



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:53 PM UTC

PDB ID : 1LOB / pdb_00001lob
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 : 2.00 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

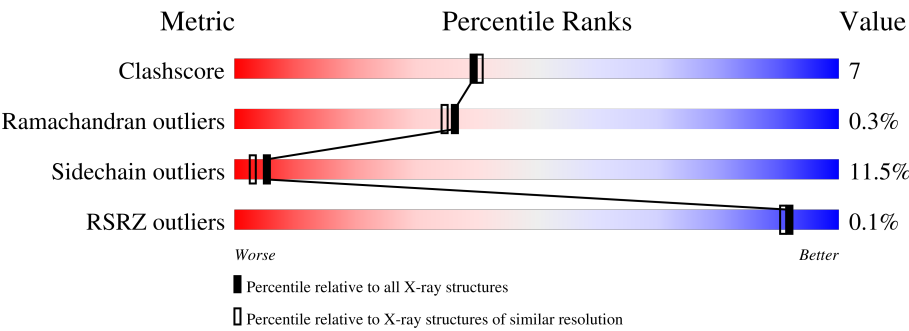
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	% 60% 29% 9% ..
1	C	181	67% 24% 8% ..
1	E	181	64% 24% 9% ..
1	G	181	70% 24% 5% .
2	B	52	69% 12% 10% 10%
2	D	52	79% 10% . 10%
2	F	52	71% 13% 6% 10%

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Mol	Chain	Length	Quality of chain
2	H	52	75% 6% 10% 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

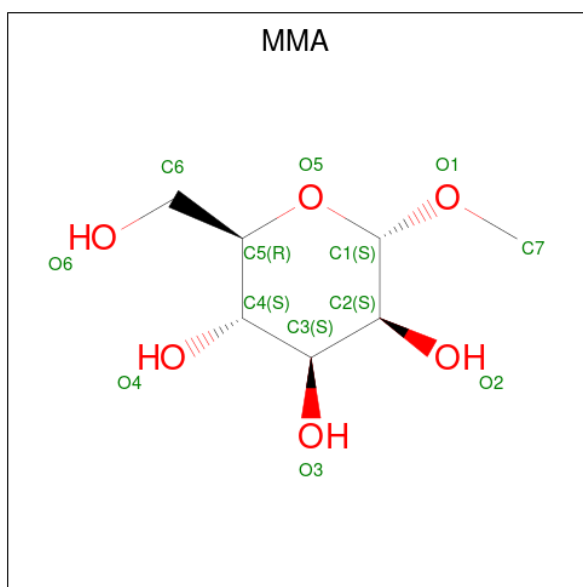
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 5 is methyl alpha-D-mannopyranoside (CCD ID: MMA) (formula: C₇H₁₄O₆).



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

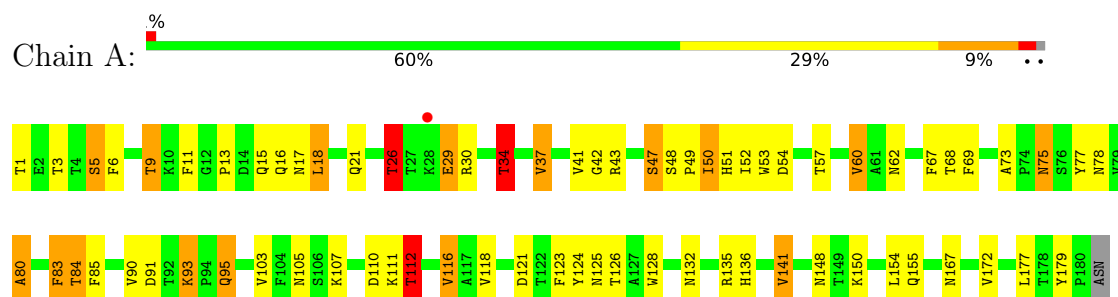
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	75	Total	O	0	0
			75	75		
6	B	14	Total	O	0	0
			14	14		
6	C	58	Total	O	0	0
			58	58		
6	D	10	Total	O	0	0
			10	10		
6	E	51	Total	O	0	0
			51	51		
6	F	13	Total	O	0	0
			13	13		
6	G	64	Total	O	0	0
			64	64		
6	H	13	Total	O	0	0
			13	13		

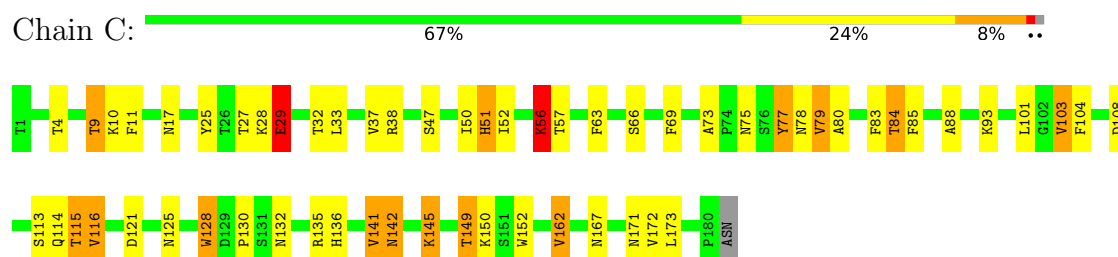
3 Residue-property plots

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.

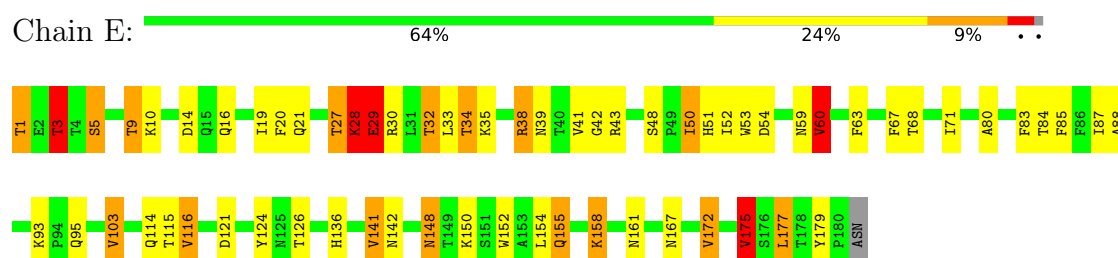
- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)



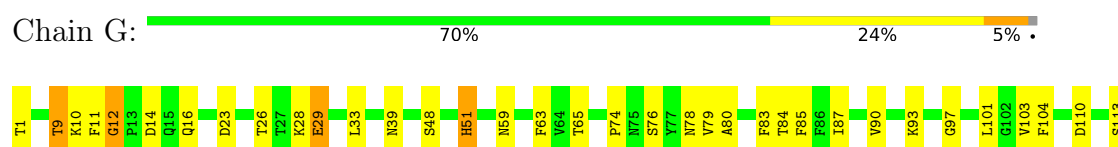
- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)



- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)

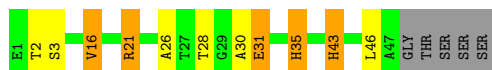


- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)

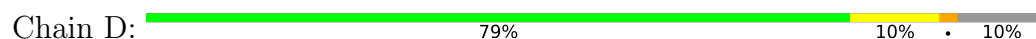




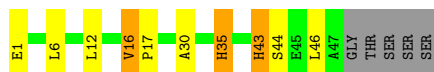
• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)



• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)



• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)



• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)



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 – 2.00 8.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.00) 79.4 (8.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.98 (at 1.97Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , (Not available) 0.176 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 95.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 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)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MN, MMA

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	1.11	7/1431 (0.5%)	1.94	53/1954 (2.7%)
1	C	1.04	6/1431 (0.4%)	1.90	35/1954 (1.8%)
1	E	1.12	8/1431 (0.6%)	1.93	50/1954 (2.6%)
1	G	1.06	4/1431 (0.3%)	1.79	31/1954 (1.6%)
2	B	1.18	3/394 (0.8%)	1.77	6/539 (1.1%)
2	D	1.18	3/389 (0.8%)	1.69	5/532 (0.9%)
2	F	1.10	2/394 (0.5%)	1.64	4/539 (0.7%)
2	H	1.42	4/389 (1.0%)	1.77	3/532 (0.6%)
All	All	1.12	37/7290 (0.5%)	1.85	187/9958 (1.9%)

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
2	H	0	1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	10	VAL	CA-CB	17.51	1.67	1.54
1	G	51	HIS	CD2-NE2	-7.85	1.29	1.37
1	E	116	VAL	CA-CB	7.68	1.65	1.54
1	A	116	VAL	CA-CB	7.57	1.64	1.54
2	D	35	HIS	CD2-NE2	-7.39	1.29	1.37
1	E	172	VAL	CA-CB	7.15	1.63	1.54
2	B	26	ALA	CA-CB	-6.82	1.42	1.53
2	H	35	HIS	CD2-NE2	-6.82	1.30	1.37
1	E	51	HIS	CD2-NE2	-6.74	1.30	1.37
2	F	35	HIS	CD2-NE2	-6.64	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	35	HIS	CD2-NE2	-6.60	1.30	1.37
2	B	43	HIS	CD2-NE2	-6.48	1.30	1.37
2	F	43	HIS	CD2-NE2	-6.46	1.30	1.37
2	D	43	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	141	VAL	CA-CB	6.23	1.62	1.54
1	G	116	VAL	CA-CB	6.21	1.62	1.54
1	A	51	HIS	CD2-NE2	-6.17	1.31	1.37
2	D	35	HIS	CG-ND1	-6.12	1.31	1.38
1	E	32	THR	CA-CB	6.08	1.61	1.53
1	C	51	HIS	CD2-NE2	-6.04	1.31	1.37
1	C	116	VAL	CA-CB	6.04	1.62	1.54
1	E	60	VAL	CA-CB	6.01	1.65	1.55
1	C	141	VAL	CA-CB	5.90	1.61	1.54
1	A	172	VAL	CA-CB	5.87	1.62	1.54
1	E	88	ALA	CA-CB	-5.84	1.46	1.53
1	A	136	HIS	CG-ND1	-5.83	1.31	1.38
1	A	60	VAL	CA-CB	5.73	1.63	1.55
1	E	136	HIS	CG-ND1	-5.71	1.31	1.38
1	C	172	VAL	CA-CB	5.62	1.61	1.54
1	A	77	TYR	CA-CB	-5.53	1.44	1.53
1	G	115	THR	CA-CB	5.37	1.67	1.53
1	G	136	HIS	CG-ND1	-5.35	1.32	1.38
2	H	35	HIS	CG-ND1	-5.27	1.32	1.38
1	C	79	VAL	CA-CB	5.20	1.61	1.54
1	C	136	HIS	CG-ND1	-5.12	1.32	1.38
2	H	43	HIS	CD2-NE2	-5.08	1.32	1.37
1	E	175	VAL	CA-CB	5.08	1.61	1.54

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	10	VAL	CA-C-O	9.45	124.85	119.94
1	E	14	ASP	CA-CB-CG	9.31	121.92	112.60
1	C	63	PHE	CA-CB-CG	9.27	123.07	113.80
1	C	103	VAL	N-CA-CB	-9.14	99.78	112.12
2	B	16	VAL	N-CA-CB	-9.12	98.44	111.21
1	E	3	THR	N-CA-CB	-9.02	94.67	111.00
1	A	26	THR	N-CA-CB	-8.93	95.30	110.83
2	F	16	VAL	N-CA-CB	-8.90	98.76	111.21
1	A	95	GLN	OE1-CD-NE2	-8.31	114.29	122.60
1	C	171	ASN	OD1-CG-ND2	-8.30	114.30	122.60
2	H	21	ARG	CA-CB-CG	-8.28	97.54	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	103	VAL	CB-CA-C	8.07	118.56	110.65
1	C	29	GLU	CB-CG-CD	7.93	126.09	112.60
1	C	56	LYS	CA-CB-CG	7.92	129.94	114.10
1	G	9	THR	N-CA-CB	-7.87	98.80	110.53
1	C	51	HIS	CB-CG-CD2	-7.73	121.16	131.20
1	E	50	ILE	CB-CG1-CD1	-7.64	97.77	113.80
1	E	167	ASN	OD1-CG-ND2	-7.59	115.01	122.60
1	A	91	ASP	CA-CB-CG	7.50	120.10	112.60
1	G	63	PHE	CA-CB-CG	7.40	121.20	113.80
1	G	59	ASN	OD1-CG-ND2	-7.39	115.21	122.60
1	A	37	VAL	N-CA-CB	-7.37	97.62	111.62
1	A	132	ASN	OD1-CG-ND2	-7.34	115.25	122.60
1	A	85	PHE	N-CA-C	-7.30	97.32	109.07
1	A	26	THR	CB-CA-C	7.20	123.12	109.37
1	E	95	GLN	OE1-CD-NE2	-7.18	115.42	122.60
1	C	172	VAL	CG1-CB-CG2	-7.15	95.07	110.80
1	C	69	PHE	CA-CB-CG	7.14	120.94	113.80
1	C	80	ALA	O-C-N	-7.10	115.81	123.26
1	A	67	PHE	CA-CB-CG	7.02	120.82	113.80
1	A	95	GLN	CG-CD-NE2	6.91	126.77	116.40
1	G	16	GLN	OE1-CD-NE2	-6.83	115.78	122.60
1	G	51	HIS	CB-CG-CD2	-6.78	122.39	131.20
1	C	142	ASN	OD1-CG-ND2	-6.77	115.83	122.60
1	E	142	ASN	OD1-CG-ND2	-6.75	115.85	122.60
1	E	155	GLN	OE1-CD-NE2	-6.74	115.86	122.60
1	C	17	ASN	CA-CB-CG	6.73	119.33	112.60
2	D	2	THR	CA-CB-OG1	-6.72	99.52	109.60
1	E	63	PHE	CA-CB-CG	6.70	120.50	113.80
1	A	93	LYS	CA-C-N	6.68	126.72	119.90
1	A	93	LYS	C-N-CA	6.68	126.72	119.90
1	E	39	ASN	OD1-CG-ND2	-6.68	115.92	122.60
1	C	51	HIS	CB-CG-ND1	6.67	132.71	122.70
1	E	80	ALA	O-C-N	-6.66	116.27	123.26
1	G	132	ASN	OD1-CG-ND2	-6.65	115.95	122.60
1	E	54	ASP	CA-CB-CG	6.59	119.19	112.60
1	E	148	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	A	148	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	C	171	ASN	CB-CG-ND2	6.55	126.22	116.40
1	A	49	PRO	CA-C-O	-6.53	113.98	121.36
1	G	39	ASN	N-CA-C	6.50	120.21	111.24
1	A	125	ASN	N-CA-C	-6.49	96.51	107.99
1	A	57	THR	CA-CB-OG1	-6.47	99.90	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	THR	N-CA-CB	-6.45	99.64	111.37
1	E	39	ASN	N-CA-C	6.42	120.25	111.39
1	A	17	ASN	CA-CB-CG	6.38	118.98	112.60
1	E	20	PHE	CA-CB-CG	-6.34	107.46	113.80
1	A	9	THR	N-CA-CB	-6.34	99.76	110.41
2	D	21	ARG	CA-CB-CG	-6.34	101.42	114.10
1	E	3	THR	CB-CA-C	6.32	121.86	109.35
1	A	155	GLN	OE1-CD-NE2	-6.28	116.32	122.60
1	C	167	ASN	OD1-CG-ND2	-6.28	116.32	122.60
2	H	31	GLU	CA-CB-CG	-6.27	101.55	114.10
1	C	84	THR	CA-CB-OG1	-6.26	100.21	109.60
1	G	85	PHE	N-CA-C	-6.23	99.55	109.59
1	C	77	TYR	N-CA-C	-6.22	104.91	113.18
1	A	50	ILE	CB-CG1-CD1	-6.22	100.74	113.80
1	A	9	THR	CA-CB-OG1	-6.12	100.41	109.60
1	G	78	ASN	OD1-CG-ND2	-6.11	116.49	122.60
2	B	21	ARG	CA-CB-CG	-6.08	101.93	114.10
1	A	54	ASP	CA-CB-CG	6.08	118.68	112.60
1	G	172	VAL	CG1-CB-CG2	-6.08	97.43	110.80
1	E	177	LEU	N-CA-C	-6.05	99.54	109.40
2	B	43	HIS	CB-CG-CD2	-6.00	123.39	131.20
1	E	85	PHE	N-CA-C	-5.99	99.47	109.24
1	E	121	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	135	ARG	N-CA-C	-5.93	102.13	110.50
1	E	71	ILE	N-CA-C	-5.92	99.89	108.17
1	G	83	PHE	N-CA-CB	-5.91	100.53	111.53
1	C	9	THR	CA-CB-OG1	-5.90	100.74	109.60
1	C	125	ASN	N-CA-C	-5.90	97.54	107.99
1	A	41	VAL	N-CA-C	-5.87	99.60	108.17
1	E	83	PHE	N-CA-CB	-5.85	100.64	111.52
1	G	87	ILE	N-CA-C	-5.82	99.75	108.12
1	A	179	TYR	N-CA-C	-5.81	102.29	110.31
1	G	80	ALA	O-C-N	-5.81	117.20	123.42
1	A	9	THR	OG1-CB-CG2	5.80	120.90	109.30
1	A	62	ASN	O-C-N	-5.77	116.47	123.16
1	G	12	GLY	CA-C-N	5.75	125.61	119.28
1	G	12	GLY	C-N-CA	5.75	125.61	119.28
1	G	177	LEU	CA-CB-CG	5.75	136.41	116.30
1	G	90	VAL	N-CA-CB	-5.73	102.74	110.54
1	A	167	ASN	OD1-CG-ND2	-5.70	116.90	122.60
2	D	2	THR	N-CA-CB	-5.70	101.82	111.50
1	E	136	HIS	O-C-N	5.70	129.10	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	135	ARG	N-CA-C	-5.68	102.07	110.48
1	G	161	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	E	27	THR	CA-C-O	-5.65	113.63	119.51
2	F	35	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	A	132	ASN	CA-CB-CG	5.62	118.22	112.60
1	E	59	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	E	85	PHE	O-C-N	-5.62	116.92	123.27
1	G	1	THR	CA-CB-OG1	-5.59	101.21	109.60
1	A	80	ALA	O-C-N	-5.58	117.44	123.42
2	B	30	ALA	N-CA-C	-5.57	105.98	112.89
1	E	38	ARG	N-CA-CB	-5.55	101.36	110.41
1	E	161	ASN	OD1-CG-ND2	-5.55	117.05	122.60
2	B	2	THR	N-CA-C	-5.54	99.87	108.90
1	A	107	LYS	N-CA-C	-5.54	106.53	113.28
1	G	51	HIS	CB-CG-ND1	5.53	130.99	122.70
1	E	93	LYS	CA-C-N	5.51	125.44	119.76
1	E	93	LYS	C-N-CA	5.51	125.44	119.76
1	A	128	TRP	CG-CD2-CE3	5.51	139.41	133.90
1	A	48	SER	CA-C-N	5.50	125.51	119.90
1	A	48	SER	C-N-CA	5.50	125.51	119.90
1	E	16	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	E	87	ILE	N-CA-C	-5.46	99.68	107.77
1	C	84	THR	CA-CB-CG2	5.46	119.79	110.50
1	C	29	GLU	N-CA-CB	-5.46	104.01	112.30
1	C	83	PHE	N-CA-CB	-5.45	101.40	111.53
1	E	48	SER	CA-C-N	5.45	125.45	119.90
1	E	48	SER	C-N-CA	5.45	125.45	119.90
1	E	141	VAL	CA-C-O	5.44	125.06	120.22
1	G	128	TRP	CE2-CD2-CG	-5.42	100.69	107.20
1	A	69	PHE	CA-CB-CG	5.42	119.22	113.80
1	C	121	ASP	CA-CB-CG	5.41	118.01	112.60
2	D	30	ALA	N-CA-C	-5.40	105.55	111.82
1	E	67	PHE	CA-CB-CG	5.38	119.19	113.80
1	E	142	ASN	CB-CG-ND2	5.38	124.48	116.40
1	G	118	VAL	N-CA-C	-5.38	100.00	107.80
1	E	167	ASN	CB-CG-ND2	5.37	124.46	116.40
1	A	118	VAL	N-CA-C	-5.33	100.07	107.80
1	A	6	PHE	CA-CB-CG	5.32	119.12	113.80
1	E	19	ILE	N-CA-C	-5.32	100.73	108.17
1	A	90	VAL	N-CA-CB	-5.31	103.84	110.47
1	A	83	PHE	O-C-N	-5.30	117.12	123.27
1	G	9	THR	CB-CA-C	5.30	118.87	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	179	TYR	CA-C-O	-5.29	115.18	120.63
1	C	47	SER	CA-C-O	-5.29	114.81	120.42
1	G	51	HIS	CA-CB-CG	-5.29	108.51	113.80
1	G	173	LEU	N-CA-C	-5.28	100.56	109.07
1	E	9	THR	CA-CB-OG1	-5.28	101.69	109.60
2	D	43	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	C	152	TRP	CG-CD1-NE1	-5.26	103.36	110.20
1	C	85	PHE	N-CA-C	-5.24	100.63	109.07
1	C	108	ASP	CA-CB-CG	5.24	117.84	112.60
1	G	59	ASN	CB-CG-ND2	5.23	124.25	116.40
1	E	38	ARG	CA-CB-CG	5.23	124.56	114.10
1	C	128	TRP	CE2-CD2-CG	-5.23	100.93	107.20
1	C	73	ALA	CA-C-N	5.22	124.40	118.97
1	C	73	ALA	C-N-CA	5.22	124.40	118.97
1	E	103	VAL	N-CA-CB	-5.21	105.09	112.12
1	A	112	THR	N-CA-CB	-5.21	100.84	110.32
1	A	42	GLY	CA-C-O	-5.21	116.88	120.94
1	A	150	LYS	CA-CB-CG	-5.21	103.69	114.10
1	A	155	GLN	N-CA-C	-5.21	99.30	108.20
1	C	9	THR	N-CA-CB	-5.20	101.93	110.40
1	E	121	ASP	N-CA-CB	-5.19	101.96	110.42
1	C	88	ALA	O-C-N	-5.18	117.14	121.54
2	B	31	GLU	CA-CB-CG	-5.17	103.75	114.10
1	A	123	PHE	CA-C-O	5.17	126.06	120.32
1	G	48	SER	CA-C-N	5.17	125.08	119.76
1	G	48	SER	C-N-CA	5.17	125.08	119.76
1	A	75	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	E	30	ARG	N-CA-C	5.16	117.65	109.50
2	F	43	HIS	CB-CG-ND1	5.14	130.42	122.70
1	E	41	VAL	CB-CA-C	-5.14	102.16	110.28
1	A	47	SER	O-C-N	-5.13	116.31	122.15
1	A	73	ALA	CA-C-N	5.12	125.16	119.32
1	A	73	ALA	C-N-CA	5.12	125.16	119.32
1	G	93	LYS	O-C-N	-5.12	117.56	121.55
1	A	51	HIS	CB-CG-CD2	-5.11	124.55	131.20
1	E	177	LEU	CA-CB-CG	5.11	134.20	116.30
1	A	93	LYS	CA-CB-CG	-5.11	103.88	114.10
1	A	34	THR	N-CA-CB	-5.10	102.00	111.13
1	E	141	VAL	CB-CA-C	5.10	116.22	110.41
1	A	121	ASP	CA-CB-CG	5.09	117.69	112.60
1	E	152	TRP	CG-CD1-NE1	-5.07	103.61	110.20
1	E	9	THR	N-CA-CB	-5.07	102.14	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	43	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	E	103	VAL	CG1-CB-CG2	-5.06	99.68	110.80
1	E	51	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	A	57	THR	CA-CB-CG2	5.04	119.07	110.50
1	G	14	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	16	GLN	N-CA-C	5.03	119.05	113.01
1	C	4	THR	N-CA-C	-5.01	99.82	108.69
1	E	179	TYR	N-CA-C	-5.01	102.76	110.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	41	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	22	0
1	C	1397	0	1346	18	0
1	E	1397	0	1346	22	0
1	G	1397	0	1346	10	0
2	B	381	0	357	10	0
2	D	376	0	351	2	0
2	F	381	0	357	8	0
2	H	376	0	351	4	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	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	B	13	0	14	0	0
5	C	13	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	13	0	14	0	0
5	G	13	0	14	0	0
6	A	75	0	0	3	0
6	B	14	0	0	2	0
6	C	58	0	0	1	0
6	D	10	0	0	0	0
6	E	51	0	0	0	0
6	F	13	0	0	0	0
6	G	64	0	0	1	0
6	H	13	0	0	0	0
All	All	7460	0	6856	76	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 7.

All (76) 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	1.52	0.92
1:A:21:GLN:HE22	1:A:43:ARG:HH21	1.30	0.79
1:E:21:GLN:HE22	1:E:43:ARG:HH21	1.35	0.75
1:E:21:GLN:HE21	1:E:43:ARG:HE	1.41	0.67
1:A:83:PHE:HB2	6:B:67:HOH:O	1.96	0.64
1:A:11:PHE:O	1:A:29:GLU:HA	1.98	0.64
1:C:11:PHE:O	1:C:29:GLU:HA	1.98	0.63
1:G:103:VAL:HG13	1:G:104:PHE:CD2	2.35	0.61
1:C:114:GLN:HA	1:C:142:ASN:HD21	1.67	0.59
1:E:124:TYR:CE2	1:E:126:THR:HG22	2.37	0.59
1:C:128:TRP:HB2	1:C:145:LYS:HG2	1.86	0.58
1:A:110:ASP:OD1	1:A:112:THR:HB	2.04	0.57
1:E:5:SER:OG	2:F:43:HIS:HD2	1.88	0.56
1:G:130:PRO:HG3	1:G:149:THR:HG21	1.87	0.54
1:E:1:THR:HA	2:F:46:LEU:O	2.07	0.54
1:A:5:SER:OG	2:B:43:HIS:HD2	1.91	0.54
1:E:21:GLN:NE2	1:E:43:ARG:HE	2.06	0.53
1:A:15:GLN:HG2	1:A:18:LEU:HD22	1.91	0.52
1:G:148:ASN:HD22	2:H:8:GLU:HG2	1.74	0.52
1:A:75:ASN:HD21	1:A:78:ASN:HD22	1.58	0.52
1:G:12:GLY:O	1:G:26:THR:HG21	2.11	0.50
1:E:28:LYS:HG2	1:E:29:GLU:HG2	1.93	0.50
1:A:34:THR:CG2	2:B:35:HIS:HD2	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:GLN:NE2	1:E:43:ARG:HH21	2.06	0.49
1:A:21:GLN:HE21	1:A:43:ARG:HE	1.59	0.49
1:C:25:TYR:CE2	1:C:27:THR:HB	2.47	0.49
1:A:52:ILE:HG23	1:A:53:TRP:HD1	1.78	0.49
1:G:167:ASN:HD21	1:G:169:ALA:HB3	1.78	0.49
1:E:148:ASN:CG	2:F:6:LEU:HD11	2.38	0.49
1:C:10:LYS:HZ2	1:C:29:GLU:HG2	1.78	0.48
1:E:53:TRP:HB3	1:E:60:VAL:HB	1.95	0.48
1:A:21:GLN:NE2	1:A:43:ARG:HE	2.10	0.48
1:E:114:GLN:HB3	2:F:17:PRO:HD3	1.95	0.48
1:E:21:GLN:HE22	1:E:43:ARG:NH2	2.08	0.48
1:G:97:GLY:HA2	2:H:27:THR:HG21	1.96	0.47
1:E:34:THR:CG2	2:F:35:HIS:HD2	2.27	0.47
1:C:103:VAL:HG13	1:C:104:PHE:CD2	2.49	0.47
1:C:75:ASN:HD22	1:C:77:TYR:HD2	1.61	0.47
2:H:41:TYR:OH	2:H:43:HIS:HB2	2.15	0.47
1:A:34:THR:HG21	2:B:28:THR:HG23	1.97	0.47
1:A:124:TYR:CE2	1:A:126:THR:HG22	2.50	0.46
1:C:128:TRP:CB	1:C:145:LYS:HG2	2.46	0.46
1:A:13:PRO:HA	1:A:26:THR:HG23	1.96	0.46
1:C:38:ARG:HG2	2:D:32:PHE:HD2	1.79	0.46
1:C:56:LYS:HD3	1:C:57:THR:HG23	1.98	0.46
1:G:65:THR:HA	2:H:41:TYR:O	2.15	0.46
1:A:34:THR:HG21	2:B:35:HIS:HD2	1.81	0.46
1:E:33:LEU:O	1:E:42:GLY:HA3	2.15	0.46
1:E:103:VAL:HG13	1:E:115:THR:HG21	1.98	0.46
1:C:38:ARG:HG2	2:D:32:PHE:CD2	2.51	0.45
1:A:111:LYS:HG3	6:A:242:HOH:O	2.18	0.44
1:G:11:PHE:O	1:G:29:GLU:HA	2.18	0.44
1:A:47:SER:O	2:B:21:ARG:NH1	2.51	0.44
1:C:113:SER:O	1:C:115:THR:HG22	2.17	0.44
1:C:130:PRO:HB2	1:C:132:ASN:HD21	1.82	0.44
1:A:95:GLN:HB3	1:A:105:ASN:OD1	2.18	0.44
1:E:158:LYS:HB3	1:E:158:LYS:HE2	1.53	0.43
2:B:35:HIS:CG	6:B:67:HOH:O	2.71	0.43
1:G:23:ASP:HB3	6:G:965:HOH:O	2.19	0.43
1:E:3:THR:HA	2:F:44:SER:O	2.18	0.43
1:A:84:THR:HG21	1:A:103:VAL:HG11	2.01	0.43
1:A:15:GLN:CG	1:A:18:LEU:HD22	2.49	0.42
1:C:66:SER:HA	1:C:162:VAL:O	2.20	0.42
1:E:21:GLN:HB2	1:E:43:ARG:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:THR:HA	2:B:46:LEU:O	2.20	0.41
1:C:78:ASN:HB3	6:C:511:HOH:O	2.19	0.41
1:E:155:GLN:NE2	1:E:158:LYS:HD3	2.35	0.41
1:C:27:THR:HG22	1:C:32:THR:OG1	2.20	0.41
1:E:38:ARG:HD3	2:F:30:ALA:O	2.21	0.41
1:E:52:ILE:HG23	1:E:53:TRP:HD1	1.85	0.41
1:A:80:ALA:HB3	2:B:31:GLU:HB2	2.03	0.41
1:E:175:VAL:HG13	2:F:6:LEU:HB3	2.02	0.40
6:A:265:HOH:O	2:B:35:HIS:HE1	2.04	0.40
1:C:130:PRO:HB2	1:C:132:ASN:ND2	2.36	0.40
6:A:265:HOH:O	2:B:35:HIS:CE1	2.73	0.40
1:G:110:ASP:O	1:G:113:SER:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	178/181 (98%)	174 (98%)	4 (2%)	0	100	100
1	C	178/181 (98%)	169 (95%)	8 (4%)	1 (1%)	21	17
1	E	178/181 (98%)	172 (97%)	4 (2%)	2 (1%)	11	7
1	G	178/181 (98%)	171 (96%)	7 (4%)	0	100	100
2	B	45/52 (86%)	43 (96%)	2 (4%)	0	100	100
2	D	45/52 (86%)	43 (96%)	2 (4%)	0	100	100
2	F	45/52 (86%)	43 (96%)	2 (4%)	0	100	100
2	H	45/52 (86%)	43 (96%)	2 (4%)	0	100	100
All	All	892/932 (96%)	858 (96%)	31 (4%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	29	GLU
1	E	28	LYS
1	C	28	LYS

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%)	135 (88%)	19 (12%)	4	3
1	C	154/155 (99%)	134 (87%)	20 (13%)	4	2
1	E	154/155 (99%)	131 (85%)	23 (15%)	3	1
1	G	154/155 (99%)	136 (88%)	18 (12%)	5	3
2	B	40/44 (91%)	38 (95%)	2 (5%)	22	20
2	D	39/44 (89%)	38 (97%)	1 (3%)	40	44
2	F	40/44 (91%)	37 (92%)	3 (8%)	12	9
2	H	39/44 (89%)	36 (92%)	3 (8%)	12	8
All	All	774/796 (97%)	685 (88%)	89 (12%)	5	3

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	5	SER
1	A	9	THR
1	A	18	LEU
1	A	26	THR
1	A	29	GLU
1	A	30	ARG
1	A	34	THR
1	A	37	VAL
1	A	50	ILE
1	A	60	VAL
1	A	68	THR
1	A	84	THR

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Mol	Chain	Res	Type
1	A	93	LYS
1	A	112	THR
1	A	116	VAL
1	A	141	VAL
1	A	154	LEU
1	A	177	LEU
2	B	3	SER
2	B	16	VAL
1	C	9	THR
1	C	29	GLU
1	C	33	LEU
1	C	37	VAL
1	C	50	ILE
1	C	51	HIS
1	C	52	ILE
1	C	56	LYS
1	C	79	VAL
1	C	84	THR
1	C	93	LYS
1	C	101	LEU
1	C	115	THR
1	C	116	VAL
1	C	141	VAL
1	C	145	LYS
1	C	149	THR
1	C	150	LYS
1	C	162	VAL
1	C	173	LEU
2	D	21	ARG
1	E	1	THR
1	E	3	THR
1	E	5	SER
1	E	9	THR
1	E	10	LYS
1	E	27	THR
1	E	28	LYS
1	E	29	GLU
1	E	32	THR
1	E	34	THR
1	E	35	LYS
1	E	50	ILE
1	E	60	VAL

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Mol	Chain	Res	Type
1	E	68	THR
1	E	84	THR
1	E	116	VAL
1	E	141	VAL
1	E	150	LYS
1	E	154	LEU
1	E	158	LYS
1	E	172	VAL
1	E	175	VAL
1	E	177	LEU
2	F	1	GLU
2	F	12	LEU
2	F	16	VAL
1	G	9	THR
1	G	10	LYS
1	G	28	LYS
1	G	29	GLU
1	G	33	LEU
1	G	51	HIS
1	G	74	PRO
1	G	76	SER
1	G	79	VAL
1	G	84	THR
1	G	101	LEU
1	G	115	THR
1	G	116	VAL
1	G	141	VAL
1	G	149	THR
1	G	162	VAL
1	G	172	VAL
1	G	177	LEU
2	H	8	GLU
2	H	10	VAL
2	H	21	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	21	GLN
1	A	78	ASN
2	B	7	ASN

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Mol	Chain	Res	Type
2	B	35	HIS
2	B	43	HIS
1	C	39	ASN
1	C	132	ASN
1	C	142	ASN
1	C	167	ASN
1	E	21	GLN
1	E	39	ASN
1	E	95	GLN
1	E	105	ASN
1	E	148	ASN
1	E	155	GLN
1	E	167	ASN
2	F	7	ASN
2	F	35	HIS
2	F	43	HIS
1	G	51	HIS
1	G	95	GLN
1	G	105	ASN
1	G	142	ASN
1	G	148	ASN
1	G	167	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	$\# Z > 2$
5	MMA	E	182	-	13,13,13	0.74	0	18,18,18	1.05	0
5	MMA	B	53	-	13,13,13	0.91	0	18,18,18	0.79	0
5	MMA	G	182	-	13,13,13	0.87	0	18,18,18	1.24	2 (11%)
5	MMA	C	182	-	13,13,13	1.05	1 (7%)	18,18,18	1.76	4 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MMA	E	182	-	-	2/4/24/24	0/1/1/1
5	MMA	B	53	-	-	0/4/24/24	0/1/1/1
5	MMA	G	182	-	-	1/4/24/24	0/1/1/1
5	MMA	C	182	-	-	0/4/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	182	MMA	O1-C1	2.58	1.44	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	182	MMA	O4-C4-C3	-3.91	101.15	110.38
5	C	182	MMA	O2-C2-C1	-2.77	103.48	110.08
5	C	182	MMA	O3-C3-C2	2.72	116.78	110.38
5	C	182	MMA	O5-C1-C2	-2.67	104.88	110.37
5	G	182	MMA	O1-C1-C2	2.35	110.85	108.14
5	G	182	MMA	O3-C3-C2	-2.17	105.27	110.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	182	MMA	C4-C5-C6-O6
5	E	182	MMA	O5-C5-C6-O6
5	G	182	MMA	O5-C5-C6-O6

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 [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%)	-0.79	1 (0%) 85 85	7, 14, 28, 44	0
1	C	180/181 (99%)	-0.56	0 100 100	8, 23, 39, 46	0
1	E	180/181 (99%)	-0.57	0 100 100	10, 19, 40, 49	0
1	G	180/181 (99%)	-0.75	0 100 100	7, 17, 32, 42	0
2	B	47/52 (90%)	-0.80	0 100 100	4, 14, 26, 35	0
2	D	47/52 (90%)	-0.62	0 100 100	10, 20, 34, 43	0
2	F	47/52 (90%)	-0.70	0 100 100	7, 19, 29, 37	0
2	H	47/52 (90%)	-0.77	0 100 100	7, 15, 31, 37	0
All	All	908/932 (97%)	-0.68	1 (0%) 92 91	4, 18, 35, 49	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	LYS	2.7

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(Å ²)	Q<0.9
3	CA	C	458	1/1	0.60	0.14	46,46,46,46	0
3	CA	E	688	1/1	0.64	0.15	36,36,36,36	0
3	CA	A	228	1/1	0.79	0.08	13,13,13,13	0
4	MN	C	459	1/1	0.87	0.06	30,30,30,30	0
3	CA	G	918	1/1	0.91	0.09	11,11,11,11	0
5	MMA	C	182	13/13	0.91	0.06	27,29,31,31	0
5	MMA	E	182	13/13	0.92	0.06	20,24,29,30	0
5	MMA	G	182	13/13	0.94	0.05	14,17,20,20	0
5	MMA	B	53	13/13	0.95	0.05	7,13,17,18	0
4	MN	E	689	1/1	0.96	0.04	27,27,27,27	0
4	MN	G	919	1/1	0.97	0.04	19,19,19,19	0
4	MN	A	229	1/1	0.98	0.05	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.