



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:06 AM UTC

PDB ID : 2XBO / pdb_00002xbo
Title : Equine Rhinitis A Virus in Complex with its Sialic Acid Receptor
Authors : Fry, E.E.; Tuthill, T.J.; Harlos, K.; Walter, T.S.; Rowlands, D.J.; Stuart, D.I.
Deposited on : 2010-04-14
Resolution : 4.00 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

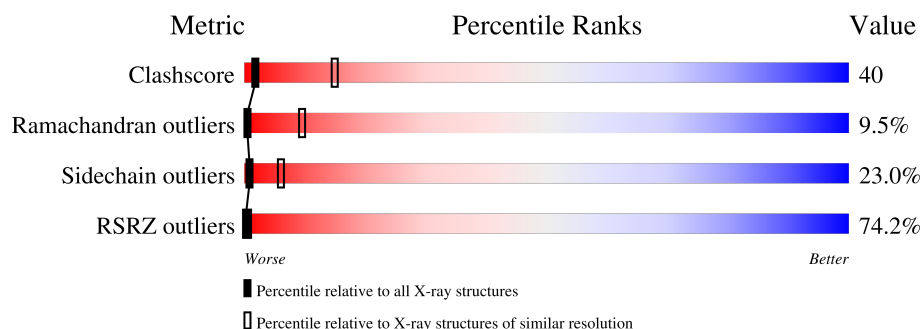
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	1	248	
2	2	230	
3	3	226	
4	4	80	
5	A	3	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5415 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 P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	247	Total	C	N	O	S	0	0	1
			1929	1240	330	351	8			

- Molecule 2 is a protein called P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	200	Total	C	N	O	S	0	0	0
			1554	997	266	284	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	85	SER	GLY	conflict	UNP B9VV85

- Molecule 3 is a protein called P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	226	Total	C	N	O	S	0	0	0
			1723	1112	279	326	6			

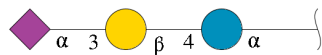
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	59	LYS	ARG	conflict	UNP B9VV85
3	107	TYR	ARG	conflict	UNP B9VV85

- Molecule 4 is a protein called P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	22	Total	C	N	O	S	0	0	1
			166	101	29	35	1			

- Molecule 5 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose.

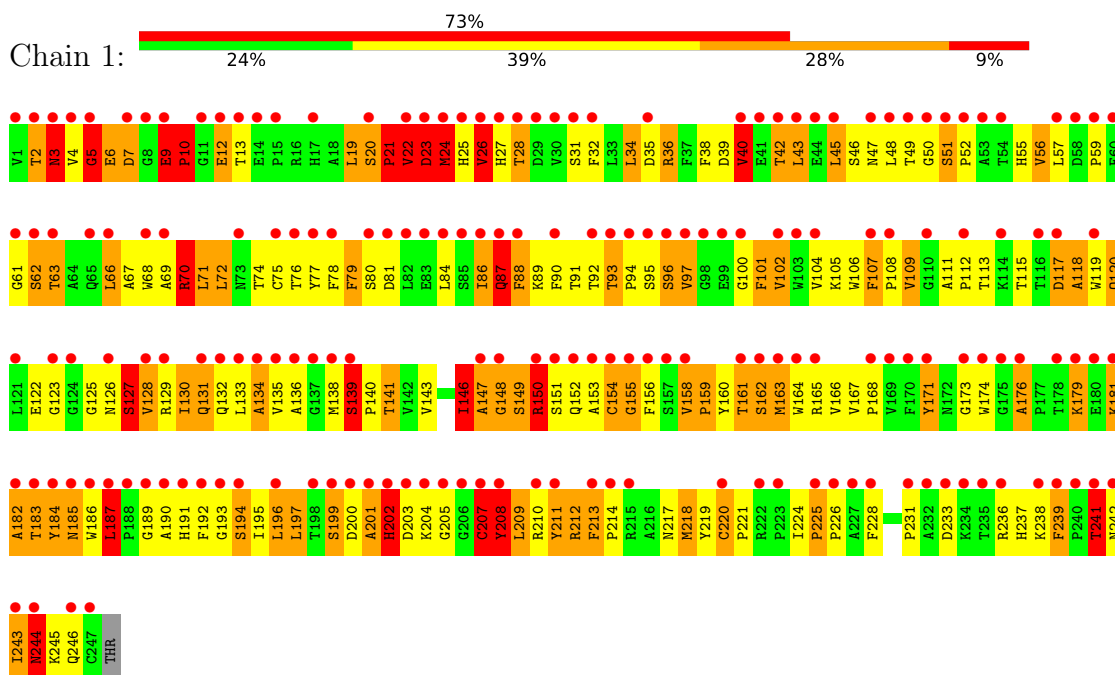


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	A	3	Total	C	N	O	0	0	0
			43	23	1	19			

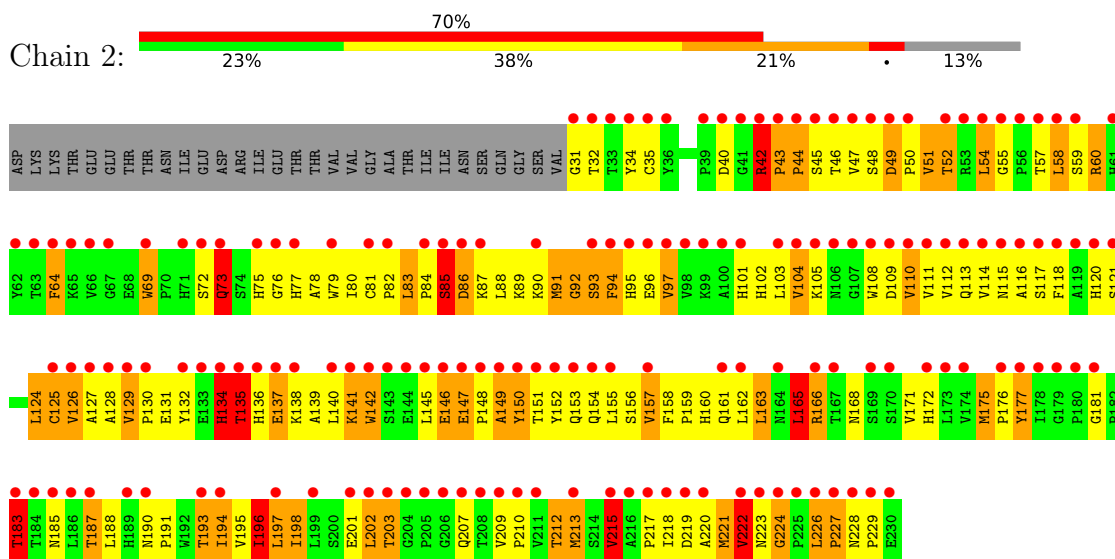
3 Residue-property plots

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: P1



• Molecule 2: P1



Chain 3:

Item	Category	Percentage
A1	Category 1	27%
P2	Category 1	27%
I3	Category 1	27%
R4	Category 1	27%
V5	Category 1	27%
V6	Category 1	27%
S7	Category 1	27%
V8	Category 1	27%
P9	Category 1	27%
E10	Category 1	27%
S11	Category 1	27%
D12	Category 1	27%
S13	Category 1	27%
F14	Category 1	27%
M15	Category 1	27%
S16	Category 1	27%
S17	Category 1	27%
V18	Category 1	27%
P19	Category 1	27%
D20	Category 1	27%
N21	Category 1	27%
S22	Category 1	27%
T23	Category 1	27%
P24	Category 1	27%
L25	Category 1	27%
Y26	Category 1	27%
V29	Category 2	68%
V30	Category 2	68%
V31	Category 2	68%
P32	Category 2	68%
P33	Category 2	68%
R34	Category 2	68%
Q35	Category 2	68%
V36	Category 2	68%
P37	Category 2	68%
G38	Category 2	68%
R39	Category 2	68%
F40	Category 2	68%
T41	Category 2	68%
N42	Category 2	68%
F43	Category 2	68%
L44	Category 2	68%
D45	Category 2	68%
V46	Category 2	68%
A47	Category 2	68%
K48	Category 2	68%
Q49	Category 2	68%
T50	Category 2	68%
Y51	Category 2	68%
S52	Category 2	68%
F53	Category 2	68%
G54	Category 2	68%
S55	Category 2	68%
L56	Category 2	68%
S57	Category 2	68%
G58	Category 2	68%
K59	Category 2	68%
P60	Category 2	68%
V61	Category 2	68%
F62	Category 3	49%
E63	Category 3	49%
V64	Category 3	49%
T65	Category 3	49%
M66	Category 3	49%
S68	Category 3	49%
G69	Category 3	49%
D70	Category 3	49%
E71	Category 3	49%
P72	Category 3	49%
L73	Category 3	49%
F74	Category 3	49%
K75	Category 3	49%
M76	Category 3	49%
D77	Category 3	49%
V78	Category 3	49%
S79	Category 3	49%
L80	Category 3	49%
S81	Category 3	49%
A82	Category 3	49%
A83	Category 3	49%
E84	Category 3	49%
L85	Category 3	49%
H86	Category 3	49%
G87	Category 3	49%
T88	Category 3	49%
V89	Category 3	49%
V90	Category 3	49%
A91	Category 3	49%
S92	Category 3	49%
L93	Category 3	49%
S94	Category 3	49%
S95	Category 3	49%
F96	Category 3	49%
P97	Category 3	49%
A98	Category 3	49%
Q99	Category 3	49%
Y100	Category 3	49%
R101	Category 3	49%
G102	Category 3	49%
S103	Category 3	49%
L104	Category 3	49%
M105	Category 3	49%
P106	Category 3	49%
V107	Category 3	49%
L108	Category 3	49%
I109	Category 3	49%
F110	Category 3	49%
T111	Category 3	49%
G112	Category 3	49%
A113	Category 3	49%
L114	Category 3	49%
A115	Category 3	49%
T116	Category 3	49%
K117	Category 3	49%
V118	Category 3	49%
G119	Category 3	49%
A120	Category 3	49%
L121	Category 3	49%
V122	Category 4	19%
A123	Category 4	19%
F124	Category 4	19%
V125	Category 4	19%
P126	Category 4	19%
P127	Category 4	19%
H128	Category 4	19%
S129	Category 4	19%
A130	Category 4	19%
K131	Category 4	19%
P132	Category 4	19%
K133	Category 4	19%
T134	Category 4	19%
R135	Category 4	19%
D136	Category 4	19%
E137	Category 4	19%
A138	Category 4	19%
M139	Category 4	19%
A140	Category 4	19%
C141	Category 4	19%
G142	Category 4	19%
H143	Category 4	19%
A144	Category 4	19%
V145	Category 4	19%
F146	Category 4	19%
D147	Category 4	19%
V148	Category 4	19%
G149	Category 4	19%
A150	Category 4	19%
M151	Category 4	19%
S152	Category 4	19%
A153	Category 4	19%
F154	Category 4	19%
S155	Category 4	1

Chain 4:

Chain A: 67% 33%

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	344.80Å 531.40Å 488.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 20.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	7.8 (20.00-4.00) 7.7 (20.00-4.00)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.247 , (Not available) 0.245 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 143.6	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.07	EDS
Total number of atoms	5415	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

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: GAL, GLC, SIA

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	1	1.17	4/1993 (0.2%)	1.77	72/2723 (2.6%)
2	2	1.27	7/1608 (0.4%)	1.76	57/2208 (2.6%)
3	3	1.25	7/1774 (0.4%)	1.67	54/2427 (2.2%)
4	4	1.25	0/168	1.56	4/226 (1.8%)
All	All	1.23	18/5543 (0.3%)	1.73	187/7584 (2.5%)

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	1	0	1
2	2	0	1
3	3	0	2
All	All	0	4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	24	MET	SD-CE	9.73	2.03	1.79
3	3	176	VAL	CA-CB	7.08	1.62	1.54
3	3	15	MET	SD-CE	6.53	1.95	1.79
3	3	176	VAL	CA-C	6.04	1.59	1.52
2	2	32	THR	CA-CB	6.03	1.61	1.53
3	3	3	ILE	CA-CB	-5.87	1.48	1.54
1	1	218	MET	SD-CE	-5.83	1.65	1.79
2	2	128	ALA	CA-C	-5.81	1.45	1.52
3	3	36	VAL	CA-CB	5.67	1.61	1.54
2	2	97	VAL	CA-CB	-5.65	1.46	1.54
1	1	147	ALA	CA-C	-5.46	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	110	VAL	CA-CB	-5.35	1.47	1.54
1	1	22	VAL	N-CA	5.29	1.52	1.46
2	2	124	LEU	CA-C	-5.29	1.45	1.52
3	3	195	ASP	CA-C	-5.29	1.47	1.53
2	2	81	CYS	N-CA	-5.19	1.40	1.46
2	2	31	GLY	N-CA	5.11	1.53	1.45
3	3	180	SER	CA-C	5.04	1.59	1.52

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	207	CYS	N-CA-C	14.31	131.30	112.12
1	1	203	ASP	N-CA-C	-11.94	92.79	110.46
2	2	94	PHE	N-CA-C	-11.91	98.32	111.07
3	3	8	VAL	CA-C-N	10.78	133.31	119.84
3	3	8	VAL	C-N-CA	10.78	133.31	119.84
2	2	138	LYS	N-CA-C	-10.74	95.75	110.68
2	2	51	VAL	N-CA-C	10.54	122.96	107.37
1	1	7	ASP	N-CA-C	-10.15	89.19	110.80
1	1	5	GLY	N-CA-C	10.08	137.08	113.18
2	2	46	THR	N-CA-C	10.03	125.64	111.30
3	3	208	VAL	CB-CA-C	-9.73	99.15	110.73
1	1	20	SER	CA-C-N	-9.55	107.90	119.84
1	1	20	SER	C-N-CA	-9.55	107.90	119.84
1	1	158	VAL	CA-C-N	9.53	129.47	120.03
1	1	158	VAL	C-N-CA	9.53	129.47	120.03
2	2	109	ASP	N-CA-C	-9.04	94.45	109.46
2	2	228	ASN	CA-C-N	9.02	131.11	119.84
2	2	228	ASN	C-N-CA	9.02	131.11	119.84
1	1	56	VAL	N-CA-C	8.99	120.75	108.17
1	1	181	LYS	N-CA-C	-8.95	98.46	110.55
2	2	226	LEU	N-CA-C	-8.88	99.91	110.13
3	3	14	PHE	N-CA-C	8.87	122.68	111.24
1	1	225	PRO	CA-C-N	8.84	130.89	119.84
1	1	225	PRO	C-N-CA	8.84	130.89	119.84
1	1	70	ARG	N-CA-C	-8.48	99.67	110.19
2	2	43	PRO	CA-C-N	8.43	130.38	119.84
2	2	43	PRO	C-N-CA	8.43	130.38	119.84
1	1	225	PRO	N-CA-C	8.36	120.90	110.70
1	1	19	LEU	N-CA-C	8.28	121.00	110.33
2	2	226	LEU	CA-C-N	8.27	130.18	119.84
2	2	226	LEU	C-N-CA	8.27	130.18	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	83	LEU	N-CA-C	8.25	120.04	109.65
3	3	1	ALA	CA-C-N	-8.24	111.41	120.14
3	3	1	ALA	C-N-CA	-8.24	111.41	120.14
1	1	187	LEU	CA-C-N	8.10	128.15	119.89
1	1	187	LEU	C-N-CA	8.10	128.15	119.89
3	3	168	ALA	N-CA-C	8.03	121.34	108.41
1	1	199	SER	N-CA-C	8.02	120.33	108.14
4	4	20	SER	N-CA-C	-8.00	97.87	108.19
3	3	88	THR	N-CA-C	7.98	127.80	110.80
3	3	122	VAL	N-CA-C	-7.87	97.11	108.36
2	2	222	VAL	N-CA-C	7.83	121.23	109.17
4	4	17	ASN	N-CA-C	7.81	127.44	110.80
1	1	233	ASP	N-CA-C	7.78	121.69	110.10
1	1	107	PHE	CA-C-N	7.67	127.60	119.85
1	1	107	PHE	C-N-CA	7.67	127.60	119.85
1	1	201	ALA	N-CA-C	-7.63	94.54	110.80
2	2	102	HIS	N-CA-C	7.58	119.18	111.07
1	1	134	ALA	N-CA-C	-7.57	103.04	111.82
1	1	113	THR	N-CA-C	7.51	126.79	110.80
3	3	222	LEU	N-CA-C	7.49	120.51	109.50
2	2	42	ARG	CA-C-N	7.47	128.08	120.38
2	2	42	ARG	C-N-CA	7.47	128.08	120.38
1	1	9	GLU	CA-C-N	7.38	129.06	119.84
1	1	9	GLU	C-N-CA	7.38	129.06	119.84
3	3	125	VAL	CA-C-N	7.35	127.95	120.38
3	3	125	VAL	C-N-CA	7.35	127.95	120.38
2	2	125	CYS	N-CA-C	-7.33	95.28	108.48
3	3	126	PRO	CA-C-N	7.26	128.92	119.84
3	3	126	PRO	C-N-CA	7.26	128.92	119.84
3	3	5	VAL	N-CA-C	7.20	119.19	108.46
2	2	48	SER	N-CA-C	-7.10	104.08	112.89
3	3	185	VAL	N-CA-C	-7.06	98.30	108.53
2	2	124	LEU	N-CA-C	-7.01	99.22	109.18
1	1	139	SER	N-CA-C	-6.97	101.29	110.07
3	3	16	SER	N-CA-C	6.94	122.95	113.37
1	1	72	LEU	N-CA-C	-6.89	104.13	112.54
2	2	55	GLY	CA-C-N	6.88	126.39	119.24
2	2	55	GLY	C-N-CA	6.88	126.39	119.24
1	1	241	THR	N-CA-C	6.86	118.20	108.74
3	3	50	THR	N-CA-C	6.82	119.19	107.93
3	3	97	PHE	N-CA-C	6.82	118.48	108.86
1	1	3	ASN	N-CA-C	6.81	125.30	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	131	ALA	CA-C-N	6.80	126.77	120.03
3	3	131	ALA	C-N-CA	6.80	126.77	120.03
1	1	66	LEU	N-CA-C	6.74	124.63	113.50
4	4	25	PHE	N-CA-C	-6.73	103.95	111.28
3	3	163	PRO	N-CA-C	-6.70	105.13	113.84
2	2	215	VAL	CB-CA-C	-6.69	101.21	111.31
1	1	190	ALA	N-CA-C	-6.68	102.23	110.65
1	1	194	SER	N-CA-C	6.67	119.08	109.14
1	1	156	PHE	N-CA-C	6.67	118.27	108.14
1	1	176	ALA	CA-C-N	6.62	126.56	119.28
1	1	176	ALA	C-N-CA	6.62	126.56	119.28
1	1	86	ILE	N-CA-C	-6.61	98.60	108.12
1	1	51	SER	CA-C-N	6.61	128.10	119.84
1	1	51	SER	C-N-CA	6.61	128.10	119.84
1	1	21	PRO	N-CA-C	6.57	125.99	112.47
1	1	148	GLY	N-CA-C	-6.56	106.73	115.40
3	3	36	VAL	CA-C-N	6.55	127.45	120.11
3	3	36	VAL	C-N-CA	6.55	127.45	120.11
2	2	150	TYR	N-CA-C	-6.55	103.37	111.75
1	1	23	ASP	N-CA-C	6.54	124.74	110.80
1	1	84	LEU	N-CA-C	6.51	120.14	109.85
2	2	128	ALA	N-CA-C	-6.49	98.62	109.07
1	1	26	VAL	N-CA-C	6.47	122.79	109.34
1	1	127	SER	N-CA-C	6.46	124.56	110.80
2	2	34	TYR	N-CA-C	6.46	120.18	109.46
1	1	197	LEU	N-CA-C	-6.44	99.22	109.59
1	1	87	GLN	N-CA-C	6.41	122.17	113.97
1	1	50	GLY	N-CA-C	-6.37	101.30	110.60
1	1	12	GLU	N-CA-C	6.37	118.32	109.15
2	2	134	HIS	N-CA-C	-6.34	97.29	110.80
2	2	113	GLN	N-CA-C	6.34	120.95	107.70
3	3	218	HIS	CA-C-N	6.29	126.31	119.90
3	3	218	HIS	C-N-CA	6.29	126.31	119.90
3	3	102	GLY	N-CA-C	6.24	119.33	111.85
2	2	142	TRP	N-CA-C	-6.22	102.28	110.43
3	3	151	ASN	N-CA-C	-6.19	98.53	109.06
3	3	38	GLY	N-CA-C	6.17	122.48	113.48
2	2	48	SER	CA-C-N	6.14	128.93	120.39
2	2	48	SER	C-N-CA	6.14	128.93	120.39
1	1	102	VAL	N-CA-C	6.10	116.65	107.80
1	1	120	GLN	N-CA-C	6.09	118.68	108.02
1	1	4	VAL	N-CA-C	6.07	121.96	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	128	VAL	N-CA-C	6.07	118.70	109.12
2	2	49	ASP	CA-C-N	6.05	126.40	119.93
2	2	49	ASP	C-N-CA	6.05	126.40	119.93
1	1	6	GLU	N-CA-C	6.04	123.66	110.80
2	2	175	MET	CA-C-N	6.04	127.38	119.84
2	2	175	MET	C-N-CA	6.04	127.38	119.84
2	2	195	VAL	N-CA-C	-6.02	99.75	108.89
1	1	159	PRO	N-CA-C	6.01	120.43	111.41
1	1	212	ARG	N-CA-C	-5.99	98.09	108.69
2	2	147	GLU	CA-C-N	5.99	125.61	119.56
2	2	147	GLU	C-N-CA	5.99	125.61	119.56
2	2	96	GLU	N-CA-C	5.98	118.57	111.33
2	2	129	VAL	CA-C-N	5.97	128.55	120.79
2	2	129	VAL	C-N-CA	5.97	128.55	120.79
1	1	9	GLU	N-CA-C	5.96	122.98	109.81
3	3	23	THR	CA-C-N	5.94	125.70	119.76
3	3	23	THR	C-N-CA	5.94	125.70	119.76
3	3	93	LEU	N-CA-C	-5.93	104.73	111.14
1	1	192	PHE	N-CA-C	5.91	120.49	113.16
1	1	155	GLY	N-CA-C	5.87	119.06	110.38
1	1	22	VAL	CB-CA-C	-5.86	101.67	111.29
1	1	213	PHE	CA-C-N	-5.86	112.52	119.84
1	1	213	PHE	C-N-CA	-5.86	112.52	119.84
3	3	116	THR	N-CA-C	5.85	119.48	110.42
1	1	34	LEU	N-CA-C	5.85	120.57	113.38
3	3	157	ASN	N-CA-C	5.84	117.81	108.41
2	2	165	LEU	N-CA-C	5.83	123.22	110.80
3	3	174	ALA	N-CA-C	5.77	123.10	110.80
2	2	90	LYS	N-CA-C	5.76	120.30	113.16
1	1	78	PHE	N-CA-C	5.71	118.52	109.50
3	3	208	VAL	N-CA-C	5.70	116.82	107.24
3	3	159	PRO	N-CA-C	5.68	119.45	111.33
1	1	52	PRO	N-CA-C	5.67	124.15	112.47
1	1	171	TYR	N-CA-C	5.63	116.63	107.23
1	1	40	VAL	N-CA-C	-5.61	100.26	108.11
1	1	131	GLN	N-CA-C	5.58	118.74	110.48
1	1	244	ASN	N-CA-C	5.57	122.66	110.80
1	1	239	PHE	CB-CA-C	-5.55	99.84	109.32
2	2	86	ASP	N-CA-C	-5.49	99.11	110.80
3	3	64	VAL	N-CA-C	-5.48	100.59	108.48
2	2	72	SER	N-CA-C	5.42	118.36	111.69
2	2	81	CYS	CA-C-N	-5.42	112.49	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	81	CYS	C-N-CA	-5.42	112.49	120.46
3	3	32	PRO	CA-C-N	5.40	125.30	119.85
3	3	32	PRO	C-N-CA	5.40	125.30	119.85
2	2	92	GLY	N-CA-C	5.37	125.91	113.18
4	4	34	ILE	N-CA-C	5.37	116.00	108.17
3	3	87	GLY	N-CA-C	5.35	119.15	112.73
2	2	196	ILE	N-CA-C	-5.33	98.37	106.42
1	1	141	THR	N-CA-C	-5.32	101.49	109.95
3	3	192	THR	N-CA-C	-5.32	101.03	109.96
3	3	125	VAL	N-CA-C	5.31	113.28	107.60
2	2	54	LEU	N-CA-C	5.29	117.25	108.20
3	3	68	SER	N-CA-C	5.29	122.07	110.80
3	3	34	ARG	N-CA-C	5.24	117.19	108.02
3	3	51	TYR	N-CA-C	5.22	118.12	109.46
2	2	224	GLY	N-CA-C	5.21	122.97	112.34
1	1	146	ILE	CB-CA-C	-5.14	102.85	111.29
2	2	135	THR	N-CA-C	5.14	121.75	110.80
3	3	141	CYS	N-CA-C	5.13	118.00	109.94
3	3	11	SER	N-CA-C	5.11	121.68	110.80
3	3	7	SER	N-CA-C	5.11	117.62	108.17
2	2	212	THR	N-CA-CB	-5.09	103.66	111.56
2	2	141	LYS	N-CA-C	-5.08	100.88	109.07
3	3	128	HIS	O-C-N	5.08	124.59	120.83
3	3	21	ASN	N-CA-C	5.05	118.24	110.42
2	2	58	LEU	N-CA-C	-5.04	100.07	110.80
3	3	196	ILE	N-CA-C	5.04	119.82	109.34
3	3	67	THR	CB-CA-C	-5.04	105.19	111.43
3	3	70	ASP	N-CA-C	5.03	119.27	113.18
2	2	219	ASP	N-CA-C	5.02	118.25	111.17
2	2	69	TRP	N-CA-C	-5.00	102.61	109.71

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	208	TYR	Sidechain
2	2	177	TYR	Sidechain
3	3	26	TYR	Sidechain
3	3	51	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	1	1929	0	1864	183	0
2	2	1554	0	1523	125	0
3	3	1723	0	1680	152	0
4	4	166	0	146	8	0
5	A	43	0	37	0	0
All	All	5415	0	5250	428	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 40.

All (428) 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)
1:1:24:MET:SD	1:1:24:MET:CE	2.03	1.44
2:2:80:ILE:HG22	2:2:82:PRO:HD3	1.29	1.11
2:2:213:MET:HE1	2:2:215:VAL:HG22	1.23	1.10
2:2:163:LEU:HD12	2:2:171:VAL:HG23	1.37	1.04
3:3:116:THR:HG23	3:3:191:LEU:HD11	1.42	1.00
2:2:213:MET:CE	2:2:215:VAL:HG22	1.96	0.95
1:1:115:THR:HG22	1:1:131:GLN:OE1	1.67	0.94
2:2:112:VAL:HG22	2:2:213:MET:HG3	1.51	0.93
2:2:126:VAL:HG22	2:2:171:VAL:HG11	1.51	0.93
1:1:88:PHE:CE1	1:1:205:GLY:HA3	2.06	0.90
1:1:109:VAL:HG11	1:1:162:SER:HA	1.55	0.88
1:1:120:GLN:HG3	1:1:129:ARG:HD3	1.54	0.86
2:2:115:ASN:O	2:2:209:VAL:HG13	1.75	0.86
1:1:146:ILE:HG22	1:1:152:GLN:HG2	1.58	0.85
3:3:103:SER:O	3:3:211:GLY:HA3	1.77	0.85
2:2:114:VAL:HG22	2:2:209:VAL:HG12	1.59	0.84
1:1:87:GLN:HE21	1:1:210:ARG:HH12	1.28	0.82
2:2:69:TRP:NE1	2:2:202:LEU:HB2	1.94	0.82
1:1:243:ILE:HG22	1:1:244:ASN:H	1.44	0.82
1:1:117:ASP:HB2	1:1:129:ARG:NH1	1.96	0.80
1:1:207:CYS:O	1:1:208:TYR:HB2	1.82	0.79
2:2:75:HIS:HA	2:2:198:ILE:HG22	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:88:PHE:HE1	1:1:205:GLY:HA3	1.49	0.78
1:1:92:THR:HG22	1:1:93:THR:H	1.49	0.78
3:3:74:PHE:HB3	3:3:185:VAL:HG23	1.63	0.78
1:1:70:ARG:O	1:1:71:LEU:HB2	1.83	0.76
2:2:105:LYS:HG3	2:2:177:TYR:CG	2.20	0.76
1:1:219:TYR:OH	3:3:34:ARG:HD2	1.86	0.75
3:3:116:THR:CG2	3:3:191:LEU:HD11	2.16	0.74
2:2:54:LEU:HB2	2:2:220:ALA:HB3	1.69	0.74
2:2:161:GLN:HB3	2:2:171:VAL:HG13	1.69	0.74
3:3:122:VAL:O	3:3:143:HIS:HB2	1.87	0.74
1:1:159:PRO:HG3	3:3:29:VAL:HG21	1.69	0.74
1:1:195:ILE:HD13	1:1:197:LEU:HD21	1.70	0.73
3:3:217:ARG:HD3	3:3:218:HIS:CD2	2.24	0.73
2:2:35:CYS:HB2	2:2:175:MET:HA	1.71	0.72
2:2:121:SER:HB2	2:2:203:THR:HG23	1.71	0.72
3:3:175:THR:HG22	3:3:177:VAL:H	1.52	0.72
1:1:77:TYR:HD1	1:1:168:PRO:HA	1.53	0.72
3:3:101:ARG:O	3:3:214:PHE:HA	1.90	0.72
3:3:100:TYR:HA	3:3:216:LEU:HD12	1.73	0.71
2:2:153:GLN:OE1	3:3:87:GLY:HA3	1.90	0.71
3:3:94:SER:O	3:3:169:VAL:HG11	1.90	0.71
3:3:119:LYS:HG2	3:3:147:ASP:HA	1.72	0.70
1:1:2:THR:HG21	1:1:9:GLU:OE1	1.92	0.69
3:3:55:SER:O	3:3:84:GLU:HA	1.92	0.69
2:2:116:ALA:HB2	2:2:209:VAL:HG13	1.75	0.69
3:3:217:ARG:HD3	3:3:218:HIS:NE2	2.07	0.69
1:1:40:VAL:HB	1:1:68:TRP:CZ2	2.27	0.69
2:2:47:VAL:HG11	2:2:223:ASN:OD1	1.92	0.69
2:2:153:GLN:CD	3:3:87:GLY:HA3	2.18	0.69
1:1:2:THR:HB	1:1:12:GLU:HB2	1.75	0.68
1:1:22:VAL:HG12	1:1:23:ASP:N	2.08	0.68
2:2:86:ASP:HB2	2:2:141:LYS:HA	1.75	0.68
1:1:136:ALA:HA	1:1:141:THR:OG1	1.93	0.68
1:1:163:MET:H	1:1:163:MET:HE2	1.58	0.68
1:1:22:VAL:HG12	1:1:23:ASP:H	1.58	0.68
1:1:191:HIS:HD2	1:1:193:GLY:H	1.41	0.67
3:3:116:THR:HG23	3:3:191:LEU:CD1	2.21	0.67
2:2:114:VAL:HG22	2:2:209:VAL:CG1	2.25	0.67
3:3:160:TYR:OH	3:3:167:MET:HG2	1.95	0.67
1:1:184:TYR:O	1:1:186:TRP:N	2.28	0.66
2:2:116:ALA:HB2	2:2:209:VAL:CG1	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:107:TYR:CE2	3:3:155:SER:HB2	2.31	0.66
1:1:75:CYS:SG	1:1:218:MET:HG2	2.35	0.66
1:1:241:THR:H	1:1:244:ASN:ND2	1.94	0.66
1:1:45:LEU:HD12	1:1:45:LEU:H	1.60	0.66
2:2:132:TYR:HB3	2:2:193:THR:HG21	1.78	0.66
1:1:87:GLN:NE2	1:1:210:ARG:HH12	1.92	0.65
2:2:79:TRP:HE3	2:2:196:ILE:HG22	1.61	0.65
2:2:97:VAL:O	2:2:101:HIS:HD2	1.79	0.65
1:1:120:GLN:CG	1:1:129:ARG:HD3	2.26	0.65
3:3:42:ASN:HD22	3:3:43:PHE:N	1.95	0.65
3:3:160:TYR:HE2	3:3:167:MET:HG3	1.61	0.65
1:1:117:ASP:HB2	1:1:129:ARG:HH11	1.60	0.65
3:3:131:ALA:HB2	3:3:182:TRP:CZ2	2.32	0.65
3:3:220:VAL:HG12	3:3:221:ASP:N	2.12	0.64
2:2:79:TRP:CE3	2:2:196:ILE:HG22	2.32	0.64
1:1:38:PHE:O	1:1:210:ARG:HA	1.98	0.64
1:1:90:PHE:CE1	1:1:94:PRO:HA	2.33	0.64
2:2:64:PHE:N	2:2:64:PHE:CD1	2.65	0.64
2:2:161:GLN:CB	2:2:171:VAL:HG13	2.27	0.63
2:2:197:LEU:HG	2:2:198:ILE:N	2.11	0.63
3:3:34:ARG:HB2	3:3:36:VAL:HG12	1.80	0.63
1:1:19:LEU:HB2	3:3:213:ASP:HB2	1.80	0.63
1:1:131:GLN:HB2	1:1:134:ALA:HB2	1.80	0.62
1:1:163:MET:HE3	1:1:164:TRP:CD1	2.35	0.62
3:3:61:TYR:HB3	3:3:205:LEU:HD23	1.80	0.62
1:1:77:TYR:CD1	1:1:168:PRO:HA	2.33	0.62
1:1:159:PRO:CG	3:3:29:VAL:HG21	2.29	0.62
1:1:120:GLN:HE21	1:1:129:ARG:HE	1.44	0.62
2:2:83:LEU:HD11	2:2:194:ILE:HD12	1.81	0.62
1:1:43:LEU:HD23	1:1:43:LEU:N	2.15	0.61
1:1:164:TRP:CZ2	1:1:187:LEU:HD21	2.34	0.61
1:1:176:ALA:HB3	1:1:183:THR:HG21	1.82	0.61
3:3:97:PHE:CD1	3:3:97:PHE:N	2.68	0.61
3:3:138:ALA:O	3:3:141:CYS:SG	2.51	0.61
2:2:220:ALA:O	2:2:221:MET:HG2	2.00	0.61
3:3:42:ASN:HD22	3:3:44:ILE:H	1.48	0.61
1:1:163:MET:HE1	1:1:189:GLY:HA3	1.82	0.61
1:1:243:ILE:HG22	1:1:244:ASN:N	2.15	0.60
1:1:224:ILE:HG13	3:3:89:TYR:CE2	2.36	0.60
1:1:236:ARG:NH1	3:3:172:ALA:O	2.34	0.60
1:1:22:VAL:O	1:1:24:MET:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:80:SER:HB2	1:1:214:PRO:O	2.01	0.60
1:1:79:PHE:HE2	3:3:31:VAL:HG11	1.67	0.60
1:1:122:GLU:HG2	1:1:123:GLY:N	2.16	0.60
2:2:185:ASN:OD1	2:2:187:THR:HB	2.02	0.59
2:2:124:LEU:HD23	2:2:198:ILE:HA	1.85	0.59
2:2:127:ALA:O	2:2:194:ILE:HA	2.01	0.59
1:1:45:LEU:HB2	1:1:202:HIS:HA	1.83	0.59
2:2:104:VAL:HG13	2:2:222:VAL:HG13	1.84	0.59
3:3:54:CYS:HB2	3:3:206:VAL:HG13	1.83	0.59
1:1:68:TRP:O	1:1:72:LEU:HG	2.03	0.58
1:1:97:VAL:HG22	1:1:204:LYS:HD2	1.84	0.58
3:3:175:THR:CG2	3:3:176:VAL:N	2.66	0.58
1:1:79:PHE:CD1	1:1:79:PHE:C	2.82	0.58
3:3:127:PRO:HD3	3:3:181:GLY:CA	2.33	0.58
1:1:181:LYS:O	1:1:182:ALA:HB3	2.04	0.58
2:2:134:HIS:O	2:2:136:HIS:N	2.35	0.58
2:2:153:GLN:NE2	3:3:87:GLY:HA3	2.18	0.58
2:2:59:SER:HA	2:2:94:PHE:HB2	1.85	0.58
1:1:55:HIS:O	1:1:194:SER:HB2	2.04	0.57
2:2:160:HIS:HD1	2:2:160:HIS:H	1.52	0.57
1:1:105:LYS:HE3	1:1:139:SER:HB2	1.86	0.57
3:3:110:PHE:CD2	3:3:148:VAL:HG11	2.40	0.57
1:1:28:THR:HB	3:3:42:ASN:HD21	1.69	0.57
1:1:132:GLN:HG3	1:1:133:LEU:HD23	1.85	0.57
1:1:239:PHE:HE1	3:3:81:SER:HB3	1.69	0.57
2:2:58:LEU:O	2:2:60:ARG:HG3	2.05	0.57
2:2:85:SER:HB3	2:2:140:LEU:HB3	1.85	0.57
2:2:126:VAL:CG2	2:2:171:VAL:HG11	2.31	0.57
2:2:147:GLU:HB3	2:2:148:PRO:HD2	1.86	0.57
3:3:113:ALA:O	3:3:116:THR:HB	2.04	0.57
1:1:109:VAL:CG1	1:1:162:SER:HA	2.31	0.57
1:1:120:GLN:HG3	1:1:129:ARG:CD	2.29	0.57
1:1:130:ILE:HG13	1:1:131:GLN:N	2.19	0.57
4:4:29:GLN:HA	4:4:34:ILE:HD11	1.87	0.57
1:1:77:TYR:HB3	1:1:166:VAL:HG21	1.85	0.57
3:3:46:VAL:O	3:3:50:THR:HB	2.05	0.57
3:3:96:PHE:C	3:3:97:PHE:CD1	2.82	0.57
2:2:97:VAL:HG12	2:2:101:HIS:CD2	2.41	0.56
3:3:184:GLN:NE2	3:3:186:TYR:HE1	2.03	0.56
2:2:110:VAL:HG12	2:2:215:VAL:HG13	1.88	0.56
3:3:15:MET:O	3:3:18:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:110:VAL:HG23	2:2:110:VAL:O	2.05	0.56
1:1:174:TRP:CE2	1:1:179:LYS:HB3	2.41	0.56
1:1:28:THR:HB	3:3:42:ASN:ND2	2.20	0.55
1:1:45:LEU:HD12	1:1:45:LEU:N	2.21	0.55
3:3:44:ILE:HG23	3:3:48:LYS:HE3	1.88	0.55
2:2:43:PRO:HA	2:2:221:MET:HE1	1.88	0.55
4:4:17:ASN:CG	4:4:17:ASN:O	2.49	0.55
2:2:140:LEU:HD22	2:2:190:ASN:ND2	2.22	0.55
2:2:97:VAL:O	2:2:101:HIS:CD2	2.59	0.55
3:3:42:ASN:ND2	3:3:44:ILE:H	2.03	0.55
1:1:43:LEU:HD23	1:1:43:LEU:H	1.73	0.54
1:1:70:ARG:O	1:1:71:LEU:CB	2.50	0.54
2:2:115:ASN:HB3	2:2:210:PRO:HG2	1.88	0.54
2:2:166:ARG:HD2	3:3:110:PHE:HD2	1.73	0.54
2:2:149:ALA:O	2:2:150:TYR:C	2.51	0.54
1:1:19:LEU:HB2	3:3:213:ASP:CB	2.37	0.54
1:1:209:LEU:HD13	1:1:211:TYR:HE1	1.71	0.54
1:1:219:TYR:CE1	3:3:36:VAL:HG13	2.42	0.54
1:1:125:GLY:O	1:1:127:SER:N	2.41	0.54
1:1:207:CYS:O	1:1:208:TYR:CB	2.55	0.54
3:3:42:ASN:HD22	3:3:42:ASN:C	2.14	0.54
3:3:120:PHE:HB3	3:3:186:TYR:O	2.08	0.54
1:1:28:THR:CB	3:3:42:ASN:HD21	2.21	0.54
1:1:77:TYR:HB3	1:1:166:VAL:CG2	2.38	0.54
2:2:42:ARG:HG3	2:2:43:PRO:HD2	1.90	0.54
2:2:118:PHE:HB2	3:3:114:ALA:HB3	1.90	0.54
1:1:105:LYS:HE3	1:1:139:SER:CB	2.38	0.53
1:1:74:THR:HG21	3:3:43:PHE:CZ	2.43	0.53
1:1:32:PHE:C	1:1:32:PHE:CD2	2.86	0.53
2:2:75:HIS:HA	2:2:198:ILE:CG2	2.37	0.53
1:1:61:GLY:O	1:1:62:SER:HB3	2.08	0.53
1:1:35:ASP:OD2	1:1:212:ARG:HD3	2.08	0.53
3:3:106:PHE:O	3:3:155:SER:HA	2.09	0.53
1:1:13:THR:HA	3:3:144:ALA:HB2	1.90	0.53
2:2:134:HIS:HD2	2:2:145:LEU:HD13	1.75	0.52
2:2:149:ALA:HA	2:2:152:TYR:CD2	2.45	0.52
3:3:127:PRO:HD3	3:3:181:GLY:HA2	1.90	0.52
2:2:137:GLU:C	2:2:139:ALA:H	2.18	0.52
3:3:18:VAL:HG12	3:3:20:ASP:H	1.74	0.52
2:2:202:LEU:HD21	2:2:209:VAL:HG23	1.92	0.52
3:3:96:PHE:HB2	3:3:97:PHE:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:191:HIS:CD2	1:1:193:GLY:H	2.26	0.52
2:2:148:PRO:O	2:2:149:ALA:HB3	2.10	0.52
2:2:149:ALA:O	2:2:153:GLN:HG3	2.10	0.52
3:3:94:SER:OG	3:3:216:LEU:HD21	2.10	0.52
1:1:7:ASP:HB2	1:1:12:GLU:OE1	2.09	0.52
1:1:219:TYR:HA	3:3:39:ARG:HA	1.90	0.52
2:2:108:TRP:HB2	2:2:175:MET:CG	2.40	0.52
2:2:149:ALA:C	2:2:151:THR:N	2.66	0.52
3:3:160:TYR:HE2	3:3:167:MET:CG	2.23	0.51
1:1:59:PRO:O	1:1:72:LEU:HD12	2.10	0.51
1:1:163:MET:HE3	1:1:164:TRP:NE1	2.25	0.51
1:1:122:GLU:HG3	1:1:127:SER:HB3	1.92	0.51
1:1:76:THR:HB	1:1:220:CYS:HB2	1.91	0.51
2:2:69:TRP:CZ3	2:2:124:LEU:HG	2.46	0.51
3:3:110:PHE:CG	3:3:148:VAL:HG11	2.46	0.51
1:1:19:LEU:HD11	3:3:160:TYR:HB3	1.92	0.51
1:1:238:LYS:HA	3:3:172:ALA:HA	1.92	0.51
2:2:160:HIS:ND1	2:2:160:HIS:N	2.59	0.51
3:3:46:VAL:O	3:3:50:THR:CG2	2.58	0.51
3:3:196:ILE:HD12	3:3:199:ASN:O	2.10	0.51
2:2:132:TYR:HB3	2:2:193:THR:CG2	2.41	0.51
2:2:137:GLU:C	2:2:139:ALA:N	2.69	0.51
1:1:106:TRP:O	1:1:139:SER:HB3	2.11	0.51
1:1:109:VAL:HB	1:1:161:THR:HB	1.91	0.51
3:3:31:VAL:HG13	3:3:32:PRO:HD2	1.93	0.51
3:3:74:PHE:O	3:3:184:GLN:HA	2.11	0.51
1:1:160:TYR:OH	1:1:167:VAL:HG23	2.11	0.50
2:2:149:ALA:HA	2:2:152:TYR:CE2	2.46	0.50
2:2:120:HIS:O	3:3:113:ALA:HB2	2.12	0.50
3:3:74:PHE:HB3	3:3:185:VAL:CG2	2.36	0.50
3:3:83:ALA:C	3:3:85:LEU:H	2.19	0.50
2:2:160:HIS:HD1	2:2:160:HIS:N	2.10	0.50
1:1:5:GLY:HA2	1:1:13:THR:O	2.11	0.50
1:1:104:VAL:HA	1:1:196:LEU:O	2.11	0.50
3:3:109:ILE:N	3:3:109:ILE:HD12	2.27	0.50
2:2:69:TRP:CE2	2:2:202:LEU:HB2	2.45	0.50
1:1:102:VAL:HA	1:1:199:SER:HB2	1.94	0.50
2:2:117:SER:H	2:2:120:HIS:CE1	2.30	0.50
2:2:151:THR:O	2:2:155:LEU:N	2.45	0.50
2:2:64:PHE:HE1	2:2:215:VAL:HG23	1.76	0.49
3:3:35:GLN:O	3:3:36:VAL:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:115:THR:OG1	1:1:133:LEU:HG	2.11	0.49
2:2:134:HIS:C	2:2:136:HIS:H	2.21	0.49
1:1:36:ARG:O	1:1:212:ARG:HA	2.11	0.49
3:3:94:SER:HB3	3:3:169:VAL:HG13	1.94	0.49
2:2:87:LYS:HG3	2:2:142:TRP:CE2	2.47	0.49
2:2:108:TRP:HB2	2:2:175:MET:HG3	1.95	0.49
3:3:65:THR:C	3:3:67:THR:H	2.21	0.49
3:3:76:MET:HG3	3:3:76:MET:O	2.13	0.49
2:2:111:VAL:HG22	2:2:172:HIS:CD2	2.47	0.49
2:2:40:ASP:HB2	2:2:42:ARG:HH21	1.78	0.48
2:2:158:PHE:O	2:2:160:HIS:ND1	2.45	0.48
1:1:74:THR:HG21	3:3:43:PHE:CE2	2.48	0.48
3:3:116:THR:HG22	3:3:117:LYS:N	2.29	0.48
1:1:89:LYS:HB2	1:1:208:TYR:HE1	1.78	0.48
2:2:58:LEU:O	2:2:60:ARG:N	2.46	0.48
2:2:59:SER:HB2	2:2:217:PRO:HB2	1.94	0.48
3:3:24:PRO:CG	4:4:31:GLN:HA	2.43	0.48
3:3:100:TYR:CE1	3:3:167:MET:HB3	2.48	0.48
3:3:173:GLU:OE1	3:3:173:GLU:HA	2.13	0.48
1:1:100:GLY:O	1:1:146:ILE:HG13	2.13	0.48
2:2:76:GLY:O	2:2:146:GLU:HA	2.12	0.48
1:1:224:ILE:N	2:2:154:GLN:OE1	2.46	0.48
2:2:126:VAL:HB	2:2:196:ILE:HG12	1.96	0.48
1:1:115:THR:CG2	1:1:131:GLN:OE1	2.53	0.48
2:2:220:ALA:C	2:2:221:MET:HG2	2.38	0.48
2:2:129:VAL:HA	2:2:130:PRO:HD3	1.61	0.48
1:1:199:SER:C	1:1:201:ALA:H	2.22	0.47
3:3:164:ALA:HB1	3:3:166:PHE:O	2.14	0.47
2:2:201:GLU:O	2:2:203:THR:HG22	2.14	0.47
1:1:181:LYS:O	1:1:182:ALA:CB	2.61	0.47
3:3:121:LEU:HG	3:3:143:HIS:CD2	2.48	0.47
1:1:107:PHE:HE1	1:1:196:LEU:HB2	1.80	0.47
3:3:84:GLU:H	3:3:84:GLU:CD	2.22	0.47
2:2:83:LEU:HA	2:2:84:PRO:HA	1.41	0.47
3:3:46:VAL:O	3:3:50:THR:HG22	2.14	0.47
1:1:66:LEU:O	1:1:67:ALA:HB3	2.15	0.47
1:1:118:ALA:CB	1:1:132:GLN:HB2	2.45	0.47
3:3:157:ASN:O	3:3:159:PRO:HD3	2.15	0.47
2:2:181:GLY:C	2:2:183:THR:H	2.21	0.47
3:3:85:LEU:HD23	3:3:85:LEU:HA	1.58	0.47
3:3:169:VAL:O	3:3:169:VAL:HG12	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:172:ALA:O	3:3:173:GLU:C	2.58	0.47
1:1:9:GLU:HA	1:1:10:PRO:HD3	1.76	0.47
3:3:220:VAL:CG1	3:3:221:ASP:N	2.78	0.47
1:1:109:VAL:O	1:1:109:VAL:HG12	2.15	0.47
1:1:231:PRO:HG2	3:3:83:ALA:HA	1.96	0.47
3:3:121:LEU:HG	3:3:143:HIS:HD2	1.79	0.47
1:1:35:ASP:HB3	4:4:17:ASN:HB3	1.97	0.46
1:1:118:ALA:HB3	1:1:132:GLN:HB2	1.96	0.46
1:1:220:CYS:HA	1:1:221:PRO:HD2	1.76	0.46
3:3:24:PRO:HG3	4:4:31:GLN:HA	1.97	0.46
1:1:115:THR:HG23	1:1:132:GLN:HB3	1.97	0.46
3:3:184:GLN:NE2	3:3:186:TYR:CE1	2.82	0.46
1:1:21:PRO:O	1:1:22:VAL:O	2.33	0.46
2:2:84:PRO:HB2	2:2:91:MET:HE3	1.96	0.46
2:2:198:ILE:HG22	2:2:198:ILE:O	2.14	0.46
3:3:48:LYS:HA	3:3:210:ALA:HB3	1.97	0.46
3:3:85:LEU:O	3:3:86:HIS:C	2.58	0.46
3:3:92:SER:O	3:3:95:SER:OG	2.33	0.46
1:1:106:TRP:HE3	1:1:140:PRO:HD2	1.81	0.46
3:3:45:ASP:O	3:3:49:GLN:HG2	2.15	0.46
3:3:80:LEU:HD12	3:3:80:LEU:HA	1.55	0.46
1:1:34:LEU:HA	1:1:34:LEU:HD23	1.72	0.46
1:1:96:SER:HB2	1:1:204:LYS:HD3	1.96	0.46
3:3:162:SER:C	3:3:164:ALA:N	2.74	0.46
1:1:80:SER:OG	1:1:213:PHE:HB3	2.16	0.46
3:3:120:PHE:HA	3:3:188:LEU:H	1.81	0.46
1:1:43:LEU:N	1:1:43:LEU:CD2	2.79	0.46
1:1:171:TYR:HA	2:2:131:GLU:OE1	2.15	0.46
2:2:157:VAL:O	2:2:157:VAL:HG13	2.15	0.46
2:2:220:ALA:C	2:2:221:MET:CG	2.88	0.46
2:2:52:THR:HB	2:2:222:VAL:HG23	1.98	0.46
1:1:166:VAL:HG22	1:1:167:VAL:N	2.29	0.45
3:3:125:VAL:HG21	3:3:132:PRO:HG3	1.97	0.45
1:1:89:LYS:HD2	1:1:90:PHE:H	1.81	0.45
1:1:120:GLN:CB	1:1:129:ARG:HD3	2.46	0.45
1:1:149:SER:O	1:1:151:SER:N	2.49	0.45
1:1:173:GLY:CA	2:2:188:LEU:O	2.63	0.45
2:2:85:SER:HA	2:2:88:LEU:HB2	1.97	0.45
3:3:124:PHE:CD1	3:3:124:PHE:C	2.93	0.45
1:1:154:CYS:SG	1:1:155:GLY:N	2.88	0.45
1:1:173:GLY:HA2	2:2:188:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:94:PHE:O	2:2:95:HIS:C	2.59	0.45
2:2:140:LEU:HD22	2:2:190:ASN:CG	2.41	0.45
1:1:151:SER:C	1:1:153:ALA:H	2.25	0.45
3:3:44:ILE:CG2	3:3:48:LYS:HE3	2.46	0.45
3:3:206:VAL:HG13	3:3:206:VAL:O	2.16	0.45
2:2:85:SER:O	2:2:86:ASP:HB3	2.17	0.45
2:2:148:PRO:O	2:2:149:ALA:CB	2.65	0.45
1:1:128:VAL:CG1	1:1:129:ARG:N	2.80	0.45
3:3:121:LEU:HD21	3:3:123:ALA:HB2	1.99	0.45
3:3:220:VAL:HG12	3:3:221:ASP:H	1.78	0.45
1:1:79:PHE:CE2	3:3:34:ARG:NH2	2.85	0.45
1:1:199:SER:OG	1:1:200:ASP:N	2.49	0.45
3:3:106:PHE:CE1	3:3:158:VAL:HG21	2.52	0.45
1:1:87:GLN:O	1:1:87:GLN:HG3	2.17	0.44
1:1:228:PHE:CE2	1:1:239:PHE:HE2	2.36	0.44
2:2:77:HIS:O	2:2:78:ALA:HB2	2.17	0.44
3:3:83:ALA:O	3:3:85:LEU:N	2.50	0.44
3:3:106:PHE:HE1	3:3:158:VAL:HG21	1.81	0.44
2:2:124:LEU:HA	2:2:197:LEU:O	2.16	0.44
3:3:48:LYS:HD3	3:3:212:PRO:HA	1.99	0.44
3:3:166:PHE:CE2	3:3:217:ARG:HG2	2.52	0.44
4:4:35:ASP:OD1	4:4:35:ASP:N	2.50	0.44
1:1:88:PHE:N	1:1:207:CYS:O	2.49	0.44
2:2:91:MET:O	2:2:93:SER:N	2.50	0.44
1:1:146:ILE:HG22	1:1:152:GLN:CG	2.40	0.44
3:3:108:PHE:HB3	3:3:204:VAL:CG1	2.48	0.44
1:1:140:PRO:HG3	3:3:25:LEU:O	2.18	0.44
2:2:165:LEU:N	2:2:165:LEU:HD23	2.33	0.44
3:3:128:HIS:HB3	3:3:129:SER:H	1.56	0.44
1:1:241:THR:HG22	1:1:242:ASN:H	1.82	0.44
1:1:119:TRP:HB3	1:1:130:ILE:HG12	2.00	0.44
3:3:70:ASP:HB3	3:3:135:ARG:H	1.82	0.44
3:3:222:LEU:HA	3:3:223:PRO:HD2	1.87	0.44
1:1:79:PHE:CE2	3:3:31:VAL:HG11	2.51	0.43
2:2:177:TYR:CZ	2:2:183:THR:HA	2.54	0.43
1:1:62:SER:O	1:1:63:THR:HB	2.18	0.43
1:1:68:TRP:O	1:1:68:TRP:HE3	2.01	0.43
3:3:175:THR:HB	3:3:178:ASN:ND2	2.33	0.43
3:3:160:TYR:CE2	3:3:167:MET:CG	3.02	0.43
1:1:47:ASN:HD22	1:1:48:LEU:H	1.67	0.43
3:3:125:VAL:HA	3:3:126:PRO:HD2	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:86:ILE:N	1:1:86:ILE:HD12	2.33	0.43
2:2:175:MET:H	2:2:175:MET:HG2	1.67	0.43
3:3:7:SER:O	3:3:8:VAL:C	2.62	0.43
3:3:60:PRO:HD2	3:3:61:TYR:CD2	2.53	0.43
3:3:132:PRO:O	3:3:133:LYS:HG3	2.19	0.43
1:1:68:TRP:CE3	1:1:68:TRP:C	2.97	0.43
3:3:175:THR:HG22	3:3:176:VAL:N	2.33	0.43
3:3:34:ARG:HB2	3:3:36:VAL:CG1	2.45	0.42
1:1:42:THR:O	1:1:42:THR:HG22	2.19	0.42
1:1:71:LEU:O	1:1:218:MET:HE1	2.19	0.42
2:2:110:VAL:HG21	2:2:175:MET:HE3	2.02	0.42
3:3:196:ILE:HD12	3:3:196:ILE:HA	1.84	0.42
1:1:69:ALA:C	1:1:70:ARG:O	2.57	0.42
1:1:148:GLY:O	1:1:150:ARG:N	2.52	0.42
2:2:95:HIS:C	2:2:95:HIS:CD2	2.96	0.42
1:1:89:LYS:HB2	1:1:208:TYR:CE1	2.55	0.42
1:1:212:ARG:NH2	3:3:18:VAL:O	2.45	0.42
1:1:40:VAL:HB	1:1:68:TRP:CE2	2.54	0.42
1:1:57:LEU:H	1:1:57:LEU:HG	1.65	0.42
1:1:71:LEU:O	1:1:218:MET:CE	2.68	0.42
1:1:101:PHE:HD1	1:1:101:PHE:HA	1.53	0.42
2:2:161:GLN:OE1	2:2:171:VAL:HA	2.19	0.42
3:3:23:THR:HA	3:3:24:PRO:HD3	1.69	0.42
3:3:44:ILE:HA	3:3:44:ILE:HD12	1.59	0.42
2:2:155:LEU:HD12	2:2:155:LEU:HA	1.50	0.42
2:2:226:LEU:HA	2:2:227:PRO:HD3	1.80	0.42
3:3:18:VAL:C	3:3:20:ASP:H	2.28	0.42
3:3:76:MET:HB3	3:3:84:GLU:HG3	2.02	0.42
1:1:81:ASP:HB2	1:1:214:PRO:HG2	2.02	0.42
3:3:30:VAL:HG22	4:4:34:ILE:HB	2.02	0.42
1:1:21:PRO:C	1:1:22:VAL:O	2.63	0.42
3:3:98:ALA:HB3	3:3:218:HIS:HB2	2.02	0.42
2:2:84:PRO:O	2:2:85:SER:O	2.37	0.41
3:3:175:THR:HG23	3:3:176:VAL:H	1.85	0.41
1:1:147:ALA:C	1:1:149:SER:H	2.27	0.41
3:3:108:PHE:O	3:3:153:ALA:HA	2.21	0.41
1:1:25:HIS:O	1:1:27:HIS:N	2.53	0.41
1:1:106:TRP:HA	1:1:195:ILE:HG22	2.02	0.41
2:2:35:CYS:O	2:2:176:PRO:HD3	2.20	0.41
2:2:175:MET:HA	2:2:176:PRO:HD3	1.86	0.41
3:3:75:GLN:HG3	3:3:184:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:148:GLY:O	1:1:149:SER:C	2.63	0.41
2:2:49:ASP:HA	2:2:50:PRO:HD2	1.93	0.41
2:2:129:VAL:HG22	2:2:158:PHE:CD1	2.56	0.41
3:3:52:SER:O	3:3:207:ALA:HB1	2.20	0.41
1:1:164:TRP:CH2	1:1:187:LEU:HD21	2.56	0.41
1:1:241:THR:N	1:1:244:ASN:ND2	2.65	0.41
3:3:36:VAL:HA	3:3:37:PRO:HD3	1.85	0.41
3:3:127:PRO:CD	3:3:181:GLY:HA2	2.50	0.41
1:1:88:PHE:CD2	1:1:88:PHE:O	2.74	0.41
1:1:111:ALA:HB1	1:1:112:PRO:HD2	2.03	0.41
1:1:168:PRO:O	1:1:168:PRO:HG2	2.20	0.41
1:1:191:HIS:HD2	1:1:193:GLY:N	2.13	0.41
2:2:80:ILE:HG22	2:2:82:PRO:CD	2.22	0.41
3:3:99:GLN:HB3	3:3:166:PHE:HB3	2.03	0.41
3:3:120:PHE:CD1	3:3:120:PHE:N	2.89	0.41
4:4:17:ASN:O	4:4:17:ASN:ND2	2.54	0.41
1:1:26:VAL:O	1:1:26:VAL:HG12	2.21	0.41
1:1:87:GLN:HA	1:1:153:ALA:HB2	2.03	0.41
1:1:241:THR:N	1:1:244:ASN:HD21	2.19	0.41
1:1:241:THR:HB	1:1:243:ILE:H	1.85	0.41
3:3:93:LEU:O	3:3:93:LEU:HD23	2.21	0.41
1:1:186:TRP:O	1:1:187:LEU:O	2.39	0.40
1:1:211:TYR:N	1:1:211:TYR:CD1	2.89	0.40
2:2:73:GLN:HA	2:2:73:GLN:NE2	2.37	0.40
1:1:74:THR:O	1:1:74:THR:HG22	2.21	0.40
1:1:199:SER:C	1:1:201:ALA:N	2.79	0.40
2:2:166:ARG:HD3	3:3:152:SER:HB3	2.03	0.40
1:1:108:PRO:CB	1:1:161:THR:HG21	2.52	0.40
1:1:211:TYR:N	1:1:211:TYR:HD1	2.19	0.40
3:3:218:HIS:HA	3:3:219:PRO:HD2	1.91	0.40
1:1:219:TYR:CD2	1:1:219:TYR:N	2.90	0.40
1:1:225:PRO:HA	1:1:226:PRO:HD3	1.71	0.40
2:2:69:TRP:CG	2:2:202:LEU:HD22	2.56	0.40
2:2:114:VAL:CG2	2:2:209:VAL:HG12	2.41	0.40
1:1:217:ASN:OD1	3:3:39:ARG:NH1	2.55	0.40
2:2:58:LEU:HD23	2:2:58:LEU:HA	1.82	0.40
3:3:46:VAL:O	3:3:50:THR:CB	2.68	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	1	245/248 (99%)	173 (71%)	41 (17%)	31 (13%)	0	4
2	2	198/230 (86%)	154 (78%)	27 (14%)	17 (9%)	0	10
3	3	224/226 (99%)	181 (81%)	28 (12%)	15 (7%)	1	15
4	4	20/80 (25%)	12 (60%)	6 (30%)	2 (10%)	0	8
All	All	687/784 (88%)	520 (76%)	102 (15%)	65 (10%)	0	9

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	5	GLY
1	1	9	GLU
1	1	10	PRO
1	1	21	PRO
1	1	22	VAL
1	1	23	ASP
1	1	26	VAL
1	1	88	PHE
1	1	126	ASN
1	1	127	SER
1	1	150	ARG
1	1	184	TYR
2	2	85	SER
2	2	92	GLY
2	2	134	HIS
2	2	135	THR
2	2	137	GLU
2	2	149	ALA
3	3	11	SER
3	3	36	VAL
3	3	129	SER
4	4	17	ASN

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Mol	Chain	Res	Type
1	1	6	GLU
1	1	109	VAL
1	1	149	SER
1	1	162	SER
1	1	185	ASN
1	1	208	TYR
1	1	243	ILE
2	2	60	ARG
2	2	73	GLN
2	2	93	SER
2	2	165	LEU
2	2	183	THR
2	2	224	GLY
2	2	229	PRO
3	3	9	PRO
3	3	15	MET
3	3	57	SER
3	3	84	GLU
1	1	62	SER
1	1	179	LYS
1	1	182	ALA
3	3	54	CYS
3	3	88	THR
3	3	127	PRO
4	4	31	GLN
1	1	3	ASN
1	1	202	HIS
1	1	244	ASN
2	2	227	PRO
3	3	131	ALA
3	3	172	ALA
3	3	174	ALA
1	1	63	THR
1	1	118	ALA
1	1	135	VAL
1	1	187	LEU
2	2	44	PRO
2	2	156	SER
3	3	139	MET
3	3	196	ILE
1	1	220	CYS
1	1	20	SER

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Mol	Chain	Res	Type
2	2	191	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	208/210 (99%)	157 (76%)	51 (24%)	1	5
2	2	176/203 (87%)	136 (77%)	40 (23%)	1	6
3	3	190/190 (100%)	149 (78%)	41 (22%)	1	6
4	4	18/65 (28%)	14 (78%)	4 (22%)	1	6
All	All	592/668 (89%)	456 (77%)	136 (23%)	1	6

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	2	THR
1	1	3	ASN
1	1	9	GLU
1	1	10	PRO
1	1	24	MET
1	1	28	THR
1	1	31	SER
1	1	36	ARG
1	1	39	ASP
1	1	40	VAL
1	1	42	THR
1	1	43	LEU
1	1	45	LEU
1	1	46	SER
1	1	49	THR
1	1	51	SER
1	1	56	VAL
1	1	70	ARG
1	1	71	LEU
1	1	79	PHE

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Mol	Chain	Res	Type
1	1	87	GLN
1	1	91	THR
1	1	93	THR
1	1	95	SER
1	1	96	SER
1	1	97	VAL
1	1	101	PHE
1	1	117	ASP
1	1	130	ILE
1	1	138	MET
1	1	139	SER
1	1	143	VAL
1	1	146	ILE
1	1	150	ARG
1	1	154	CYS
1	1	158	VAL
1	1	161	THR
1	1	163	MET
1	1	165	ARG
1	1	183	THR
1	1	185	ASN
1	1	187	LEU
1	1	196	LEU
1	1	202	HIS
1	1	207	CYS
1	1	209	LEU
1	1	211	TYR
1	1	237	HIS
1	1	241	THR
1	1	245	LYS
1	1	246	GLN
2	2	42	ARG
2	2	44	PRO
2	2	45	SER
2	2	51	VAL
2	2	52	THR
2	2	57	THR
2	2	64	PHE
2	2	73	GLN
2	2	85	SER
2	2	89	LYS
2	2	91	MET

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Mol	Chain	Res	Type
2	2	103	LEU
2	2	104	VAL
2	2	125	CYS
2	2	126	VAL
2	2	135	THR
2	2	146	GLU
2	2	157	VAL
2	2	159	PRO
2	2	162	LEU
2	2	163	LEU
2	2	165	LEU
2	2	166	ARG
2	2	168	ASN
2	2	183	THR
2	2	187	THR
2	2	193	THR
2	2	194	ILE
2	2	196	ILE
2	2	197	LEU
2	2	198	ILE
2	2	202	LEU
2	2	203	THR
2	2	207	GLN
2	2	212	THR
2	2	213	MET
2	2	215	VAL
2	2	218	ILE
2	2	221	MET
2	2	222	VAL
3	3	13	SER
3	3	23	THR
3	3	30	VAL
3	3	34	ARG
3	3	41	THR
3	3	42	ASN
3	3	44	ILE
3	3	50	THR
3	3	52	SER
3	3	56	ILE
3	3	59	LYS
3	3	64	VAL
3	3	70	ASP

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Mol	Chain	Res	Type
3	3	71	GLU
3	3	76	MET
3	3	80	LEU
3	3	81	SER
3	3	84	GLU
3	3	90	VAL
3	3	97	PHE
3	3	124	PHE
3	3	133	LYS
3	3	139	MET
3	3	141	CYS
3	3	142	ILE
3	3	150	LEU
3	3	151	ASN
3	3	152	SER
3	3	161	SER
3	3	173	GLU
3	3	175	THR
3	3	176	VAL
3	3	178	ASN
3	3	179	VAL
3	3	183	LEU
3	3	188	LEU
3	3	191	LEU
3	3	196	ILE
3	3	209	SER
3	3	213	ASP
3	3	216	LEU
4	4	21	ILE
4	4	22	VAL
4	4	27	MET
4	4	35	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	47	ASN
1	1	65	GLN
1	1	87	GLN
1	1	120	GLN
1	1	132	GLN
1	1	191	HIS

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Mol	Chain	Res	Type
1	1	244	ASN
2	2	73	GLN
2	2	95	HIS
2	2	101	HIS
2	2	134	HIS
2	2	136	HIS
2	2	172	HIS
2	2	228	ASN
3	3	42	ASN
3	3	49	GLN
3	3	99	GLN
3	3	184	GLN
4	4	17	ASN
4	4	24	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

3 monosaccharides 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	$\# Z > 2$
5	GLC	A	1	5	12,12,12	0.69	0	17,17,17	0.68	0
5	GAL	A	2	5	11,11,12	0.64	0	15,15,17	0.64	0
5	SIA	A	3	5	20,20,21	1.12	3 (15%)	21,28,31	1.28	3 (14%)

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	GLC	A	1	5	-	2/2/22/22	0/1/1/1
5	GAL	A	2	5	-	2/2/19/22	0/1/1/1
5	SIA	A	3	5	-	2/18/34/38	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3	SIA	C7-C6	-2.31	1.50	1.52
5	A	3	SIA	C4-C5	-2.28	1.51	1.53
5	A	3	SIA	C6-C5	-2.05	1.49	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3	SIA	C8-C7-C6	-3.22	107.00	113.05
5	A	3	SIA	O1B-C1-C2	2.38	118.89	112.71
5	A	3	SIA	O1A-C1-C2	-2.07	118.39	122.85

There are no chirality outliers.

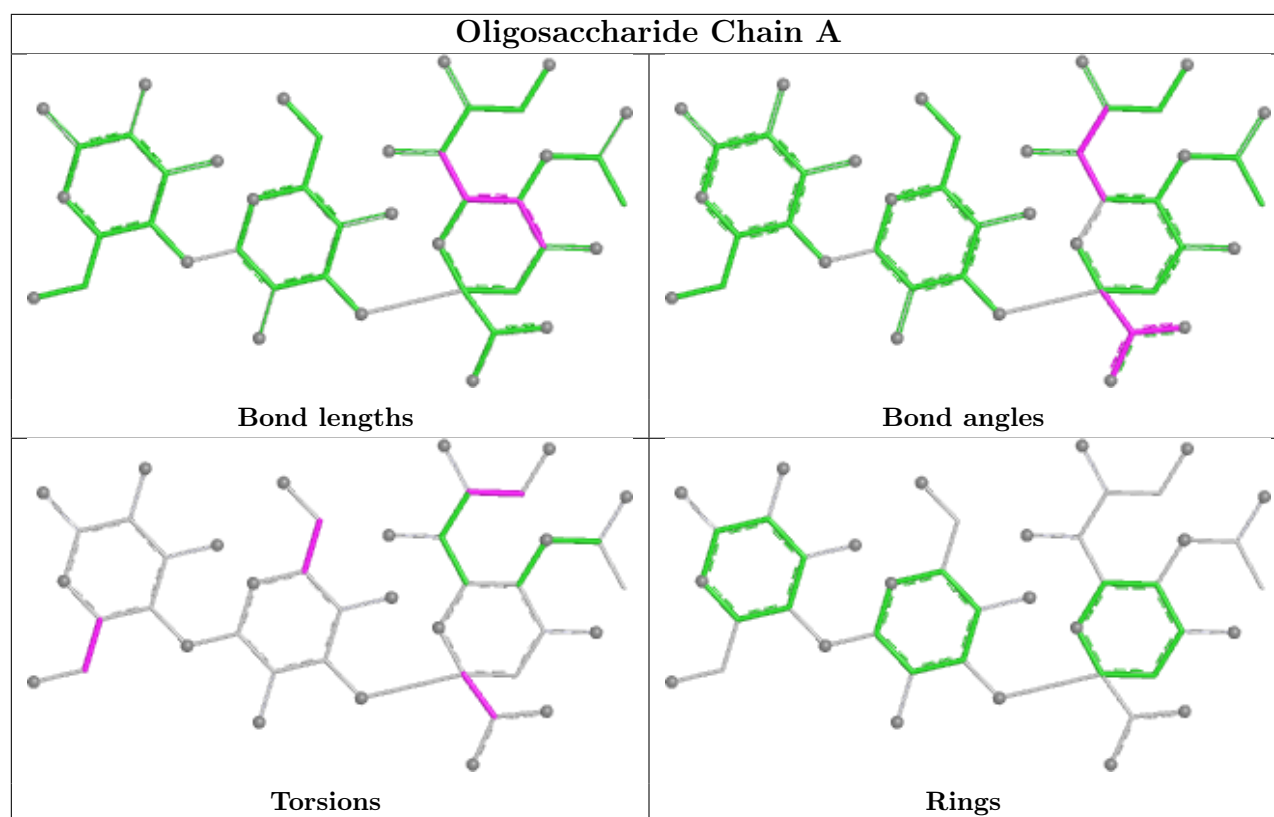
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2	GAL	O5-C5-C6-O6
5	A	1	GLC	O5-C5-C6-O6
5	A	2	GAL	C4-C5-C6-O6
5	A	1	GLC	C4-C5-C6-O6
5	A	3	SIA	O8-C8-C9-O9
5	A	3	SIA	O1A-C1-C2-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	1	247/248 (99%)	3.03	182 (73%) 0 1	2, 10, 44, 101	0
2	2	200/230 (86%)	3.06	160 (80%) 0 0	2, 6, 43, 88	0
3	3	226/226 (100%)	2.85	154 (68%) 0 1	2, 4, 26, 61	0
4	4	22/80 (27%)	4.40	20 (90%) 0 0	15, 37, 55, 71	0
All	All	695/784 (88%)	3.02	516 (74%) 0 0	2, 6, 44, 101	0

All (516) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	3	145	VAL	10.8
4	4	24	ASN	9.4
1	1	44	GLU	8.8
1	1	176	ALA	8.2
3	3	116	THR	8.2
2	2	216	ALA	8.1
2	2	147	GLU	7.7
1	1	96	SER	7.6
3	3	144	ALA	7.6
2	2	169	SER	7.5
4	4	31	GLN	7.4
2	2	136	HIS	7.4
1	1	227	ALA	7.3
2	2	137	GLU	7.1
1	1	181	LYS	7.1
2	2	105	LYS	7.1
1	1	76	THR	7.0
2	2	35	CYS	6.7
4	4	32	ASN	6.7
3	3	134	THR	6.7
1	1	110	GLY	6.6

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Mol	Chain	Res	Type	RSRZ
3	3	161	SER	6.5
1	1	157	SER	6.4
4	4	37	ASP	6.4
2	2	135	THR	6.3
3	3	168	ALA	6.3
1	1	2	THR	6.3
3	3	212	PRO	6.2
2	2	172	HIS	6.2
2	2	225	PRO	6.2
3	3	149	GLY	6.2
3	3	71	GLU	6.2
1	1	95	SER	6.1
1	1	185	ASN	6.0
3	3	69	GLY	6.0
4	4	28	GLN	6.0
1	1	97	VAL	5.9
4	4	23	GLN	5.9
3	3	137	GLU	5.7
1	1	247	CYS	5.7
3	3	65	THR	5.7
2	2	153	GLN	5.7
1	1	63	THR	5.6
1	1	233	ASP	5.6
1	1	204	LYS	5.6
1	1	134	ALA	5.6
3	3	70	ASP	5.6
1	1	3	ASN	5.5
3	3	181	GLY	5.5
3	3	20	ASP	5.5
1	1	54	THR	5.5
2	2	56	PRO	5.5
3	3	72	PRO	5.4
2	2	151	THR	5.4
1	1	244	ASN	5.3
2	2	59	SER	5.3
3	3	91	ALA	5.3
3	3	98	ALA	5.3
2	2	81	CYS	5.2
1	1	5	GLY	5.2
2	2	208	THR	5.2
3	3	200	SER	5.2
3	3	102	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
3	3	180	SER	5.2
1	1	189	GLY	5.1
2	2	120	HIS	5.1
2	2	224	GLY	5.1
2	2	72	SER	5.0
3	3	122	VAL	5.0
2	2	149	ALA	5.0
4	4	18	SER	5.0
1	1	126	ASN	5.0
1	1	11	GLY	5.0
1	1	201	ALA	4.9
3	3	87	GLY	4.9
3	3	85	LEU	4.9
2	2	44	PRO	4.9
1	1	124	GLY	4.9
3	3	68	SER	4.9
3	3	187	ALA	4.8
2	2	230	GLU	4.8
3	3	47	ALA	4.8
2	2	117	SER	4.8
3	3	169	VAL	4.8
2	2	185	ASN	4.7
1	1	4	VAL	4.7
1	1	77	TYR	4.7
2	2	96	GLU	4.7
3	3	163	PRO	4.7
1	1	136	ALA	4.7
2	2	176	PRO	4.6
3	3	165	ASP	4.6
2	2	181	GLY	4.6
3	3	128	HIS	4.6
1	1	137	GLY	4.6
2	2	144	GLU	4.6
2	2	90	LYS	4.6
3	3	35	GLN	4.6
2	2	63	THR	4.5
2	2	86	ASP	4.5
1	1	223	PRO	4.5
2	2	223	ASN	4.5
3	3	66	ASN	4.5
3	3	210	ALA	4.5
1	1	246	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	1	93	THR	4.4
1	1	90	PHE	4.4
3	3	112	GLY	4.4
2	2	148	PRO	4.4
2	2	49	ASP	4.4
1	1	61	GLY	4.4
3	3	209	SER	4.4
4	4	36	ALA	4.4
1	1	148	GLY	4.4
2	2	119	ALA	4.3
1	1	158	VAL	4.3
1	1	30	VAL	4.3
1	1	26	VAL	4.3
3	3	57	SER	4.3
1	1	57	LEU	4.3
3	3	26	TYR	4.3
3	3	14	PHE	4.3
1	1	114	LYS	4.3
1	1	151	SER	4.3
2	2	121	SER	4.3
1	1	14	GLU	4.3
1	1	58	ASP	4.2
1	1	188	PRO	4.2
3	3	155	SER	4.2
3	3	132	PRO	4.2
1	1	41	GLU	4.2
1	1	62	SER	4.2
1	1	131	GLN	4.2
1	1	205	GLY	4.2
1	1	83	GLU	4.1
4	4	20	SER	4.1
1	1	24	MET	4.1
2	2	125	CYS	4.1
1	1	42	THR	4.1
2	2	170	SER	4.1
1	1	164	TRP	4.1
3	3	88	THR	4.1
2	2	100	ALA	4.1
2	2	204	GLY	4.1
4	4	16	GLY	4.0
2	2	95	HIS	4.0
1	1	29	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	1	161	THR	4.0
2	2	184	THR	4.0
2	2	31	GLY	4.0
1	1	81	ASP	4.0
3	3	67	THR	4.0
4	4	29	GLN	4.0
3	3	203	ARG	4.0
1	1	65	GLN	3.9
1	1	236	ARG	3.9
4	4	30	TYR	3.9
4	4	35	ASP	3.9
2	2	229	PRO	3.9
3	3	82	ALA	3.9
3	3	197	ALA	3.9
1	1	52	PRO	3.9
2	2	218	ILE	3.9
2	2	61	HIS	3.9
1	1	222	ARG	3.9
3	3	173	GLU	3.9
1	1	7	ASP	3.8
2	2	193	THR	3.8
2	2	94	PHE	3.8
2	2	43	PRO	3.8
3	3	167	MET	3.8
2	2	133	GLU	3.8
1	1	116	THR	3.8
2	2	32	THR	3.8
2	2	55	GLY	3.7
2	2	217	PRO	3.7
3	3	215	SER	3.7
2	2	179	GLY	3.7
1	1	50	GLY	3.7
1	1	173	GLY	3.7
3	3	103	SER	3.7
3	3	170	TYR	3.7
3	3	42	ASN	3.7
3	3	113	ALA	3.7
2	2	45	SER	3.7
2	2	48	SER	3.7
1	1	100	GLY	3.7
2	2	82	PRO	3.7
1	1	8	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	1	150	ARG	3.6
4	4	27	MET	3.6
1	1	199	SER	3.6
1	1	240	PRO	3.6
2	2	106	ASN	3.6
2	2	58	LEU	3.6
2	2	65	LYS	3.6
1	1	203	ASP	3.5
3	3	166	PHE	3.5
1	1	228	PHE	3.5
4	4	34	ILE	3.5
3	3	22	SER	3.5
2	2	213	MET	3.5
3	3	21	ASN	3.5
2	2	77	HIS	3.5
3	3	55	SER	3.5
2	2	84	PRO	3.5
1	1	123	GLY	3.5
1	1	129	ARG	3.5
3	3	46	VAL	3.5
2	2	34	TYR	3.5
2	2	75	HIS	3.4
3	3	143	HIS	3.4
1	1	15	PRO	3.4
3	3	130	ALA	3.4
1	1	220	CYS	3.4
1	1	22	VAL	3.4
3	3	86	HIS	3.4
1	1	51	SER	3.4
1	1	168	PRO	3.4
1	1	60	PHE	3.4
1	1	107	PHE	3.4
1	1	213	PHE	3.4
1	1	82	LEU	3.4
3	3	24	PRO	3.4
3	3	105	ASN	3.4
1	1	102	VAL	3.4
3	3	121	LEU	3.4
1	1	200	ASP	3.4
3	3	95	SER	3.4
1	1	192	PHE	3.4
2	2	46	THR	3.4

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Mol	Chain	Res	Type	RSRZ
2	2	115	ASN	3.4
1	1	183	THR	3.4
2	2	116	ALA	3.4
3	3	63	GLU	3.4
3	3	127	PRO	3.4
1	1	47	ASN	3.4
1	1	243	ILE	3.4
2	2	129	VAL	3.3
2	2	197	LEU	3.3
1	1	153	ALA	3.3
3	3	80	LEU	3.3
2	2	202	LEU	3.3
3	3	222	LEU	3.3
4	4	19	GLY	3.3
1	1	174	TRP	3.3
2	2	164	ASN	3.3
3	3	202	GLY	3.3
2	2	207	GLN	3.3
3	3	1	ALA	3.3
1	1	210	ARG	3.3
1	1	207	CYS	3.3
4	4	17	ASN	3.3
1	1	53	ALA	3.2
2	2	152	TYR	3.2
3	3	81	SER	3.2
3	3	148	VAL	3.2
3	3	172	ALA	3.2
1	1	138	MET	3.2
1	1	238	LYS	3.2
3	3	129	SER	3.2
1	1	94	PRO	3.2
2	2	219	ASP	3.2
2	2	215	VAL	3.2
1	1	225	PRO	3.2
2	2	150	TYR	3.2
1	1	31	SER	3.2
1	1	139	SER	3.2
1	1	180	GLU	3.2
2	2	62	TYR	3.2
3	3	174	ALA	3.1
2	2	73	GLN	3.1
3	3	43	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
2	2	67	GLY	3.1
2	2	127	ALA	3.1
1	1	49	THR	3.1
1	1	119	TRP	3.1
2	2	138	LYS	3.1
1	1	117	ASP	3.1
1	1	198	THR	3.1
3	3	111	THR	3.1
2	2	107	GLY	3.1
1	1	182	ALA	3.1
2	2	110	VAL	3.1
1	1	17	HIS	3.1
2	2	222	VAL	3.1
2	2	206	GLY	3.0
1	1	43	LEU	3.0
3	3	13	SER	3.0
3	3	175	THR	3.0
3	3	192	THR	3.0
2	2	101	HIS	3.0
2	2	112	VAL	3.0
3	3	44	ILE	3.0
3	3	89	TYR	3.0
1	1	48	LEU	3.0
1	1	35	ASP	3.0
3	3	90	VAL	3.0
1	1	20	SER	3.0
3	3	162	SER	3.0
1	1	154	CYS	3.0
3	3	138	ALA	3.0
2	2	108	TRP	3.0
1	1	108	PRO	3.0
1	1	231	PRO	3.0
2	2	57	THR	3.0
1	1	171	TYR	3.0
2	2	39	PRO	3.0
3	3	114	ALA	3.0
3	3	204	VAL	3.0
1	1	92	THR	3.0
1	1	178	THR	3.0
1	1	179	LYS	3.0
1	1	9	GLU	3.0
2	2	194	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	2	52	THR	2.9
3	3	193	SER	2.9
2	2	186	LEU	2.9
3	3	142	ILE	2.9
3	3	50	THR	2.9
1	1	1	VAL	2.9
3	3	118	ALA	2.9
3	3	99	GLN	2.9
2	2	114	VAL	2.9
2	2	134	HIS	2.9
4	4	21	ILE	2.9
4	4	22	VAL	2.9
2	2	146	GLU	2.9
2	2	132	TYR	2.9
3	3	33	PRO	2.9
3	3	198	VAL	2.9
4	4	33	SER	2.9
3	3	196	ILE	2.9
3	3	120	PHE	2.9
1	1	23	ASP	2.9
1	1	25	HIS	2.8
1	1	187	LEU	2.8
3	3	188	LEU	2.8
1	1	193	GLY	2.8
1	1	184	TYR	2.8
3	3	159	PRO	2.8
2	2	141	LYS	2.8
2	2	54	LEU	2.8
1	1	59	PRO	2.8
2	2	190	ASN	2.8
1	1	12	GLU	2.8
1	1	194	SER	2.8
1	1	175	GLY	2.8
2	2	66	VAL	2.8
2	2	97	VAL	2.8
2	2	177	TYR	2.8
3	3	54	CYS	2.8
3	3	223	PRO	2.8
1	1	128	VAL	2.8
3	3	101	ARG	2.8
1	1	152	GLN	2.8
2	2	87	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
3	3	51	TYR	2.8
1	1	104	VAL	2.8
2	2	209	VAL	2.8
1	1	235	THR	2.8
2	2	93	SER	2.8
1	1	27	HIS	2.8
3	3	217	ARG	2.7
2	2	155	LEU	2.7
3	3	226	GLN	2.7
3	3	147	ASP	2.7
3	3	221	ASP	2.7
1	1	206	GLY	2.7
3	3	117	LYS	2.7
2	2	142	TRP	2.7
2	2	130	PRO	2.7
1	1	169	VAL	2.7
3	3	97	PHE	2.7
3	3	135	ARG	2.7
3	3	164	ALA	2.7
2	2	69	TRP	2.7
2	2	205	PRO	2.7
1	1	133	LEU	2.7
2	2	42	ARG	2.7
3	3	77	ASP	2.6
2	2	166	ARG	2.6
1	1	121	LEU	2.6
1	1	186	TRP	2.6
3	3	41	THR	2.6
1	1	191	HIS	2.6
1	1	234	LYS	2.6
1	1	45	LEU	2.6
2	2	111	VAL	2.6
3	3	34	ARG	2.6
1	1	147	ALA	2.6
3	3	176	VAL	2.6
1	1	239	PHE	2.5
2	2	201	GLU	2.5
3	3	141	CYS	2.5
1	1	80	SER	2.5
1	1	84	LEU	2.5
1	1	162	SER	2.5
1	1	135	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	3	125	VAL	2.5
3	3	211	GLY	2.5
3	3	49	GLN	2.5
2	2	228	ASN	2.5
2	2	220	ALA	2.5
1	1	78	PHE	2.5
3	3	151	ASN	2.5
3	3	23	THR	2.5
2	2	40	ASP	2.5
1	1	156	PHE	2.5
1	1	103	TRP	2.5
2	2	98	VAL	2.5
3	3	177	VAL	2.5
2	2	33	THR	2.5
3	3	45	ASP	2.5
2	2	203	THR	2.5
2	2	118	PHE	2.5
3	3	110	PHE	2.5
2	2	79	TRP	2.5
1	1	28	THR	2.4
2	2	187	THR	2.4
1	1	242	ASN	2.4
2	2	145	LEU	2.4
3	3	189	THR	2.4
2	2	47	VAL	2.4
2	2	76	GLY	2.4
1	1	190	ALA	2.4
1	1	170	PHE	2.4
1	1	208	TYR	2.4
3	3	107	TYR	2.4
1	1	241	THR	2.4
1	1	99	GLU	2.4
2	2	161	GLN	2.4
1	1	112	PRO	2.4
3	3	195	ASP	2.4
2	2	226	LEU	2.4
2	2	109	ASP	2.4
3	3	6	VAL	2.4
1	1	196	LEU	2.4
2	2	113	GLN	2.4
2	2	128	ALA	2.4
3	3	190	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
3	3	219	PRO	2.3
1	1	85	SER	2.3
2	2	53	ARG	2.3
3	3	218	HIS	2.3
1	1	32	PHE	2.3
3	3	40	PHE	2.3
3	3	75	GLN	2.3
1	1	69	ALA	2.3
1	1	226	PRO	2.3
2	2	104	VAL	2.3
3	3	11	SER	2.3
2	2	103	LEU	2.3
1	1	98	GLY	2.3
3	3	79	SER	2.3
3	3	160	TYR	2.3
1	1	132	GLN	2.3
3	3	84	GLU	2.2
1	1	232	ALA	2.2
2	2	199	LEU	2.2
2	2	211	VAL	2.2
2	2	227	PRO	2.2
3	3	19	PRO	2.2
2	2	143	SER	2.2
3	3	119	LYS	2.2
1	1	40	VAL	2.2
2	2	174	VAL	2.2
2	2	210	PRO	2.2
2	2	189	HIS	2.2
1	1	68	TRP	2.2
2	2	162	LEU	2.2
2	2	167	THR	2.2
2	2	178	ILE	2.2
1	1	87	GLN	2.2
3	3	185	VAL	2.2
1	1	73	ASN	2.2
2	2	50	PRO	2.2
1	1	202	HIS	2.2
2	2	85	SER	2.2
2	2	140	LEU	2.2
2	2	126	VAL	2.2
1	1	155	GLY	2.2
1	1	214	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
3	3	133	LYS	2.2
3	3	92	SER	2.2
3	3	78	VAL	2.2
1	1	163	MET	2.1
2	2	64	PHE	2.1
2	2	36	TYR	2.1
1	1	75	CYS	2.1
3	3	30	VAL	2.1
3	3	36	VAL	2.1
1	1	215	ARG	2.1
3	3	194	THR	2.1
2	2	154	GLN	2.1
3	3	124	PHE	2.1
3	3	199	ASN	2.1
3	3	4	ARG	2.1
1	1	211	TYR	2.1
2	2	71	HIS	2.1
2	2	183	THR	2.1
2	2	157	VAL	2.1
3	3	216	LEU	2.1
3	3	2	PRO	2.1
1	1	165	ARG	2.0
2	2	99	LYS	2.0
3	3	93	LEU	2.0
1	1	13	THR	2.0
2	2	180	PRO	2.0
2	2	173	LEU	2.0
3	3	62	PHE	2.0
2	2	41	GLY	2.0
1	1	66	LEU	2.0
1	1	86	ILE	2.0
3	3	61	TYR	2.0
1	1	88	PHE	2.0

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

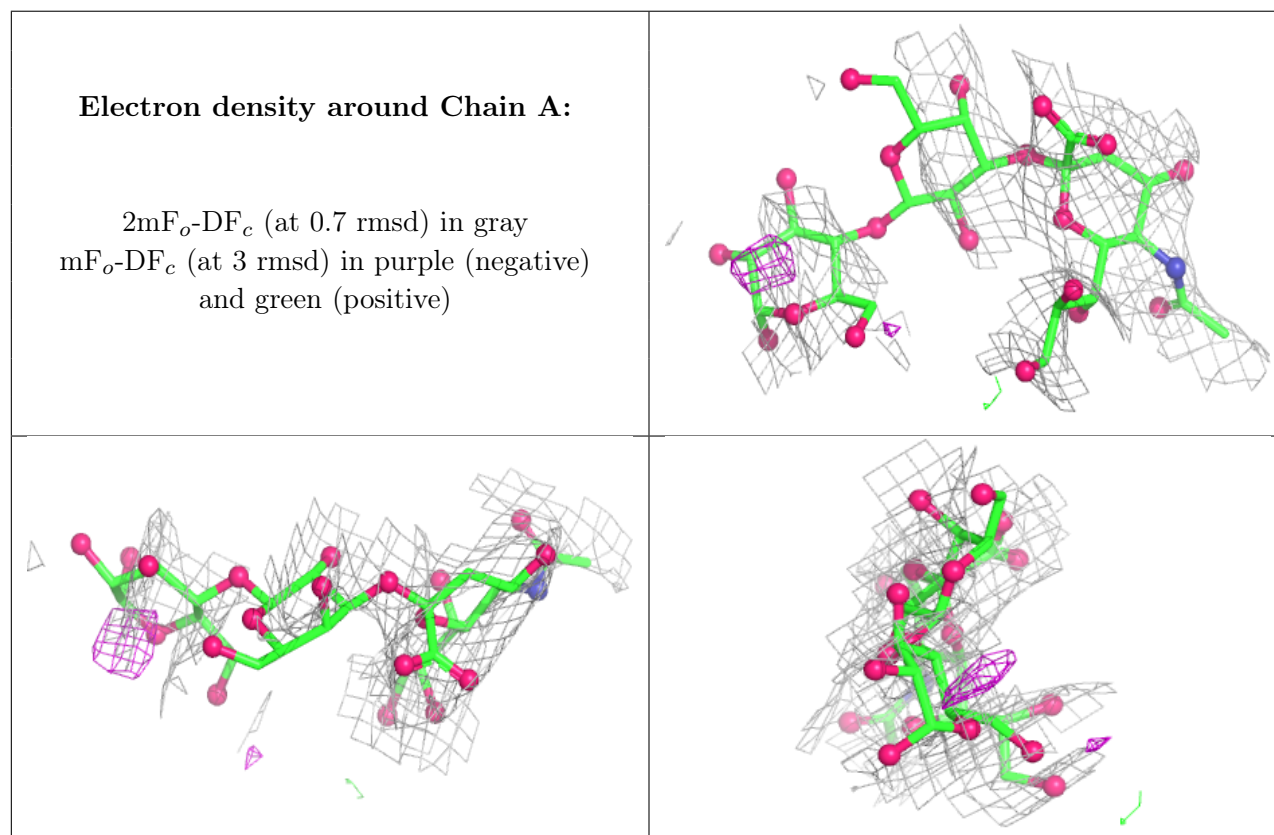
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [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
5	GLC	A	1	12/12	-	-	62,73,74,75	12
5	GAL	A	2	11/12	-	-	35,47,53,55	11
5	SIA	A	3	20/21	-	-	3,18,26,27	20

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.