2.01	0.42
1:C:167:ASN:ND2	1:C:170:THR:HG23	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:182:GYP:H7C3	3:C:182:GYP:C5	2.51	0.41
1:E:38:ARG:HD3	2:F:32:PHE:HE1	1.82	0.41
1:G:167:ASN:ND2	1:G:170:THR:H	2.18	0.41
1:E:52:ILE:HD13	2:F:20:VAL:HG21	2.01	0.41
1:C:33:LEU:HD12	1:C:33:LEU:HA	1.86	0.41
1:C:89:PRO:HD2	1:C:115:THR:HG22	2.02	0.41
1:G:35:LYS:HD3	1:G:35:LYS:HA	1.90	0.41
1:G:75:ASN:N	1:G:75:ASN:ND2	2.68	0.41
1:G:88:ALA:HB2	1:G:115:THR:HB	2.03	0.41
1:A:49:PRO:HG2	1:C:16:GLN:O	2.20	0.41
1:A:68:THR:HA	1:A:160:ALA:O	2.20	0.41
2:D:17:PRO:HD2	2:D:20:VAL:HG12	2.02	0.41
1:A:19:ILE:O	1:A:44:ALA:HA	2.21	0.41
1:C:178:THR:HB	2:D:3:SER:OG	2.21	0.40
1:E:35:LYS:HA	1:E:35:LYS:HE2	2.02	0.40
1:C:123:PHE:CD2	3:C:182:GYP:H6C1	2.56	0.40
1:G:12:GLY:O	1:G:26:THR:HG21	2.22	0.40
2:B:10:VAL:HG12	2:B:12:LEU:HD12	2.04	0.40
1:E:66:SER:HB3	1:E:163:VAL:HG22	2.02	0.40
2:F:17:PRO:HG2	2:F:20:VAL:HG12	2.02	0.40
1:A:34:THR:HG22	1:A:35:LYS:O	2.22	0.40
2:B:33:ALA:O	2:B:35:HIS:CD2	2.75	0.40
1:G:47:SER:O	2:H:21:ARG:NH1	2.54	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	178/181 (98%)	172 (97%)	5 (3%)	1 (1%)	21	23
1	C	178/181 (98%)	164 (92%)	13 (7%)	1 (1%)	21	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	178/181 (98%)	165 (93%)	11 (6%)	2 (1%)	11	10
1	G	178/181 (98%)	164 (92%)	10 (6%)	4 (2%)	5	3
2	B	45/52 (86%)	43 (96%)	2 (4%)	0	100	100
2	D	45/52 (86%)	44 (98%)	1 (2%)	0	100	100
2	F	45/52 (86%)	41 (91%)	4 (9%)	0	100	100
2	H	45/52 (86%)	43 (96%)	2 (4%)	0	100	100
All	All	892/932 (96%)	836 (94%)	48 (5%)	8 (1%)	14	14

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	28	LYS
1	C	28	LYS
1	G	39	ASN
1	E	28	LYS
1	E	111	LYS
1	A	99	GLY
1	G	130	PRO
1	G	8	ILE

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	154/155 (99%)	129 (84%)	25 (16%)	2	2
1	C	154/155 (99%)	135 (88%)	19 (12%)	4	4
1	E	154/155 (99%)	126 (82%)	28 (18%)	2	1
1	G	154/155 (99%)	127 (82%)	27 (18%)	2	1
2	B	40/44 (91%)	39 (98%)	1 (2%)	42	56
2	D	39/44 (89%)	36 (92%)	3 (8%)	12	13
2	F	40/44 (91%)	37 (92%)	3 (8%)	12	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	39/44 (89%)	38 (97%)	1 (3%)	40 55
All	All	774/796 (97%)	667 (86%)	107 (14%)	3 3

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	5	SER
1	A	9	THR
1	A	18	LEU
1	A	30	ARG
1	A	35	LYS
1	A	37	VAL
1	A	45	LEU
1	A	47	SER
1	A	50	ILE
1	A	52	ILE
1	A	57	THR
1	A	60	VAL
1	A	66	SER
1	A	68	THR
1	A	81	ASP
1	A	84	THR
1	A	93	LYS
1	A	111	LYS
1	A	126	THR
1	A	130	PRO
1	A	131	SER
1	A	152	TRP
1	A	154	LEU
1	A	177	LEU
2	B	16	VAL
1	C	23	ASP
1	C	33	LEU
1	C	41	VAL
1	C	45	LEU
1	C	50	ILE
1	C	52	ILE
1	C	56	LYS
1	C	64	VAL
1	C	79	VAL
1	C	81	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	93	LYS
1	C	101	LEU
1	C	116	VAL
1	C	131	SER
1	C	141	VAL
1	C	145	LYS
1	C	149	THR
1	C	162	VAL
1	C	178	THR
2	D	7	ASN
2	D	8	GLU
2	D	36	GLU
1	E	3	THR
1	E	9	THR
1	E	14	ASP
1	E	18	LEU
1	E	28	LYS
1	E	29	GLU
1	E	32	THR
1	E	34	THR
1	E	37	VAL
1	E	38	ARG
1	E	50	ILE
1	E	52	ILE
1	E	57	THR
1	E	60	VAL
1	E	68	THR
1	E	72	ASP
1	E	76	SER
1	E	81	ASP
1	E	96	THR
1	E	103	VAL
1	E	111	LYS
1	E	131	SER
1	E	146	SER
1	E	150	LYS
1	E	154	LEU
1	E	158	LYS
1	E	175	VAL
1	E	177	LEU
2	F	12	LEU
2	F	14	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	16	VAL
1	G	7	SER
1	G	10	LYS
1	G	28	LYS
1	G	29	GLU
1	G	33	LEU
1	G	40	THR
1	G	41	VAL
1	G	45	LEU
1	G	51	HIS
1	G	54	ASP
1	G	66	SER
1	G	75	ASN
1	G	76	SER
1	G	77	TYR
1	G	79	VAL
1	G	81	ASP
1	G	93	LYS
1	G	101	LEU
1	G	106	SER
1	G	115	THR
1	G	116	VAL
1	G	141	VAL
1	G	143	SER
1	G	149	THR
1	G	159	GLU
1	G	162	VAL
1	G	177	LEU
2	H	10	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	39	ASN
1	A	59	ASN
1	A	161	ASN
2	B	35	HIS
1	C	142	ASN
1	E	21	GLN
1	E	95	GLN
1	E	105	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	125	ASN
1	E	148	ASN
2	F	35	HIS
2	F	43	HIS
1	G	75	ASN
1	G	78	ASN
1	G	161	ASN
1	G	167	ASN
2	H	7	ASN

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 [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GYP	C	182	-	13,13,13	0.80	0	18,18,18	1.65	3 (16%)
3	GYP	E	182	-	13,13,13	0.95	1 (7%)	18,18,18	1.64	4 (22%)
3	GYP	A	182	-	13,13,13	0.92	0	18,18,18	1.68	4 (22%)
3	GYP	G	182	-	13,13,13	0.70	0	18,18,18	1.14	1 (5%)

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
3	GYP	C	182	-	-	1/4/24/24	0/1/1/1
3	GYP	E	182	-	-	2/4/24/24	0/1/1/1
3	GYP	A	182	-	-	0/4/24/24	0/1/1/1
3	GYP	G	182	-	-	1/4/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	182	GYP	O1-C1	2.06	1.43	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	182	GYP	C4-C3-C2	-4.30	103.28	110.83
3	A	182	GYP	C7-O1-C1	-4.27	106.77	113.26
3	E	182	GYP	C6-C5-C4	-4.22	102.67	113.02
3	C	182	GYP	O1-C1-C2	-3.52	104.08	108.14
3	E	182	GYP	C4-C3-C2	-3.35	104.94	110.83
3	A	182	GYP	C1-O5-C5	2.93	119.45	113.72
3	G	182	GYP	C1-O5-C5	2.44	118.49	113.72
3	C	182	GYP	O3-C3-C4	2.29	115.77	110.38
3	E	182	GYP	O5-C5-C4	2.26	113.78	109.70
3	E	182	GYP	O3-C3-C2	2.20	115.55	110.38
3	A	182	GYP	O2-C2-C1	-2.14	104.98	110.08
3	A	182	GYP	O2-C2-C3	-2.01	105.63	110.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	182	GYP	O5-C1-O1-C7
3	G	182	GYP	O5-C1-O1-C7
3	E	182	GYP	O5-C5-C6-O6
3	E	182	GYP	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	182	GYP	3	0
3	E	182	GYP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	180/181 (99%)	-0.88	0 100 100	11, 22, 35, 48	0
1	C	180/181 (99%)	-0.74	0 100 100	12, 30, 46, 57	0
1	E	180/181 (99%)	-0.74	0 100 100	13, 27, 44, 57	0
1	G	180/181 (99%)	-0.82	0 100 100	16, 26, 41, 51	0
2	B	47/52 (90%)	-0.93	0 100 100	6, 20, 31, 46	0
2	D	47/52 (90%)	-0.85	0 100 100	12, 28, 38, 41	0
2	F	47/52 (90%)	-0.77	0 100 100	9, 29, 41, 49	0
2	H	47/52 (90%)	-0.90	0 100 100	15, 23, 33, 39	0
All	All	908/932 (97%)	-0.81	0 100 100	6, 26, 42, 57	0

There are no RSRZ outliers to report.

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
4	CA	A	228	1/1	0.77	0.07	27,27,27,27	0
4	CA	C	458	1/1	0.85	0.15	36,36,36,36	0
5	MN	F	689	1/1	0.87	0.32	29,29,29,29	0
4	CA	E	688	1/1	0.89	0.07	56,56,56,56	0
3	GYP	C	182	13/13	0.90	0.06	40,43,46,49	0
4	CA	G	918	1/1	0.91	0.04	33,33,33,33	0
3	GYP	E	182	13/13	0.91	0.07	32,38,45,46	0
3	GYP	G	182	13/13	0.95	0.05	27,30,32,34	0
5	MN	C	459	1/1	0.95	0.04	41,41,41,41	0
3	GYP	A	182	13/13	0.95	0.05	18,22,25,28	0
5	MN	G	919	1/1	0.96	0.03	28,28,28,28	0
5	MN	A	229	1/1	0.99	0.03	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.