



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:07 PM GMT

PDB ID : 1J4T
Title : Structure of Artocarpin: a Lectin with Mannose Specificity (Form 2)
Authors : Pratap, J.V.; Jeyaprakash, A.A.; Rani, P.G.; Sekar, K.; Surolia, A.; Vijayan, M.
Deposited on : 2001-10-30
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

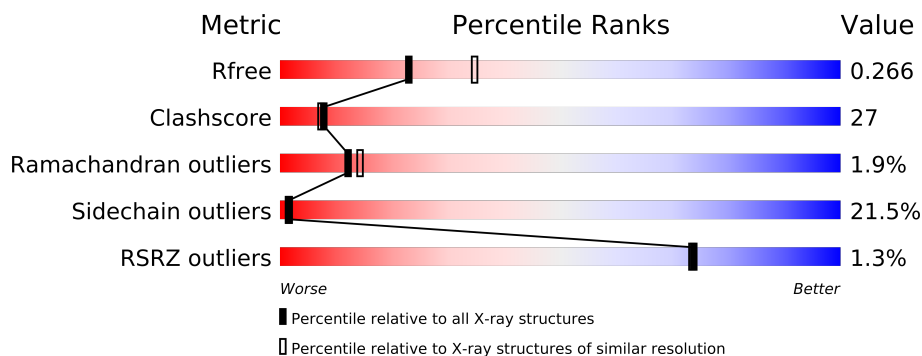
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	149	
1	B	149	
1	C	149	
1	D	149	
1	E	149	
1	F	149	
1	G	149	
1	H	149	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9922 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Artocarpin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	B	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	C	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	D	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	E	149	Total	C	N	O	S	0	0	0
			1128	724	181	222	1			
1	F	149	Total	C	N	O	S	0	0	0
			1128	724	181	222	1			
1	G	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	H	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
A	9	SER	PRO	CONFLICT	UNP Q7M1T4
A	20	GLU	ASP	CONFLICT	UNP Q7M1T4
A	49	ASP	GLU	CONFLICT	UNP Q7M1T4
A	70	LYS	ARG	CONFLICT	UNP Q7M1T4
A	84	GLY	ALA	CONFLICT	UNP Q7M1T4
A	145	ILE	VAL	CONFLICT	UNP Q7M1T4
A	148	SER	ALA	CONFLICT	UNP Q7M1T4
B	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
B	9	SER	PRO	CONFLICT	UNP Q7M1T4
B	20	GLU	ASP	CONFLICT	UNP Q7M1T4
B	49	ASP	GLU	CONFLICT	UNP Q7M1T4
B	70	LYS	ARG	CONFLICT	UNP Q7M1T4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	84	GLY	ALA	CONFLICT	UNP Q7M1T4
B	145	ILE	VAL	CONFLICT	UNP Q7M1T4
B	148	SER	ALA	CONFLICT	UNP Q7M1T4
C	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
C	9	SER	PRO	CONFLICT	UNP Q7M1T4
C	20	GLU	ASP	CONFLICT	UNP Q7M1T4
C	49	ASP	GLU	CONFLICT	UNP Q7M1T4
C	70	LYS	ARG	CONFLICT	UNP Q7M1T4
C	84	GLY	ALA	CONFLICT	UNP Q7M1T4
C	145	ILE	VAL	CONFLICT	UNP Q7M1T4
C	148	SER	ALA	CONFLICT	UNP Q7M1T4
D	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
D	9	SER	PRO	CONFLICT	UNP Q7M1T4
D	20	GLU	ASP	CONFLICT	UNP Q7M1T4
D	49	ASP	GLU	CONFLICT	UNP Q7M1T4
D	70	LYS	ARG	CONFLICT	UNP Q7M1T4
D	84	GLY	ALA	CONFLICT	UNP Q7M1T4
D	145	ILE	VAL	CONFLICT	UNP Q7M1T4
D	148	SER	ALA	CONFLICT	UNP Q7M1T4
E	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
E	9	SER	PRO	CONFLICT	UNP Q7M1T4
E	20	GLU	ASP	CONFLICT	UNP Q7M1T4
E	49	ASP	GLU	CONFLICT	UNP Q7M1T4
E	70	LYS	ARG	CONFLICT	UNP Q7M1T4
E	84	GLY	ALA	CONFLICT	UNP Q7M1T4
E	145	ILE	VAL	CONFLICT	UNP Q7M1T4
E	148	SER	ALA	CONFLICT	UNP Q7M1T4
F	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
F	9	SER	PRO	CONFLICT	UNP Q7M1T4
F	20	GLU	ASP	CONFLICT	UNP Q7M1T4
F	49	ASP	GLU	CONFLICT	UNP Q7M1T4
F	70	LYS	ARG	CONFLICT	UNP Q7M1T4
F	84	GLY	ALA	CONFLICT	UNP Q7M1T4
F	145	ILE	VAL	CONFLICT	UNP Q7M1T4
F	148	SER	ALA	CONFLICT	UNP Q7M1T4
G	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
G	9	SER	PRO	CONFLICT	UNP Q7M1T4
G	20	GLU	ASP	CONFLICT	UNP Q7M1T4
G	49	ASP	GLU	CONFLICT	UNP Q7M1T4
G	70	LYS	ARG	CONFLICT	UNP Q7M1T4
G	84	GLY	ALA	CONFLICT	UNP Q7M1T4
G	145	ILE	VAL	CONFLICT	UNP Q7M1T4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	148	SER	ALA	CONFLICT	UNP Q7M1T4
H	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
H	9	SER	PRO	CONFLICT	UNP Q7M1T4
H	20	GLU	ASP	CONFLICT	UNP Q7M1T4
H	49	ASP	GLU	CONFLICT	UNP Q7M1T4
H	70	LYS	ARG	CONFLICT	UNP Q7M1T4
H	84	GLY	ALA	CONFLICT	UNP Q7M1T4
H	145	ILE	VAL	CONFLICT	UNP Q7M1T4
H	148	SER	ALA	CONFLICT	UNP Q7M1T4

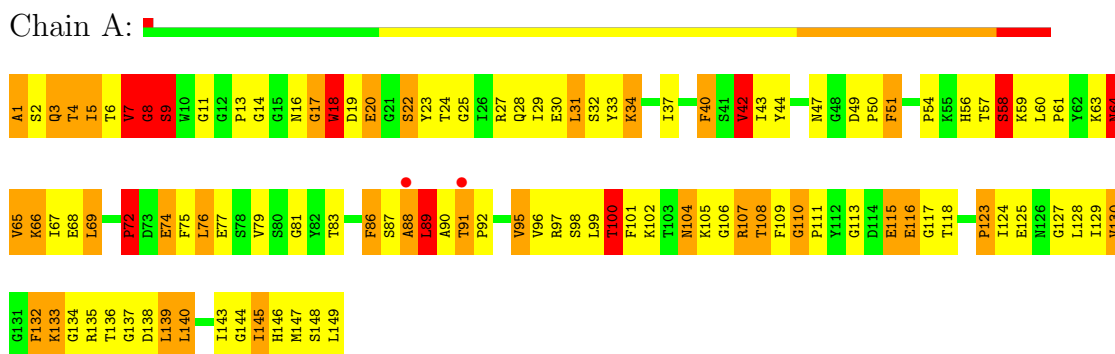
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	118	Total O 118 118	0	0
2	B	123	Total O 123 123	0	0
2	C	121	Total O 121 121	0	0
2	D	121	Total O 121 121	0	0
2	E	93	Total O 93 93	0	0
2	F	115	Total O 115 115	0	0
2	G	102	Total O 102 102	0	0
2	H	81	Total O 81 81	0	0

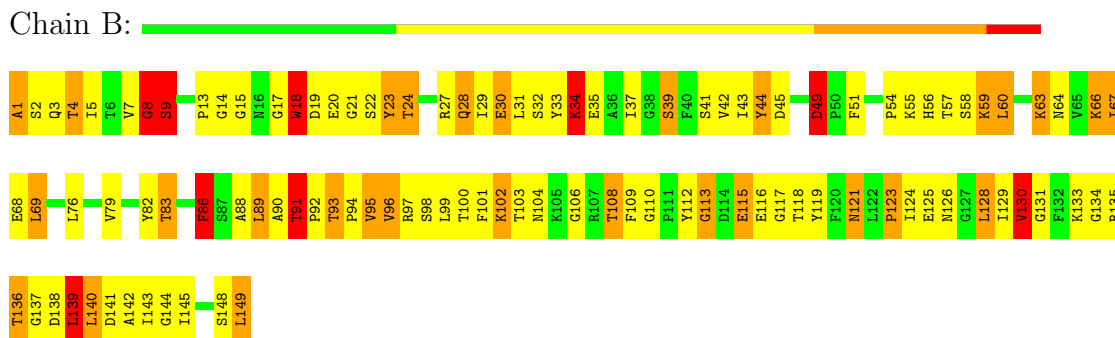
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

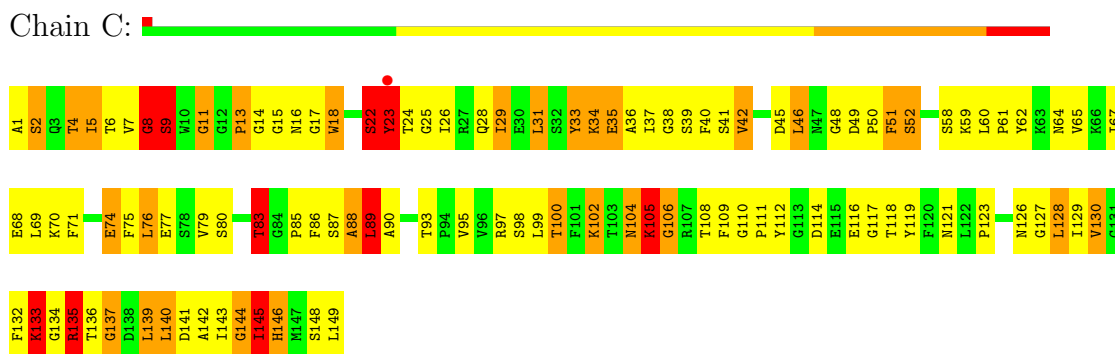
• Molecule 1: Artocarpin



• Molecule 1: Artocarpin



• Molecule 1: Artocarpin



• Molecule 1: Artocarpin

I129	I130	I131	I132	I133	I134	I135	I136	I137	I138	I139	I140	I141	I142	I143	I144	I145	I146	I147	I148	I149	I150	I151	I152	I153	I154	I155	I156	I157	I158	I159	I160	I161	I162	I163	I164	I165	I166	I167	I168	I169	I170	I171	I172	I173	I174	I175	I176	I177	I178	I179	I180	I181	I182	I183	I184	I185	I186	I187	I188	I189	I190	I191	I192	I193	I194	I195	I196	I197	I198	I199	I200	I201	I202	I203	I204	I205	I206	I207	I208	I209	I210	I211	I212	I213	I214	I215	I216	I217	I218	I219	I220	I221	I222	I223	I224	I225	I226	I227	I228	I229	I230	I231	I232	I233	I234	I235	I236	I237	I238	I239	I240	I241	I242	I243	I244	I245	I246	I247	I248	I249	I250	I251	I252	I253	I254	I255	I256	I257	I258	I259	I260	I261	I262	I263	I264	I265	I266	I267	I268	I269	I270	I271	I272	I273	I274	I275	I276	I277	I278	I279	I280	I281	I282	I283	I284	I285	I286	I287	I288	I289	I290	I291	I292	I293	I294	I295	I296	I297	I298	I299	I300	I301	I302	I303	I304	I305	I306	I307	I308	I309	I310	I311	I312	I313	I314	I315	I316	I317	I318	I319	I320	I321	I322	I323	I324	I325	I326	I327	I328	I329	I330	I331	I332	I333	I334	I335	I336	I337	I338	I339	I340	I341	I342	I343	I344	I345	I346	I347	I348	I349	I350	I351	I352	I353	I354	I355	I356	I357	I358	I359	I360	I361	I362	I363	I364	I365	I366	I367	I368	I369	I370	I371	I372	I373	I374	I375	I376	I377	I378	I379	I380	I381	I382	I383	I384	I385	I386	I387	I388	I389	I390	I391	I392	I393	I394	I395	I396	I397	I398	I399	I400	I401	I402	I403	I404	I405	I406	I407	I408	I409	I410	I411	I412	I413	I414	I415	I416	I417	I418	I419	I420	I421	I422	I423	I424	I425	I426	I427	I428	I429	I430	I431	I432	I433	I434	I435	I436	I437	I438	I439	I440	I441	I442	I443	I444	I445	I446	I447	I448	I449	I450	I451	I452	I453	I454	I455	I456	I457	I458	I459	I460	I461	I462	I463	I464	I465	I466	I467	I468	I469	I470	I471	I472	I473	I474	I475	I476	I477	I478	I479	I480	I481	I482	I483	I484	I485	I486	I487	I488	I489	I490	I491	I492	I493	I494	I495	I496	I497	I498	I499	I500	I501	I502	I503	I504	I505	I506	I507	I508	I509	I510	I511	I512	I513	I514	I515	I516	I517	I518	I519	I520	I521	I522	I523	I524	I525	I526	I527	I528	I529	I530	I531	I532	I533	I534	I535	I536	I537	I538	I539	I540	I541	I542	I543	I544	I545	I546	I547	I548	I549	I550	I551	I552	I553	I554	I555	I556	I557	I558	I559	I560	I561	I562	I563	I564	I565	I566	I567	I568	I569	I570	I571	I572	I573	I574	I575	I576	I577	I578	I579	I580	I581	I582	I583	I584	I585	I586	I587	I588	I589	I590	I591	I592	I593	I594	I595	I596	I597	I598	I599	I600	I601	I602	I603	I604	I605	I606	I607	I608	I609	I610	I611	I612	I613	I614	I615	I616	I617	I618	I619	I620	I621	I622	I623	I624	I625	I626	I627	I628	I629	I630	I631	I632	I633	I634	I635	I636	I637	I638	I639	I64
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Chain E:

A142	I143	H146	M147	S148	L149																																																
K70	F75	L76	E77	G81	Y82	T83	G84	P85	F86	S87	A88	L89	A90	T91	P92	T93	P94	Y95	S98	L99	T100	F101	K102	T103	N104	K105	G106	R107	T108	F109	G110	G113	D114	E115	E116	G117	T118	P123	I124	E125	N126	G127	V130	K133	G134	R135	T136	G137	D138	L139	L140	P141	
A1	T4	I5	T6	V7	G8	S9	W10	G11	G12	P13	G14	G15	N16	G17	W18	D19	E20	G21	S22	Y23	T24	G25	I26	R27	Q28	I29	S32	Y33	K34	I37	Y42	I43	Y44	G48	D49	P50	F51	S52	G53	P54	K55	H56	T57	L60	P61	Y62	K63	M64	V65	K66	I67	E68	L69

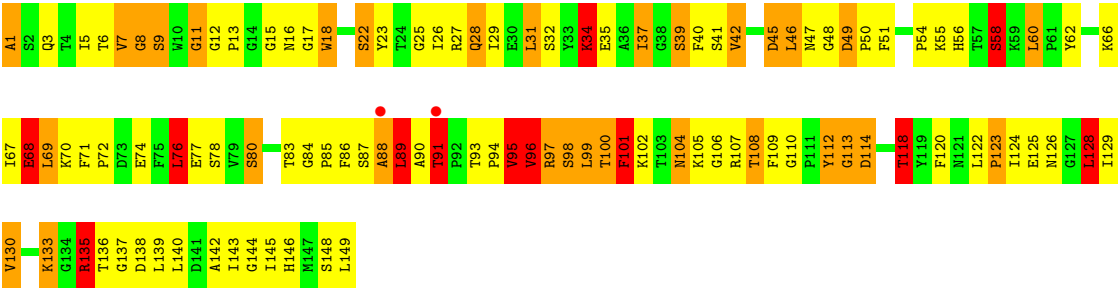
Chain F:

G131	E68	A1
F132	L69	S2
K133	K70	Q3
G134	F71	T4
R135	F72	V7
T136	D73	S8
G137	E74	G9
D138	F75	S9
L139	L76	G14
L140	E77	G15
D141	S78	H16
	V79	G17
G144	S80	W18
I145	E81	D19
H146	H82	E20
M147	T83	G21
S148		S22
L149	S87	Y23
	A88	T24
	L89	G25
	A90	I26
	T91	R27
		Q28
	P94	I29
	V95	E30
	R97	L31
	S98	S32
	I99	Y33
	T100	K34
	F101	E35
	K102	A36
	T103	I37
	N104	G38
	K105	S39
	G106	F40
	R107	S41
	T108	V42
	F109	I43
	G110	Y44
	P111	D45
	Y112	L46
	G113	N47
	D114	G48
	E115	F51
	H116	S52
	T118	G53
	Y119	P54
	F120	K55
	N121	H56
	L122	T57
	P123	S58
	I124	K59
	E125	L60
	N126	P61
	G127	Y62
	L128	K63
	I129	T64
	K130	S65

Chain G:

R135	L69	A1
T136	K70	S2
L139	F71	Q3
L140	P72	T4
D141	D73	I5
A142	E74	T6
A143	F75	V7
G144	L76	G8
I145	E77	S9
H146	S78	W10
H147	V79	G11
S148	S80	
L149	G81	G15
	Y82	M16
	T83	G17
		M18
	F86	D19
	S87	E20
	A88	
	L89	Y23
	A90	T24
	T91	G25
	P92	I26
	T93	K27
	P94	Q28
	V95	I29
	V96	E30
	R97	L31
	S98	S32
	L99	Y33
	T100	K34
	F101	E35
	K102	A36
	T103	I37
	N104	G38
	K105	S39
	G106	F40
	R107	S41
	T108	V42
	F109	I43
		Y44
	E116	D45
	G117	L46
	T118	
	Y119	D49
	F120	P50
	N121	F51
	L122	
	P123	P54
	I124	K55
	E125	
	G126	K59
	T127	L60
	L128	P61
	I129	Y62
	V130	K63
	G131	
	F132	K66
	K133	I67
	C134	S68

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.69Å 72.19Å 92.63Å 90.00° 101.15° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 10.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.40) 83.5 (10.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.41Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.191 , 0.258 0.207 , 0.266	Depositor DCC
R_{free} test set	1536 reflections (4.18%)	DCC
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 46.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 36759 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9922	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.61 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.0588e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	1.08	4/1155 (0.3%)	2.09	74/1569 (4.7%)
1	B	1.03	6/1155 (0.5%)	2.09	66/1569 (4.2%)
1	C	1.06	5/1155 (0.4%)	2.21	79/1569 (5.0%)
1	D	0.97	5/1155 (0.4%)	2.31	82/1569 (5.2%)
1	E	0.99	3/1151 (0.3%)	2.40	77/1565 (4.9%)
1	F	1.50	6/1151 (0.5%)	2.31	70/1565 (4.5%)
1	G	1.52	3/1155 (0.3%)	2.20	68/1569 (4.3%)
1	H	0.96	1/1155 (0.1%)	2.31	73/1569 (4.7%)
All	All	1.16	33/9232 (0.4%)	2.24	589/12544 (4.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	8
1	B	1	4
1	C	1	8
1	D	0	5
1	E	1	5
1	F	0	7
1	G	1	5
1	H	1	4
All	All	6	46

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	70	LYS	CD-CE	39.71	2.50	1.51
1	F	70	LYS	CD-CE	37.27	2.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	33	TYR	C-N	11.14	1.59	1.34
1	A	34	LYS	C-N	10.43	1.58	1.34
1	C	33	TYR	C-N	9.15	1.55	1.34
1	F	34	LYS	C-N	8.37	1.53	1.34
1	F	90	ALA	C-N	-8.32	1.15	1.34
1	A	68	GLU	CD-OE1	6.63	1.32	1.25
1	B	89	LEU	C-N	-6.58	1.19	1.34
1	C	68	GLU	CD-OE1	6.46	1.32	1.25
1	E	68	GLU	CD-OE2	6.42	1.32	1.25
1	C	133	LYS	CE-NZ	6.37	1.65	1.49
1	E	33	TYR	C-N	6.25	1.48	1.34
1	B	59	LYS	C-O	-6.16	1.11	1.23
1	D	8	GLY	C-N	-6.10	1.20	1.34
1	C	22	SER	C-N	-6.08	1.20	1.34
1	B	68	GLU	CD-OE1	6.01	1.32	1.25
1	F	9	SER	C-N	-5.96	1.20	1.34
1	H	68	GLU	CG-CD	5.96	1.60	1.51
1	F	70	LYS	CE-NZ	-5.91	1.34	1.49
1	F	22	SER	C-N	-5.79	1.20	1.34
1	E	133	LYS	CE-NZ	5.72	1.63	1.49
1	C	68	GLU	CD-OE2	5.69	1.31	1.25
1	A	68	GLU	CD-OE2	5.66	1.31	1.25
1	B	34	LYS	CE-NZ	5.61	1.63	1.49
1	D	34	LYS	CE-NZ	5.58	1.62	1.49
1	G	70	LYS	CE-NZ	-5.51	1.35	1.49
1	B	68	GLU	CD-OE2	5.44	1.31	1.25
1	D	33	TYR	C-N	-5.41	1.21	1.34
1	D	68	GLU	CD-OE2	5.35	1.31	1.25
1	A	68	GLU	CB-CG	-5.25	1.42	1.52
1	G	96	VAL	CA-CB	5.04	1.65	1.54
1	D	34	LYS	C-N	-5.04	1.22	1.34

All (589) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	34	LYS	O-C-N	-36.39	64.47	122.70
1	G	70	LYS	CD-CE-NZ	-35.79	29.38	111.70
1	F	70	LYS	CD-CE-NZ	-35.17	30.80	111.70
1	D	34	LYS	O-C-N	-28.27	77.46	122.70
1	H	9	SER	O-C-N	-27.94	77.99	122.70
1	E	34	LYS	CA-C-N	22.48	166.66	117.20
1	H	89	LEU	O-C-N	-19.77	91.07	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	9	SER	CA-C-N	18.79	158.54	117.20
1	C	89	LEU	O-C-N	-18.52	93.07	122.70
1	C	9	SER	O-C-N	-18.40	93.26	122.70
1	F	9	SER	O-C-N	-17.72	94.35	122.70
1	D	8	GLY	C-N-CA	17.15	164.58	121.70
1	D	8	GLY	O-C-N	-16.94	95.60	122.70
1	B	9	SER	O-C-N	-16.78	95.85	122.70
1	E	8	GLY	O-C-N	-16.09	96.96	122.70
1	A	33	TYR	O-C-N	-15.50	97.90	122.70
1	D	34	LYS	CA-C-N	15.37	151.01	117.20
1	A	34	LYS	O-C-N	-14.96	98.76	122.70
1	F	90	ALA	O-C-N	-14.56	99.40	122.70
1	E	8	GLY	C-N-CA	14.16	157.10	121.70
1	B	8	GLY	O-C-N	-14.02	100.28	122.70
1	F	89	LEU	CA-CB-CG	13.90	147.26	115.30
1	D	33	TYR	O-C-N	-13.73	100.74	122.70
1	E	34	LYS	CB-CA-C	-13.32	83.77	110.40
1	B	34	LYS	O-C-N	-12.86	102.12	122.70
1	G	8	GLY	O-C-N	-12.60	102.54	122.70
1	H	90	ALA	O-C-N	12.29	142.36	122.70
1	E	33	TYR	C-N-CA	-11.85	92.07	121.70
1	C	23	TYR	O-C-N	-11.29	104.63	122.70
1	H	90	ALA	CA-C-N	-11.27	92.41	117.20
1	D	9	SER	O-C-N	-11.03	105.05	122.70
1	E	9	SER	O-C-N	-10.89	105.27	122.70
1	H	89	LEU	CB-CG-CD1	10.81	129.38	111.00
1	D	22	SER	O-C-N	-9.93	106.82	122.70
1	C	8	GLY	O-C-N	-9.69	107.19	122.70
1	E	34	LYS	C-N-CA	9.66	145.85	121.70
1	F	70	LYS	CG-CD-CE	9.62	140.76	111.90
1	B	8	GLY	C-N-CA	9.53	145.52	121.70
1	B	33	TYR	C-N-CA	-9.24	98.59	121.70
1	E	8	GLY	CA-C-N	9.20	137.44	117.20
1	B	89	LEU	C-N-CA	9.09	144.42	121.70
1	H	8	GLY	O-C-N	-8.91	108.44	122.70
1	A	33	TYR	CA-C-N	8.84	136.64	117.20
1	F	89	LEU	C-N-CA	8.83	143.78	121.70
1	F	9	SER	CA-C-N	8.81	136.58	117.20
1	A	8	GLY	O-C-N	-8.75	108.70	122.70
1	C	89	LEU	C-N-CA	8.73	143.53	121.70
1	H	135	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	G	8	GLY	C-N-CA	8.30	142.45	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	34	LYS	O-C-N	-8.20	109.58	122.70
1	C	22	SER	O-C-N	-8.17	109.62	122.70
1	H	9	SER	C-N-CA	8.13	142.03	121.70
1	G	88	ALA	O-C-N	-8.10	109.75	122.70
1	B	89	LEU	O-C-N	-8.05	109.83	122.70
1	H	135	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	C	128	LEU	CA-CB-CG	8.01	133.73	115.30
1	E	81	GLY	N-CA-C	7.97	133.03	113.10
1	F	33	TYR	O-C-N	-7.90	110.06	122.70
1	F	22	SER	O-C-N	-7.87	110.11	122.70
1	D	9	SER	N-CA-C	-7.81	89.91	111.00
1	D	8	GLY	CA-C-N	7.78	134.31	117.20
1	G	9	SER	N-CA-C	-7.75	90.07	111.00
1	C	9	SER	CA-C-N	7.75	134.24	117.20
1	H	149	LEU	CA-CB-CG	7.71	133.03	115.30
1	C	89	LEU	CA-C-N	7.70	134.14	117.20
1	C	8	GLY	C-N-CA	7.66	140.84	121.70
1	C	89	LEU	CA-CB-CG	7.62	132.83	115.30
1	A	99	LEU	CA-CB-CG	7.61	132.80	115.30
1	H	9	SER	N-CA-C	-7.54	90.63	111.00
1	F	89	LEU	O-C-N	-7.50	110.70	122.70
1	H	8	GLY	C-N-CA	7.45	140.31	121.70
1	E	81	GLY	O-C-N	-7.41	110.84	122.70
1	B	89	LEU	CA-CB-CG	7.34	132.19	115.30
1	D	129	ILE	O-C-N	-7.30	111.01	122.70
1	D	123	PRO	O-C-N	-7.27	111.07	122.70
1	C	149	LEU	CA-CB-CG	7.27	132.01	115.30
1	B	9	SER	CA-C-N	7.25	133.16	117.20
1	B	69	LEU	CA-CB-CG	7.13	131.70	115.30
1	C	49	ASP	CB-CG-OD1	7.09	124.68	118.30
1	E	9	SER	N-CA-C	-7.03	92.02	111.00
1	A	81	GLY	O-C-N	-7.02	111.47	122.70
1	H	146	HIS	O-C-N	-6.97	111.55	122.70
1	F	38	GLY	O-C-N	-6.95	111.58	122.70
1	D	22	SER	C-N-CA	6.94	139.05	121.70
1	B	89	LEU	CB-CA-C	6.93	123.36	110.20
1	G	29	ILE	O-C-N	-6.92	111.62	122.70
1	H	113	GLY	O-C-N	-6.89	111.67	122.70
1	B	41	SER	O-C-N	-6.89	111.68	122.70
1	D	34	LYS	C-N-CA	6.86	138.85	121.70
1	A	17	GLY	O-C-N	-6.85	111.75	122.70
1	A	4	THR	O-C-N	-6.84	111.76	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	95	VAL	O-C-N	-6.83	111.77	122.70
1	C	99	LEU	O-C-N	-6.79	111.84	122.70
1	D	83	THR	O-C-N	-6.78	111.67	123.20
1	H	99	LEU	CA-CB-CG	6.78	130.89	115.30
1	E	101	PHE	O-C-N	-6.75	111.89	122.70
1	D	9	SER	CA-C-N	6.75	132.05	117.20
1	D	33	TYR	CA-C-N	6.75	132.05	117.20
1	A	37	ILE	O-C-N	-6.73	111.75	123.20
1	A	133	LYS	O-C-N	-6.72	111.78	123.20
1	E	123	PRO	O-C-N	-6.67	112.02	122.70
1	G	4	THR	O-C-N	-6.67	112.03	122.70
1	F	89	LEU	CB-CG-CD2	-6.66	99.67	111.00
1	A	113	GLY	O-C-N	-6.66	112.04	122.70
1	C	95	VAL	O-C-N	-6.66	112.05	122.70
1	G	15	GLY	O-C-N	-6.64	112.07	122.70
1	F	29	ILE	O-C-N	-6.61	112.13	122.70
1	G	33	TYR	O-C-N	-6.59	112.16	122.70
1	F	130	VAL	O-C-N	-6.57	112.03	123.20
1	C	139	LEU	O-C-N	-6.57	112.19	122.70
1	B	143	ILE	O-C-N	-6.55	112.06	123.20
1	H	90	ALA	C-N-CA	-6.54	105.35	121.70
1	G	76	LEU	O-C-N	-6.52	112.26	122.70
1	D	128	LEU	CA-CB-CG	6.52	130.30	115.30
1	G	6	THR	O-C-N	-6.50	112.30	122.70
1	D	24	THR	O-C-N	-6.50	112.15	123.20
1	E	55	LYS	O-C-N	-6.49	112.33	122.70
1	C	129	ILE	O-C-N	-6.48	112.33	122.70
1	F	69	LEU	O-C-N	-6.48	112.33	122.70
1	B	139	LEU	CA-CB-CG	6.47	130.19	115.30
1	H	88	ALA	O-C-N	-6.42	112.42	122.70
1	A	9	SER	N-CA-C	-6.42	93.66	111.00
1	H	32	SER	O-C-N	-6.42	112.43	122.70
1	F	91	THR	N-CA-C	-6.41	93.69	111.00
1	G	99	LEU	O-C-N	-6.41	112.44	122.70
1	C	22	SER	C-N-CA	6.39	137.67	121.70
1	C	106	GLY	O-C-N	-6.39	112.48	122.70
1	C	114	ASP	O-C-N	-6.38	112.50	122.70
1	H	46	LEU	O-C-N	-6.37	112.52	122.70
1	B	106	GLY	O-C-N	-6.36	112.52	122.70
1	B	134	GLY	O-C-N	-6.36	112.53	122.70
1	E	100	THR	O-C-N	-6.34	112.55	122.70
1	A	127	GLY	O-C-N	-6.34	112.55	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	LEU	CA-CB-CG	6.32	129.84	115.30
1	D	100	THR	O-C-N	-6.32	112.59	122.70
1	H	120	PHE	O-C-N	-6.29	112.64	122.70
1	C	99	LEU	CA-CB-CG	6.28	129.75	115.30
1	F	134	GLY	O-C-N	-6.28	112.65	122.70
1	H	135	ARG	O-C-N	-6.28	112.66	122.70
1	A	68	GLU	O-C-N	-6.27	112.67	122.70
1	E	17	GLY	O-C-N	-6.25	112.70	122.70
1	A	13	PRO	O-C-N	-6.23	112.60	123.20
1	G	51	PHE	O-C-N	-6.23	112.73	122.70
1	B	89	LEU	CB-CG-CD1	-6.23	100.41	111.00
1	H	98	SER	O-C-N	-6.23	112.73	122.70
1	E	62	TYR	O-C-N	-6.23	112.73	122.70
1	F	89	LEU	CB-CA-C	6.23	122.03	110.20
1	D	114	ASP	O-C-N	-6.22	112.75	122.70
1	G	121	ASN	O-C-N	-6.22	112.75	122.70
1	A	146	HIS	O-C-N	-6.21	112.77	122.70
1	B	144	GLY	O-C-N	-6.20	112.78	122.70
1	F	140	LEU	O-C-N	-6.19	112.79	122.70
1	B	86	PHE	O-C-N	-6.18	112.81	122.70
1	C	135	ARG	O-C-N	-6.16	112.84	122.70
1	B	29	ILE	O-C-N	-6.15	112.86	122.70
1	E	141	ASP	O-C-N	-6.15	112.86	122.70
1	F	76	LEU	O-C-N	-6.14	112.87	122.70
1	D	108	THR	O-C-N	-6.14	112.88	122.70
1	F	55	LYS	O-C-N	-6.13	112.88	122.70
1	H	128	LEU	O-C-N	-6.13	112.89	122.70
1	B	133	LYS	O-C-N	-6.13	112.78	123.20
1	H	91	THR	N-CA-C	-6.13	94.46	111.00
1	E	146	HIS	O-C-N	-6.12	112.91	122.70
1	F	95	VAL	O-C-N	-6.12	112.91	122.70
1	D	87	SER	O-C-N	-6.12	112.92	122.70
1	E	104	ASN	O-C-N	-6.11	112.93	122.70
1	F	3	GLN	O-C-N	-6.09	112.96	122.70
1	H	54	PRO	O-C-N	-6.09	112.96	122.70
1	D	101	PHE	O-C-N	-6.08	112.97	122.70
1	F	27	ARG	O-C-N	-6.08	112.97	122.70
1	C	130	VAL	O-C-N	-6.07	112.88	123.20
1	H	45	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	14	GLY	O-C-N	-6.06	112.90	123.20
1	C	126	ASN	O-C-N	-6.06	112.90	123.20
1	A	74	GLU	O-C-N	-6.05	113.01	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	70	LYS	O-C-N	-6.05	113.01	122.70
1	G	66	LYS	O-C-N	-6.05	113.01	122.70
1	H	80	SER	O-C-N	-6.05	112.91	123.20
1	G	101	PHE	O-C-N	-6.05	113.02	122.70
1	G	106	GLY	O-C-N	-6.04	113.04	122.70
1	D	65	VAL	O-C-N	-6.04	113.04	122.70
1	H	102	LYS	O-C-N	-6.04	113.04	122.70
1	C	137	GLY	N-CA-C	-6.03	98.02	113.10
1	D	18	TRP	O-C-N	-6.03	113.06	122.70
1	D	80	SER	O-C-N	-6.03	112.95	123.20
1	F	115	GLU	O-C-N	-6.03	113.06	122.70
1	F	144	GLY	O-C-N	-6.03	113.06	122.70
1	H	11	GLY	O-C-N	-6.00	113.00	123.20
1	C	24	THR	O-C-N	-5.98	113.03	123.20
1	C	77	GLU	O-C-N	-5.97	113.15	122.70
1	C	144	GLY	O-C-N	-5.97	113.15	122.70
1	E	77	GLU	O-C-N	-5.96	113.16	122.70
1	A	33	TYR	C-N-CA	5.96	136.59	121.70
1	D	97	ARG	O-C-N	-5.96	113.17	122.70
1	B	119	TYR	O-C-N	-5.95	113.18	122.70
1	A	137	GLY	N-CA-C	-5.94	98.26	113.10
1	C	51	PHE	O-C-N	-5.94	113.20	122.70
1	D	22	SER	CA-C-N	5.93	130.25	117.20
1	B	15	GLY	O-C-N	-5.92	113.22	122.70
1	D	117	GLY	O-C-N	-5.92	113.23	122.70
1	E	87	SER	O-C-N	-5.91	113.24	122.70
1	B	88	ALA	O-C-N	-5.90	113.26	122.70
1	B	121	ASN	O-C-N	-5.89	113.28	122.70
1	G	40	PHE	O-C-N	-5.89	113.28	122.70
1	G	62	TYR	O-C-N	-5.88	113.28	122.70
1	A	99	LEU	O-C-N	-5.88	113.30	122.70
1	D	19	ASP	O-C-N	-5.87	113.30	122.70
1	H	99	LEU	O-C-N	-5.87	113.31	122.70
1	D	25	GLY	O-C-N	-5.87	113.31	122.70
1	D	84	GLY	N-CA-C	-5.87	98.43	113.10
1	E	130	VAL	O-C-N	-5.87	113.22	123.20
1	F	15	GLY	O-C-N	-5.87	113.31	122.70
1	C	40	PHE	O-C-N	-5.86	113.33	122.70
1	C	41	SER	O-C-N	-5.86	113.33	122.70
1	C	83	THR	O-C-N	-5.84	113.27	123.20
1	E	52	SER	O-C-N	-5.84	113.28	123.20
1	F	25	GLY	O-C-N	-5.83	113.38	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	VAL	O-C-N	-5.82	113.30	123.20
1	F	82	TYR	O-C-N	-5.82	113.39	122.70
1	H	6	THR	O-C-N	-5.81	113.40	122.70
1	A	16	ASN	O-C-N	-5.81	113.33	123.20
1	G	130	VAL	O-C-N	-5.81	113.33	123.20
1	E	27	ARG	O-C-N	-5.80	113.41	122.70
1	D	55	LYS	O-C-N	-5.80	113.42	122.70
1	G	81	GLY	O-C-N	-5.80	113.42	122.70
1	E	9	SER	CA-C-N	5.79	129.95	117.20
1	E	69	LEU	O-C-N	-5.79	113.43	122.70
1	H	124	ILE	O-C-N	-5.79	113.44	122.70
1	B	101	PHE	O-C-N	-5.78	113.44	122.70
1	B	137	GLY	O-C-N	-5.78	113.45	122.70
1	G	55	LYS	O-C-N	-5.78	113.45	122.70
1	B	24	THR	O-C-N	-5.78	113.38	123.20
1	B	130	VAL	O-C-N	-5.78	113.38	123.20
1	B	123	PRO	O-C-N	-5.78	113.46	122.70
1	C	18	TRP	O-C-N	-5.78	113.46	122.70
1	C	148	SER	O-C-N	-5.78	113.46	122.70
1	G	144	GLY	O-C-N	-5.77	113.47	122.70
1	E	88	ALA	O-C-N	-5.76	113.48	122.70
1	F	19	ASP	O-C-N	-5.76	113.48	122.70
1	A	132	PHE	O-C-N	-5.76	113.48	122.70
1	G	38	GLY	O-C-N	-5.76	113.49	122.70
1	E	136	THR	O-C-N	-5.76	113.41	123.20
1	B	137	GLY	N-CA-C	-5.75	98.72	113.10
1	A	20	GLU	O-C-N	-5.75	113.42	123.20
1	E	133	LYS	O-C-N	-5.75	113.43	123.20
1	C	15	GLY	O-C-N	-5.74	113.51	122.70
1	D	120	PHE	O-C-N	-5.74	113.52	122.70
1	C	9	SER	N-CA-C	-5.74	95.51	111.00
1	A	125	GLU	O-C-N	-5.73	113.53	122.70
1	H	144	GLY	O-C-N	-5.73	113.53	122.70
1	B	125	GLU	O-C-N	-5.72	113.55	122.70
1	H	69	LEU	CA-CB-CG	5.71	128.44	115.30
1	A	14	GLY	O-C-N	-5.70	113.50	123.20
1	C	37	ILE	O-C-N	-5.70	113.50	123.20
1	H	129	ILE	O-C-N	-5.70	113.58	122.70
1	B	14	GLY	O-C-N	-5.70	113.51	123.20
1	C	52	SER	O-C-N	-5.70	113.51	123.20
1	D	113	GLY	O-C-N	-5.70	113.58	122.70
1	G	94	PRO	O-C-N	-5.70	113.59	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	76	LEU	O-C-N	-5.70	113.59	122.70
1	A	95	VAL	O-C-N	-5.69	113.60	122.70
1	H	101	PHE	O-C-N	-5.68	113.61	122.70
1	B	17	GLY	O-C-N	-5.68	113.61	122.70
1	B	23	TYR	O-C-N	-5.68	113.61	122.70
1	G	149	LEU	CA-CB-CG	5.68	128.37	115.30
1	G	5	ILE	O-C-N	-5.68	113.61	122.70
1	D	3	GLN	O-C-N	-5.68	113.62	122.70
1	F	63	LYS	O-C-N	-5.68	113.61	122.70
1	D	142	ALA	O-C-N	-5.68	113.62	122.70
1	C	127	GLY	O-C-N	-5.67	113.62	122.70
1	E	15	GLY	O-C-N	-5.67	113.62	122.70
1	B	113	GLY	O-C-N	-5.67	113.63	122.70
1	C	42	VAL	O-C-N	-5.67	113.63	122.70
1	F	88	ALA	O-C-N	-5.67	113.63	122.70
1	D	95	VAL	O-C-N	-5.66	113.64	122.70
1	A	31	LEU	O-C-N	-5.66	113.64	122.70
1	C	48	GLY	O-C-N	-5.66	113.65	122.70
1	F	21	GLY	O-C-N	-5.65	113.65	122.70
1	B	117	GLY	O-C-N	-5.65	113.66	122.70
1	D	102	LYS	O-C-N	-5.65	113.66	122.70
1	E	63	LYS	O-C-N	-5.65	113.66	122.70
1	C	74	GLU	O-C-N	-5.65	113.66	122.70
1	C	38	GLY	O-C-N	-5.64	113.67	122.70
1	H	5	ILE	O-C-N	-5.64	113.67	122.70
1	E	107	ARG	O-C-N	-5.64	113.67	122.70
1	A	107	ARG	O-C-N	-5.64	113.67	122.70
1	G	70	LYS	O-C-N	-5.64	113.67	122.70
1	F	45	ASP	O-C-N	-5.64	113.68	122.70
1	E	50	PRO	O-C-N	-5.64	113.68	122.70
1	H	106	GLY	O-C-N	-5.63	113.69	122.70
1	A	115	GLU	O-C-N	-5.63	113.69	122.70
1	B	63	LYS	O-C-N	-5.63	113.70	122.70
1	C	45	ASP	O-C-N	-5.63	113.70	122.70
1	E	114	ASP	O-C-N	-5.63	113.70	122.70
1	G	42	VAL	O-C-N	-5.62	113.71	122.70
1	H	48	GLY	O-C-N	-5.62	113.71	122.70
1	A	27	ARG	O-C-N	-5.61	113.72	122.70
1	C	61	PRO	O-C-N	-5.61	113.72	122.70
1	D	90	ALA	O-C-N	-5.61	113.72	122.70
1	F	72	PRO	O-C-N	-5.61	113.72	122.70
1	C	29	ILE	O-C-N	-5.61	113.73	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	141	ASP	O-C-N	-5.61	113.73	122.70
1	G	67	ILE	O-C-N	-5.61	113.73	122.70
1	G	86	PHE	O-C-N	-5.60	113.73	122.70
1	F	52	SER	O-C-N	-5.60	113.69	123.20
1	A	101	PHE	O-C-N	-5.59	113.76	122.70
1	E	90	ALA	O-C-N	-5.59	113.76	122.70
1	G	128	LEU	CA-CB-CG	5.58	128.14	115.30
1	E	106	GLY	O-C-N	-5.58	113.77	122.70
1	A	88	ALA	O-C-N	-5.58	113.78	122.70
1	C	2	SER	O-C-N	-5.58	113.78	122.70
1	D	145	ILE	O-C-N	-5.58	113.78	122.70
1	F	48	GLY	O-C-N	-5.57	113.78	122.70
1	C	16	ASN	O-C-N	-5.57	113.73	123.20
1	G	141	ASP	O-C-N	-5.56	113.80	122.70
1	A	44	TYR	O-C-N	-5.56	113.80	122.70
1	F	23	TYR	O-C-N	-5.56	113.81	122.70
1	H	105	LYS	O-C-N	-5.56	113.75	123.20
1	D	128	LEU	O-C-N	-5.56	113.81	122.70
1	H	126	ASN	O-C-N	-5.55	113.76	123.20
1	A	123	PRO	O-C-N	-5.55	113.82	122.70
1	B	18	TRP	O-C-N	-5.55	113.82	122.70
1	C	133	LYS	O-C-N	-5.55	113.77	123.20
1	F	133	LYS	O-C-N	-5.55	113.77	123.20
1	H	3	GLN	O-C-N	-5.55	113.83	122.70
1	G	77	GLU	O-C-N	-5.54	113.83	122.70
1	B	44	TYR	O-C-N	-5.54	113.83	122.70
1	B	115	GLU	O-C-N	-5.54	113.84	122.70
1	D	57	THR	O-C-N	-5.54	113.84	122.70
1	D	135	ARG	O-C-N	-5.54	113.83	122.70
1	E	135	ARG	O-C-N	-5.54	113.84	122.70
1	C	28	GLN	O-C-N	-5.54	113.84	122.70
1	D	11	GLY	O-C-N	-5.53	113.80	123.20
1	D	30	GLU	O-C-N	-5.53	113.85	122.70
1	G	24	THR	O-C-N	-5.53	113.79	123.20
1	G	107	ARG	O-C-N	-5.53	113.85	122.70
1	G	133	LYS	O-C-N	-5.52	113.81	123.20
1	H	17	GLY	O-C-N	-5.52	113.87	122.70
1	H	112	TYR	O-C-N	-5.52	113.82	123.20
1	H	95	VAL	O-C-N	-5.52	113.87	122.70
1	H	89	LEU	CA-C-N	5.51	129.33	117.20
1	G	95	VAL	O-C-N	-5.51	113.88	122.70
1	A	51	PHE	O-C-N	-5.51	113.88	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	23	TYR	O-C-N	-5.51	113.89	122.70
1	F	120	PHE	O-C-N	-5.51	113.89	122.70
1	D	51	PHE	O-C-N	-5.50	113.89	122.70
1	F	146	HIS	O-C-N	-5.50	113.90	122.70
1	D	107	ARG	O-C-N	-5.50	113.90	122.70
1	H	133	LYS	O-C-N	-5.49	113.86	123.20
1	F	123	PRO	O-C-N	-5.49	113.91	122.70
1	B	124	ILE	O-C-N	-5.49	113.92	122.70
1	G	127	GLY	O-C-N	-5.49	113.92	122.70
1	D	76	LEU	O-C-N	-5.48	113.93	122.70
1	A	86	PHE	O-C-N	-5.48	113.94	122.70
1	G	46	LEU	O-C-N	-5.48	113.93	122.70
1	D	59	LYS	O-C-N	-5.47	113.94	122.70
1	G	129	ILE	N-CA-C	-5.47	96.23	111.00
1	C	76	LEU	O-C-N	-5.47	113.95	122.70
1	B	99	LEU	O-C-N	-5.46	113.96	122.70
1	B	100	THR	O-C-N	-5.46	113.96	122.70
1	E	18	TRP	O-C-N	-5.46	113.97	122.70
1	F	105	LYS	O-C-N	-5.46	113.92	123.20
1	G	17	GLY	O-C-N	-5.46	113.97	122.70
1	B	138	ASP	O-C-N	-5.45	113.98	122.70
1	G	143	ILE	O-C-N	-5.45	113.94	123.20
1	F	89	LEU	CA-C-N	-5.44	105.23	117.20
1	B	67	ILE	O-C-N	-5.43	114.01	122.70
1	D	4	THR	O-C-N	-5.43	114.01	122.70
1	F	40	PHE	O-C-N	-5.43	114.01	122.70
1	A	72	PRO	O-C-N	-5.43	114.02	122.70
1	A	22	SER	O-C-N	-5.42	114.03	122.70
1	A	40	PHE	O-C-N	-5.42	114.03	122.70
1	C	140	LEU	O-C-N	-5.42	114.03	122.70
1	G	140	LEU	O-C-N	-5.41	114.04	122.70
1	C	79	VAL	O-C-N	-5.41	114.05	122.70
1	F	128	LEU	O-C-N	-5.41	114.05	122.70
1	C	11	GLY	O-C-N	-5.41	114.01	123.20
1	D	143	ILE	CB-CA-C	-5.41	100.79	111.60
1	C	68	GLU	O-C-N	-5.40	114.06	122.70
1	C	80	SER	O-C-N	-5.40	114.02	123.20
1	H	137	GLY	N-CA-C	-5.40	99.60	113.10
1	D	67	ILE	O-C-N	-5.39	114.07	122.70
1	E	137	GLY	O-C-N	-5.39	114.07	122.70
1	G	36	ALA	O-C-N	-5.39	114.07	122.70
1	E	13	PRO	O-C-N	-5.39	114.04	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	TRP	O-C-N	-5.39	114.08	122.70
1	H	96	VAL	O-C-N	-5.38	114.09	122.70
1	G	131	GLY	O-C-N	-5.38	114.09	122.70
1	G	11	GLY	O-C-N	-5.38	114.05	123.20
1	A	134	GLY	O-C-N	-5.38	114.09	122.70
1	F	135	ARG	O-C-N	-5.38	114.09	122.70
1	A	2	SER	O-C-N	-5.38	114.10	122.70
1	B	129	ILE	N-CA-C	-5.38	96.48	111.00
1	G	105	LYS	O-C-N	-5.38	114.06	123.20
1	D	13	PRO	O-C-N	-5.37	114.06	123.20
1	H	129	ILE	N-CA-C	-5.37	96.49	111.00
1	E	124	ILE	O-C-N	-5.37	114.11	122.70
1	E	66	LYS	O-C-N	-5.37	114.11	122.70
1	G	61	PRO	O-C-N	-5.37	114.11	122.70
1	F	100	THR	O-C-N	-5.37	114.11	122.70
1	G	41	SER	O-C-N	-5.37	114.11	122.70
1	A	11	GLY	O-C-N	-5.36	114.09	123.20
1	A	76	LEU	O-C-N	-5.36	114.12	122.70
1	A	117	GLY	O-C-N	-5.36	114.13	122.70
1	H	62	TYR	O-C-N	-5.36	114.13	122.70
1	E	108	THR	O-C-N	-5.35	114.13	122.70
1	E	140	LEU	O-C-N	-5.35	114.13	122.70
1	C	145	ILE	O-C-N	-5.35	114.14	122.70
1	E	113	GLY	O-C-N	-5.35	114.14	122.70
1	B	45	ASP	O-C-N	-5.34	114.15	122.70
1	C	119	TYR	O-C-N	-5.34	114.15	122.70
1	C	141	ASP	O-C-N	-5.34	114.15	122.70
1	E	115	GLU	O-C-N	-5.34	114.15	122.70
1	A	63	LYS	O-C-N	-5.34	114.16	122.70
1	C	36	ALA	O-C-N	-5.34	114.16	122.70
1	G	30	GLU	O-C-N	-5.34	114.16	122.70
1	H	123	PRO	O-C-N	-5.34	114.16	122.70
1	D	139	LEU	O-C-N	-5.33	114.17	122.70
1	E	75	PHE	O-C-N	-5.33	114.17	122.70
1	E	16	ASN	O-C-N	-5.33	114.15	123.20
1	C	105	LYS	O-C-N	-5.32	114.16	123.20
1	F	32	SER	O-C-N	-5.32	114.19	122.70
1	E	11	GLY	O-C-N	-5.32	114.16	123.20
1	H	51	PHE	O-C-N	-5.32	114.20	122.70
1	F	107	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	6	THR	O-C-N	-5.31	114.20	122.70
1	C	100	THR	O-C-N	-5.31	114.21	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	79	VAL	O-C-N	-5.31	114.21	122.70
1	A	140	LEU	O-C-N	-5.31	114.21	122.70
1	C	85	PRO	O-C-N	-5.31	114.21	122.70
1	A	97	ARG	O-C-N	-5.30	114.21	122.70
1	H	58	SER	O-C-N	-5.30	114.21	122.70
1	C	17	GLY	O-C-N	-5.30	114.22	122.70
1	A	29	ILE	O-C-N	-5.30	114.22	122.70
1	B	103	THR	O-C-N	-5.30	114.22	122.70
1	A	8	GLY	C-N-CA	5.30	134.95	121.70
1	E	126	ASN	O-C-N	-5.30	114.19	123.20
1	A	139	LEU	CA-CB-CG	5.29	127.48	115.30
1	E	67	ILE	O-C-N	-5.29	114.23	122.70
1	E	102	LYS	O-C-N	-5.29	114.24	122.70
1	B	140	LEU	O-C-N	-5.29	114.24	122.70
1	G	139	LEU	O-C-N	-5.29	114.24	122.70
1	F	4	THR	O-C-N	-5.28	114.25	122.70
1	E	22	SER	O-C-N	-5.28	114.26	122.70
1	F	62	TYR	O-C-N	-5.27	114.26	122.70
1	D	32	SER	O-C-N	-5.27	114.26	122.70
1	F	30	GLU	O-C-N	-5.27	114.27	122.70
1	D	89	LEU	CB-CG-CD1	-5.27	102.04	111.00
1	F	119	TYR	O-C-N	-5.27	114.27	122.70
1	A	50	PRO	O-C-N	-5.26	114.28	122.70
1	D	31	LEU	O-C-N	-5.26	114.28	122.70
1	F	14	GLY	O-C-N	-5.26	114.25	123.20
1	D	45	ASP	O-C-N	-5.25	114.29	122.70
1	A	64	ASN	O-C-N	-5.25	114.29	122.70
1	D	74	GLU	O-C-N	-5.25	114.30	122.70
1	E	142	ALA	O-C-N	-5.25	114.29	122.70
1	F	79	VAL	O-C-N	-5.25	114.30	122.70
1	D	94	PRO	O-C-N	-5.25	114.30	122.70
1	G	102	LYS	O-C-N	-5.25	114.30	122.70
1	A	129	ILE	O-C-N	-5.25	114.30	122.70
1	E	37	ILE	O-C-N	-5.25	114.28	123.20
1	A	24	THR	O-C-N	-5.25	114.28	123.20
1	A	69	LEU	O-C-N	-5.24	114.31	122.70
1	E	81	GLY	CA-C-N	5.24	128.74	117.20
1	B	95	VAL	O-C-N	-5.24	114.32	122.70
1	E	143	ILE	O-C-N	-5.24	114.30	123.20
1	E	7	VAL	O-C-N	-5.23	114.31	123.20
1	B	30	GLU	O-C-N	-5.23	114.33	122.70
1	D	40	PHE	O-C-N	-5.23	114.33	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	SER	O-C-N	-5.23	114.33	122.70
1	E	103	THR	O-C-N	-5.23	114.33	122.70
1	D	62	TYR	O-C-N	-5.22	114.34	122.70
1	A	89	LEU	N-CA-C	-5.22	96.90	111.00
1	F	117	GLY	O-C-N	-5.22	114.35	122.70
1	H	23	TYR	O-C-N	-5.22	114.35	122.70
1	H	89	LEU	N-CA-C	-5.22	96.91	111.00
1	B	91	THR	N-CA-C	-5.21	96.92	111.00
1	B	128	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	65	VAL	O-C-N	-5.21	114.36	122.70
1	B	21	GLY	O-C-N	-5.21	114.36	122.70
1	F	36	ALA	O-C-N	-5.20	114.38	122.70
1	F	125	GLU	O-C-N	-5.20	114.38	122.70
1	E	32	SER	O-C-N	-5.20	114.38	122.70
1	C	117	GLY	O-C-N	-5.20	114.39	122.70
1	D	126	ASN	O-C-N	-5.19	114.37	123.20
1	G	120	PHE	O-C-N	-5.19	114.39	122.70
1	B	136	THR	O-C-N	-5.19	114.38	123.20
1	D	128	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	E	76	LEU	O-C-N	-5.19	114.40	122.70
1	C	88	ALA	O-C-N	-5.19	114.40	122.70
1	D	38	GLY	O-C-N	-5.18	114.41	122.70
1	E	48	GLY	O-C-N	-5.18	114.41	122.70
1	B	3	GLN	O-C-N	-5.18	114.41	122.70
1	G	92	PRO	O-C-N	-5.17	114.42	122.70
1	D	5	ILE	O-C-N	-5.17	114.42	122.70
1	H	97	ARG	O-C-N	-5.17	114.42	122.70
1	H	45	ASP	N-CA-C	-5.17	97.04	111.00
1	C	134	GLY	O-C-N	-5.17	114.43	122.70
1	D	137	GLY	N-CA-C	-5.17	100.18	113.10
1	G	31	LEU	O-C-N	-5.17	114.44	122.70
1	C	90	ALA	N-CA-C	5.16	124.94	111.00
1	F	37	ILE	O-C-N	-5.16	114.42	123.20
1	H	85	PRO	O-C-N	-5.16	114.45	122.70
1	G	63	LYS	O-C-N	-5.16	114.45	122.70
1	G	72	PRO	O-C-N	-5.15	114.45	122.70
1	H	31	LEU	O-C-N	-5.15	114.46	122.70
1	F	58	SER	O-C-N	-5.15	114.46	122.70
1	D	146	HIS	O-C-N	-5.15	114.46	122.70
1	A	25	GLY	O-C-N	-5.14	114.47	122.70
1	A	57	THR	O-C-N	-5.14	114.47	122.70
1	A	147	MET	O-C-N	-5.14	114.47	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	25	GLY	O-C-N	-5.14	114.47	122.70
1	B	49	ASP	CB-CG-OD1	5.14	122.93	118.30
1	G	80	SER	O-C-N	-5.14	114.46	123.20
1	C	31	LEU	O-C-N	-5.14	114.48	122.70
1	G	134	GLY	O-C-N	-5.14	114.48	122.70
1	A	42	VAL	O-C-N	-5.13	114.49	122.70
1	A	124	ILE	O-C-N	-5.13	114.49	122.70
1	F	113	GLY	O-C-N	-5.13	114.49	122.70
1	F	137	GLY	O-C-N	-5.13	114.49	122.70
1	C	106	GLY	N-CA-C	5.13	125.92	113.10
1	C	6	THR	O-C-N	-5.13	114.50	122.70
1	A	100	THR	O-C-N	-5.12	114.50	122.70
1	E	65	VAL	CB-CA-C	-5.12	101.67	111.40
1	D	99	LEU	O-C-N	-5.12	114.50	122.70
1	C	25	GLY	O-C-N	-5.12	114.51	122.70
1	E	134	GLY	O-C-N	-5.12	114.51	122.70
1	E	127	GLY	O-C-N	-5.12	114.51	122.70
1	A	136	THR	O-C-N	-5.11	114.51	123.20
1	B	34	LYS	N-CA-CB	5.11	119.80	110.60
1	G	3	GLN	O-C-N	-5.11	114.52	122.70
1	H	70	LYS	O-C-N	-5.11	114.52	122.70
1	F	127	GLY	O-C-N	-5.11	114.53	122.70
1	C	121	ASN	O-C-N	-5.11	114.53	122.70
1	G	125	GLU	O-C-N	-5.11	114.53	122.70
1	H	55	LYS	O-C-N	-5.10	114.53	122.70
1	B	79	VAL	CB-CA-C	-5.10	101.71	111.40
1	D	63	LYS	O-C-N	-5.10	114.54	122.70
1	D	141	ASP	O-C-N	-5.10	114.54	122.70
1	H	108	THR	O-C-N	-5.09	114.55	122.70
1	B	128	LEU	CB-CG-CD1	-5.09	102.34	111.00
1	C	26	ILE	O-C-N	-5.09	114.56	122.70
1	G	109	PHE	O-C-N	-5.09	114.55	123.20
1	E	33	TYR	CA-C-N	-5.09	106.01	117.20
1	B	90	ALA	O-C-N	-5.08	114.56	122.70
1	F	78	SER	O-C-N	-5.08	114.57	122.70
1	C	34	LYS	O-C-N	-5.08	114.57	122.70
1	F	111	PRO	O-C-N	-5.08	114.57	122.70
1	A	5	ILE	O-C-N	-5.08	114.57	122.70
1	D	103	THR	O-C-N	-5.08	114.57	122.70
1	E	6	THR	O-C-N	-5.07	114.58	122.70
1	A	106	GLY	O-C-N	-5.07	114.59	122.70
1	H	15	GLY	O-C-N	-5.07	114.59	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	SER	O-C-N	-5.07	114.60	122.70
1	B	37	ILE	O-C-N	-5.06	114.59	123.20
1	C	102	LYS	O-C-N	-5.06	114.60	122.70
1	A	79	VAL	O-C-N	-5.06	114.61	122.70
1	E	29	ILE	O-C-N	-5.06	114.61	122.70
1	H	45	ASP	O-C-N	-5.06	114.61	122.70
1	A	66	LYS	O-C-N	-5.05	114.61	122.70
1	B	19	ASP	O-C-N	-5.05	114.61	122.70
1	H	39	SER	O-C-N	-5.05	114.62	122.70
1	H	130	VAL	O-C-N	-5.05	114.62	123.20
1	C	90	ALA	C-N-CA	-5.05	109.08	121.70
1	D	70	LYS	O-C-N	-5.04	114.64	122.70
1	H	78	SER	O-C-N	-5.04	114.63	122.70
1	E	85	PRO	O-C-N	-5.04	114.64	122.70
1	B	27	ARG	O-C-N	-5.03	114.65	122.70
1	E	28	GLN	O-C-N	-5.03	114.65	122.70
1	F	24	THR	O-C-N	-5.03	114.65	123.20
1	C	146	HIS	O-C-N	-5.03	114.66	122.70
1	F	83	THR	O-C-N	-5.03	114.66	123.20
1	H	41	SER	O-C-N	-5.03	114.66	122.70
1	G	28	GLN	O-C-N	-5.02	114.66	122.70
1	G	135	ARG	O-C-N	-5.02	114.66	122.70
1	D	130	VAL	O-C-N	-5.02	114.66	123.20
1	E	61	PRO	O-C-N	-5.02	114.67	122.70
1	D	58	SER	O-C-N	-5.02	114.67	122.70
1	H	114	ASP	O-C-N	-5.02	114.67	122.70
1	E	4	THR	O-C-N	-5.01	114.68	122.70
1	F	28	GLN	O-C-N	-5.01	114.68	122.70
1	D	37	ILE	O-C-N	-5.01	114.68	123.20
1	G	124	ILE	O-C-N	-5.01	114.68	122.70
1	A	7	VAL	O-C-N	-5.01	114.68	123.20
1	D	6	THR	O-C-N	-5.01	114.68	122.70
1	D	28	GLN	O-C-N	-5.01	114.68	122.70
1	D	41	SER	O-C-N	-5.01	114.68	122.70
1	D	39	SER	O-C-N	-5.01	114.69	122.70
1	A	98	SER	O-C-N	-5.01	114.69	122.70

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	AYA	CA
1	B	1	AYA	CA

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Mol	Chain	Res	Type	Atom
1	C	1	AYA	CA
1	E	1	AYA	CA
1	G	1	AYA	CA
1	H	1	AYA	CA

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	AYA	Mainchain
1	A	115	GLU	Mainchain
1	A	34	LYS	Mainchain
1	A	42	VAL	Mainchain
1	A	72	PRO	Mainchain
1	A	8	GLY	Mainchain,Peptide
1	A	9	SER	Mainchain
1	B	1	AYA	Mainchain
1	B	34	LYS	Mainchain
1	B	8	GLY	Mainchain
1	B	9	SER	Mainchain
1	C	109	PHE	Mainchain
1	C	144	GLY	Mainchain
1	C	23	TYR	Mainchain
1	C	34	LYS	Mainchain
1	C	7	VAL	Mainchain
1	C	8	GLY	Mainchain
1	C	89	LEU	Mainchain
1	C	9	SER	Mainchain
1	D	1	AYA	Mainchain
1	D	23	TYR	Mainchain
1	D	34	LYS	Mainchain
1	D	8	GLY	Mainchain,Peptide
1	E	34	LYS	Mainchain,Peptide
1	E	8	GLY	Peptide
1	E	9	SER	Mainchain
1	E	99	LEU	Mainchain
1	F	23	TYR	Mainchain
1	F	7	VAL	Mainchain
1	F	8	GLY	Mainchain
1	F	88	ALA	Mainchain
1	F	89	LEU	Mainchain
1	F	9	SER	Mainchain
1	F	90	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	G	3	GLN	Mainchain
1	G	33	TYR	Mainchain
1	G	7	VAL	Mainchain
1	G	8	GLY	Mainchain
1	G	89	LEU	Mainchain
1	H	1	AYA	Mainchain
1	H	118	THR	Mainchain
1	H	89	LEU	Mainchain
1	H	9	SER	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1132	0	1084	69	0
1	B	1132	0	1083	59	0
1	C	1132	0	1084	58	0
1	D	1132	0	1080	86	0
1	E	1128	0	1071	48	0
1	F	1128	0	1067	69	0
1	G	1132	0	1081	55	0
1	H	1132	0	1082	72	0
2	A	118	0	0	7	0
2	B	123	0	0	9	0
2	C	121	0	0	4	0
2	D	121	0	0	7	0
2	E	93	0	0	4	0
2	F	115	0	0	6	0
2	G	102	0	0	6	0
2	H	81	0	0	6	0
All	All	9922	0	8632	481	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (481) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:8:GLY:HA2	1:D:123:PRO:HG2	1.22	1.18
1:D:18:TRP:HZ3	1:D:136:THR:HG23	0.98	1.10
1:D:18:TRP:CZ3	1:D:136:THR:HG23	1.89	1.07
1:A:61:PRO:HD2	2:A:181:HOH:O	1.57	1.04
1:E:60:LEU:HD11	1:E:89:LEU:HD11	1.47	0.97
1:F:28:GLN:HG2	1:F:43:ILE:HB	1.47	0.95
1:D:20:GLU:HG2	1:D:54:PRO:HD2	1.50	0.92
1:D:74:GLU:HA	1:D:104:ASN:HD21	1.33	0.92
1:D:99:LEU:HD11	1:D:143:ILE:HD11	1.51	0.91
1:C:8:GLY:CA	1:D:123:PRO:HG2	2.00	0.90
1:A:92:PRO:HD2	2:A:240:HOH:O	1.72	0.88
1:H:86:PHE:CZ	1:H:88:ALA:HB3	2.10	0.86
1:G:123:PRO:HG2	1:H:8:GLY:HA2	1.55	0.86
1:C:60:LEU:HD11	1:C:89:LEU:HD11	1.56	0.86
1:G:8:GLY:HA2	1:H:123:PRO:HB2	1.55	0.86
1:H:74:GLU:HA	1:H:104:ASN:HD21	1.42	0.84
1:D:18:TRP:HZ3	1:D:136:THR:CG2	1.88	0.84
1:D:60:LEU:HD12	1:D:139:LEU:HD13	1.59	0.83
1:D:14:GLY:O	1:D:135:ARG:HG2	1.78	0.82
1:G:34:LYS:HG3	2:G:246:HOH:O	1.78	0.82
1:F:79:VAL:HG13	1:F:101:PHE:CE1	2.14	0.82
1:C:74:GLU:HA	1:C:104:ASN:HD21	1.43	0.82
2:B:212:HOH:O	1:D:1:AYA:HM3	1.82	0.80
1:E:86:PHE:HD2	1:E:89:LEU:HB2	1.46	0.78
1:E:86:PHE:CD2	1:E:89:LEU:HB2	2.19	0.78
1:F:60:LEU:H	1:F:60:LEU:HD22	1.48	0.78
1:D:60:LEU:HD12	1:D:139:LEU:CD1	2.14	0.78
1:E:123:PRO:HG2	1:F:8:GLY:HA2	1.66	0.78
1:F:67:ILE:HG23	1:F:109:PHE:CD2	2.19	0.77
1:G:18:TRP:HZ3	1:G:136:THR:HG1	1.32	0.77
1:F:75:PHE:H	1:F:104:ASN:ND2	1.83	0.76
1:A:133:LYS:HE3	1:A:144:GLY:HA3	1.66	0.76
1:A:89:LEU:O	1:A:91:THR:HG22	1.86	0.76
1:D:41:SER:OG	1:D:55:LYS:HD3	1.86	0.76
1:D:75:PHE:H	1:D:104:ASN:ND2	1.84	0.75
1:H:18:TRP:HZ3	1:H:136:THR:OG1	1.71	0.74
1:E:52:SER:HB2	2:E:153:HOH:O	1.87	0.74
1:A:102:LYS:HG2	1:A:108:THR:HB	1.70	0.73
1:D:60:LEU:CD1	1:D:139:LEU:HD13	2.17	0.73
1:H:91:THR:HG21	1:H:95:VAL:HG21	1.69	0.73
1:G:74:GLU:HA	1:G:104:ASN:HD21	1.54	0.73
1:F:7:VAL:HG12	1:F:145:ILE:HG22	1.69	0.73
1:A:100:THR:HG22	1:A:111:PRO:HA	1.70	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:8:GLY:HA2	1:D:123:PRO:CG	2.12	0.73
1:B:20:GLU:HG2	1:B:54:PRO:HD2	1.69	0.72
1:C:35:GLU:HG3	1:C:86:PHE:CZ	2.24	0.72
1:E:48:GLY:HA3	2:E:172:HOH:O	1.89	0.72
1:C:133:LYS:HE2	2:C:218:HOH:O	1.90	0.72
1:F:20:GLU:HG2	1:F:54:PRO:HD2	1.71	0.72
1:H:109:PHE:HB3	1:H:112:TYR:OH	1.90	0.71
1:D:89:LEU:HA	2:D:223:HOH:O	1.90	0.71
1:C:4:THR:HG21	1:C:146:HIS:HB3	1.73	0.71
1:A:88:ALA:C	1:A:90:ALA:H	1.90	0.71
1:B:39:SER:HB3	1:B:57:THR:HA	1.73	0.71
1:H:18:TRP:HZ3	1:H:136:THR:HG1	1.38	0.70
1:E:60:LEU:CD1	1:E:89:LEU:HD11	2.20	0.70
1:B:28:GLN:HG2	1:B:43:ILE:HG13	1.74	0.70
1:G:133:LYS:HE3	1:H:125:GLU:OE2	1.92	0.69
1:C:65:VAL:HG21	1:C:112:TYR:CE1	2.28	0.68
1:H:135:ARG:HD2	2:H:205:HOH:O	1.95	0.67
1:C:74:GLU:HB2	1:C:105:LYS:HG3	1.75	0.67
1:A:60:LEU:H	1:A:60:LEU:HD22	1.59	0.67
1:F:67:ILE:HG23	1:F:109:PHE:CE2	2.30	0.67
1:H:71:PHE:CD1	1:H:72:PRO:HA	2.30	0.66
1:D:78:SER:HB3	1:D:102:LYS:HB2	1.77	0.66
1:F:34:LYS:HD2	1:F:62:TYR:HA	1.76	0.66
1:B:30:GLU:OE2	1:B:66:LYS:HG3	1.95	0.66
1:F:79:VAL:HG13	1:F:101:PHE:HE1	1.57	0.66
1:F:89:LEU:O	1:F:91:THR:HG22	1.94	0.66
1:A:92:PRO:HD3	2:A:256:HOH:O	1.95	0.66
1:H:18:TRP:CZ3	1:H:136:THR:OG1	2.48	0.66
1:D:136:THR:HG22	1:D:140:LEU:HD12	1.78	0.66
1:G:83:THR:HG22	1:G:118:THR:HG23	1.77	0.66
1:G:18:TRP:HZ3	1:G:136:THR:OG1	1.78	0.66
1:F:74:GLU:HA	1:F:104:ASN:HD21	1.60	0.65
1:C:18:TRP:HH2	1:C:140:LEU:CD1	2.09	0.65
1:E:82:TYR:HB2	1:E:98:SER:HB3	1.79	0.65
1:C:5:ILE:HD13	1:D:5:ILE:HD12	1.77	0.65
1:G:104:ASN:HD22	1:G:104:ASN:H	1.45	0.65
1:D:74:GLU:OE2	1:D:103:THR:HG21	1.98	0.64
1:D:60:LEU:HD11	1:D:89:LEU:HD11	1.78	0.64
1:E:123:PRO:HG2	1:F:8:GLY:CA	2.26	0.64
1:H:58:SER:HB2	1:H:138:ASP:O	1.98	0.64
1:D:60:LEU:CD1	1:D:89:LEU:HD11	2.28	0.63
1:F:20:GLU:HB2	1:F:132:PHE:O	1.98	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:99:LEU:HD11	1:D:143:ILE:CD1	2.28	0.63
1:B:1:AYA:H	1:D:128:LEU:HD21	1.63	0.63
1:A:1:AYA:HM3	1:C:128:LEU:HD11	1.81	0.63
1:D:74:GLU:OE2	1:D:107:ARG:HD3	1.99	0.63
1:B:89:LEU:O	1:B:91:THR:HG22	1.99	0.63
1:A:132:PHE:CE1	1:A:145:ILE:HD11	2.33	0.63
1:F:34:LYS:CD	1:F:62:TYR:HA	2.29	0.63
1:A:20:GLU:HG2	1:A:54:PRO:HD2	1.80	0.63
1:F:1:AYA:HM2	1:H:128:LEU:HG	1.81	0.62
1:D:37:ILE:O	1:D:139:LEU:HG	1.99	0.62
1:C:86:PHE:CZ	1:C:88:ALA:HB3	2.35	0.62
1:G:116:GLU:HB3	2:G:203:HOH:O	1.97	0.62
1:E:82:TYR:CE2	1:E:115:GLU:HG2	2.34	0.61
1:E:81:GLY:O	1:E:98:SER:HB3	2.00	0.61
1:A:40:PHE:O	1:A:56:HIS:HB2	2.00	0.61
1:B:102:LYS:HD3	1:B:108:THR:HB	1.81	0.61
1:C:11:GLY:HA2	1:C:83:THR:HG21	1.83	0.61
1:A:8:GLY:HA2	1:B:123:PRO:HD2	1.82	0.61
1:H:60:LEU:HD21	2:H:227:HOH:O	2.01	0.60
1:B:130:VAL:HG11	1:B:148:SER:OG	2.01	0.60
1:F:34:LYS:HB2	1:F:62:TYR:CD1	2.35	0.60
1:A:60:LEU:HD11	1:A:89:LEU:HD11	1.83	0.60
1:D:98:SER:HA	1:D:112:TYR:O	2.01	0.60
1:D:59:LYS:HG3	2:D:186:HOH:O	2.00	0.59
1:G:18:TRP:HH2	1:G:140:LEU:HD13	1.66	0.59
1:B:135:ARG:HB2	1:B:141:ASP:HB2	1.85	0.59
1:D:67:ILE:HG23	1:D:109:PHE:CD2	2.37	0.59
1:E:20:GLU:HG2	1:E:54:PRO:HD2	1.84	0.59
1:H:28:GLN:NE2	1:H:66:LYS:HE3	2.17	0.59
1:A:123:PRO:HD2	1:B:8:GLY:HA2	1.84	0.59
1:H:74:GLU:OE2	1:H:107:ARG:HD3	2.03	0.59
1:D:136:THR:CG2	1:D:140:LEU:HD12	2.34	0.58
1:D:13:PRO:HB3	2:D:162:HOH:O	2.02	0.58
1:B:128:LEU:HD12	1:D:2:SER:HB3	1.85	0.58
1:D:74:GLU:CA	1:D:104:ASN:HD21	2.11	0.58
1:C:135:ARG:CG	1:C:142:ALA:HB3	2.34	0.58
1:E:133:LYS:NZ	2:E:166:HOH:O	2.37	0.58
1:B:98:SER:HA	1:B:112:TYR:O	2.03	0.58
1:H:28:GLN:HE22	1:H:66:LYS:HE3	1.68	0.58
1:A:49:ASP:HB3	2:A:172:HOH:O	2.03	0.58
1:A:18:TRP:CD1	1:A:19:ASP:N	2.72	0.58
1:B:23:TYR:HE2	1:B:51:PHE:CE2	2.21	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1:AYA:HM3	2:D:150:HOH:O	2.04	0.57
1:A:18:TRP:HD1	1:A:19:ASP:N	2.02	0.57
1:C:135:ARG:HG3	1:C:142:ALA:HB3	1.84	0.57
1:D:58:SER:HB2	1:D:138:ASP:O	2.04	0.57
1:D:18:TRP:HH2	1:D:140:LEU:HD11	1.69	0.57
1:D:136:THR:HG22	1:D:140:LEU:HA	1.86	0.57
1:G:139:LEU:HD23	2:G:212:HOH:O	2.03	0.57
1:F:96:VAL:HG21	1:F:140:LEU:HD23	1.86	0.57
1:H:86:PHE:CE2	1:H:88:ALA:HB3	2.39	0.57
1:D:75:PHE:N	1:D:104:ASN:ND2	2.52	0.57
1:D:99:LEU:CD1	1:D:143:ILE:HD11	2.32	0.57
1:H:27:ARG:HD3	1:H:71:PHE:CD2	2.40	0.57
1:F:104:ASN:HD22	1:F:104:ASN:H	1.51	0.57
1:F:8:GLY:O	1:F:9:SER:HB2	2.04	0.57
1:G:18:TRP:C	1:G:18:TRP:CD1	2.78	0.57
1:G:78:SER:HB3	1:G:102:LYS:HB3	1.86	0.57
1:G:135:ARG:HB2	1:G:142:ALA:HB3	1.87	0.57
1:G:121:ASN:HB3	2:G:214:HOH:O	2.04	0.57
1:C:60:LEU:CD1	1:C:89:LEU:HD11	2.31	0.56
1:B:83:THR:O	1:B:118:THR:HG22	2.05	0.56
1:B:35:GLU:HB2	1:B:86:PHE:CZ	2.40	0.56
1:D:36:ALA:HB3	1:D:139:LEU:HD21	1.88	0.56
1:A:74:GLU:HA	1:A:104:ASN:HD21	1.70	0.56
1:G:139:LEU:HD23	1:G:139:LEU:N	2.20	0.56
1:H:138:ASP:HB2	1:H:139:LEU:HD12	1.88	0.56
1:C:11:GLY:HA2	1:C:83:THR:CG2	2.36	0.56
1:A:17:GLY:HA2	1:A:135:ARG:HG2	1.87	0.56
1:C:46:LEU:HB2	1:C:51:PHE:HB2	1.88	0.56
1:B:93:THR:CG2	2:B:195:HOH:O	2.53	0.56
1:H:104:ASN:HD22	1:H:104:ASN:H	1.52	0.56
1:H:26:ILE:HG23	1:H:42:VAL:HG23	1.87	0.56
1:D:11:GLY:HA2	1:D:83:THR:OG1	2.06	0.55
1:D:132:PHE:CE1	1:D:145:ILE:HD12	2.41	0.55
1:D:74:GLU:HG3	1:D:105:LYS:HG2	1.88	0.55
1:G:74:GLU:OE2	1:G:107:ARG:HD3	2.06	0.55
1:A:88:ALA:C	1:A:90:ALA:N	2.60	0.55
1:B:22:SER:HB2	2:B:156:HOH:O	2.07	0.55
1:A:28:GLN:NE2	1:A:66:LYS:HE3	2.21	0.55
1:A:28:GLN:NE2	1:A:66:LYS:CE	2.69	0.55
1:F:23:TYR:O	1:F:130:VAL:HG22	2.07	0.55
1:C:67:ILE:O	1:C:67:ILE:HG22	2.06	0.55
1:F:19:ASP:HA	1:F:133:LYS:HB2	1.87	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:75:PHE:H	1:E:104:ASN:ND2	2.04	0.55
1:B:102:LYS:CD	1:B:108:THR:HB	2.36	0.55
1:E:104:ASN:N	1:E:104:ASN:HD22	2.03	0.55
1:G:34:LYS:NZ	1:G:34:LYS:HB3	2.22	0.54
1:H:13:PRO:HD2	1:H:93:THR:OG1	2.07	0.54
1:A:7:VAL:HG12	1:A:145:ILE:HG22	1.88	0.54
1:A:23:TYR:HE2	1:A:51:PHE:CE2	2.25	0.54
1:A:104:ASN:H	1:A:104:ASN:HD22	1.54	0.54
1:E:11:GLY:HA2	1:E:83:THR:CG2	2.36	0.54
1:E:60:LEU:H	1:E:60:LEU:HD22	1.72	0.54
1:H:101:PHE:N	1:H:101:PHE:CD1	2.74	0.54
1:G:18:TRP:CZ3	1:G:136:THR:OG1	2.54	0.54
1:F:1:AYA:HM3	2:H:153:HOH:O	2.07	0.54
1:H:28:GLN:HB2	1:H:68:GLU:HA	1.89	0.53
1:A:23:TYR:CE2	1:A:51:PHE:CD2	2.95	0.53
1:G:139:LEU:HD23	1:G:139:LEU:H	1.74	0.53
1:C:11:GLY:HA3	1:C:142:ALA:HA	1.90	0.53
1:G:104:ASN:HD22	1:G:104:ASN:N	2.05	0.53
1:B:92:PRO:HD3	2:B:245:HOH:O	2.07	0.53
1:E:114:ASP:O	1:E:116:GLU:N	2.42	0.53
1:F:74:GLU:HG3	1:F:105:LYS:HG2	1.91	0.53
1:D:40:PHE:O	1:D:56:HIS:HB2	2.09	0.53
1:D:96:VAL:HG12	1:D:140:LEU:O	2.09	0.53
1:H:18:TRP:HH2	1:H:140:LEU:CD1	2.22	0.53
1:F:104:ASN:HD22	1:F:104:ASN:N	2.07	0.53
1:A:89:LEU:HG	1:A:139:LEU:HD21	1.91	0.53
1:C:18:TRP:CZ3	1:C:136:THR:OG1	2.55	0.53
1:A:60:LEU:N	1:A:60:LEU:HD22	2.23	0.52
1:H:18:TRP:CD1	1:H:18:TRP:C	2.81	0.52
1:B:97:ARG:O	1:B:113:GLY:HA3	2.09	0.52
1:G:125:GLU:OE2	1:H:133:LYS:HE3	2.09	0.52
1:D:89:LEU:CD1	1:D:139:LEU:HD22	2.39	0.52
1:C:35:GLU:HG3	1:C:86:PHE:HZ	1.74	0.52
1:H:11:GLY:HA3	1:H:142:ALA:HA	1.91	0.52
1:C:31:LEU:HA	1:C:39:SER:O	2.10	0.52
1:D:14:GLY:O	1:D:135:ARG:CG	2.53	0.52
1:B:23:TYR:CE2	1:B:51:PHE:CE2	2.98	0.52
1:B:135:ARG:HD2	2:B:268:HOH:O	2.08	0.52
1:E:11:GLY:HA2	1:E:83:THR:HG23	1.91	0.52
1:E:60:LEU:HD11	1:E:89:LEU:CD1	2.30	0.52
1:D:100:THR:HG22	1:D:111:PRO:HA	1.92	0.52
1:A:5:ILE:HG13	1:B:149:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:20:GLU:OE1	1:D:44:TYR:OH	2.27	0.52
1:G:83:THR:HG22	1:G:118:THR:CG2	2.40	0.52
1:D:132:PHE:CE1	1:D:145:ILE:CD1	2.93	0.52
1:F:58:SER:HB2	1:F:138:ASP:O	2.11	0.51
1:A:28:GLN:NE2	1:A:43:ILE:HD12	2.25	0.51
1:F:32:SER:HA	1:F:63:LYS:O	2.10	0.51
1:G:130:VAL:HG21	1:G:148:SER:HB3	1.93	0.51
1:D:86:PHE:CD2	1:D:89:LEU:HG	2.46	0.51
1:D:33:TYR:CD1	1:D:33:TYR:N	2.79	0.51
1:D:60:LEU:HD11	1:D:89:LEU:CD1	2.41	0.51
1:D:86:PHE:HD2	1:D:89:LEU:HG	1.75	0.50
1:G:36:ALA:HA	1:G:97:ARG:HA	1.93	0.50
1:H:35:GLU:HA	1:H:114:ASP:OD2	2.11	0.50
1:H:31:LEU:HA	1:H:39:SER:O	2.11	0.50
1:G:33:TYR:O	1:G:62:TYR:HB3	2.12	0.50
1:B:18:TRP:CZ3	1:B:136:THR:OG1	2.63	0.50
1:D:18:TRP:C	1:D:18:TRP:CD1	2.85	0.50
1:C:22:SER:C	1:C:23:TYR:CD1	2.85	0.50
1:H:135:ARG:HG3	1:H:142:ALA:HB3	1.93	0.50
1:F:41:SER:HB3	1:F:55:LYS:HA	1.94	0.50
1:F:100:THR:HG22	2:F:202:HOH:O	2.10	0.50
1:F:47:ASN:ND2	1:H:22:SER:H	2.09	0.50
1:C:60:LEU:HD11	1:C:89:LEU:CD1	2.35	0.49
1:F:27:ARG:HB2	1:F:43:ILE:HG22	1.93	0.49
1:C:22:SER:O	1:C:23:TYR:CD1	2.65	0.49
1:C:75:PHE:H	1:C:104:ASN:ND2	2.10	0.49
1:E:42:VAL:HG13	1:E:44:TYR:CE2	2.47	0.49
1:B:89:LEU:HD11	1:B:139:LEU:CD2	2.43	0.49
1:F:106:GLY:HA2	2:F:209:HOH:O	2.11	0.49
1:E:62:TYR:CD1	1:E:62:TYR:N	2.80	0.49
1:B:18:TRP:HH2	1:B:140:LEU:CD1	2.26	0.49
1:H:12:GLY:HA2	1:H:94:PRO:HG2	1.94	0.49
1:D:71:PHE:HE2	2:D:177:HOH:O	1.96	0.49
1:C:18:TRP:HH2	1:C:140:LEU:HD13	1.78	0.49
1:F:47:ASN:HD21	1:H:22:SER:H	1.61	0.49
1:E:60:LEU:CG	1:E:89:LEU:HD11	2.43	0.49
1:G:63:LYS:CB	2:G:246:HOH:O	2.61	0.49
1:B:96:VAL:HG13	1:B:140:LEU:O	2.13	0.49
1:B:18:TRP:CD1	1:B:56:HIS:NE2	2.81	0.49
1:H:83:THR:HG22	1:H:118:THR:O	2.12	0.49
1:H:74:GLU:OE1	1:H:107:ARG:NH1	2.45	0.48
1:F:89:LEU:HD11	1:F:139:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:18:TRP:CG	1:F:56:HIS:CE1	3.01	0.48
1:C:97:ARG:NH1	1:C:116:GLU:HG3	2.27	0.48
1:E:84:GLY:O	1:E:95:VAL:HG12	2.14	0.48
1:D:36:ALA:HB3	1:D:139:LEU:CD2	2.43	0.48
1:D:94:PRO:HD2	2:D:236:HOH:O	2.12	0.48
1:G:102:LYS:HD3	1:G:108:THR:HB	1.95	0.48
1:A:3:GLN:HG3	1:B:126:ASN:ND2	2.28	0.48
1:G:8:GLY:N	1:H:123:PRO:O	2.46	0.48
1:F:21:GLY:O	1:F:131:GLY:HA3	2.14	0.48
1:E:18:TRP:CG	1:E:56:HIS:CE1	3.02	0.48
1:A:89:LEU:O	1:A:90:ALA:C	2.51	0.48
1:H:67:ILE:HG12	1:H:109:PHE:CD2	2.48	0.48
1:A:60:LEU:H	1:A:60:LEU:CD2	2.25	0.48
1:D:18:TRP:CH2	1:D:140:LEU:HD11	2.49	0.47
1:C:13:PRO:HD2	1:C:93:THR:OG1	2.14	0.47
1:B:44:TYR:CE1	1:B:131:GLY:HA2	2.49	0.47
1:H:71:PHE:CE1	1:H:72:PRO:HB3	2.50	0.47
1:E:18:TRP:CD1	1:E:18:TRP:C	2.87	0.47
1:F:17:GLY:HA2	1:F:135:ARG:HG2	1.96	0.47
1:D:7:VAL:CG1	1:D:8:GLY:N	2.77	0.47
1:E:5:ILE:HG13	1:F:149:LEU:HD13	1.96	0.47
1:G:95:VAL:HG13	1:G:140:LEU:O	2.14	0.47
1:H:27:ARG:HH21	1:H:50:PRO:N	2.11	0.47
1:B:34:LYS:NZ	2:B:170:HOH:O	2.26	0.47
1:B:18:TRP:CH2	1:B:140:LEU:CD1	2.98	0.47
1:F:33:TYR:HD2	1:F:113:GLY:H	1.62	0.47
1:A:4:THR:HG21	1:A:22:SER:OG	2.14	0.47
1:E:1:AYA:OT	1:G:71:PHE:CE2	2.68	0.47
1:A:23:TYR:HE2	1:A:51:PHE:CD2	2.32	0.47
1:G:71:PHE:C	1:G:71:PHE:CD1	2.88	0.47
1:F:31:LEU:C	1:F:31:LEU:HD12	2.35	0.47
1:G:75:PHE:H	1:G:104:ASN:ND2	2.13	0.47
1:G:11:GLY:HA2	1:G:83:THR:OG1	2.15	0.47
1:A:132:PHE:CE1	1:A:145:ILE:CD1	2.98	0.47
1:G:35:GLU:HB3	1:G:97:ARG:HH21	1.79	0.47
1:A:148:SER:HA	1:B:5:ILE:HD11	1.97	0.47
1:H:27:ARG:HH21	1:H:49:ASP:C	2.18	0.47
1:H:58:SER:OG	1:H:60:LEU:HB2	2.15	0.47
1:H:40:PHE:O	1:H:56:HIS:HB2	2.15	0.47
1:D:99:LEU:HA	1:D:99:LEU:HD12	1.78	0.46
1:C:58:SER:OG	1:C:60:LEU:HD12	2.15	0.46
1:E:24:THR:O	1:G:2:SER:OG	2.33	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:60:LEU:CD2	1:F:60:LEU:H	2.24	0.46
1:D:74:GLU:HA	1:D:104:ASN:ND2	2.16	0.46
1:F:110:GLY:HA2	2:F:210:HOH:O	2.14	0.46
1:C:74:GLU:CA	1:C:104:ASN:HD21	2.19	0.46
1:A:58:SER:HB2	1:A:138:ASP:O	2.16	0.46
1:A:67:ILE:HG23	1:A:109:PHE:CE2	2.51	0.46
1:D:31:LEU:C	1:D:31:LEU:HD12	2.36	0.46
1:B:93:THR:HG22	2:B:195:HOH:O	2.15	0.46
1:A:28:GLN:NE2	1:A:66:LYS:HE2	2.30	0.46
1:A:67:ILE:HG23	1:A:109:PHE:CD2	2.51	0.46
1:G:17:GLY:HA2	1:G:135:ARG:HG2	1.97	0.46
1:C:46:LEU:HD23	1:C:46:LEU:HA	1.86	0.46
1:F:98:SER:HA	1:F:112:TYR:O	2.15	0.46
1:B:18:TRP:C	1:B:18:TRP:CD1	2.89	0.46
1:G:139:LEU:CD2	1:G:139:LEU:N	2.78	0.46
1:H:27:ARG:NH2	1:H:50:PRO:N	2.64	0.46
1:B:135:ARG:HG3	1:B:142:ALA:HB3	1.98	0.46
1:D:7:VAL:HG13	1:D:8:GLY:N	2.31	0.46
1:H:16:ASN:O	1:H:135:ARG:HA	2.15	0.45
1:F:71:PHE:HE1	1:H:1:AYA:HM3	1.81	0.45
1:H:99:LEU:O	1:H:100:THR:HG22	2.16	0.45
1:G:4:THR:HG21	1:G:146:HIS:ND1	2.31	0.45
1:C:64:ASN:HB3	2:C:172:HOH:O	2.17	0.45
1:F:76:LEU:HD11	1:F:101:PHE:HB3	1.99	0.45
1:F:75:PHE:H	1:F:104:ASN:HD21	1.57	0.45
1:H:18:TRP:CH2	1:H:140:LEU:CD1	3.00	0.45
1:B:109:PHE:HB3	1:B:112:TYR:OH	2.16	0.45
1:H:96:VAL:HG12	1:H:140:LEU:O	2.16	0.45
1:F:90:ALA:HA	2:F:248:HOH:O	2.16	0.45
1:F:58:SER:HB2	1:F:60:LEU:HD23	1.98	0.45
1:A:28:GLN:HB3	1:A:43:ILE:HB	1.98	0.45
1:E:62:TYR:HD1	1:E:62:TYR:N	2.14	0.45
1:B:23:TYR:O	1:B:130:VAL:HG22	2.16	0.45
1:A:74:GLU:HG3	1:A:105:LYS:HB2	1.99	0.45
1:F:44:TYR:O	1:F:51:PHE:N	2.45	0.45
1:G:130:VAL:O	1:G:130:VAL:CG1	2.64	0.45
1:C:97:ARG:HH12	1:C:116:GLU:CD	2.20	0.45
1:E:37:ILE:HG21	1:E:140:LEU:HD23	1.99	0.45
1:G:24:THR:O	1:G:24:THR:HG22	2.17	0.45
1:D:18:TRP:CZ3	1:D:136:THR:CG2	2.77	0.45
1:F:18:TRP:CD1	1:F:18:TRP:C	2.89	0.45
1:A:104:ASN:HD22	1:A:104:ASN:N	2.15	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:37:ILE:HD12	1:H:99:LEU:HD22	1.99	0.45
1:G:26:ILE:HG22	1:G:69:LEU:HD12	1.98	0.44
1:A:89:LEU:CG	1:A:139:LEU:HD21	2.47	0.44
1:A:89:LEU:HA	1:A:89:LEU:HD22	1.63	0.44
1:F:34:LYS:HB2	1:F:62:TYR:CG	2.52	0.44
1:A:18:TRP:CD1	1:A:18:TRP:C	2.91	0.44
1:D:54:PRO:HG2	2:D:164:HOH:O	2.16	0.44
1:E:18:TRP:CD1	1:E:56:HIS:CE1	3.05	0.44
1:A:116:GLU:HG3	2:A:208:HOH:O	2.17	0.44
1:C:71:PHE:CD1	1:C:71:PHE:C	2.91	0.44
1:H:84:GLY:HA2	2:H:202:HOH:O	2.17	0.44
1:E:87:SER:O	1:E:90:ALA:N	2.44	0.44
1:B:18:TRP:HZ3	1:B:136:THR:OG1	1.99	0.44
1:C:18:TRP:HZ3	1:C:136:THR:N	2.16	0.44
1:B:32:SER:HB3	1:B:64:ASN:ND2	2.33	0.44
1:H:97:ARG:O	1:H:113:GLY:HA3	2.17	0.44
1:B:104:ASN:OD1	1:B:104:ASN:N	2.51	0.44
1:A:110:GLY:HA3	2:A:203:HOH:O	2.18	0.44
1:E:60:LEU:HD21	1:E:89:LEU:HD11	2.00	0.44
1:F:68:GLU:HB3	2:F:154:HOH:O	2.18	0.44
1:G:31:LEU:HD12	1:G:31:LEU:C	2.38	0.44
1:A:30:GLU:HG2	1:A:66:LYS:HG3	2.00	0.43
1:B:67:ILE:HG22	1:B:69:LEU:HD22	1.99	0.43
1:A:96:VAL:HG22	1:A:140:LEU:O	2.17	0.43
1:D:103:THR:HG23	1:D:105:LYS:H	1.84	0.43
1:F:74:GLU:OE2	1:F:107:ARG:HD3	2.17	0.43
1:C:87:SER:O	1:C:88:ALA:C	2.56	0.43
1:B:89:LEU:HD11	1:B:139:LEU:HD22	2.00	0.43
1:E:134:GLY:O	1:E:135:ARG:HG3	2.18	0.43
1:C:8:GLY:O	1:C:9:SER:HB2	2.18	0.43
1:E:34:LYS:HB2	1:E:62:TYR:CD1	2.53	0.43
1:C:97:ARG:NH1	1:C:116:GLU:CG	2.82	0.43
1:G:18:TRP:CH2	1:G:140:LEU:CD1	3.02	0.43
1:F:71:PHE:O	2:F:182:HOH:O	2.21	0.43
1:F:18:TRP:CH2	1:F:140:LEU:HD11	2.54	0.43
1:D:86:PHE:CZ	1:D:88:ALA:HB3	2.53	0.43
1:B:39:SER:HB3	1:B:57:THR:CA	2.47	0.43
1:C:5:ILE:HG13	1:D:149:LEU:HD13	2.00	0.43
1:D:67:ILE:HG23	1:D:109:PHE:CE2	2.54	0.43
1:A:77:GLU:O	1:A:77:GLU:HG2	2.17	0.43
1:F:24:THR:HG22	1:F:24:THR:O	2.19	0.43
1:E:33:TYR:HE1	1:E:65:VAL:HG22	1.84	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:105:LYS:HB3	1:C:105:LYS:HE2	1.62	0.43
1:D:43:ILE:HG12	1:D:52:SER:HB3	2.01	0.43
1:B:31:LEU:HA	1:B:39:SER:O	2.19	0.43
1:A:132:PHE:HE1	1:A:145:ILE:HD11	1.82	0.43
1:G:59:LYS:O	1:G:60:LEU:C	2.57	0.43
1:D:139:LEU:HD12	1:D:139:LEU:HA	1.78	0.42
1:B:1:AYA:HM2	1:D:128:LEU:HD21	2.01	0.42
1:B:34:LYS:HG2	1:B:35:GLU:CD	2.39	0.42
1:A:75:PHE:H	1:A:104:ASN:ND2	2.16	0.42
1:D:18:TRP:HH2	1:D:140:LEU:CD1	2.33	0.42
1:C:104:ASN:HD22	1:C:104:ASN:N	2.17	0.42
1:A:20:GLU:CG	1:A:54:PRO:HD2	2.47	0.42
1:E:75:PHE:H	1:E:104:ASN:HD21	1.66	0.42
1:D:69:LEU:HA	1:D:69:LEU:HD12	1.79	0.42
1:B:32:SER:HA	1:B:63:LYS:O	2.19	0.42
1:C:50:PRO:HG2	1:C:50:PRO:O	2.19	0.42
1:H:122:LEU:HA	1:H:122:LEU:HD12	1.77	0.42
1:G:100:THR:HG21	2:G:224:HOH:O	2.18	0.42
1:F:46:LEU:HD12	1:F:46:LEU:HA	1.70	0.42
1:H:96:VAL:CG1	1:H:140:LEU:O	2.67	0.42
1:B:121:ASN:ND2	1:B:123:PRO:HG3	2.35	0.42
1:B:13:PRO:HB2	2:B:160:HOH:O	2.20	0.42
1:G:20:GLU:HG2	1:G:54:PRO:HD2	2.00	0.42
1:E:81:GLY:O	1:E:82:TYR:HB2	2.20	0.42
1:B:23:TYR:N	1:B:23:TYR:CD1	2.87	0.42
1:B:93:THR:HA	1:B:94:PRO:HD3	1.99	0.42
1:G:8:GLY:HA2	1:H:123:PRO:CB	2.36	0.42
1:D:37:ILE:HA	1:D:37:ILE:HD13	1.87	0.42
1:H:27:ARG:CZ	1:H:50:PRO:HG3	2.50	0.42
1:F:34:LYS:HD3	1:F:62:TYR:HA	2.02	0.42
1:C:93:THR:HG23	2:C:200:HOH:O	2.20	0.42
1:H:74:GLU:HA	1:H:104:ASN:ND2	2.21	0.42
1:A:47:ASN:OD1	1:C:23:TYR:CE1	2.73	0.42
1:C:59:LYS:NZ	2:C:188:HOH:O	2.51	0.42
1:G:140:LEU:HD11	1:G:142:ALA:O	2.20	0.42
1:H:27:ARG:NH2	1:H:45:ASP:OD1	2.53	0.42
1:H:60:LEU:HA	1:H:60:LEU:HD12	1.70	0.42
1:A:23:TYR:CE2	1:A:51:PHE:CE2	3.06	0.42
1:G:20:GLU:OE1	1:G:44:TYR:OH	2.25	0.42
1:A:32:SER:HA	1:A:64:ASN:HA	2.02	0.42
1:B:82:TYR:HE1	1:B:115:GLU:OE1	2.02	0.42
1:C:33:TYR:O	1:C:62:TYR:HB3	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:104:ASN:HD22	1:C:104:ASN:H	1.66	0.42
1:F:29:ILE:HB	1:F:67:ILE:HD12	2.01	0.42
1:D:65:VAL:HG21	1:D:112:TYR:CE1	2.55	0.42
1:H:26:ILE:HG23	1:H:42:VAL:CG2	2.49	0.42
1:E:60:LEU:HD23	1:E:139:LEU:HD12	2.01	0.41
1:A:18:TRP:CE2	1:A:56:HIS:CD2	3.07	0.41
1:H:46:LEU:O	1:H:47:ASN:C	2.59	0.41
1:B:49:ASP:HB3	2:B:230:HOH:O	2.20	0.41
1:F:58:SER:HB2	1:F:60:LEU:CD2	2.50	0.41
1:H:67:ILE:HG23	1:H:109:PHE:CE2	2.55	0.41
1:B:1:AYA:H	1:D:128:LEU:CD2	2.30	0.41
1:A:74:GLU:OE2	1:A:107:ARG:HD3	2.20	0.41
1:E:42:VAL:CG1	1:E:44:TYR:CZ	3.03	0.41
1:D:45:ASP:CG	1:D:71:PHE:CZ	2.93	0.41
1:F:121:ASN:O	1:F:123:PRO:HD3	2.20	0.41
1:G:96:VAL:HG22	1:G:140:LEU:HD23	2.02	0.41
1:F:35:GLU:O	1:F:97:ARG:NE	2.53	0.41
1:H:130:VAL:HG21	1:H:148:SER:HB3	2.02	0.41
1:D:89:LEU:HD11	1:D:139:LEU:HD13	2.02	0.41
1:C:135:ARG:HG3	1:C:142:ALA:CB	2.49	0.41
1:D:109:PHE:N	1:D:109:PHE:CD1	2.88	0.41
1:H:12:GLY:CA	1:H:94:PRO:HG2	2.49	0.41
1:D:129:ILE:HG12	1:D:145:ILE:HG12	2.03	0.41
1:E:34:LYS:HB2	1:E:62:TYR:CG	2.55	0.41
1:A:31:LEU:HD12	1:A:65:VAL:HG12	2.03	0.41
1:F:129:ILE:HG21	1:F:129:ILE:HD13	1.81	0.41
1:D:74:GLU:CG	1:D:105:LYS:HG2	2.51	0.41
1:H:7:VAL:HG13	1:H:8:GLY:N	2.35	0.41
1:F:36:ALA:HA	1:F:97:ARG:HA	2.01	0.41
1:B:58:SER:OG	1:B:60:LEU:HB2	2.21	0.41
1:A:96:VAL:HG21	1:A:140:LEU:HD23	2.02	0.41
1:C:33:TYR:C	1:C:62:TYR:HB3	2.41	0.41
1:F:82:TYR:CD1	1:F:115:GLU:HG2	2.56	0.41
1:C:29:ILE:HG12	1:C:42:VAL:HG13	2.02	0.41
1:H:71:PHE:CD1	1:H:72:PRO:CA	3.02	0.41
1:A:128:LEU:HD21	1:C:1:AYA:CT	2.51	0.41
1:E:89:LEU:O	1:E:90:ALA:HB3	2.21	0.41
1:G:119:TYR:CE2	1:G:121:ASN:HB2	2.56	0.41
1:F:71:PHE:CE1	1:H:1:AYA:HM3	2.55	0.41
1:H:29:ILE:HD11	1:H:76:LEU:HD21	2.02	0.41
1:B:4:THR:HG23	1:B:5:ILE:O	2.21	0.41
1:E:37:ILE:HG23	1:E:37:ILE:HD12	1.82	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:60:LEU:HB3	1:F:61:PRO:HD2	2.02	0.40
1:A:87:SER:O	1:A:90:ALA:HA	2.21	0.40
1:C:123:PRO:HD2	1:D:8:GLY:HA2	2.03	0.40
1:E:125:GLU:HG3	2:E:226:HOH:O	2.20	0.40
1:D:6:THR:HG23	1:D:146:HIS:ND1	2.36	0.40
1:G:104:ASN:ND2	1:G:104:ASN:N	2.70	0.40
1:E:82:TYR:CD2	1:E:115:GLU:HG2	2.55	0.40
1:H:25:GLY:HA2	2:H:153:HOH:O	2.22	0.40
1:A:64:ASN:ND2	2:A:244:HOH:O	2.53	0.40
1:C:132:PHE:CE1	1:C:145:ILE:HD11	2.57	0.40
1:D:129:ILE:HG22	1:D:130:VAL:N	2.36	0.40
1:A:47:ASN:HD21	1:C:22:SER:H	1.67	0.40
1:E:18:TRP:CD1	1:E:19:ASP:N	2.90	0.40
1:H:100:THR:CG2	2:H:196:HOH:O	2.69	0.40
1:E:89:LEU:HD22	1:E:89:LEU:HA	1.68	0.40
1:G:95:VAL:HG11	1:G:139:LEU:HG	2.04	0.40
1:F:121:ASN:C	1:F:123:PRO:HD3	2.41	0.40
1:A:31:LEU:HD12	1:A:31:LEU:C	2.42	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	147/149 (99%)	133 (90%)	12 (8%)	2 (1%)	16	22
1	B	147/149 (99%)	136 (92%)	8 (5%)	3 (2%)	11	13
1	C	147/149 (99%)	131 (89%)	11 (8%)	5 (3%)	6	4
1	D	147/149 (99%)	132 (90%)	12 (8%)	3 (2%)	11	13
1	E	147/149 (99%)	131 (89%)	12 (8%)	4 (3%)	8	7
1	F	147/149 (99%)	135 (92%)	11 (8%)	1 (1%)	30	43
1	G	147/149 (99%)	139 (95%)	6 (4%)	2 (1%)	16	22
1	H	147/149 (99%)	128 (87%)	17 (12%)	2 (1%)	16	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1176/1192 (99%)	1065 (91%)	89 (8%)	22 (2%)	12	14

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	110	GLY
1	B	9	SER
1	B	110	GLY
1	C	9	SER
1	C	110	GLY
1	D	110	GLY
1	E	110	GLY
1	F	9	SER
1	H	110	GLY
1	C	70	LYS
1	D	130	VAL
1	G	90	ALA
1	B	34	LYS
1	C	106	GLY
1	E	34	LYS
1	E	81	GLY
1	D	34	LYS
1	H	34	LYS
1	G	34	LYS
1	E	13	PRO
1	C	137	GLY

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	120/122 (98%)	95 (79%)	25 (21%)	2	2
1	B	120/122 (98%)	93 (78%)	27 (22%)	1	1
1	C	120/122 (98%)	95 (79%)	25 (21%)	2	2
1	D	120/122 (98%)	93 (78%)	27 (22%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	119/122 (98%)	95 (80%)	24 (20%)	2	2
1	F	119/122 (98%)	95 (80%)	24 (20%)	2	2
1	G	120/122 (98%)	96 (80%)	24 (20%)	2	2
1	H	120/122 (98%)	90 (75%)	30 (25%)	1	1
All	All	958/976 (98%)	752 (78%)	206 (22%)	1	1

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	7	VAL
1	A	9	SER
1	A	18	TRP
1	A	42	VAL
1	A	58	SER
1	A	59	LYS
1	A	64	ASN
1	A	69	LEU
1	A	72	PRO
1	A	76	LEU
1	A	83	THR
1	A	86	PHE
1	A	89	LEU
1	A	91	THR
1	A	95	VAL
1	A	100	THR
1	A	104	ASN
1	A	108	THR
1	A	116	GLU
1	A	118	THR
1	A	130	VAL
1	A	143	ILE
1	A	145	ILE
1	A	149	LEU
1	B	4	THR
1	B	7	VAL
1	B	18	TRP
1	B	24	THR
1	B	28	GLN
1	B	34	LYS
1	B	39	SER

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Mol	Chain	Res	Type
1	B	42	VAL
1	B	49	ASP
1	B	55	LYS
1	B	59	LYS
1	B	60	LEU
1	B	66	LYS
1	B	76	LEU
1	B	83	THR
1	B	86	PHE
1	B	91	THR
1	B	93	THR
1	B	95	VAL
1	B	96	VAL
1	B	102	LYS
1	B	108	THR
1	B	116	GLU
1	B	130	VAL
1	B	139	LEU
1	B	145	ILE
1	B	149	LEU
1	C	2	SER
1	C	4	THR
1	C	5	ILE
1	C	13	PRO
1	C	22	SER
1	C	35	GLU
1	C	46	LEU
1	C	52	SER
1	C	69	LEU
1	C	76	LEU
1	C	83	THR
1	C	98	SER
1	C	100	THR
1	C	102	LYS
1	C	104	ASN
1	C	105	LYS
1	C	108	THR
1	C	111	PRO
1	C	118	THR
1	C	130	VAL
1	C	133	LYS
1	C	135	ARG

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Mol	Chain	Res	Type
1	C	139	LEU
1	C	143	ILE
1	C	145	ILE
1	D	7	VAL
1	D	16	ASN
1	D	18	TRP
1	D	22	SER
1	D	34	LYS
1	D	42	VAL
1	D	49	ASP
1	D	69	LEU
1	D	76	LEU
1	D	80	SER
1	D	93	THR
1	D	95	VAL
1	D	96	VAL
1	D	98	SER
1	D	100	THR
1	D	103	THR
1	D	104	ASN
1	D	108	THR
1	D	118	THR
1	D	120	PHE
1	D	130	VAL
1	D	135	ARG
1	D	138	ASP
1	D	143	ILE
1	D	145	ILE
1	D	148	SER
1	D	149	LEU
1	E	5	ILE
1	E	7	VAL
1	E	13	PRO
1	E	18	TRP
1	E	24	THR
1	E	49	ASP
1	E	57	THR
1	E	69	LEU
1	E	76	LEU
1	E	89	LEU
1	E	93	THR
1	E	95	VAL

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Mol	Chain	Res	Type
1	E	103	THR
1	E	104	ASN
1	E	108	THR
1	E	115	GLU
1	E	118	THR
1	E	125	GLU
1	E	130	VAL
1	E	138	ASP
1	E	141	ASP
1	E	143	ILE
1	E	148	SER
1	E	149	LEU
1	F	7	VAL
1	F	18	TRP
1	F	28	GLN
1	F	34	LYS
1	F	42	VAL
1	F	43	ILE
1	F	57	THR
1	F	60	LEU
1	F	70	LYS
1	F	72	PRO
1	F	76	LEU
1	F	80	SER
1	F	87	SER
1	F	89	LEU
1	F	94	PRO
1	F	95	VAL
1	F	102	LYS
1	F	104	ASN
1	F	130	VAL
1	F	133	LYS
1	F	141	ASP
1	F	145	ILE
1	F	148	SER
1	F	149	LEU
1	G	2	SER
1	G	4	THR
1	G	9	SER
1	G	18	TRP
1	G	34	LYS
1	G	49	ASP

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Mol	Chain	Res	Type
1	G	70	LYS
1	G	72	PRO
1	G	76	LEU
1	G	83	THR
1	G	86	PHE
1	G	89	LEU
1	G	96	VAL
1	G	100	THR
1	G	102	LYS
1	G	104	ASN
1	G	105	LYS
1	G	108	THR
1	G	120	PHE
1	G	125	GLU
1	G	130	VAL
1	G	133	LYS
1	G	139	LEU
1	G	145	ILE
1	H	7	VAL
1	H	18	TRP
1	H	22	SER
1	H	28	GLN
1	H	34	LYS
1	H	37	ILE
1	H	42	VAL
1	H	49	ASP
1	H	58	SER
1	H	60	LEU
1	H	68	GLU
1	H	69	LEU
1	H	76	LEU
1	H	77	GLU
1	H	80	SER
1	H	87	SER
1	H	89	LEU
1	H	91	THR
1	H	95	VAL
1	H	96	VAL
1	H	98	SER
1	H	100	THR
1	H	101	PHE
1	H	104	ASN

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Mol	Chain	Res	Type
1	H	108	THR
1	H	118	THR
1	H	128	LEU
1	H	135	ARG
1	H	143	ILE
1	H	145	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	28	GLN
1	A	47	ASN
1	A	104	ASN
1	B	16	ASN
1	B	47	ASN
1	B	64	ASN
1	B	126	ASN
1	C	16	ASN
1	C	28	GLN
1	C	47	ASN
1	C	104	ASN
1	D	28	GLN
1	D	104	ASN
1	E	47	ASN
1	E	56	HIS
1	E	104	ASN
1	F	47	ASN
1	F	64	ASN
1	F	104	ASN
1	G	47	ASN
1	G	104	ASN
1	H	47	ASN
1	H	104	ASN
1	H	121	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	AYA	A	1	1	7,7,8	7.77	2 (28%)	6,8,10	28.34	5 (83%)
1	AYA	B	1	1	7,7,8	7.23	3 (42%)	6,8,10	29.98	6 (100%)
1	AYA	C	1	1	7,7,8	6.57	3 (42%)	6,8,10	30.21	5 (83%)
1	AYA	D	1	1	7,7,8	6.49	3 (42%)	6,8,10	29.16	3 (50%)
1	AYA	E	1	1	7,7,8	6.88	2 (28%)	6,8,10	31.34	3 (50%)
1	AYA	F	1	1	7,7,8	6.10	3 (42%)	6,8,10	30.99	6 (100%)
1	AYA	G	1	1	7,7,8	8.35	3 (42%)	6,8,10	29.30	3 (50%)
1	AYA	H	1	1	7,7,8	7.79	3 (42%)	6,8,10	34.31	5 (83%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	AYA	A	1	1	1/1/2/4	0/4/6/8	0/0/0/0
1	AYA	B	1	1	1/1/2/4	0/4/6/8	0/0/0/0
1	AYA	C	1	1	1/1/2/4	1/4/6/8	0/0/0/0
1	AYA	D	1	1	-	0/4/6/8	0/0/0/0
1	AYA	E	1	1	1/1/2/4	0/4/6/8	0/0/0/0
1	AYA	F	1	1	-	0/4/6/8	0/0/0/0
1	AYA	G	1	1	1/1/2/4	0/4/6/8	0/0/0/0
1	AYA	H	1	1	1/1/2/4	0/4/6/8	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1	AYA	O-C	21.47	1.26	1.11
1	A	1	AYA	O-C	20.28	1.25	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	1	AYA	O-C	19.90	1.25	1.11
1	B	1	AYA	O-C	18.73	1.24	1.11
1	E	1	AYA	O-C	17.65	1.23	1.11
1	C	1	AYA	O-C	16.95	1.23	1.11
1	D	1	AYA	O-C	15.97	1.22	1.11
1	F	1	AYA	O-C	14.97	1.21	1.11
1	F	1	AYA	CA-C	4.78	1.57	1.48
1	D	1	AYA	CA-C	4.76	1.57	1.48
1	E	1	AYA	CA-C	4.29	1.56	1.48
1	H	1	AYA	CA-C	4.22	1.56	1.48
1	G	1	AYA	CA-N	-4.15	1.40	1.46
1	D	1	AYA	CA-N	3.33	1.50	1.46
1	F	1	AYA	CA-N	3.00	1.50	1.46
1	H	1	AYA	OT-CT	3.00	1.29	1.23
1	A	1	AYA	CA-C	2.92	1.53	1.48
1	C	1	AYA	CA-C	2.80	1.53	1.48
1	G	1	AYA	CA-C	2.77	1.53	1.48
1	C	1	AYA	CM-CT	2.46	1.55	1.50
1	B	1	AYA	CM-CT	2.33	1.55	1.50
1	B	1	AYA	CA-C	2.24	1.52	1.48

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1	AYA	CB-CA-C	82.08	145.07	108.46
1	E	1	AYA	CB-CA-C	74.66	141.76	108.46
1	F	1	AYA	CB-CA-C	73.69	141.33	108.46
1	C	1	AYA	CB-CA-C	71.46	140.34	108.46
1	B	1	AYA	CB-CA-C	71.18	140.21	108.46
1	G	1	AYA	CB-CA-C	69.46	139.44	108.46
1	D	1	AYA	CB-CA-C	68.74	139.12	108.46
1	A	1	AYA	CB-CA-C	66.84	138.27	108.46
1	D	1	AYA	CB-CA-N	17.32	136.60	110.24
1	C	1	AYA	CB-CA-N	17.21	136.45	110.24
1	G	1	AYA	CB-CA-N	16.85	135.89	110.24
1	A	1	AYA	CB-CA-N	16.70	135.66	110.24
1	E	1	AYA	CB-CA-N	15.71	134.16	110.24
1	B	1	AYA	CB-CA-N	15.53	133.88	110.24
1	H	1	AYA	CB-CA-N	15.48	133.81	110.24
1	F	1	AYA	CB-CA-N	15.39	133.68	110.24
1	D	1	AYA	CA-N-CT	8.74	140.09	121.44
1	F	1	AYA	CA-N-CT	8.42	139.41	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1	AYA	CA-N-CT	8.28	139.12	121.44
1	E	1	AYA	CA-N-CT	8.13	138.80	121.44
1	A	1	AYA	CA-N-CT	7.90	138.30	121.44
1	C	1	AYA	CA-N-CT	7.66	137.80	121.44
1	G	1	AYA	CA-N-CT	6.17	134.61	121.44
1	B	1	AYA	OT-CT-N	-5.78	109.83	121.90
1	B	1	AYA	CA-N-CT	5.23	132.60	121.44
1	B	1	AYA	CM-CT-N	4.27	124.45	116.11
1	F	1	AYA	CM-CT-N	3.86	123.65	116.11
1	H	1	AYA	OT-CT-N	-2.82	116.01	121.90
1	C	1	AYA	OT-CT-CM	-2.72	116.72	122.04
1	C	1	AYA	CM-CT-N	2.60	121.18	116.11
1	B	1	AYA	OT-CT-CM	-2.57	117.03	122.04
1	F	1	AYA	OT-CT-N	-2.44	116.82	121.90
1	F	1	AYA	OT-CT-CM	-2.20	117.75	122.04
1	A	1	AYA	CM-CT-N	2.16	120.33	116.11
1	A	1	AYA	OT-CT-CM	-2.13	117.89	122.04
1	H	1	AYA	CM-CT-N	2.10	120.22	116.11

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	G	1	AYA	CA
1	A	1	AYA	CA
1	C	1	AYA	CA
1	H	1	AYA	CA
1	B	1	AYA	CA
1	E	1	AYA	CA

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	1	AYA	OT-CT-N-CA

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	149/149 (100%)	-0.64	2 (1%) 74 73	7, 20, 37, 60	0
1	B	149/149 (100%)	-0.54	0 100 100	11, 24, 37, 46	0
1	C	149/149 (100%)	-0.65	1 (0%) 84 84	7, 22, 34, 57	0
1	D	149/149 (100%)	-0.33	3 (2%) 62 59	11, 26, 44, 66	0
1	E	149/149 (100%)	-0.53	2 (1%) 74 73	8, 23, 47, 61	0
1	F	149/149 (100%)	-0.38	5 (3%) 43 41	9, 26, 44, 63	0
1	G	149/149 (100%)	-0.71	0 100 100	10, 21, 33, 52	0
1	H	149/149 (100%)	-0.42	2 (1%) 74 73	11, 26, 40, 60	0
All	All	1192/1192 (100%)	-0.52	15 (1%) 74 73	7, 24, 43, 66	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	91	THR	6.7
1	A	88	ALA	4.4
1	F	91	THR	4.3
1	D	91	THR	4.0
1	F	89	LEU	3.9
1	D	89	LEU	3.7
1	E	91	THR	3.6
1	H	88	ALA	3.5
1	A	91	THR	3.4
1	C	23	TYR	3.4
1	F	88	ALA	3.1
1	D	90	ALA	3.0
1	E	88	ALA	2.9
1	F	90	ALA	2.1
1	F	23	TYR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	AYA	A	1	8/9	0.13	1.14	24,26,31,35	0
1	AYA	C	1	8/9	0.12	0.92	18,23,29,34	0
1	AYA	E	1	8/9	0.11	0.32	12,20,22,22	0
1	AYA	G	1	8/9	0.10	0.19	22,26,31,31	0
1	AYA	B	1	8/9	0.12	0.16	30,33,37,38	0
1	AYA	F	1	8/9	0.10	-0.28	17,23,32,32	0
1	AYA	D	1	8/9	0.11	-0.32	22,28,32,34	0
1	AYA	H	1	8/9	0.08	-0.88	23,25,30,32	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.