



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:01 AM UTC

PDB ID : 7XGX / pdb_00007xgx
Title : Glucosyltransferase
Authors : Chen, T.T.; Ouyang, S.Y.
Deposited on : 2022-04-07
Resolution : 2.39 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

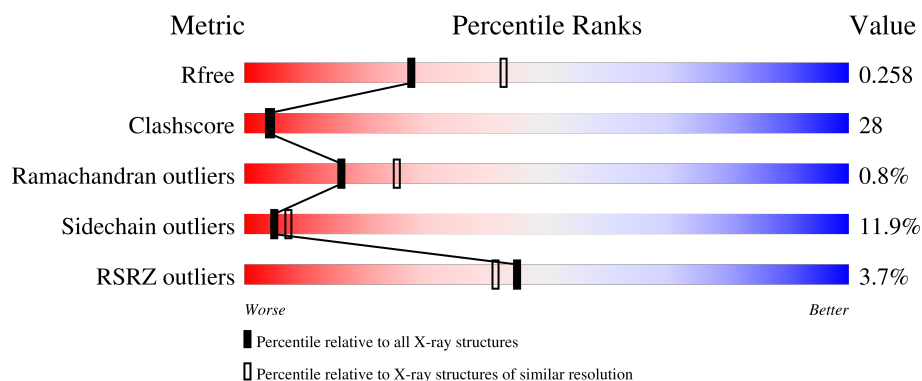
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	655	4% 53% 31% 8% • 7%
1	B	655	3% 48% 33% 8% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9711 atoms, of which 44 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 Lgt2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	0	0
			4801	3040	828	907	26			
1	B	591	Total	C	N	O	S	0	0	0
			4674	2964	802	882	26			

There are 38 discrepancies between the modelled and reference sequences:

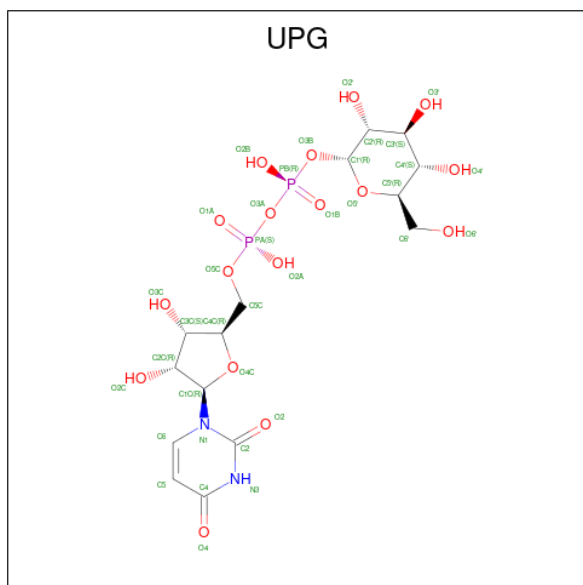
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP A0A2S6F0H5
A	-17	GLY	-	expression tag	UNP A0A2S6F0H5
A	-16	SER	-	expression tag	UNP A0A2S6F0H5
A	-15	SER	-	expression tag	UNP A0A2S6F0H5
A	-14	HIS	-	expression tag	UNP A0A2S6F0H5
A	-13	HIS	-	expression tag	UNP A0A2S6F0H5
A	-12	HIS	-	expression tag	UNP A0A2S6F0H5
A	-11	HIS	-	expression tag	UNP A0A2S6F0H5
A	-10	HIS	-	expression tag	UNP A0A2S6F0H5
A	-9	HIS	-	expression tag	UNP A0A2S6F0H5
A	-8	SER	-	expression tag	UNP A0A2S6F0H5
A	-7	SER	-	expression tag	UNP A0A2S6F0H5
A	-6	GLY	-	expression tag	UNP A0A2S6F0H5
A	-5	LEU	-	expression tag	UNP A0A2S6F0H5
A	-4	VAL	-	expression tag	UNP A0A2S6F0H5
A	-3	PRO	-	expression tag	UNP A0A2S6F0H5
A	-2	ARG	-	expression tag	UNP A0A2S6F0H5
A	-1	GLY	-	expression tag	UNP A0A2S6F0H5
A	0	SER	-	expression tag	UNP A0A2S6F0H5
B	-18	MET	-	initiating methionine	UNP A0A2S6F0H5
B	-17	GLY	-	expression tag	UNP A0A2S6F0H5
B	-16	SER	-	expression tag	UNP A0A2S6F0H5
B	-15	SER	-	expression tag	UNP A0A2S6F0H5
B	-14	HIS	-	expression tag	UNP A0A2S6F0H5
B	-13	HIS	-	expression tag	UNP A0A2S6F0H5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP A0A2S6F0H5
B	-11	HIS	-	expression tag	UNP A0A2S6F0H5
B	-10	HIS	-	expression tag	UNP A0A2S6F0H5
B	-9	HIS	-	expression tag	UNP A0A2S6F0H5
B	-8	SER	-	expression tag	UNP A0A2S6F0H5
B	-7	SER	-	expression tag	UNP A0A2S6F0H5
B	-6	GLY	-	expression tag	UNP A0A2S6F0H5
B	-5	LEU	-	expression tag	UNP A0A2S6F0H5
B	-4	VAL	-	expression tag	UNP A0A2S6F0H5
B	-3	PRO	-	expression tag	UNP A0A2S6F0H5
B	-2	ARG	-	expression tag	UNP A0A2S6F0H5
B	-1	GLY	-	expression tag	UNP A0A2S6F0H5
B	0	SER	-	expression tag	UNP A0A2S6F0H5

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total 52	O 52	0	0
3	B	68	Total 68	O 68	0	0

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.

Chain A:

Row	Col 1	Col 2	Col 3	Col 4	Col 5
1	V613	V518	G443	R308	T192
2	E614	S519	E444	E309	E193
3	R615	R520	E445	A318	I194
4	T616	L521	N446	S319	L195
5	Q617	N522			
6	S618		K449	V322	K199
7	L619	E525	L450	R323	K218
8	ARG	K526	S451	W324	N227
9	THR		L452	I325	I129
10	ASP	I530	P453	S326	M130
11		K531	N454	D340	S231
12	L624	K532	L455	T345	A232
13	S625	Y533	R456		M233
14					P134
15	W626	S639	Q461	K348	K235
16	M627	L540	A462		K236
17	P628	L541		E353	I237
18	S629	Y542	S467		D239
19	E630	K543	V470	H359	E242
20	Q631	V544	L473	P360	L146
21	R633	L545	G474	L362	L148
22	L634	M547	V475	L363	Q149
23	S635		Q476	M364	E152
24	K636	P552	R477	N365	P250
25		V555		G366	L255
26		T556	N481	S367	V256
27			V482		Y257
28		L560	E486	V374	R259
29			D487	K395	E160
30		L563	P564		K161
31		T565	P489	I399	L162
32		G566		K264	Y163
33		E567	Q492	K402	E164
34		P568	E493	R403	C165
35		T569	A494	I404	I166
36		R570		A405	R167
37		Y571	Q497	G406	D168
38		I572	G498	S407	K169
39			N499	L408	L170
40		L575	T500	I409	P171
41		K576	V501	L282	I172
42		Q577	V502	D283	P173
43		R578	L503	T416	G104
44		S579	T504	E417	S174
45		A580	N505	K421	K175
46			A506	Q290	F176
47		L583	L507	G291	E177
48			V508	E426	E178
49		T596	A509	D293	I179
50			G510	R429	L180
51		W606	L511		L181
52		L607	V512	M433	P182
53		T608	H513	Y436	I183
54		S609	G514	H437	V184
55		S610	N515	Q301	K187
56		E611	D516	K305	L117
57		N612	N517	A306	L118
58				R307	
59					
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Chain B:

3% 48% 33% 8% 10%

MET GLY SER HIS HIS HIS HIS SER SER SER GLY LEU VAL PRO ARG ARG GLY SER MET MET SER E3 Q4 Y5 W6 R7 F8 K9 L10 M11 T12 G15 C16 M17 Q18 M19 E20 A21 R22 T23 R24 L25 T26 V27 K28 K29 R30 LYS LEU LEU SER PHE PHE PRO GLU GLU S39 I40 M41 M42

M597	F598	T599	I603	P604	M605	M606	T607	T608	S609	S610	E611	E612	VAL	GLU	ARG	THR	GLN	SER	LEU	ARG	THR	ASP	GLY	L624	S625	W626	M627	P628	S629	E630	GLN	ALA	ARG	LEU	SER	LYS													
A506	L439	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
D285	L439	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
E286	L440	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
C289	L441	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
D293	E444	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
K307	E445	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
N314	E446	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
D320	E451	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
W324	E452	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
D340	E455	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
N341	E456	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
P342	T460	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
K343	Q461	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
L344	Q461	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
T345	S464	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
K348	N465	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
K351	S467	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
Y356	S468	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
H359	S470	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
P360	S471	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
L363	S472	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
K364	S473	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
K365	S474	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
G366	S475	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
S367	S476	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
A368	S477	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
L369	S478	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
V370	S479	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
G373	S480	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567	P568	T569	R570	K576	I582	L583	V592	K595	T596
V374	S481	V508	A509	Y510	L511	V512	H513	H514	M515	D516	N517	V518	S519	R520	N522	S523	S524	E525	K526	N527	N528	L529	K532	L541	Y542	K543	P544	L545	V546	S550	G551	P552	C553	I559	L562	L563	P564	T565	G566	E567</									

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.06Å 75.86Å 126.64Å 90.00° 90.24° 90.00°	Depositor
Resolution (Å)	32.22 – 2.39 32.22 – 2.39	Depositor EDS
% Data completeness (in resolution range)	95.3 (32.22-2.39) 95.1 (32.22-2.39)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.215 , 0.265 0.227 , 0.258	Depositor DCC
R_{free} test set	1988 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.013 for -k,-h,-l 0.014 for k,h,-l 0.149 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9711	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.12	34/4887 (0.7%)	0.91	26/6603 (0.4%)
1	B	1.04	32/4760 (0.7%)	0.96	30/6435 (0.5%)
All	All	1.08	66/9647 (0.7%)	0.94	56/13038 (0.4%)

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	LYS	C-O	-7.62	1.17	1.24
1	B	543	LYS	C-O	-7.46	1.17	1.24
1	A	544	PRO	C-O	-7.10	1.15	1.24
1	B	452	LEU	C-O	-6.87	1.18	1.24
1	A	14	GLY	C-O	-6.62	1.19	1.24
1	B	546	VAL	N-CA	-6.44	1.39	1.46
1	B	9	LYS	C-O	-6.28	1.16	1.24
1	B	133	GLU	CA-C	-6.22	1.45	1.52
1	B	232	ALA	C-O	-6.20	1.16	1.24
1	A	453	PRO	C-O	-6.19	1.17	1.24
1	A	452	LEU	C-O	-6.16	1.18	1.24
1	B	252	VAL	C-O	-6.09	1.16	1.24
1	B	365	MET	C-O	-6.09	1.16	1.23
1	B	460	THR	C-O	-6.05	1.17	1.24
1	A	462	ALA	C-O	-5.94	1.17	1.24
1	A	361	VAL	C-O	-5.89	1.17	1.24
1	A	488	ALA	C-O	-5.83	1.19	1.24
1	A	540	LEU	C-O	-5.82	1.16	1.24
1	A	546	VAL	C-O	-5.74	1.17	1.24
1	B	456	ARG	C-O	-5.74	1.17	1.24
1	A	236	LYS	C-O	-5.73	1.17	1.24
1	A	546	VAL	N-CA	-5.71	1.39	1.46
1	B	551	GLY	C-O	-5.68	1.16	1.24
1	A	542	TYR	C-O	-5.64	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	MET	C-O	-5.63	1.18	1.24
1	A	436	TYR	N-CA	-5.56	1.39	1.46
1	A	8	PHE	C-O	-5.55	1.17	1.24
1	B	550	SER	C-O	-5.46	1.17	1.24
1	A	307	MET	C-O	-5.46	1.17	1.24
1	B	78	GLN	C-O	-5.45	1.19	1.24
1	A	362	LEU	C-O	-5.44	1.17	1.24
1	A	541	LEU	C-O	-5.42	1.17	1.24
1	B	553	CYS	C-O	-5.41	1.17	1.24
1	B	234	PRO	C-O	-5.41	1.17	1.23
1	B	249	ALA	CA-C	-5.33	1.46	1.52
1	B	450	LEU	C-O	-5.32	1.17	1.24
1	B	250	PRO	CA-C	-5.30	1.47	1.52
1	B	341	MET	C-O	-5.30	1.17	1.24
1	A	456	ARG	C-O	-5.29	1.18	1.24
1	A	365	MET	C-O	-5.29	1.17	1.23
1	B	340	ASP	C-O	-5.28	1.17	1.24
1	A	454	MET	C-O	-5.26	1.17	1.24
1	A	552	PRO	C-O	-5.22	1.18	1.24
1	B	454	MET	C-O	-5.22	1.18	1.24
1	B	541	LEU	C-O	-5.21	1.17	1.24
1	A	232	ALA	C-O	-5.20	1.17	1.24
1	B	247	GLN	C-O	-5.20	1.18	1.24
1	B	307	MET	C-O	-5.18	1.18	1.24
1	B	544	PRO	C-O	-5.17	1.17	1.24
1	A	433	MET	C-O	-5.16	1.17	1.23
1	A	437	HIS	C-O	-5.13	1.18	1.24
1	B	379	GLU	C-O	-5.12	1.18	1.24
1	A	475	VAL	C-O	-5.12	1.17	1.24
1	A	120	GLN	C-O	-5.11	1.18	1.24
1	B	343	MET	C-O	-5.09	1.17	1.23
1	A	555	VAL	C-O	-5.08	1.17	1.24
1	B	363	LEU	C-O	-5.07	1.17	1.23
1	A	363	LEU	C-O	-5.06	1.17	1.23
1	A	455	LEU	C-O	-5.06	1.18	1.24
1	B	380	ASN	C-O	-5.06	1.18	1.24
1	A	231	SER	C-O	-5.05	1.18	1.24
1	B	455	LEU	C-O	-5.05	1.18	1.24
1	B	520	ARG	CA-C	-5.05	1.46	1.52
1	A	123	ARG	C-O	-5.05	1.18	1.24
1	A	340	ASP	C-O	-5.04	1.17	1.24
1	A	309	GLU	C-O	-5.01	1.17	1.24

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ASP	N-CA-C	19.88	153.15	110.80
1	A	29	LYS	CB-CA-C	-17.82	79.61	109.55
1	A	5	TYR	N-CA-C	14.91	130.57	112.38
1	B	47	ASP	CB-CA-C	-14.75	81.06	110.42
1	B	17	ASN	CB-CA-C	13.42	135.70	109.66
1	A	565	THR	N-CA-C	12.12	128.01	113.23
1	B	17	ASN	N-CA-C	-11.31	91.98	109.85
1	B	73	ILE	N-CA-C	11.26	132.77	109.34
1	A	46	ASN	CB-CA-C	11.23	124.22	109.28
1	B	133	GLU	N-CA-C	-11.14	85.18	109.81
1	A	5	TYR	CB-CA-C	-11.00	87.12	110.32
1	A	109	PHE	N-CA-C	10.74	133.68	110.80
1	B	565	THR	CB-CA-C	-10.06	90.40	110.42
1	B	248	ASN	N-CA-C	9.93	124.78	112.87
1	B	133	GLU	CB-CA-C	8.69	127.28	110.17
1	B	527	GLU	N-CA-C	-8.53	101.94	111.07
1	A	41	ASN	N-CA-C	8.10	128.05	110.80
1	B	565	THR	N-CA-C	7.84	127.49	110.80
1	A	29	LYS	N-CA-C	7.81	123.87	113.72
1	B	132	ASP	N-CA-C	7.79	127.39	110.80
1	A	632	ALA	CA-C-N	7.73	136.31	121.54
1	A	632	ALA	C-N-CA	7.73	136.31	121.54
1	B	46	ASN	CB-CA-C	7.68	126.04	110.38
1	A	547	MET	N-CA-C	7.53	120.36	111.71
1	A	39	SER	N-CA-C	7.48	121.37	111.28
1	B	546	VAL	N-CA-C	-7.39	105.91	112.12
1	B	10	LEU	N-CA-C	-7.12	103.45	111.14
1	B	484	ALA	CA-C-N	7.07	126.78	119.64
1	B	484	ALA	C-N-CA	7.07	126.78	119.64
1	A	632	ALA	N-CA-C	6.95	121.35	113.01
1	A	44	PHE	N-CA-C	6.83	121.21	113.01
1	B	284	PHE	CB-CA-C	-6.81	96.86	110.42
1	A	40	ILE	N-CA-C	-6.66	104.27	110.53
1	A	5	TYR	CA-C-N	6.52	131.55	121.19
1	A	5	TYR	C-N-CA	6.52	131.55	121.19
1	B	109	PHE	N-CA-C	6.50	119.83	108.52
1	B	73	ILE	CB-CA-C	-6.39	100.81	111.29
1	A	632	ALA	CB-CA-C	6.29	122.99	110.17
1	B	17	ASN	CA-C-N	6.25	131.13	121.19
1	B	17	ASN	C-N-CA	6.25	131.13	121.19
1	A	120	GLN	N-CA-C	-6.16	104.64	111.36
1	A	18	GLN	N-CA-C	6.15	118.52	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	MET	N-CA-C	6.04	119.92	112.54
1	B	252	VAL	CB-CA-C	-6.03	102.77	111.34
1	A	564	PRO	N-CA-C	5.85	122.47	113.75
1	A	29	LYS	CA-C-N	5.76	132.54	121.54
1	A	29	LYS	C-N-CA	5.76	132.54	121.54
1	B	341	MET	N-CA-C	5.45	116.27	109.57
1	B	563	LEU	CA-C-N	5.35	125.67	119.47
1	B	563	LEU	C-N-CA	5.35	125.67	119.47
1	B	133	GLU	C-N-CD	-5.21	103.63	125.00
1	B	158	GLN	CB-CA-C	5.16	120.69	110.42
1	A	108	THR	N-CA-C	-5.09	100.22	108.41
1	A	232	ALA	N-CA-C	5.07	117.70	111.82
1	B	564	PRO	N-CA-C	5.03	121.10	113.81
1	A	109	PHE	CB-CA-C	-5.00	100.47	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4801	0	4854	243	0
1	B	4674	0	4717	288	0
2	A	36	22	22	1	0
2	B	36	22	22	1	0
3	A	52	0	0	1	0
3	B	68	0	0	6	0
All	All	9667	44	9615	531	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 28.

All (531) 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:A:129:ILE:CD1	1:A:192:THR:HG23	1.49	1.41
1:B:249:ALA:CB	1:B:250:PRO:CD	2.15	1.23
1:B:249:ALA:CB	1:B:250:PRO:HD2	1.71	1.21
1:B:249:ALA:HB1	1:B:250:PRO:CD	1.70	1.19
1:A:129:ILE:CD1	1:A:192:THR:CG2	2.20	1.19
1:A:114:VAL:HG12	1:A:172:ILE:HG22	1.25	1.15
1:A:129:ILE:HD12	1:A:192:THR:CG2	1.81	1.11
1:B:249:ALA:HB1	1:B:250:PRO:HD3	1.27	1.11
1:B:109:PHE:CD1	1:B:167:ARG:HA	1.86	1.09
1:B:249:ALA:HB3	1:B:250:PRO:HD2	1.30	1.07
1:A:17:ASN:OD1	1:A:20:GLU:HG2	1.52	1.07
1:A:129:ILE:HD11	1:A:192:THR:CG2	1.84	1.02
1:A:105:ALA:HB1	1:A:166:ILE:HD11	1.43	1.00
1:A:515:MET:HA	1:A:518:VAL:HG13	1.39	1.00
1:A:543:LYS:HB3	1:A:544:PRO:HD3	1.42	1.00
1:B:567:GLU:HG2	1:B:568:PRO:HD2	1.43	1.00
1:A:247:GLN:CD	1:A:345:THR:HG21	1.87	0.99
1:B:44:PHE:HD1	1:B:44:PHE:N	1.55	0.98
1:B:482:VAL:HG23	1:B:510:TYR:CB	1.92	0.97
1:B:515:MET:HE2	1:B:518:VAL:CG1	1.96	0.96
1:A:129:ILE:HD11	1:A:192:THR:HG23	1.00	0.96
1:B:126:CYS:HB3	1:B:134:PRO:HG3	1.48	0.94
1:B:140:GLU:HG2	1:B:374:VAL:HG23	1.49	0.94
1:B:482:VAL:HG23	1:B:510:TYR:HB3	1.47	0.93
1:B:24:LEU:HD23	1:B:61:PHE:HE2	1.34	0.90
1:B:515:MET:HA	1:B:518:VAL:HG12	1.54	0.90
1:B:562:LEU:HG	1:B:582:ILE:HD11	1.52	0.89
1:A:104:GLY:O	1:A:108:THR:HG23	1.71	0.89
1:A:19:ASN:O	1:A:23:ARG:HB2	1.72	0.88
1:B:626:TRP:HB2	3:B:807:HOH:O	1.72	0.88
1:B:18:GLN:O	1:B:22:THR:HG23	1.76	0.85
1:A:567:GLU:HG2	1:A:568:PRO:HD2	1.59	0.84
1:B:567:GLU:HG2	1:B:568:PRO:CD	2.08	0.84
1:B:478:PHE:O	1:B:482:VAL:HG12	1.77	0.83
1:A:249:ALA:HB1	1:A:250:PRO:HD3	1.59	0.83
1:B:46:ASN:O	1:B:373:GLY:HA2	1.79	0.83
1:B:167:ARG:HG3	1:B:168:ASP:N	1.92	0.83
1:A:23:ARG:NE	1:A:61:PHE:CE1	2.45	0.83
1:B:515:MET:HE2	1:B:518:VAL:HG13	1.59	0.83
1:A:486:GLU:OE1	1:A:486:GLU:N	2.11	0.82
1:B:284:PHE:CG	1:B:284:PHE:O	2.34	0.81
1:A:627:MET:HE3	1:A:628:PRO:CD	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:PHE:O	1:A:109:PHE:CD1	2.33	0.81
1:A:18:GLN:O	1:A:22:THR:HG23	1.80	0.81
1:B:8:PHE:O	1:B:12:THR:HB	1.82	0.79
1:B:452:LEU:HB3	1:B:453:PRO:HD3	1.64	0.79
1:A:518:VAL:HA	1:A:521:LEU:HD23	1.65	0.79
1:B:24:LEU:HD23	1:B:61:PHE:CE2	2.19	0.78
1:B:29:LYS:O	1:B:30:ARG:HD3	1.84	0.78
1:A:567:GLU:HG2	1:A:568:PRO:CD	2.13	0.78
1:A:513:HIS:CD2	1:A:513:HIS:H	2.01	0.78
1:A:114:VAL:HG12	1:A:172:ILE:CG2	2.11	0.77
1:A:24:LEU:CD1	1:A:28:LEU:HD22	2.15	0.77
1:B:109:PHE:CE1	1:B:167:ARG:HB2	2.20	0.77
1:B:129:ILE:HD11	1:B:188:LYS:O	1.86	0.76
1:B:73:ILE:HG22	1:B:73:ILE:O	1.84	0.76
1:B:109:PHE:CE1	1:B:167:ARG:CB	2.68	0.76
1:B:109:PHE:HE1	1:B:167:ARG:CB	1.99	0.76
1:B:154:TYR:HE2	1:B:179:ILE:HG21	1.50	0.76
1:A:109:PHE:CD1	1:A:109:PHE:C	2.64	0.76
1:A:444:GLU:OE2	1:A:444:GLU:HA	1.86	0.76
1:B:162:LEU:O	1:B:166:ILE:HG22	1.86	0.75
1:B:543:LYS:HB3	1:B:544:PRO:HD3	1.66	0.75
1:B:429:ARG:HD3	1:B:477:ARG:HH12	1.51	0.75
1:A:426:GLU:OE1	1:A:429:ARG:NH1	2.20	0.74
1:B:15:GLY:O	1:B:57:MET:HE2	1.87	0.74
1:B:109:PHE:CE1	1:B:167:ARG:HA	2.22	0.74
1:A:249:ALA:HB1	1:A:250:PRO:CD	2.18	0.74
1:B:429:ARG:HG2	1:B:477:ARG:NH2	2.03	0.74
1:A:114:VAL:CG1	1:A:172:ILE:HG22	2.12	0.74
1:B:135:ASN:ND2	1:B:138:GLN:H	1.86	0.74
1:A:247:GLN:OE1	1:A:345:THR:CG2	2.36	0.73
1:B:429:ARG:HG2	1:B:477:ARG:HH22	1.53	0.73
1:A:172:ILE:HG13	1:A:172:ILE:O	1.89	0.73
1:B:542:TYR:CD2	1:B:628:PRO:HG3	2.23	0.73
1:A:515:MET:HA	1:A:518:VAL:CG1	2.17	0.73
1:B:196:ASN:C	1:B:196:ASN:HD22	1.96	0.73
1:A:67:TRP:HE1	1:A:71:GLN:HE21	1.35	0.72
1:A:442:ASP:O	1:A:446:ASN:HB2	1.89	0.72
1:A:627:MET:HE3	1:A:628:PRO:HD2	1.72	0.72
1:B:41:ASN:CG	1:B:41:ASN:O	2.32	0.72
1:B:29:LYS:HE2	1:B:42:LYS:HE2	1.69	0.72
1:A:24:LEU:HD13	1:A:28:LEU:HD22	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HD23	1:A:61:PHE:HE2	1.54	0.71
1:A:109:PHE:C	1:A:109:PHE:HD1	1.97	0.71
1:A:249:ALA:CB	1:A:250:PRO:CD	2.68	0.71
1:B:477:ARG:HE	1:B:481:MET:CE	2.03	0.71
1:A:175:LYS:HB3	1:A:178:GLU:HG2	1.72	0.71
1:A:508:VAL:HG21	1:A:526:LYS:HG2	1.73	0.71
1:B:46:ASN:O	1:B:373:GLY:CA	2.38	0.71
1:A:6:TRP:CZ2	1:A:40:ILE:HB	2.26	0.71
1:A:247:GLN:CD	1:A:345:THR:CG2	2.64	0.71
1:A:567:GLU:OE1	1:A:568:PRO:O	2.08	0.71
1:A:23:ARG:O	1:A:26:THR:HG22	1.92	0.70
1:A:116:LYS:HD2	1:A:116:LYS:C	2.17	0.70
1:B:126:CYS:CB	1:B:134:PRO:HG3	2.21	0.70
1:B:154:TYR:CD1	1:B:158:GLN:HG2	2.27	0.69
1:B:513:HIS:H	1:B:513:HIS:CD2	2.08	0.69
1:B:543:LYS:HB3	1:B:544:PRO:CD	2.22	0.69
1:A:627:MET:HE3	1:A:628:PRO:HD3	1.73	0.68
1:B:155:SER:H	1:B:158:GLN:HE22	1.40	0.68
1:B:117:LEU:HD21	1:B:177:GLU:HG2	1.75	0.68
1:A:155:SER:O	1:A:158:GLN:NE2	2.22	0.68
1:A:521:LEU:HD12	1:A:525:GLU:HG3	1.77	0.67
1:B:515:MET:HA	1:B:518:VAL:CG1	2.24	0.67
1:B:112:SER:OG	1:B:166:ILE:HD12	1.95	0.67
1:A:110:GLY:HA2	1:A:115:VAL:HG11	1.76	0.66
1:B:522:ASN:OD1	1:B:522:ASN:N	2.26	0.66
1:A:42:LYS:O	1:A:42:LYS:HD3	1.95	0.66
1:A:624:LEU:HD22	2:A:701:UPG:O1B	1.94	0.66
1:A:73:ILE:O	1:A:76:ASN:HB2	1.96	0.66
1:B:109:PHE:CE1	1:B:167:ARG:CA	2.78	0.66
1:B:379:GLU:HG2	1:B:583:LEU:CD1	2.26	0.66
1:A:247:GLN:OE1	1:A:345:THR:HG23	1.95	0.66
1:A:109:PHE:CE1	1:A:111:LYS:HB2	2.31	0.66
1:B:44:PHE:N	1:B:44:PHE:CD1	2.29	0.66
1:A:23:ARG:O	1:A:26:THR:CG2	2.44	0.65
1:A:609:SER:O	1:A:613:VAL:HG23	1.96	0.65
1:B:117:LEU:HD23	1:B:176:PHE:HE1	1.62	0.65
1:B:227:ASN:HA	1:B:307:MET:HE3	1.77	0.65
1:A:238:LYS:O	1:A:242:GLU:HG3	1.96	0.65
1:B:186:ARG:HH21	1:B:189:GLU:HB3	1.62	0.65
1:B:162:LEU:O	1:B:162:LEU:HD12	1.96	0.65
1:B:562:LEU:HG	1:B:582:ILE:CD1	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:GLU:HA	1:A:614:GLU:OE1	1.96	0.65
1:B:109:PHE:HD1	1:B:167:ARG:HA	1.56	0.64
1:B:158:GLN:OE1	1:B:159:ALA:N	2.31	0.64
1:B:129:ILE:HG12	1:B:191:HIS:HB2	1.78	0.64
1:B:135:ASN:OD1	1:B:138:GLN:NE2	2.29	0.64
1:A:46:ASN:O	1:A:47:ASP:OD2	2.13	0.64
1:A:129:ILE:CD1	1:A:192:THR:HG21	2.24	0.64
1:A:17:ASN:O	1:A:21:ALA:CB	2.46	0.64
1:A:155:SER:C	1:A:158:GLN:HE22	2.05	0.64
1:B:482:VAL:HG23	1:B:510:TYR:HB2	1.80	0.64
1:B:154:TYR:CE2	1:B:179:ILE:HG21	2.31	0.64
1:A:104:GLY:HA2	1:A:107:ILE:CG2	2.28	0.63
1:B:129:ILE:HG13	1:B:192:THR:HG23	1.81	0.63
1:B:201:ASN:O	1:B:562:LEU:HD13	1.97	0.63
1:B:370:VAL:CG1	1:B:378:MET:HB2	2.28	0.63
1:B:515:MET:HE2	1:B:518:VAL:CG2	2.28	0.63
1:A:292:GLU:OE2	1:A:402:LYS:HE3	1.99	0.63
1:A:259:ARG:NH2	1:A:264:LYS:HG3	2.13	0.63
1:B:42:LYS:HA	1:B:44:PHE:CE1	2.34	0.63
1:A:319:SER:OG	1:A:323:ARG:NH2	2.30	0.62
1:A:482:VAL:CG2	1:A:507:LEU:HA	2.29	0.62
1:B:444:GLU:HB3	3:B:829:HOH:O	1.99	0.62
1:B:529:LEU:HA	1:B:532:LYS:HZ1	1.64	0.62
1:A:129:ILE:HD12	1:A:192:THR:HG21	1.79	0.61
1:A:475:VAL:HG21	1:A:492:GLN:HE21	1.65	0.61
1:B:117:LEU:HD23	1:B:176:PHE:CE1	2.34	0.61
1:A:170:LYS:HB2	1:A:171:PRO:HD2	1.81	0.61
1:B:543:LYS:CB	1:B:544:PRO:CD	2.78	0.61
1:A:24:LEU:O	1:A:28:LEU:N	2.31	0.61
1:A:154:TYR:CE2	1:A:162:LEU:HD13	2.35	0.61
1:B:53:LEU:O	1:B:57:MET:HB2	2.01	0.61
1:B:123:ARG:NH2	1:B:133:GLU:OE1	2.34	0.61
1:B:430:LEU:HD23	1:B:541:LEU:HD13	1.82	0.61
1:A:105:ALA:CB	1:A:166:ILE:HD11	2.27	0.60
1:B:479:ALA:HB1	1:B:485:PRO:HA	1.84	0.60
1:A:23:ARG:HE	1:A:61:PHE:HE1	1.36	0.60
1:B:359:HIS:CG	1:B:360:PRO:HD2	2.37	0.60
1:A:257:TYR:CE1	1:A:281:LEU:HG	2.36	0.60
1:B:605:ASN:O	1:B:608:THR:HG22	2.01	0.60
1:A:66:GLU:OE2	1:A:66:GLU:HA	2.01	0.60
1:B:484:ALA:HB1	1:B:486:GLU:OE1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:O	1:A:117:LEU:HG	2.02	0.59
1:B:272:GLN:O	1:B:276:GLU:HG3	2.02	0.59
1:A:161:LYS:HZ3	1:A:173:PRO:HG2	1.68	0.59
1:A:452:LEU:HB3	1:A:453:PRO:HD3	1.83	0.59
1:A:606:TRP:O	1:A:607:ILE:HG12	2.01	0.59
1:B:43:LEU:H	1:B:43:LEU:HD22	1.67	0.59
1:B:222:CYS:SG	1:B:241:LEU:HD21	2.42	0.59
1:B:515:MET:O	1:B:518:VAL:HG13	2.03	0.59
1:B:515:MET:HE2	1:B:518:VAL:HG11	1.82	0.59
1:B:369:LEU:O	1:B:610:SER:HB2	2.02	0.59
1:A:359:HIS:CG	1:A:360:PRO:HD2	2.37	0.59
1:A:367:SER:OG	1:A:607:ILE:N	2.31	0.59
1:B:74:LEU:O	1:B:77:ILE:HD12	2.02	0.59
1:B:367:SER:OG	1:B:607:ILE:N	2.31	0.58
1:B:529:LEU:HA	1:B:532:LYS:NZ	2.18	0.58
1:B:528:ASN:O	1:B:532:LYS:HD3	2.02	0.58
1:A:515:MET:HG2	1:A:518:VAL:CG2	2.33	0.58
1:A:324:TRP:CE2	1:A:404:ILE:HG21	2.39	0.58
1:B:627:MET:HE3	1:B:628:PRO:HD2	1.86	0.58
1:A:40:ILE:CG2	1:A:44:PHE:HE1	2.17	0.58
1:A:318:ALA:O	1:A:322:VAL:HG23	2.04	0.57
1:B:482:VAL:HG21	1:B:506:ALA:O	2.03	0.57
1:B:446:ASN:O	1:B:447:ASN:C	2.46	0.57
1:B:513:HIS:CD2	1:B:513:HIS:N	2.72	0.57
1:A:625:SER:O	1:A:631:GLN:NE2	2.36	0.57
1:A:161:LYS:HZ3	1:A:173:PRO:CG	2.17	0.57
1:A:494:ALA:HB1	1:A:499:ASN:HB3	1.87	0.57
1:A:17:ASN:O	1:A:21:ALA:HB2	2.04	0.57
1:A:417:GLU:O	1:A:421:LYS:HG3	2.04	0.57
1:B:505:ASN:HB3	1:B:515:MET:HE3	1.86	0.57
1:A:164:GLU:HG3	1:A:167:ARG:HH11	1.68	0.57
1:B:238:LYS:O	1:B:242:GLU:HG3	2.04	0.57
1:A:162:LEU:O	1:A:166:ILE:HG23	2.04	0.57
1:A:513:HIS:H	1:A:513:HIS:HD2	1.51	0.57
1:B:516:ASP:O	1:B:519:SER:HB3	2.05	0.56
1:B:129:ILE:HG13	1:B:192:THR:CG2	2.34	0.56
1:A:148:LEU:O	1:A:148:LEU:HD23	2.06	0.56
1:A:611:GLU:CD	1:A:611:GLU:H	2.12	0.56
1:B:186:ARG:NH2	1:B:189:GLU:HB3	2.20	0.56
1:B:546:VAL:HA	3:B:842:HOH:O	2.05	0.56
1:A:24:LEU:HD12	1:A:28:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:HIS:CD2	1:A:513:HIS:N	2.72	0.56
1:A:40:ILE:HG21	1:A:44:PHE:HE1	1.71	0.56
1:A:148:LEU:O	1:A:152:GLU:HG2	2.06	0.56
1:B:129:ILE:HG12	1:B:191:HIS:CB	2.36	0.56
1:A:117:LEU:HD23	1:A:176:PHE:HE1	1.69	0.56
1:A:170:LYS:HB2	1:A:171:PRO:CD	2.35	0.56
1:B:140:GLU:HG2	1:B:374:VAL:CG2	2.32	0.56
1:B:174:SER:O	1:B:175:LYS:HG2	2.06	0.56
1:B:229:PRO:O	1:B:263:THR:HG23	2.06	0.56
1:B:605:ASN:O	1:B:608:THR:CG2	2.54	0.56
1:A:3:GLU:O	1:A:3:GLU:HG3	2.04	0.56
1:A:493:GLU:O	1:A:497:GLN:HG2	2.06	0.56
1:B:170:LYS:HB3	1:B:171:PRO:HD2	1.87	0.56
1:B:222:CYS:SG	1:B:255:LEU:HD13	2.45	0.55
1:A:74:LEU:C	1:A:76:ASN:H	2.14	0.55
1:B:24:LEU:O	1:B:28:LEU:HB2	2.07	0.55
1:B:520:ARG:HD2	1:B:520:ARG:C	2.31	0.55
1:B:186:ARG:HA	1:B:186:ARG:NE	2.21	0.55
1:A:499:ASN:O	1:A:502:VAL:HG13	2.07	0.55
1:B:606:TRP:C	1:B:607:ILE:HG12	2.32	0.55
1:B:78:GLN:HB2	1:B:79:PRO:HD2	1.87	0.54
1:B:446:ASN:O	1:B:447:ASN:O	2.25	0.54
1:A:477:ARG:O	1:A:481:MET:HG3	2.07	0.54
1:A:120:GLN:HE21	1:A:120:GLN:HA	1.72	0.54
1:A:142:ILE:O	1:A:146:LEU:HD22	2.06	0.54
1:B:513:HIS:H	1:B:513:HIS:HD2	1.52	0.54
1:A:17:ASN:OD1	1:A:20:GLU:CG	2.41	0.54
1:B:112:SER:OG	1:B:114:VAL:HG23	2.08	0.54
1:B:604:PRO:HB2	1:B:608:THR:HG21	1.90	0.54
1:B:515:MET:HG2	1:B:518:VAL:HG11	1.89	0.54
1:B:433:MET:HE3	1:B:472:PHE:HD1	1.72	0.54
1:B:612:GLU:OE1	1:B:612:GLU:HA	2.08	0.53
1:A:161:LYS:NZ	1:A:173:PRO:HG2	2.23	0.53
1:A:522:ASN:H	1:A:525:GLU:CD	2.17	0.53
1:A:556:THR:O	1:A:560:LEU:HG	2.08	0.53
1:B:284:PHE:O	1:B:284:PHE:CD1	2.61	0.53
1:A:259:ARG:HH22	1:A:264:LYS:HG3	1.71	0.53
1:B:56:TYR:O	1:B:58:ALA:N	2.41	0.53
1:B:109:PHE:CD1	1:B:167:ARG:CA	2.75	0.53
1:A:619:LEU:O	1:A:619:LEU:HD12	2.08	0.53
1:A:120:GLN:HA	1:A:120:GLN:NE2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ALA:CB	1:A:499:ASN:HB3	2.39	0.53
1:B:416:THR:CG2	1:B:450:LEU:HD23	2.39	0.53
1:B:493:GLU:O	1:B:497:GLN:HB2	2.09	0.53
1:A:405:ALA:O	1:A:409:ILE:HG13	2.09	0.53
1:B:157:GLU:O	1:B:160:GLU:N	2.42	0.53
1:B:430:LEU:HD23	1:B:541:LEU:CD1	2.39	0.53
1:A:117:LEU:O	1:A:121:ASN:OD1	2.26	0.52
1:A:181:LEU:HB3	1:A:182:PRO:HD3	1.91	0.52
1:A:488:ALA:N	1:A:489:PRO:HD2	2.24	0.52
1:B:104:GLY:O	1:B:108:THR:HG23	2.09	0.52
1:B:434:PRO:HD2	1:B:474:GLY:N	2.24	0.52
1:B:514:GLY:O	1:B:517:ASN:HB2	2.09	0.52
1:A:195:LEU:HD12	1:A:579:ASP:O	2.09	0.52
1:B:109:PHE:HE1	1:B:167:ARG:HB2	1.62	0.52
1:B:117:LEU:O	1:B:121:ASN:HB2	2.09	0.52
1:A:117:LEU:HD23	1:A:176:PHE:CE1	2.45	0.52
1:B:265:LYS:HE2	3:B:849:HOH:O	2.09	0.52
1:B:5:TYR:CD2	1:B:378:MET:HE1	2.44	0.52
1:B:363:LEU:CD1	1:B:559:ILE:HD11	2.40	0.52
1:A:470:VAL:O	1:A:473:ILE:O	2.28	0.52
1:B:236:LYS:H	1:B:236:LYS:CE	2.22	0.52
1:B:509:ALA:HB2	1:B:515:MET:HG2	1.92	0.52
1:A:233:MET:HE1	1:A:255:LEU:HD11	1.90	0.52
1:B:515:MET:CE	1:B:518:VAL:HG13	2.36	0.52
1:A:543:LYS:CB	1:A:544:PRO:HD3	2.22	0.51
1:B:135:ASN:O	1:B:136:LEU:C	2.49	0.51
1:A:125:ILE:HD11	1:A:184:VAL:HG13	1.92	0.51
1:A:42:LYS:HD3	1:A:42:LYS:C	2.34	0.51
1:A:543:LYS:HB3	1:A:544:PRO:CD	2.29	0.51
1:B:482:VAL:CG2	1:B:510:TYR:CB	2.80	0.51
1:A:6:TRP:CH2	1:A:40:ILE:HB	2.45	0.51
1:A:515:MET:HG2	1:A:518:VAL:HG22	1.93	0.51
1:B:186:ARG:HA	1:B:186:ARG:HE	1.76	0.51
1:B:370:VAL:HG13	1:B:378:MET:HB2	1.93	0.51
1:B:433:MET:HE3	1:B:472:PHE:CD1	2.45	0.50
1:B:154:TYR:CE1	1:B:162:LEU:HD23	2.46	0.50
1:A:218:LYS:HD2	1:A:353:GLU:HG2	1.93	0.50
1:B:344:LEU:N	1:B:597:ASN:O	2.41	0.50
1:B:367:SER:O	1:B:608:THR:HG23	2.11	0.50
1:B:389:ASN:HB2	1:B:592:VAL:HG12	1.93	0.50
1:B:416:THR:HG22	1:B:450:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HD21	1:A:49:PHE:CZ	2.47	0.50
1:A:174:SER:C	1:A:175:LYS:HG3	2.37	0.50
1:A:567:GLU:HG2	1:A:568:PRO:N	2.26	0.50
1:A:116:LYS:C	1:A:116:LYS:CD	2.85	0.50
1:A:516:ASP:OD1	1:A:517:ASN:N	2.45	0.50
1:B:29:LYS:C	1:B:30:ARG:HG2	2.36	0.49
1:B:314:ASN:ND2	3:B:807:HOH:O	2.44	0.49
1:B:434:PRO:HG2	1:B:474:GLY:HA2	1.93	0.49
1:A:612:GLU:C	1:A:614:GLU:H	2.20	0.49
1:B:73:ILE:O	1:B:75:SER:N	2.45	0.49
1:B:603:ILE:HB	1:B:604:PRO:HD2	1.95	0.49
1:A:481:MET:HE3	1:A:533:TYR:OH	2.13	0.49
1:B:52:ARG:NH1	1:B:80:LEU:HD21	2.28	0.49
1:B:477:ARG:HE	1:B:481:MET:HE1	1.78	0.49
1:B:567:GLU:CG	1:B:568:PRO:HD2	2.29	0.49
1:B:196:ASN:C	1:B:196:ASN:ND2	2.69	0.49
1:B:488:ALA:HB3	1:B:489:PRO:HD3	1.94	0.49
1:A:227:ASN:HA	1:A:307:MET:HE3	1.95	0.48
1:B:148:LEU:HD23	1:B:148:LEU:O	2.13	0.48
1:A:24:LEU:HD23	1:A:61:PHE:CE2	2.41	0.48
1:A:154:TYR:HB3	1:A:159:ALA:HB2	1.94	0.48
1:A:348:LYS:HD2	1:A:348:LYS:HA	1.49	0.48
1:A:520:ARG:HD2	1:A:520:ARG:N	2.29	0.48
1:A:289:CYS:HB3	1:A:293:ASP:HB3	1.96	0.48
1:A:504:THR:HG23	1:A:530:ILE:HD11	1.94	0.48
1:B:140:GLU:HG3	1:B:144:ARG:HD2	1.96	0.48
1:A:72:GLN:O	1:A:73:ILE:HG23	2.14	0.48
1:B:125:ILE:HG12	1:B:188:LYS:HB2	1.95	0.48
1:B:516:ASP:OD1	1:B:516:ASP:N	2.42	0.48
1:B:606:TRP:O	1:B:607:ILE:HG12	2.14	0.48
1:A:149:GLN:OE1	1:A:149:GLN:HA	2.13	0.48
1:A:296:LEU:HD11	1:A:405:ALA:CB	2.44	0.48
1:A:395:LYS:O	1:A:399:ILE:HG13	2.14	0.48
1:B:320:ASP:HB3	1:B:550:SER:O	2.14	0.48
1:B:324:TRP:CE2	1:B:404:ILE:HG21	2.49	0.48
1:A:170:LYS:CB	1:A:171:PRO:CD	2.91	0.47
1:A:429:ARG:HD3	1:A:477:ARG:NH2	2.28	0.47
1:A:606:TRP:C	1:A:607:ILE:HG12	2.39	0.47
1:B:74:LEU:CD2	1:B:77:ILE:HD11	2.45	0.47
1:B:141:TYR:CD1	1:B:570:ARG:HD2	2.49	0.47
1:B:155:SER:H	1:B:158:GLN:NE2	2.09	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:MET:SD	1:A:473:ILE:HG22	2.54	0.47
1:A:5:TYR:O	1:A:5:TYR:CG	2.65	0.47
1:A:515:MET:CA	1:A:518:VAL:HG13	2.28	0.47
1:A:20:GLU:HA	1:A:23:ARG:HB2	1.97	0.47
1:A:194:ILE:HD11	1:A:577:GLN:NE2	2.29	0.47
1:A:516:ASP:O	1:A:519:SER:OG	2.33	0.47
1:B:56:TYR:C	1:B:58:ALA:H	2.21	0.47
1:A:42:LYS:C	1:A:42:LYS:CD	2.87	0.47
1:B:470:VAL:O	1:B:473:ILE:O	2.33	0.47
1:B:516:ASP:O	1:B:519:SER:CB	2.62	0.47
1:B:604:PRO:HB2	1:B:608:THR:CG2	2.44	0.47
1:B:259:ARG:HH22	1:B:264:LYS:HG3	1.80	0.47
1:A:416:THR:HG22	1:A:450:LEU:HD23	1.97	0.47
1:B:40:ILE:O	1:B:42:LYS:N	2.44	0.47
1:B:374:VAL:HG23	1:B:374:VAL:O	2.15	0.47
1:A:161:LYS:HD2	1:A:161:LYS:C	2.40	0.47
1:B:126:CYS:O	1:B:130:LEU:HG	2.15	0.47
1:A:114:VAL:CG2	1:A:166:ILE:HG22	2.45	0.46
1:A:626:TRP:HA	1:A:631:GLN:CG	2.45	0.46
1:B:130:LEU:O	1:B:576:LYS:HG3	2.15	0.46
1:B:501:ILE:HD12	1:B:501:ILE:H	1.81	0.46
1:A:126:CYS:HB3	1:A:134:PRO:CG	2.45	0.46
1:A:515:MET:HB3	1:A:515:MET:HE3	1.64	0.46
1:B:356:TYR:O	1:B:595:LYS:NZ	2.40	0.46
1:B:465:ASN:ND2	1:B:468:SER:OG	2.40	0.46
1:B:482:VAL:CG2	1:B:510:TYR:HB2	2.45	0.46
1:A:235:LYS:HE2	1:A:239:ASP:OD1	2.16	0.46
1:A:259:ARG:HB2	1:A:283:ASP:OD2	2.15	0.46
1:B:56:TYR:C	1:B:58:ALA:N	2.71	0.46
1:B:130:LEU:C	1:B:576:LYS:HG3	2.40	0.46
1:B:234:PRO:HB3	1:B:236:LYS:NZ	2.30	0.46
1:A:164:GLU:HG3	1:A:167:ARG:NH1	2.31	0.46
1:B:122:ALA:HB2	1:B:146:LEU:HD12	1.97	0.46
1:B:154:TYR:HD1	1:B:158:GLN:HG2	1.79	0.46
1:A:161:LYS:HZ1	1:A:162:LEU:HD12	1.80	0.46
1:A:482:VAL:O	1:A:482:VAL:HG13	2.16	0.46
1:A:104:GLY:CA	1:A:107:ILE:HG22	2.46	0.46
1:B:236:LYS:H	1:B:236:LYS:HE2	1.80	0.46
1:B:433:MET:CE	1:B:472:PHE:CD1	2.99	0.46
1:B:129:ILE:CG1	1:B:192:THR:HG23	2.45	0.46
1:B:494:ALA:O	1:B:498:GLY:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:ASN:CG	1:B:525:GLU:HB2	2.41	0.46
1:A:374:VAL:HG12	1:A:374:VAL:O	2.16	0.45
1:A:421:LYS:HB3	1:A:421:LYS:HE2	1.71	0.45
1:B:123:ARG:NH1	1:B:127:GLU:OE2	2.47	0.45
1:B:439:LEU:HD23	1:B:439:LEU:C	2.40	0.45
1:B:609:SER:OG	1:B:611:GLU:HG2	2.16	0.45
1:A:141:TYR:CE1	1:A:570:ARG:HG3	2.52	0.45
1:A:257:TYR:HE1	1:A:281:LEU:HG	1.79	0.45
1:B:135:ASN:CG	1:B:138:GLN:HE21	2.24	0.45
1:B:162:LEU:HD12	1:B:162:LEU:C	2.41	0.45
1:A:23:ARG:HA	1:A:26:THR:HG22	1.98	0.45
1:B:257:TYR:CE1	1:B:281:LEU:HD13	2.51	0.45
1:A:52:ARG:HG2	1:A:67:TRP:CZ2	2.51	0.45
1:A:175:LYS:HB3	1:A:178:GLU:CG	2.46	0.45
1:A:74:LEU:C	1:A:76:ASN:N	2.75	0.45
1:A:531:LYS:N	1:A:531:LYS:HD3	2.31	0.45
1:A:271:VAL:HG11	1:B:356:TYR:CZ	2.51	0.45
1:B:20:GLU:O	1:B:24:LEU:HB2	2.16	0.45
1:A:76:ASN:N	1:A:76:ASN:HD22	2.15	0.45
1:A:540:LEU:O	3:A:801:HOH:O	2.21	0.45
1:B:3:GLU:O	1:B:7:ARG:HB2	2.17	0.45
1:A:40:ILE:CG2	1:A:44:PHE:CE1	2.98	0.45
1:B:40:ILE:HD12	1:B:40:ILE:N	2.32	0.45
1:B:161:LYS:HE3	1:B:161:LYS:HB3	1.85	0.45
1:B:611:GLU:O	1:B:612:GLU:CB	2.64	0.45
1:A:104:GLY:HA2	1:A:107:ILE:HG22	1.99	0.45
1:A:583:LEU:HD23	1:A:583:LEU:HA	1.80	0.45
1:B:429:ARG:HD3	1:B:477:ARG:NH1	2.27	0.45
1:A:172:ILE:HD11	1:A:177:GLU:OE2	2.17	0.45
1:B:344:LEU:HG	1:B:599:THR:OG1	2.17	0.45
1:B:102:ILE:HD11	1:B:159:ALA:HA	1.99	0.44
1:B:110:GLY:HA2	1:B:115:VAL:HG11	1.99	0.44
1:B:164:GLU:O	1:B:168:ASP:HB2	2.17	0.44
1:B:236:LYS:H	1:B:236:LYS:CD	2.30	0.44
1:B:370:VAL:HG13	1:B:370:VAL:O	2.18	0.44
1:B:433:MET:CE	1:B:472:PHE:CE1	3.00	0.44
1:A:148:LEU:HD23	1:A:152:GLU:HG2	1.98	0.44
1:A:227:ASN:OD1	1:A:634:LEU:HD12	2.17	0.44
1:B:289:CYS:HB3	1:B:293:ASP:HB3	1.98	0.44
1:B:115:VAL:CG1	1:B:119:LYS:HG3	2.47	0.44
1:B:146:LEU:HD21	1:B:184:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:LEU:HD21	1:B:450:LEU:HD13	1.99	0.44
1:A:111:LYS:HD3	1:A:111:LYS:N	2.33	0.44
1:B:174:SER:O	1:B:175:LYS:CG	2.66	0.44
1:B:40:ILE:O	1:B:40:ILE:HG22	2.16	0.44
1:B:286:GLU:OE1	1:B:286:GLU:HA	2.16	0.44
1:A:46:ASN:O	1:A:47:ASP:CG	2.60	0.43
1:A:233:MET:HE1	1:A:255:LEU:CD1	2.48	0.43
1:A:109:PHE:HE1	1:A:111:LYS:HB2	1.82	0.43
1:A:501:ILE:HD13	1:A:501:ILE:H	1.83	0.43
1:A:23:ARG:O	1:A:24:LEU:C	2.58	0.43
1:A:175:LYS:CB	1:A:178:GLU:HG2	2.45	0.43
1:A:290:GLN:O	1:A:293:ASP:HB2	2.17	0.43
1:B:6:TRP:CH2	1:B:42:LYS:HD3	2.53	0.43
1:A:109:PHE:HE1	1:A:111:LYS:HG2	1.84	0.43
1:A:166:ILE:HG13	1:A:167:ARG:N	2.33	0.43
1:A:611:GLU:O	1:A:614:GLU:HG2	2.19	0.43
1:B:439:LEU:HD23	1:B:439:LEU:O	2.18	0.43
1:A:125:ILE:HG21	1:A:142:ILE:HG21	1.99	0.43
1:B:227:ASN:HA	1:B:307:MET:CE	2.46	0.43
1:B:484:ALA:HB1	1:B:486:GLU:CD	2.44	0.43
1:A:187:ILE:HD13	1:A:187:ILE:N	2.34	0.43
1:B:363:LEU:HD11	1:B:559:ILE:HD11	2.01	0.43
1:A:30:ARG:O	1:A:30:ARG:HG2	2.18	0.43
1:A:499:ASN:OD1	1:A:501:ILE:HG12	2.18	0.43
1:B:130:LEU:O	1:B:576:LYS:HE3	2.19	0.43
1:B:348:LYS:HE2	1:B:348:LYS:HB3	1.84	0.43
1:B:366:GLY:HA3	1:B:604:PRO:O	2.19	0.43
1:A:109:PHE:O	1:A:109:PHE:CG	2.61	0.43
1:B:135:ASN:C	1:B:135:ASN:HD22	2.27	0.43
1:B:430:LEU:HD22	1:B:433:MET:HE2	2.00	0.43
1:B:521:LEU:HD23	1:B:521:LEU:HA	1.75	0.43
1:A:22:THR:O	1:A:23:ARG:C	2.61	0.42
1:A:195:LEU:HD23	1:A:199:LYS:HB2	2.01	0.42
1:A:511:LEU:HD23	1:A:511:LEU:HA	1.78	0.42
1:A:482:VAL:HG22	1:A:506:ALA:O	2.19	0.42
1:B:17:ASN:O	1:B:21:ALA:N	2.42	0.42
1:B:430:LEU:HD13	1:B:430:LEU:O	2.19	0.42
1:A:102:ILE:HG12	1:A:163:TYR:HB2	2.01	0.42
1:A:521:LEU:N	1:A:521:LEU:HD22	2.34	0.42
1:B:283:ASP:OD1	1:B:283:ASP:O	2.37	0.42
1:B:563:LEU:HB3	1:B:564:PRO:CD	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LYS:NZ	1:A:162:LEU:HD12	2.35	0.42
1:A:452:LEU:CB	1:A:453:PRO:HD3	2.49	0.42
1:A:521:LEU:HA	1:A:525:GLU:OE2	2.19	0.42
1:B:314:ASN:CG	3:B:807:HOH:O	2.63	0.42
1:B:515:MET:HG2	1:B:518:VAL:CG1	2.48	0.42
1:A:504:THR:HG23	1:A:530:ILE:CD1	2.50	0.42
1:A:626:TRP:HA	1:A:631:GLN:HG2	2.01	0.42
1:B:73:ILE:O	1:B:73:ILE:CG2	2.51	0.42
1:B:107:ILE:HD13	1:B:107:ILE:HG21	1.81	0.42
1:B:283:ASP:C	1:B:285:ASP:H	2.26	0.42
1:B:466:LEU:O	1:B:470:VAL:HG23	2.20	0.42
1:A:110:GLY:CA	1:A:115:VAL:HG11	2.47	0.42
1:B:461:GLN:O	1:B:464:SER:OG	2.35	0.42
1:A:572:ILE:HG21	1:A:575:LEU:HG	2.01	0.42
1:B:115:VAL:HG12	1:B:119:LYS:HG3	2.02	0.42
1:B:627:MET:HE3	1:B:628:PRO:CD	2.48	0.42
1:A:130:LEU:O	1:A:576:LYS:HG3	2.20	0.42
1:B:17:ASN:HB3	1:B:20:GLU:OE1	2.19	0.42
1:A:23:ARG:O	1:A:26:THR:HG23	2.17	0.42
1:A:293:ASP:OD2	1:A:326:SER:OG	2.35	0.42
1:B:40:ILE:O	1:B:40:ILE:CG2	2.68	0.42
1:B:52:ARG:CZ	1:B:80:LEU:HD11	2.50	0.42
1:B:611:GLU:O	1:B:612:GLU:HB2	2.19	0.42
1:A:23:ARG:C	1:A:26:THR:HG22	2.44	0.41
1:B:283:ASP:O	1:B:285:ASP:N	2.53	0.41
1:B:515:MET:CE	1:B:518:VAL:CG1	2.83	0.41
2:B:701:UPG:H3'	2:B:701:UPG:H5C2	2.02	0.41
1:A:519:SER:C	1:A:520:ARG:HD2	2.45	0.41
1:B:74:LEU:HD22	1:B:77:ILE:HD11	2.01	0.41
1:B:125:ILE:O	1:B:129:ILE:HB	2.20	0.41
1:B:461:GLN:HA	1:B:464:SER:HG	1.84	0.41
1:B:512:VAL:O	1:B:512:VAL:HG23	2.20	0.41
1:A:23:ARG:NE	1:A:61:PHE:CZ	2.88	0.41
1:B:29:LYS:O	1:B:30:ARG:CD	2.63	0.41
1:B:24:LEU:HD22	1:B:24:LEU:HA	1.83	0.41
1:B:541:LEU:HA	1:B:541:LEU:HD23	1.75	0.41
1:A:125:ILE:HD13	1:A:125:ILE:HA	1.74	0.41
1:A:359:HIS:ND1	1:A:360:PRO:HD2	2.35	0.41
1:A:512:VAL:O	1:A:512:VAL:CG2	2.69	0.41
1:B:114:VAL:HG21	1:B:166:ILE:HA	2.01	0.41
1:B:348:LYS:O	1:B:348:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:PHE:CE2	1:A:301:GLN:NE2	2.88	0.41
1:B:113:PRO:HG2	1:B:170:LYS:O	2.21	0.41
1:B:543:LYS:N	1:B:544:PRO:HD2	2.35	0.41
1:B:158:GLN:O	1:B:162:LEU:HB2	2.20	0.41
1:A:23:ARG:HA	1:A:26:THR:CG2	2.51	0.41
1:A:40:ILE:N	1:A:40:ILE:CD1	2.83	0.41
1:B:119:LYS:HG2	1:B:143:PHE:CD1	2.56	0.41
1:B:133:GLU:HA	1:B:134:PRO:HD2	1.82	0.41
1:B:439:LEU:C	1:B:439:LEU:CD2	2.94	0.41
1:B:512:VAL:O	1:B:512:VAL:CG2	2.69	0.41
1:B:515:MET:HE2	1:B:518:VAL:HG22	2.01	0.41
1:A:129:ILE:HD12	1:A:129:ILE:HA	1.69	0.40
1:A:512:VAL:O	1:A:512:VAL:HG23	2.20	0.40
1:B:44:PHE:HD1	1:B:44:PHE:H	0.69	0.40
1:A:110:GLY:HA2	1:A:115:VAL:CG1	2.49	0.40
1:A:442:ASP:O	1:A:446:ASN:CB	2.65	0.40
1:A:509:ALA:O	1:A:512:VAL:O	2.39	0.40
1:A:563:LEU:HA	1:A:564:PRO:HD3	1.83	0.40
1:B:29:LYS:CE	1:B:42:LYS:HE2	2.44	0.40
1:B:45:GLU:H	1:B:45:GLU:HG2	1.70	0.40
1:B:439:LEU:CD2	1:B:450:LEU:HD13	2.52	0.40
1:B:567:GLU:HA	1:B:568:PRO:HD3	1.73	0.40
1:A:12:THR:HG23	1:A:13:GLU:HG3	2.04	0.40
1:A:266:GLU:OE1	1:A:266:GLU:HA	2.21	0.40
1:B:157:GLU:HA	1:B:160:GLU:HG3	2.04	0.40
1:B:167:ARG:HG3	1:B:168:ASP:OD2	2.22	0.40
1:B:611:GLU:H	1:B:611:GLU:CD	2.27	0.40
1:A:17:ASN:O	1:A:21:ALA:HB3	2.20	0.40
1:B:11:MET:HE3	1:B:11:MET:HB2	1.67	0.40
1:B:157:GLU:O	1:B:158:GLN:C	2.65	0.40
1:B:254:LYS:HD2	1:B:282:LEU:HD12	2.04	0.40
1:B:273:TRP:CH2	1:B:279:ILE:HD13	2.57	0.40
1:B:532:LYS:HE2	1:B:532:LYS:HB2	1.95	0.40
1:B:567:GLU:CG	1:B:568:PRO:CD	2.91	0.40
1:A:75:SER:C	1:A:76:ASN:HD22	2.30	0.40
1:B:140:GLU:CG	1:B:374:VAL:HG23	2.35	0.40
1:B:195:LEU:HD22	1:B:199:LYS:HB3	2.03	0.40
1:B:525:GLU:O	1:B:529:LEU:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	599/655 (92%)	561 (94%)	33 (6%)	5 (1%)	16	25
1	B	583/655 (89%)	543 (93%)	35 (6%)	5 (1%)	14	22
All	All	1182/1310 (90%)	1104 (93%)	68 (6%)	10 (1%)	16	25

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	249	ALA
1	B	249	ALA
1	B	565	THR
1	B	519	SER
1	B	57	MET
1	B	284	PHE
1	A	30	ARG
1	A	566	GLY
1	A	613	VAL

5.3.2 Protein sidechains [i](#)

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	533/578 (92%)	470 (88%)	63 (12%)	5	7
1	B	519/578 (90%)	457 (88%)	62 (12%)	5	7
All	All	1052/1156 (91%)	927 (88%)	125 (12%)	5	7

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	5	TYR
1	A	10	LEU
1	A	23	ARG
1	A	24	LEU
1	A	27	VAL
1	A	28	LEU
1	A	38	GLU
1	A	40	ILE
1	A	41	ASN
1	A	42	LYS
1	A	46	ASN
1	A	73	ILE
1	A	74	LEU
1	A	81	THR
1	A	111	LYS
1	A	116	LYS
1	A	119	LYS
1	A	125	ILE
1	A	129	ILE
1	A	133	GLU
1	A	145	LEU
1	A	146	LEU
1	A	162	LEU
1	A	165	CYS
1	A	166	ILE
1	A	167	ARG
1	A	169	LYS
1	A	170	LYS
1	A	175	LYS
1	A	178	GLU
1	A	180	LEU
1	A	187	ILE
1	A	199	LYS
1	A	279	ILE
1	A	284	PHE
1	A	305	LYS
1	A	407	SER
1	A	444	GLU
1	A	449	LYS
1	A	461	GLN
1	A	467	SER

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Mol	Chain	Res	Type
1	A	476	GLN
1	A	482	VAL
1	A	501	ILE
1	A	502	VAL
1	A	513	HIS
1	A	515	MET
1	A	518	VAL
1	A	522	ASN
1	A	525	GLU
1	A	531	LYS
1	A	539	SER
1	A	567	GLU
1	A	596	THR
1	A	607	ILE
1	A	609	SER
1	A	610	SER
1	A	614	GLU
1	A	615	ARG
1	A	618	SER
1	A	624	LEU
1	A	634	LEU
1	B	12	THR
1	B	23	ARG
1	B	24	LEU
1	B	25	ILE
1	B	26	THR
1	B	27	VAL
1	B	39	SER
1	B	44	PHE
1	B	46	ASN
1	B	52	ARG
1	B	73	ILE
1	B	102	ILE
1	B	107	ILE
1	B	112	SER
1	B	114	VAL
1	B	123	ARG
1	B	125	ILE
1	B	129	ILE
1	B	133	GLU
1	B	135	ASN
1	B	136	LEU

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Mol	Chain	Res	Type
1	B	148	LEU
1	B	158	GLN
1	B	162	LEU
1	B	166	ILE
1	B	178	GLU
1	B	184	VAL
1	B	196	ASN
1	B	235	LYS
1	B	241	LEU
1	B	264	LYS
1	B	307	MET
1	B	345	THR
1	B	351	LYS
1	B	374	VAL
1	B	420	SER
1	B	439	LEU
1	B	441	LYS
1	B	464	SER
1	B	475	VAL
1	B	496	GLN
1	B	503	LEU
1	B	507	LEU
1	B	511	LEU
1	B	513	HIS
1	B	515	MET
1	B	516	ASP
1	B	518	VAL
1	B	520	ARG
1	B	522	ASN
1	B	524	SER
1	B	525	GLU
1	B	529	LEU
1	B	543	LYS
1	B	546	VAL
1	B	567	GLU
1	B	569	THR
1	B	599	THR
1	B	608	THR
1	B	612	GLU
1	B	624	LEU
1	B	629	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	76	ASN
1	A	120	GLN
1	A	121	ASN
1	A	438	GLN
1	A	492	GLN
1	A	513	HIS
1	A	517	ASN
1	A	537	GLN
1	B	121	ASN
1	B	135	ASN
1	B	138	GLN
1	B	196	ASN
1	B	248	ASN
1	B	461	GLN
1	B	492	GLN
1	B	513	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
2	UPG	B	701	-	37,38,38	1.10	2 (5%)	55,58,58	2.13	12 (21%)
2	UPG	A	701	-	37,38,38	1.19	6 (16%)	55,58,58	2.15	9 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UPG	B	701	-	-	2/23/59/59	0/3/3/3
2	UPG	A	701	-	-	3/23/59/59	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	UPG	C6-N1	-2.62	1.31	1.38
2	A	701	UPG	C6-N1	-2.42	1.32	1.38
2	A	701	UPG	C2-N1	2.41	1.42	1.38
2	B	701	UPG	PB-O2B	-2.37	1.44	1.55
2	A	701	UPG	PB-O2B	-2.34	1.44	1.55
2	A	701	UPG	PB-O1B	-2.15	1.43	1.50
2	A	701	UPG	PA-O1A	-2.15	1.43	1.50
2	A	701	UPG	O4C-C4C	-2.11	1.40	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	UPG	O2-C2-N1	-7.76	112.70	122.80
2	A	701	UPG	O2-C2-N1	-7.25	113.36	122.80
2	A	701	UPG	C4-N3-C2	-6.83	118.14	126.61
2	B	701	UPG	C4-N3-C2	-6.48	118.57	126.61
2	B	701	UPG	N3-C2-N1	6.17	122.93	114.89
2	A	701	UPG	N3-C2-N1	5.71	122.33	114.89
2	A	701	UPG	O4-C4-C5	-4.31	117.72	125.16
2	B	701	UPG	O4-C4-C5	-4.30	117.75	125.16
2	A	701	UPG	O5'-C1'-O3B	-4.06	106.06	111.36
2	B	701	UPG	O4-C4-N3	3.18	123.89	119.27
2	A	701	UPG	C5-C4-N3	2.93	118.90	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	UPG	C6-N1-C2	-2.85	117.52	121.00
2	A	701	UPG	O4-C4-N3	2.83	123.37	119.27
2	B	701	UPG	O4C-C1C-N1	2.69	114.46	108.36
2	B	701	UPG	C5-C4-N3	2.55	118.36	114.80
2	B	701	UPG	C1'-O5'-C5'	2.35	118.31	113.72
2	B	701	UPG	O2B-PB-O1B	2.32	123.23	112.44
2	B	701	UPG	C1C-N1-C2	2.31	121.74	117.59
2	B	701	UPG	O5C-PA-O1A	-2.08	100.69	108.94
2	A	701	UPG	O3A-PA-O1A	-2.06	104.50	110.70
2	A	701	UPG	C1'-O5'-C5'	2.04	117.69	113.72

There are no chirality outliers.

All (5) torsion outliers are listed below:

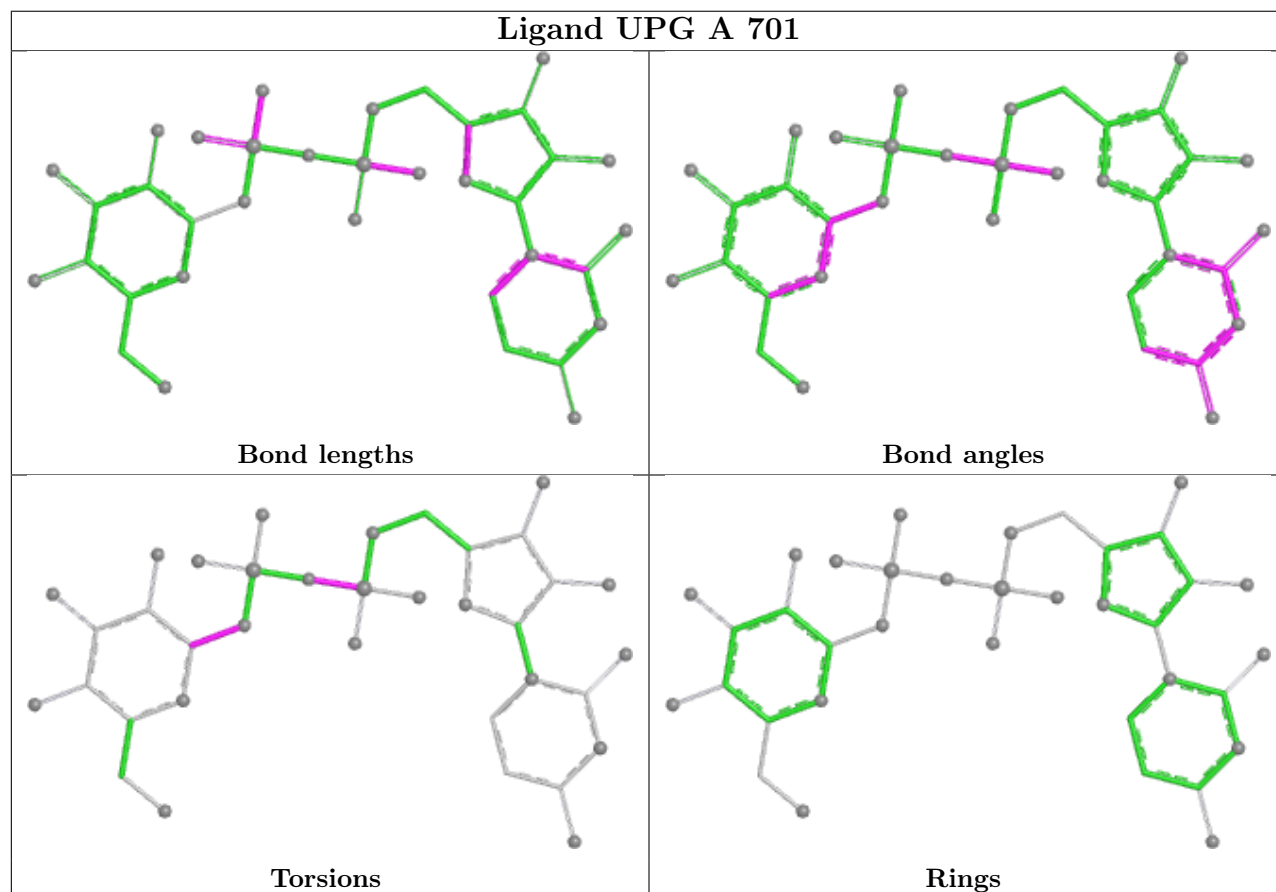
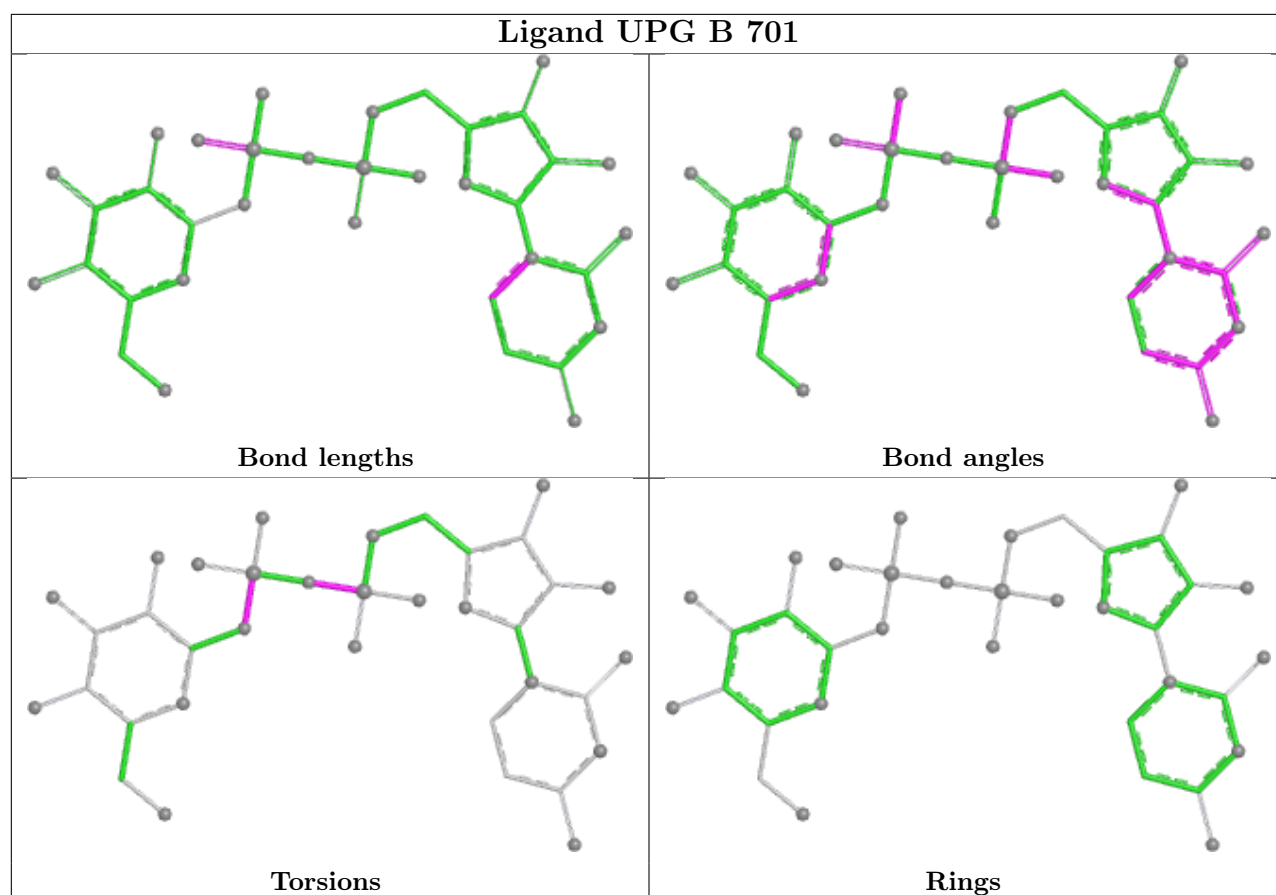
Mol	Chain	Res	Type	Atoms
2	A	701	UPG	PB-O3A-PA-O1A
2	A	701	UPG	O5'-C1'-O3B-PB
2	B	701	UPG	C1'-O3B-PB-O1B
2	A	701	UPG	PB-O3A-PA-O2A
2	B	701	UPG	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	UPG	1	0
2	A	701	UPG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	607/655 (92%)	0.45	23 (3%) 44 40	38, 63, 96, 120	0
1	B	591/655 (90%)	0.46	21 (3%) 46 42	37, 60, 97, 109	0
All	All	1198/1310 (91%)	0.45	44 (3%) 45 41	37, 62, 97, 120	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	521	LEU	4.6
1	A	109	PHE	4.0
1	B	44	PHE	3.9
1	B	47	ASP	3.5
1	A	5	TYR	3.3
1	B	40	ILE	3.2
1	A	623	GLY	3.0
1	A	44	PHE	2.9
1	B	12	THR	2.9
1	B	43	LEU	2.9
1	A	126	CYS	2.8
1	A	31	LYS	2.8
1	B	518	VAL	2.6
1	A	627	MET	2.6
1	B	515	MET	2.6
1	A	131	MET	2.6
1	B	117	LEU	2.5
1	B	46	ASN	2.5
1	A	482	VAL	2.5
1	B	10	LEU	2.5
1	A	616	THR	2.5
1	B	100	PRO	2.4
1	A	345	THR	2.4
1	A	67	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	580	ALA	2.4
1	B	166	ILE	2.4
1	B	627	MET	2.4
1	A	29	LYS	2.4
1	B	525	GLU	2.4
1	A	111	LYS	2.3
1	B	565	THR	2.3
1	A	630	GLU	2.3
1	A	80	LEU	2.2
1	A	443	CYS	2.2
1	A	566	GLY	2.2
1	A	114	VAL	2.2
1	B	567	GLU	2.2
1	B	136	LEU	2.2
1	A	619	LEU	2.1
1	A	41	ASN	2.1
1	B	167	ARG	2.1
1	B	159	ALA	2.0
1	A	615	ARG	2.0
1	B	495	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

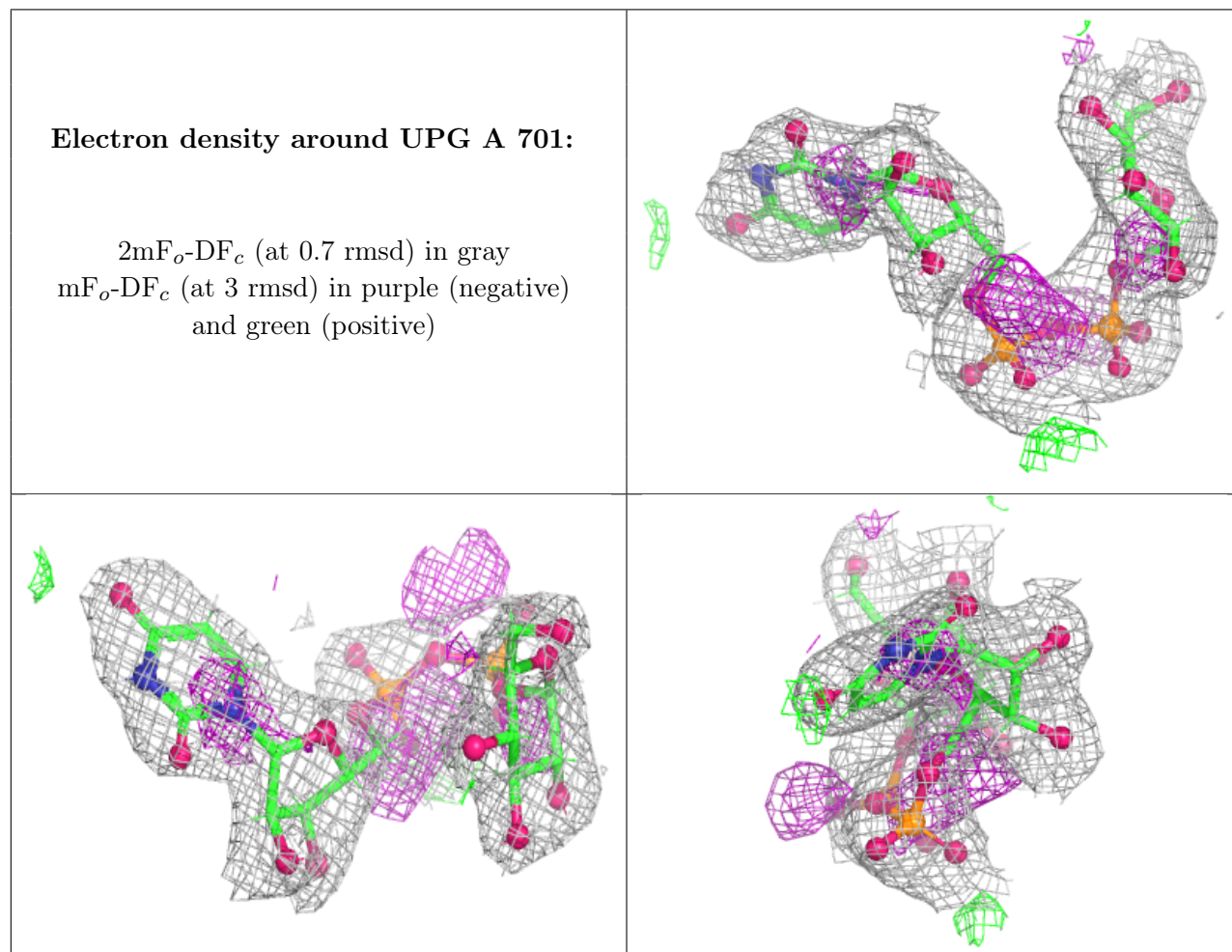
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

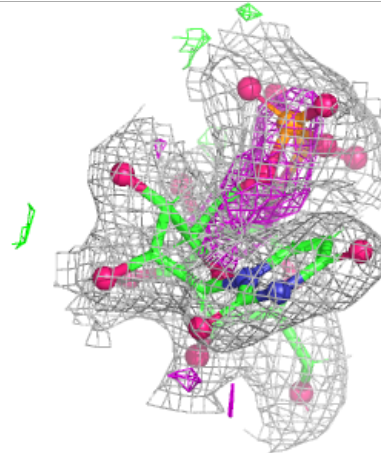
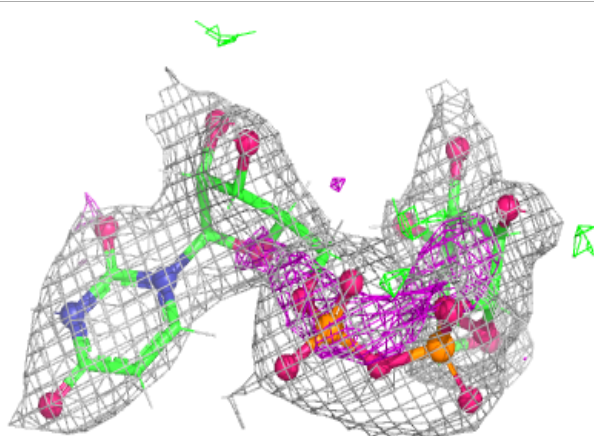
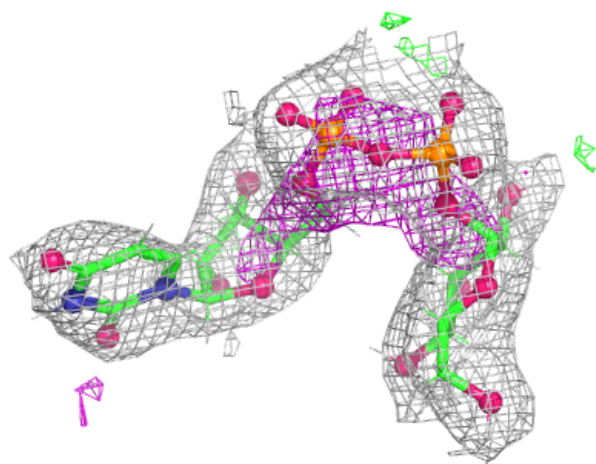
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UPG	A	701	36/36	0.90	0.08	41,62,76,79	0
2	UPG	B	701	36/36	0.91	0.09	44,61,73,77	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around UPG B 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.