



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:50 AM GMT

PDB ID : 3UBN
Title : Influenza hemagglutinin from the 2009 pandemic in complex with ligand 6SLN
Authors : Xu, R.; Wilson, I.A.
Deposited on : 2011-10-24
Resolution : 2.51 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>

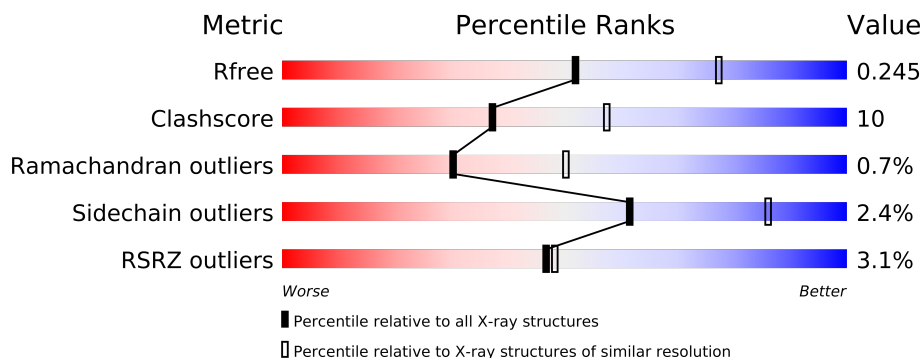
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.51 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	329	
1	C	329	
1	E	329	
1	G	329	
1	I	329	
1	K	329	
2	B	177	
2	D	177	
2	F	177	
2	H	177	
2	J	177	
2	L	177	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24203 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2522	1595	432	482	13			
1	C	319	Total	C	N	O	S	0	0	0
			2495	1579	428	475	13			
1	E	323	Total	C	N	O	S	0	0	0
			2522	1595	432	482	13			
1	G	321	Total	C	N	O	S	0	0	0
			2508	1586	430	479	13			
1	I	319	Total	C	N	O	S	0	0	0
			2495	1579	428	475	13			
1	K	319	Total	C	N	O	S	0	0	0
			2492	1578	428	473	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
A	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
A	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
A	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
C	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
C	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
C	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
C	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
E	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
E	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
E	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
E	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
G	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
G	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
G	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
G	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
I	9	PRO	-	EXPRESSION TAG	UNP C3W5S1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
I	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
I	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
K	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
K	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
K	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
K	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	0	0	0
			1405	881	237	281	6			
2	D	171	Total	C	N	O	S	0	0	0
			1380	866	234	274	6			
2	F	170	Total	C	N	O	S	0	0	0
			1371	861	233	271	6			
2	H	170	Total	C	N	O	S	0	0	0
			1371	861	233	271	6			
2	J	170	Total	C	N	O	S	0	0	0
			1371	861	233	271	6			
2	L	170	Total	C	N	O	S	0	0	0
			1371	861	233	271	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	EXPRESSION TAG	UNP C3W5S1
B	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
B	177	ARG	-	EXPRESSION TAG	UNP C3W5S1
D	175	SER	-	EXPRESSION TAG	UNP C3W5S1
D	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
D	177	ARG	-	EXPRESSION TAG	UNP C3W5S1
F	175	SER	-	EXPRESSION TAG	UNP C3W5S1
F	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
F	177	ARG	-	EXPRESSION TAG	UNP C3W5S1
H	175	SER	-	EXPRESSION TAG	UNP C3W5S1
H	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
H	177	ARG	-	EXPRESSION TAG	UNP C3W5S1
J	175	SER	-	EXPRESSION TAG	UNP C3W5S1
J	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
J	177	ARG	-	EXPRESSION TAG	UNP C3W5S1

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Chain	Residue	Modelled	Actual	Comment	Reference
L	175	SER	-	EXPRESSION TAG	UNP C3W5S1
L	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
L	177	ARG	-	EXPRESSION TAG	UNP C3W5S1

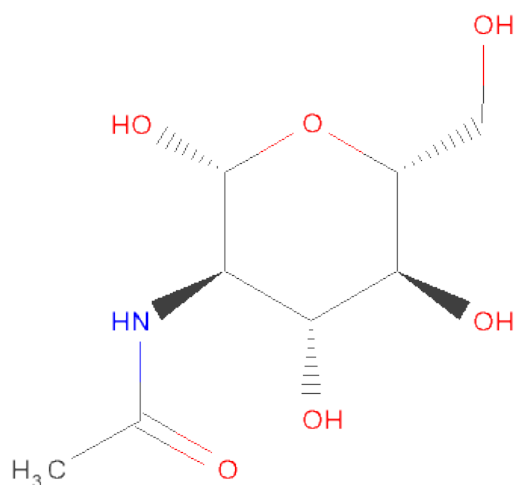
- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			46	25	2	19		
3	C	3	Total	C	N	O	0	0
			46	25	2	19		
3	E	3	Total	C	N	O	0	0
			46	25	2	19		
3	I	3	Total	C	N	O	0	0
			46	25	2	19		
3	K	3	Total	C	N	O	0	0
			46	25	2	19		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
A	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
A	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
A	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
C	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
C	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
C	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
C	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
E	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
E	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
E	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
E	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
I	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
I	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
I	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
I	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
K	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
K	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
K	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
K	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	J	1	Total	C	N	O	0	0
			14	8	1	5		
4	K	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	2	Total	C	N	O	0	0
			31	17	1	13		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
G	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
G	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
G	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	2	Total	C	N	O	0	0
			28	16	2	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
G	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
G	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
G	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	55	Total	O	0	0
			55	55		
7	B	28	Total	O	0	0
			28	28		
7	C	60	Total	O	0	0
			60	60		
7	D	31	Total	O	0	0
			31	31		
7	E	33	Total	O	0	0
			33	33		
7	F	22	Total	O	0	0
			22	22		
7	G	63	Total	O	0	0
			63	63		
7	H	27	Total	O	0	0
			27	27		
7	I	44	Total	O	0	0
			44	44		
7	J	36	Total	O	0	0
			36	36		

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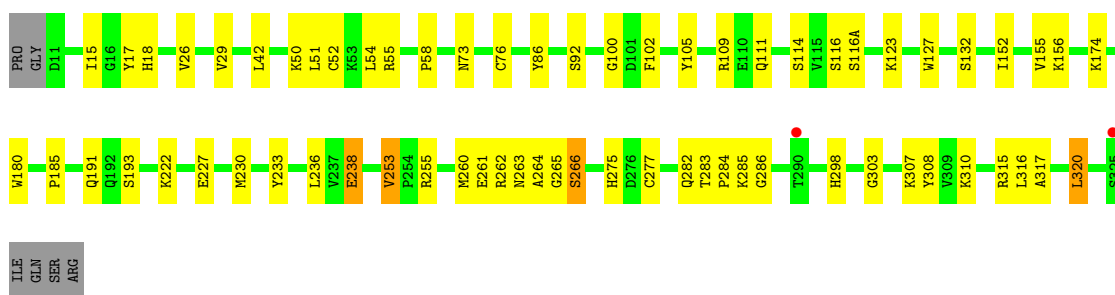
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	K	51	Total 51	O 51	0	0
7	L	35	Total 35	O 35	0	0

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.

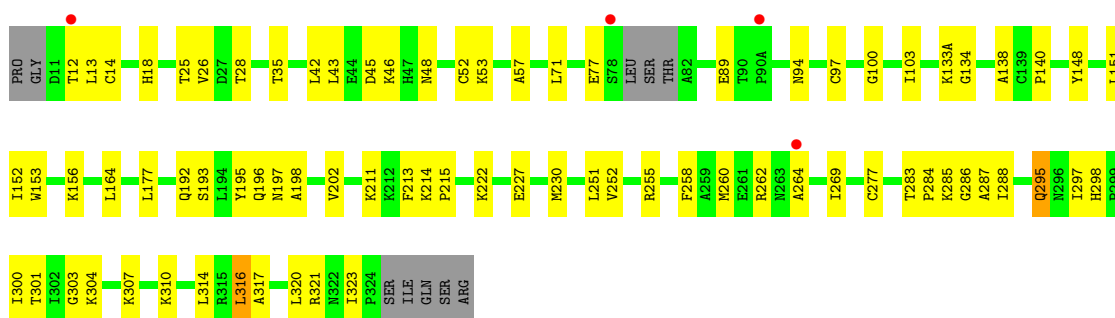
• Molecule 1: Hemagglutinin HA1

Chain A: 



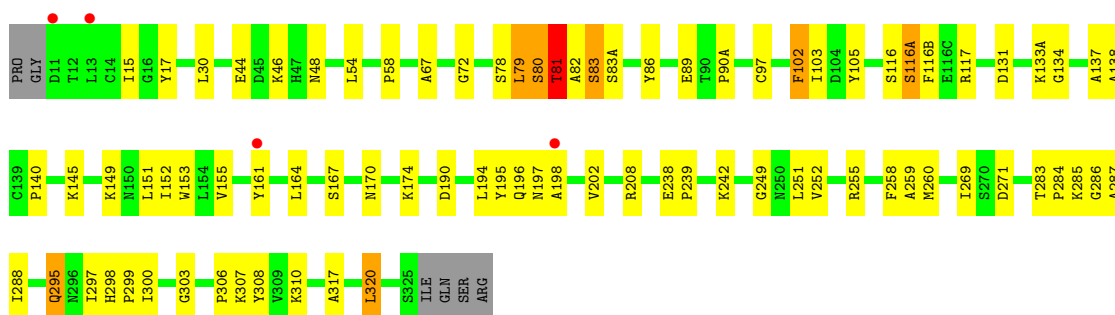
• Molecule 1: Hemagglutinin HA1

Chain C: 



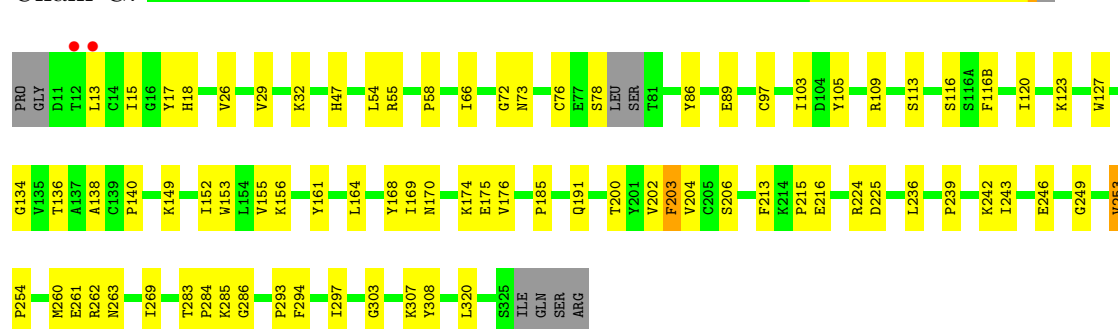
• Molecule 1: Hemagglutinin HA1

Chain E: 



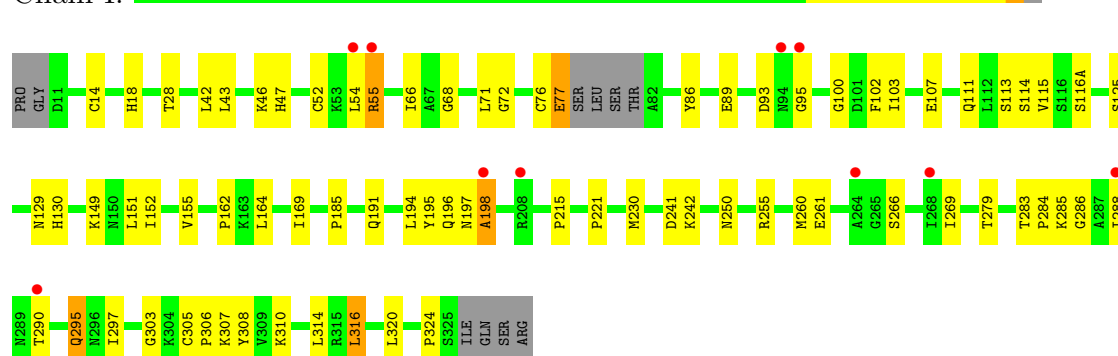
- Molecule 1: Hemagglutinin HA1

Chain G:



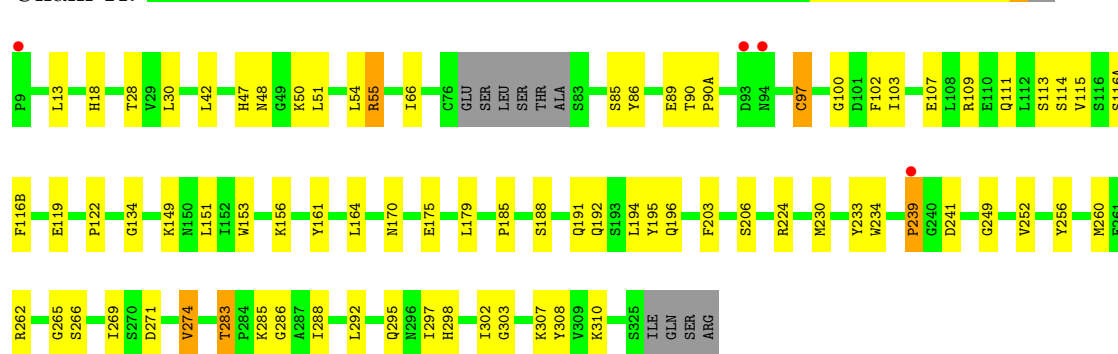
- Molecule 1: Hemagglutinin HA1

Chain I:



- Molecule 1: Hemagglutinin HA1

Chain K:



- Molecule 2: Hemagglutinin HA2

Chain B:



- Molecule 2: Hemagglutinin HA2

K121	V122	K123	S124	K125	V126	K127	V128	K129	V130	K131	V132	K133	V134	K135	V136	K137	V138	K139	V140	K141	V142	K143	V144	K145	V146	K147	V148	K149	V150	K151	V152	K153	V154	K155	V156	K157	V158	K159	V160	K161	V162	K163	V164	K165	V166	K167	V168	K169	V170	K171	V172	K173	V174	K175	V176	K177	V178	K179	V180	K181	V182	K183	V184	K185	V186	K187	V188	K189	V190	K191	V192	K193	V194	K195	V196	K197	V198	K199	V200	K201	V202	K203	V204	K205	V206	K207	V208	K209	V210	K211	V212	K213	V214	K215	V216	K217	V218	K219	V220	K221	V222	K223	V224	K225	V226	K227	V228	K229	V230	K231	V232	K233	V234	K235	V236	K237	V238	K239	V240	K241	V242	K243	V244	K245	V246	K247	V248	K249	V250	K251	V252	K253	V254	K255	V256	K257	V258	K259	V260	K261	V262	K263	V264	K265	V266	K267	V268	K269	V270	K271	V272	K273	V274	K275	V276	K277	V278	K279	V280	K281	V282	K283	V284	K285	V286	K287	V288	K289	V290	K291	V292	K293	V294	K295	V296	K297	V298	K299	V300	K301	V302	K303	V304	K305	V306	K307	V308	K309	V310	K311	V312	K313	V314	K315	V316	K317	V318	K319	V320	K321	V322	K323	V324	K325	V326	K327	V328	K329	V330	K331	V332	K333	V334	K335	V336	K337	V338	K339	V340	K341	V342	K343	V344	K345	V346	K347	V348	K349	V350	K351	V352	K353	V354	K355	V356	K357	V358	K359	V360	K361	V362	K363	V364	K365	V366	K367	V368	K369	V370	K371	V372	K373	V374	K375	V376	K377	V378	K379	V380	K381	V382	K383	V384	K385	V386	K387	V388	K389	V390	K391	V392	K393	V394	K395	V396	K397	V398	K399	V399	K401	V402	K403	V404	K405	V406	K407	V408	K409	V410	K411	V412	K413	V414	K415	V416	K417	V418	K419	V420	K421	V422	K423	V424	K425	V426	K427	V428	K429	V430	K431	V432	K433	V434	K435	V436	K437	V438	K439	V440	K441	V442	K443	V444	K445	V446	K447	V448	K449	V450	K451	V452	K453	V454	K455	V456	K457	V458	K459	V460	K461	V462	K463	V464	K465	V466	K467	V468	K469	V470	K471	V472	K473	V474	K475	V476	K477	V478	K479	V480	K481	V482	K483	V484	K485	V486	K487	V488	K489	V490	K491	V492	K493	V494	K495	V496	K497	V498	K499	V499	K501	V502	K503	V504	K505	V506	K507	V508	K509	V510	K511	V512	K513	V514	K515	V516	K517	V518	K519	V520	K521	V522	K523	V524	K525	V526	K527	V528	K529	V530	K531	V532	K533	V534	K535	V536	K537	V538	K539	V540	K541	V542	K543	V544	K545	V546	K547	V548	K549	V550	K551	V552	K553	V554	K555	V556	K557	V558	K559	V560	K561	V562	K563	V564	K565	V566	K567	V568	K569	V570	K571	V572	K573	V574	K575	V576	K577	V578	K579	V580	K581	V582	K583	V584	K585	V586	K587	V588	K589	V590	K591	V592	K593	V594	K595	V596	K597	V598	K599	V599	K601	V602	K603	V604	K605	V606	K607	V608	K609	V610	K611	V612	K613	V614	K615	V616	K617	V618	K619	V620	K621	V622	K623	V624	K625	V626	K627	V628	K629	V630	K631
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G136	F140	F141	H142	K143	C144	D145	E150	G155	D158	F159	P160	K161	F162	S163	E164	F165	A166	K167	L168	R169	GLU	GLU	ILE	ASP	SER	GLY	ARG
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H111	D112	S113	N114	V115	V122	R123	S124	Q125	I133	G134	N135	E139	F140	V141	H142	K143	G144	V152	K153	N154	G155	T156	V157	D158	V159	P160	E164	K167	L168	N169	GLU	GLU	ILE	ILE	ASP	SER	GLY	ARG
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D158	Y159	P160	K161	Y162	S163	R170	GLU	GLU	ILE	ASP	SER	GLY	ARG
------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----

Category	Count
C148	148
M149	149
V152	152
Y159	159
P160	160
R170	170
GLU, GLU, ILE, ASP, SER, GLY, ARG	6

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.00Å 116.71Å 119.66Å 60.61° 77.05° 80.38°	Depositor
Resolution (Å)	49.68 – 2.51 49.68 – 2.51	Depositor EDS
% Data completeness (in resolution range)	94.2 (49.68-2.51) 94.3 (49.68-2.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.205 , 0.253 0.199 , 0.245	Depositor DCC
R_{free} test set	4909 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 99214 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24203	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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: SIA, GAL, NAG

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	0.22	0/2586	0.40	0/3516
1	C	0.22	0/2558	0.40	0/3476
1	E	0.22	0/2586	0.43	0/3516
1	G	0.22	0/2571	0.40	0/3494
1	I	0.22	0/2558	0.41	0/3476
1	K	0.22	0/2556	0.40	0/3473
2	B	0.22	0/1433	0.35	0/1931
2	D	0.22	0/1408	0.35	0/1897
2	F	0.22	0/1399	0.36	0/1885
2	H	0.22	0/1399	0.36	0/1885
2	J	0.23	0/1399	0.37	0/1885
2	L	0.23	0/1399	0.36	0/1885
All	All	0.22	0/23852	0.39	0/32319

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2522	0	2464	47	0
1	C	2495	0	2437	50	0
1	E	2522	0	2467	74	0
1	G	2508	0	2450	56	0
1	I	2495	0	2439	54	0
1	K	2492	0	2438	55	0
2	B	1405	0	1324	28	0
2	D	1380	0	1303	44	0
2	F	1371	0	1297	33	0
2	H	1371	0	1297	38	0
2	J	1371	0	1296	35	0
2	L	1371	0	1297	31	0
3	A	46	0	40	0	0
3	C	46	0	40	1	0
3	E	46	0	40	2	0
3	I	46	0	40	0	0
3	K	46	0	40	1	0
4	A	56	0	52	0	0
4	C	28	0	26	1	0
4	E	14	0	13	1	0
4	J	14	0	13	0	0
4	K	14	0	13	0	0
5	G	31	0	26	0	0
6	G	28	0	25	2	0
7	A	55	0	0	1	0
7	B	28	0	0	0	0
7	C	60	0	0	1	0
7	D	31	0	0	0	0
7	E	33	0	0	0	0
7	F	22	0	0	1	0
7	G	63	0	0	0	0
7	H	27	0	0	0	0
7	I	44	0	0	0	0
7	J	36	0	0	1	0
7	K	51	0	0	0	0
7	L	35	0	0	1	0
All	All	24203	0	22877	470	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 10.

All (470) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:79:LEU:HA	1:E:80:SER:CB	1.81	1.10
1:E:79:LEU:HA	1:E:80:SER:HB3	1.26	1.10
2:J:59:MET:HA	2:J:60:ASN:HB3	1.03	1.03
1:E:82:ALA:HB3	1:E:83:SER:HB2	1.41	1.00
2:J:59:MET:HA	2:J:60:ASN:CB	1.91	0.97
2:J:59:MET:CA	2:J:60:ASN:HB3	1.94	0.96
1:E:79:LEU:CA	1:E:80:SER:HB3	2.02	0.89
1:E:82:ALA:CB	1:E:83:SER:HB2	2.02	0.88
2:H:97:GLU:HG2	2:L:58:LYS:HD2	1.57	0.87
1:E:283:THR:HG22	1:E:285:LYS:H	1.37	0.87
1:I:283:THR:HG22	1:I:285:LYS:H	1.38	0.87
1:G:283:THR:HG22	1:G:285:LYS:H	1.41	0.85
1:C:283:THR:HG22	1:C:285:LYS:H	1.42	0.84
2:H:58:LYS:HD2	2:J:97:GLU:HG2	1.58	0.83
2:B:97:GLU:HG2	2:F:58:LYS:HD2	1.62	0.81
2:F:164:GLU:O	2:F:167:LYS:HG2	1.82	0.79
1:E:298:HIS:HD2	1:E:300:ILE:H	1.30	0.79
1:A:283:THR:HG22	1:A:285:LYS:H	1.45	0.79
1:E:72:GLY:HA3	1:E:149:LYS:H	1.48	0.77
1:A:283:THR:HB	1:A:286:GLY:O	1.87	0.75
1:I:283:THR:HB	1:I:286:GLY:O	1.87	0.74
2:H:24:TYR:CE1	2:H:153:LYS:HG3	2.22	0.74
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.73	0.71
1:E:190:ASP:O	1:E:194:LEU:HB2	1.92	0.69
2:L:23:GLY:HA3	2:L:36:ALA:HA	1.74	0.69
2:H:62:GLN:HE21	1:I:310:LYS:HZ3	1.40	0.69
1:K:114:SER:HB2	1:K:266:SER:HB2	1.75	0.69
2:H:167:LYS:HG3	2:H:170:ARG:HH12	1.59	0.68
1:K:283:THR:HG23	1:K:285:LYS:H	1.59	0.67
2:H:167:LYS:HG3	2:H:170:ARG:NH1	2.10	0.67
1:C:25:THR:HG22	1:C:35:THR:HG22	1.77	0.67
1:G:283:THR:HB	1:G:286:GLY:O	1.94	0.66
1:I:303:GLY:HA2	2:J:63:PHE:CE1	2.30	0.66
2:J:23:GLY:HA3	2:J:36:ALA:HA	1.75	0.66
2:L:131:LYS:NZ	2:L:133:ILE:HG22	2.11	0.66
1:I:283:THR:HG23	1:I:284:PRO:HD2	1.78	0.66
1:E:298:HIS:CD2	1:E:300:ILE:H	2.12	0.65
1:E:72:GLY:HA3	1:E:149:LYS:N	2.12	0.65
2:J:9:PHE:O	2:J:135:ASN:HA	1.96	0.65
1:K:307:LYS:HG3	2:L:92:TRP:CE2	2.32	0.64
1:K:13:LEU:HB2	2:L:149:MET:HE1	1.79	0.64
1:E:174:LYS:HE3	1:E:259:ALA:HB1	1.79	0.64
2:J:119:TYR:CE1	2:J:136:GLY:HA2	2.33	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:89:GLU:O	1:I:269:ILE:HA	1.98	0.64
2:H:53:ASN:O	2:H:57:GLU:HG2	1.97	0.64
2:D:161:LYS:HD2	2:D:162:TYR:CZ	2.34	0.63
1:G:262:ARG:HG2	1:G:262:ARG:HH11	1.64	0.63
1:E:283:THR:HB	1:E:286:GLY:O	1.99	0.62
1:K:114:SER:HB2	1:K:266:SER:CB	2.29	0.62
2:B:75:LYS:NZ	2:B:79:ASN:HD21	1.98	0.61
1:I:28:THR:HG22	2:J:104:ASN:HB3	1.80	0.61
1:K:170:ASN:HB3	1:K:239:PRO:O	2.00	0.61
2:H:23:GLY:HA3	2:H:36:ALA:HA	1.83	0.61
1:E:82:ALA:CB	1:E:83:SER:CB	2.78	0.61
1:I:169:ILE:HD13	1:I:242:LYS:HB2	1.83	0.60
1:E:80:SER:O	1:E:81:THR:HG23	2.01	0.60
1:C:303:GLY:HA2	2:D:63:PHE:CE1	2.36	0.60
1:E:310:LYS:HG2	2:F:89:LEU:HD11	1.83	0.60
1:C:283:THR:HB	1:C:286:GLY:O	2.02	0.59
1:A:283:THR:HG23	1:A:284:PRO:HD2	1.83	0.59
2:H:9:PHE:O	2:H:135:ASN:HA	2.02	0.59
1:G:253:VAL:HG22	1:G:254:PRO:HD2	1.85	0.59
2:H:123:ARG:HH12	2:J:123:ARG:HH21	1.50	0.59
1:G:97:CYS:O	1:G:224:ARG:HD3	2.02	0.59
1:A:236:LEU:HD13	1:A:262:ARG:NH1	2.18	0.58
2:B:41:THR:O	2:B:45:ILE:HG13	2.02	0.58
2:J:59:MET:CA	2:J:60:ASN:CB	2.69	0.58
2:B:75:LYS:HZ3	2:B:79:ASN:HD21	1.50	0.58
2:D:149:MET:O	2:D:152:VAL:HG22	2.04	0.58
1:E:283:THR:HG23	1:E:284:PRO:HD2	1.86	0.58
1:A:303:GLY:HA2	2:B:63:PHE:CE1	2.39	0.58
1:E:167:SER:OG	1:E:242:LYS:HE2	2.04	0.58
2:B:123:ARG:NH1	2:D:123:ARG:HH22	2.02	0.58
2:D:65:ALA:O	2:D:66:VAL:HG12	2.04	0.57
1:G:15:ILE:HD11	2:H:122:VAL:HG21	1.86	0.57
1:G:283:THR:HG23	1:G:284:PRO:HD2	1.85	0.57
2:D:9:PHE:O	2:D:135:ASN:HA	2.04	0.57
1:A:174:LYS:HD2	1:A:261:GLU:HG3	1.87	0.57
1:E:202:VAL:HG11	1:E:251:LEU:HD13	1.86	0.57
1:I:115:VAL:HG12	1:I:116(A):SER:H	1.70	0.57
2:F:30:GLN:HE21	2:F:145:ASP:HB2	1.70	0.57
2:J:119:TYR:HE1	2:J:136:GLY:HA2	1.69	0.57
1:A:116:SER:HB3	1:A:263:ASN:HD21	1.70	0.56
1:E:44:GLU:OE2	1:E:46:LYS:HG2	2.06	0.56
2:J:160:PRO:HA	2:J:163:SER:OG	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:87:GLY:HA3	2:F:88:PHE:CZ	2.41	0.56
2:H:123:ARG:HH12	2:J:123:ARG:NH2	2.03	0.56
1:K:303:GLY:HA2	2:L:63:PHE:CE1	2.41	0.56
1:G:307:LYS:HE2	2:H:61:THR:HG22	1.87	0.56
2:D:53:ASN:O	2:D:57:GLU:HG2	2.05	0.56
1:C:214:LYS:HG3	1:C:215:PRO:HD2	1.87	0.56
1:G:13:LEU:HD11	2:H:24:TYR:HB3	1.87	0.56
1:G:127:TRP:CH2	1:G:253:VAL:HG21	2.41	0.56
1:E:151:LEU:HB3	1:E:252:VAL:HG12	1.87	0.56
1:I:54:LEU:C	1:I:55:ARG:HG3	2.25	0.56
1:K:206:SER:HB2	1:K:241:ASP:OD2	2.06	0.56
1:E:79:LEU:HA	1:E:80:SER:OG	2.04	0.55
2:J:88:PHE:CZ	2:L:87:GLY:HA3	2.41	0.55
1:C:140:PRO:HD2	4:C:333:NAG:H83	1.89	0.55
1:I:52:CYS:HB2	1:I:279:THR:HG22	1.88	0.55
1:C:300:ILE:HA	2:D:66:VAL:HG11	1.88	0.55
1:K:115:VAL:HG11	1:K:116(B):PHE:HB2	1.88	0.55
1:G:303:GLY:HA2	2:H:63:PHE:CE1	2.41	0.55
1:K:283:THR:HG22	1:K:286:GLY:H	1.72	0.55
1:G:200:THR:OG1	1:G:215:PRO:HG3	2.07	0.55
1:I:307:LYS:HG3	2:J:92:TRP:CE2	2.41	0.55
1:G:170:ASN:HB3	1:G:239:PRO:O	2.07	0.54
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.42	0.54
2:D:159:TYR:HB3	2:D:160:PRO:HD3	1.89	0.54
2:L:4:GLY:O	2:L:8:GLY:HA3	2.06	0.54
1:C:288:ILE:HD13	1:C:295:GLN:HG3	1.90	0.54
1:A:111:GLN:O	1:A:262:ARG:HD2	2.07	0.54
1:I:290:THR:HG23	1:I:306:PRO:HD3	1.89	0.54
1:I:197:ASN:O	1:I:198:ALA:HB3	2.07	0.54
2:D:47:GLU:HB3	1:E:30:LEU:HG	1.87	0.54
1:G:116(B):PHE:HE1	1:G:260:MET:HE2	1.72	0.54
1:E:307:LYS:HG3	2:F:92:TRP:CE2	2.42	0.54
2:F:23:GLY:HA3	2:F:36:ALA:HA	1.90	0.54
2:B:5:ALA:HB3	2:B:112:ASP:OD2	2.08	0.54
1:K:18:HIS:HB2	2:L:20:GLY:O	2.08	0.54
2:L:30:GLN:OE1	2:L:145:ASP:HB2	2.08	0.53
1:E:208:ARG:NH2	1:E:238:GLU:H	2.06	0.53
2:D:124:SER:O	2:D:127:LYS:HE3	2.08	0.53
1:K:107:GLU:O	1:K:111:GLN:HG3	2.08	0.53
1:E:140:PRO:HD2	4:E:333:NAG:H83	1.90	0.53
1:G:72:GLY:O	1:G:149:LYS:HG2	2.08	0.53
1:C:152:ILE:HD11	1:C:255:ARG:HD2	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:58:PRO:HB3	1:A:86:TYR:CE1	2.44	0.53
2:H:88:PHE:CZ	2:J:87:GLY:HA3	2.44	0.53
2:H:159:TYR:HB3	2:H:160:PRO:HD3	1.89	0.53
1:E:82:ALA:HB1	1:E:83:SER:CA	2.39	0.53
1:G:203:PHE:HD1	1:G:204:VAL:N	2.07	0.53
2:D:158:ASP:OD1	2:D:161:LYS:HB2	2.08	0.53
1:C:18:HIS:HB2	2:D:20:GLY:O	2.08	0.53
1:A:310:LYS:HE3	2:B:89:LEU:HD21	1.90	0.53
1:C:301:THR:H	2:D:66:VAL:HG11	1.74	0.52
2:L:1:GLY:HA3	7:L:280:HOH:O	2.09	0.52
1:E:283:THR:HG22	1:E:285:LYS:N	2.16	0.52
1:C:13:LEU:HD22	2:D:152:VAL:HG21	1.91	0.52
2:B:74:GLU:HB3	2:B:77:ILE:HD11	1.91	0.52
2:B:161:LYS:HE3	2:B:162:TYR:CE1	2.43	0.52
1:E:116(A):SER:O	1:E:260:MET:HA	2.09	0.52
1:E:90(A):PRO:HD2	1:E:271:ASP:OD1	2.09	0.52
1:A:152:ILE:HG13	1:A:255:ARG:HB2	1.90	0.52
1:G:283:THR:CG2	1:G:285:LYS:HG2	2.39	0.52
2:D:131:LYS:HE3	2:D:141:TYR:OH	2.10	0.52
1:G:47:HIS:HB3	1:G:297:ILE:HD13	1.92	0.51
1:E:72:GLY:CA	1:E:149:LYS:H	2.21	0.51
1:E:303:GLY:HA2	2:F:63:PHE:CE1	2.45	0.51
1:E:103:ILE:HD12	1:E:103:ILE:N	2.25	0.51
1:I:116(A):SER:HB3	1:I:261:GLU:HG2	1.92	0.51
2:H:123:ARG:HH22	2:J:123:ARG:HH22	1.58	0.51
1:A:155:VAL:HG12	1:A:156:LYS:N	2.24	0.51
2:L:131:LYS:HZ2	2:L:133:ILE:HG22	1.74	0.51
2:B:88:PHE:CZ	2:D:87:GLY:HA3	2.46	0.51
1:C:52:CYS:HB3	1:C:277:CYS:O	2.10	0.51
2:J:47:GLU:HB3	1:K:30:LEU:HG	1.93	0.51
1:E:195:TYR:O	1:E:196:GLN:HB3	2.11	0.51
1:A:116(A):SER:O	1:A:260:MET:HA	2.11	0.51
2:L:127:LYS:HG3	2:L:128:ASN:H	1.75	0.51
1:E:170:ASN:HB3	1:E:239:PRO:O	2.11	0.51
2:D:119:TYR:CE1	2:D:136:GLY:HA2	2.46	0.51
2:L:44:ALA:HA	2:L:110:TYR:OH	2.11	0.51
2:H:164:GLU:H	2:H:164:GLU:CD	2.14	0.51
2:J:58:LYS:O	2:L:94:TYR:HD1	1.94	0.51
1:E:308:TYR:CD2	2:F:89:LEU:HD13	2.45	0.50
1:A:307:LYS:HE2	2:B:61:THR:HG22	1.93	0.50
2:D:59:MET:HG3	2:D:61:THR:HG23	1.93	0.50
1:A:58:PRO:HB3	1:A:86:TYR:CZ	2.46	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:159:TYR:HB3	2:B:160:PRO:HD3	1.92	0.50
1:A:50:LYS:HG2	1:A:275:HIS:ND1	2.27	0.50
1:C:26:VAL:HG21	1:C:317:ALA:HB2	1.94	0.50
1:E:295:GLN:O	1:E:308:TYR:HA	2.12	0.50
1:K:116(A):SER:O	1:K:260:MET:HA	2.12	0.50
2:D:132:GLU:HG2	2:D:138:PHE:CE2	2.46	0.50
1:C:28:THR:HG22	2:D:104:ASN:HB3	1.94	0.49
1:C:89:GLU:O	1:C:269:ILE:HA	2.12	0.49
1:E:48:ASN:HD21	1:E:287:ALA:HB3	1.76	0.49
1:G:89:GLU:O	1:G:269:ILE:HA	2.12	0.49
1:E:117:ARG:HD3	1:E:258:PHE:CE1	2.47	0.49
1:I:114:SER:HB2	1:I:266:SER:HB2	1.94	0.49
2:D:158:ASP:OD2	2:D:160:PRO:HD2	2.13	0.49
1:C:42:LEU:HD11	1:C:316:LEU:HG	1.93	0.49
1:E:131:ASP:HB3	1:E:155:VAL:HG23	1.95	0.49
1:E:82:ALA:HB1	1:E:83:SER:HA	1.94	0.49
1:C:304:LYS:HE2	2:D:61:THR:O	2.12	0.49
1:K:119:GLU:CD	1:K:122:PRO:HA	2.33	0.49
1:A:310:LYS:HG3	2:B:89:LEU:HD11	1.94	0.49
1:K:47:HIS:HB3	1:K:297:ILE:HD13	1.94	0.49
1:K:86:TYR:HA	1:K:113:SER:O	2.12	0.49
2:D:23:GLY:HA3	2:D:36:ALA:HA	1.95	0.49
1:E:320:LEU:HD23	1:E:320:LEU:N	2.27	0.49
1:C:283:THR:HG23	1:C:284:PRO:HD2	1.93	0.49
1:I:42:LEU:HD11	1:I:316:LEU:HG	1.95	0.49
1:K:66:ILE:HD12	1:K:109:ARG:HG2	1.95	0.49
2:H:87:GLY:HA3	2:L:88:PHE:CZ	2.48	0.48
1:K:161:TYR:CZ	1:K:249:GLY:HA2	2.48	0.48
1:E:152:ILE:HG13	1:E:255:ARG:HB2	1.96	0.48
1:A:265:GLY:O	1:A:266:SER:HB3	2.12	0.48
1:C:103:ILE:N	1:C:103:ILE:HD12	2.28	0.48
2:F:17:MET:SD	2:F:23:GLY:HA3	2.53	0.48
1:E:152:ILE:HD11	1:E:255:ARG:HD2	1.94	0.48
1:K:28:THR:HG22	2:L:104:ASN:HB3	1.96	0.48
2:D:94:TYR:CZ	2:D:98:LEU:HD11	2.49	0.48
2:F:169:ASN:OD1	2:F:169:ASN:N	2.43	0.48
2:F:125:GLN:NE2	2:F:155:GLY:HA2	2.28	0.48
1:E:82:ALA:CB	1:E:83:SER:CA	2.91	0.48
1:I:307:LYS:HE2	2:J:61:THR:HG22	1.96	0.48
1:E:103:ILE:H	1:E:103:ILE:HD12	1.77	0.48
1:K:156:LYS:HD2	1:K:196:GLN:HE21	1.79	0.48
6:G:431:NAG:H62	6:G:432:NAG:H82	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:130:HIS:CE1	1:I:164:LEU:HB3	2.49	0.48
2:F:6:ILE:HG13	2:F:112:ASP:HA	1.95	0.48
1:E:137:ALA:O	1:E:140:PRO:HD3	2.14	0.48
2:B:17:MET:SD	2:B:23:GLY:HA3	2.54	0.48
2:D:17:MET:C	2:D:19:ASP:H	2.16	0.48
1:C:45:ASP:O	1:C:46:LYS:HD2	2.14	0.48
1:E:283:THR:CG2	1:E:285:LYS:H	2.19	0.48
2:H:62:GLN:NE2	1:I:310:LYS:HZ3	2.10	0.48
1:I:68:GLY:HA3	1:I:95:GLY:HA2	1.95	0.47
1:G:105:TYR:CZ	1:G:109:ARG:HD2	2.49	0.47
2:H:75:LYS:HE3	2:H:79:ASN:HD21	1.79	0.47
1:K:48:ASN:O	1:K:50:LYS:HG3	2.14	0.47
1:I:71:LEU:HD22	1:I:151:LEU:HD11	1.96	0.47
1:I:18:HIS:HB2	2:J:20:GLY:O	2.14	0.47
2:H:45:ILE:O	2:H:49:THR:HG23	2.14	0.47
1:G:103:ILE:HD12	1:G:103:ILE:N	2.28	0.47
2:F:159:TYR:N	2:F:160:PRO:HD2	2.29	0.47
1:I:100:GLY:HA3	1:I:230:MET:O	2.14	0.47
1:E:58:PRO:HB3	1:E:86:TYR:CZ	2.48	0.47
1:G:293:PRO:HG2	1:G:294:PHE:CD2	2.49	0.47
1:A:105:TYR:CE2	1:A:109:ARG:HD2	2.50	0.47
1:I:130:HIS:CE1	1:I:162:PRO:HG2	2.49	0.47
1:G:18:HIS:HB2	2:H:20:GLY:O	2.14	0.47
1:G:202:VAL:HB	1:G:213:PHE:HB2	1.96	0.47
1:A:73:ASN:HB3	1:A:76:CYS:SG	2.55	0.47
1:E:82:ALA:HB1	1:E:83:SER:CB	2.44	0.47
1:G:116(B):PHE:CE1	1:G:260:MET:HE2	2.48	0.47
1:E:48:ASN:ND2	1:E:287:ALA:HB3	2.29	0.47
1:G:78:SER:HB2	1:G:149:LYS:NZ	2.29	0.47
1:I:68:GLY:CA	1:I:95:GLY:HA2	2.44	0.47
1:A:185:PRO:HG2	1:A:191:GLN:OE1	2.14	0.47
1:G:185:PRO:HG2	1:G:191:GLN:OE1	2.14	0.47
1:C:156:LYS:HE2	1:C:193:SER:O	2.15	0.47
1:C:195:TYR:O	1:C:196:GLN:HB3	2.14	0.47
2:J:94:TYR:O	2:J:98:LEU:HB2	2.15	0.47
2:H:133:ILE:HD13	2:H:139:GLU:HB2	1.97	0.47
1:C:316:LEU:HD22	7:C:335:HOH:O	2.14	0.47
1:I:129:ASN:HB3	1:I:162:PRO:HG3	1.97	0.47
1:I:76:CYS:O	1:I:77:GLU:C	2.54	0.47
1:I:66:ILE:HG13	1:I:89:GLU:OE2	2.14	0.47
1:K:66:ILE:HG13	1:K:89:GLU:OE2	2.15	0.47
1:C:100:GLY:HA3	1:C:230:MET:O	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:151:LEU:HB3	1:C:252:VAL:HG12	1.98	0.46
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.95	0.46
1:E:164:LEU:C	1:E:164:LEU:HD12	2.36	0.46
1:I:107:GLU:O	1:I:111:GLN:HG3	2.16	0.46
1:C:202:VAL:HB	1:C:213:PHE:HB2	1.95	0.46
1:A:307:LYS:HG3	2:B:92:TRP:CE2	2.50	0.46
1:K:54:LEU:HB3	1:K:85:SER:HB2	1.95	0.46
1:A:54:LEU:O	1:A:55:ARG:HB2	2.14	0.46
2:B:161:LYS:HE3	2:B:162:TYR:CZ	2.50	0.46
1:G:164:LEU:O	1:G:246:GLU:HA	2.15	0.46
2:F:106:ARG:HD3	7:F:427:HOH:O	2.15	0.46
1:K:164:LEU:HD12	1:K:164:LEU:C	2.36	0.46
1:I:288:ILE:HG21	1:I:297:ILE:HD12	1.97	0.46
2:J:5:ALA:HB3	2:J:112:ASP:OD2	2.16	0.46
2:D:19:ASP:HB3	2:D:36:ALA:HB2	1.97	0.46
1:G:216:GLU:HB3	1:K:203:PHE:HE2	1.79	0.46
1:E:89:GLU:O	1:E:269:ILE:HA	2.15	0.46
1:G:308:TYR:CD2	2:H:89:LEU:HD13	2.51	0.46
1:E:116(B):PHE:CE1	1:E:260:MET:HE2	2.50	0.46
1:I:164:LEU:C	1:I:164:LEU:HD12	2.36	0.46
2:D:88:PHE:CZ	2:F:87:GLY:HA3	2.51	0.46
2:D:145:ASP:OD2	2:D:147:THR:HG22	2.16	0.46
2:H:125:GLN:OE1	2:H:155:GLY:HA2	2.16	0.46
1:G:175:GLU:OE1	1:G:236:LEU:HD13	2.16	0.46
1:C:45:ASP:C	1:C:297:ILE:HD11	2.36	0.46
1:A:17:TYR:CZ	2:B:6:ILE:HG23	2.51	0.46
2:F:4:GLY:O	2:F:8:GLY:HA3	2.16	0.46
2:F:9:PHE:O	2:F:135:ASN:HA	2.16	0.46
1:A:320:LEU:H	1:A:320:LEU:HD23	1.81	0.46
1:C:298:HIS:CE1	1:C:300:ILE:HB	2.51	0.45
1:K:185:PRO:HG2	1:K:191:GLN:OE1	2.16	0.45
1:I:47:HIS:HB3	1:I:288:ILE:HG22	1.98	0.45
1:C:12:THR:OG1	2:D:27:GLN:HG2	2.16	0.45
1:A:123:LYS:HE2	1:A:132:SER:O	2.16	0.45
1:G:73:ASN:HB3	1:G:76:CYS:SG	2.56	0.45
2:B:97:GLU:HG2	2:F:58:LYS:CD	2.42	0.45
1:E:317:ALA:O	2:F:107:THR:HG21	2.15	0.45
2:H:168:LEU:HD23	2:H:168:LEU:O	2.16	0.45
2:F:30:GLN:NE2	2:F:145:ASP:HB2	2.30	0.45
1:E:197:ASN:O	1:E:198:ALA:HB3	2.17	0.45
1:E:46:LYS:N	1:E:297:ILE:HD11	2.31	0.45
2:L:148:CYS:O	2:L:152:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:164:LEU:O	1:E:164:LEU:HD12	2.17	0.45
1:C:71:LEU:O	1:C:148:TYR:HB3	2.16	0.45
1:G:134:GLY:HA3	1:G:153:TRP:HB3	1.97	0.45
1:G:320:LEU:HB3	2:H:111:HIS:CG	2.52	0.45
2:L:159:TYR:N	2:L:160:PRO:HD2	2.30	0.45
1:A:238:GLU:HG2	1:A:238:GLU:H	1.54	0.45
2:J:159:TYR:N	2:J:160:PRO:HD2	2.32	0.45
1:A:18:HIS:HB2	2:B:20:GLY:O	2.16	0.45
1:C:164:LEU:HD12	1:C:164:LEU:C	2.37	0.45
1:I:86:TYR:HA	1:I:113:SER:O	2.17	0.45
1:K:51:LEU:HB2	1:K:274:VAL:HA	1.99	0.45
1:A:15:ILE:HD11	2:B:122:VAL:HG21	1.98	0.45
1:C:177:LEU:HB3	1:C:258:PHE:HB2	1.99	0.45
2:J:127:LYS:HG2	2:J:128:ASN:N	2.32	0.45
1:C:53:LYS:HG2	1:C:57:ALA:HA	1.98	0.45
1:A:180:TRP:CE2	1:A:233:TYR:HB2	2.51	0.45
2:D:125:GLN:NE2	2:D:155:GLY:HA2	2.32	0.45
2:L:51:LYS:HE3	2:L:103:GLU:OE2	2.17	0.45
1:G:116:SER:HB3	1:G:263:ASN:OD1	2.16	0.45
2:J:158:ASP:CG	2:J:161:LYS:HB2	2.38	0.44
2:F:119:TYR:CE1	2:F:136:GLY:HA2	2.51	0.44
1:K:149:LYS:HE2	1:K:256:TYR:HE1	1.82	0.44
1:G:66:ILE:HG13	1:G:89:GLU:OE2	2.17	0.44
1:A:238:GLU:HG2	7:A:352:HOH:O	2.17	0.44
1:K:151:LEU:HB3	1:K:252:VAL:HG12	1.99	0.44
1:I:195:TYR:O	1:I:196:GLN:HB3	2.18	0.44
1:G:97:CYS:HB2	1:G:138:ALA:O	2.16	0.44
1:E:320:LEU:HD23	1:E:320:LEU:H	1.82	0.44
2:L:127:LYS:HG3	2:L:128:ASN:N	2.33	0.44
1:I:114:SER:HB2	1:I:266:SER:CB	2.47	0.44
1:K:103:ILE:HG12	1:K:233:TYR:CE2	2.52	0.44
1:K:308:TYR:CD2	2:L:89:LEU:HD13	2.53	0.44
2:L:67:GLY:O	2:L:68:LYS:HE3	2.18	0.44
1:C:43:LEU:HB2	1:C:314:LEU:HB2	2.00	0.44
1:G:169:ILE:HD12	1:G:169:ILE:N	2.33	0.44
1:G:161:TYR:CZ	1:G:249:GLY:HA2	2.53	0.44
1:A:156:LYS:HE2	1:A:193:SER:O	2.17	0.44
1:E:288:ILE:CD1	1:E:295:GLN:HG3	2.47	0.44
2:H:123:ARG:HH22	2:J:123:ARG:NH2	2.15	0.44
1:I:316:LEU:HD22	7:J:189:HOH:O	2.17	0.44
1:A:114:SER:HB2	1:A:266:SER:CB	2.48	0.44
1:A:51:LEU:HA	1:A:282:GLN:NE2	2.32	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:3:PHE:CZ	2:J:2:LEU:HG	2.53	0.44
2:L:133:ILE:HD13	2:L:139:GLU:HB2	2.00	0.44
1:E:288:ILE:HD11	1:E:306:PRO:HD2	1.99	0.44
1:I:116(A):SER:HB3	1:I:261:GLU:CG	2.48	0.44
2:D:18:VAL:O	2:D:18:VAL:HG22	2.18	0.43
1:K:54:LEU:O	1:K:55:ARG:HG3	2.18	0.43
1:K:97:CYS:O	1:K:224:ARG:HD3	2.19	0.43
2:B:2:LEU:HG	2:F:3:PHE:CZ	2.54	0.43
1:A:114:SER:OG	1:A:263:ASN:HB2	2.19	0.43
1:I:305:CYS:O	2:J:61:THR:HG21	2.18	0.43
1:E:145:LYS:NZ	3:E:330:SIA:H31	2.32	0.43
1:I:185:PRO:HG2	1:I:191:GLN:OE1	2.19	0.43
1:K:175:GLU:OE1	1:K:262:ARG:NH1	2.48	0.43
1:E:67:ALA:HB2	1:E:105:TYR:CE1	2.53	0.43
1:G:54:LEU:O	1:G:55:ARG:HB2	2.17	0.43
1:E:15:ILE:HD12	1:E:15:ILE:N	2.32	0.43
2:H:68:LYS:HB3	2:H:70:PHE:CE2	2.54	0.43
2:D:121:LYS:O	2:D:125:GLN:HG3	2.18	0.43
1:E:102:PHE:O	1:E:105:TYR:HB2	2.18	0.43
2:D:125:GLN:CD	2:D:155:GLY:HA2	2.39	0.43
1:A:308:TYR:CD2	2:B:89:LEU:HD13	2.54	0.43
1:E:133(A):LYS:O	3:E:330:SIA:H113	2.19	0.43
2:D:81:ASN:OD1	2:F:80:LEU:HD13	2.19	0.43
2:J:51:LYS:HE3	2:J:103:GLU:OE2	2.19	0.43
1:K:283:THR:OG1	1:K:298:HIS:HB3	2.18	0.43
2:B:127:LYS:HB2	2:B:159:TYR:CE1	2.53	0.43
2:F:3:PHE:CE1	2:F:113:SER:HB2	2.53	0.43
1:A:26:VAL:HB	2:B:104:ASN:ND2	2.34	0.43
1:K:179:LEU:HD23	1:K:234:TRP:HB3	2.01	0.43
2:D:4:GLY:O	2:D:8:GLY:HA3	2.19	0.43
1:K:283:THR:HG22	1:K:286:GLY:O	2.19	0.43
1:K:89:GLU:O	1:K:269:ILE:HA	2.18	0.43
1:G:120:ILE:HG13	1:G:168:TYR:CD1	2.53	0.43
1:G:206:SER:HA	1:I:221:PRO:HG2	2.01	0.43
2:H:93:THR:O	2:H:97:GLU:HB2	2.19	0.43
1:K:54:LEU:HD21	1:K:302:ILE:HG22	2.01	0.43
2:J:3:PHE:CE2	2:J:113:SER:HB2	2.53	0.43
1:I:241:ASP:OD1	1:I:242:LYS:N	2.50	0.42
2:D:131:LYS:HB3	2:D:141:TYR:CZ	2.54	0.42
2:F:75:LYS:HD3	2:F:75:LYS:HA	1.79	0.42
1:K:288:ILE:O	1:K:288:ILE:HG13	2.18	0.42
1:I:308:TYR:CD2	2:J:89:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:16:GLY:O	2:H:18:VAL:HG23	2.20	0.42
1:A:52:CYS:HB3	1:A:277:CYS:O	2.18	0.42
1:C:197:ASN:O	1:C:198:ALA:HB3	2.18	0.42
1:G:155:VAL:HG12	1:G:156:LYS:N	2.34	0.42
1:G:253:VAL:HA	1:G:254:PRO:HD3	1.93	0.42
1:I:116(A):SER:O	1:I:260:MET:HA	2.20	0.42
1:C:307:LYS:HE2	2:D:61:THR:HG22	2.00	0.42
1:K:288:ILE:HG21	1:K:297:ILE:HD12	2.00	0.42
1:A:127:TRP:CZ2	1:A:253:VAL:HG11	2.54	0.42
2:F:41:THR:O	2:F:45:ILE:HG13	2.19	0.42
1:I:72:GLY:HA3	1:I:149:LYS:H	1.85	0.42
1:C:14:CYS:O	2:D:24:TYR:HA	2.19	0.42
1:K:100:GLY:HA3	1:K:230:MET:O	2.19	0.42
1:I:14:CYS:O	2:J:24:TYR:HA	2.19	0.42
1:G:262:ARG:HG2	1:G:262:ARG:NH1	2.32	0.42
1:K:149:LYS:HE2	1:K:256:TYR:CE1	2.55	0.42
1:K:194:LEU:HD11	3:K:601:SIA:H91	2.00	0.42
1:G:86:TYR:HA	1:G:113:SER:O	2.18	0.42
2:B:18:VAL:O	2:B:18:VAL:HG22	2.19	0.42
2:H:158:ASP:OD1	2:H:160:PRO:HD2	2.19	0.42
1:C:321:ARG:HD2	1:C:323:ILE:HD11	2.01	0.42
1:K:188:SER:O	1:K:192:GLN:HG2	2.20	0.42
2:L:132:GLU:HG2	2:L:138:PHE:CE2	2.55	0.42
1:G:170:ASN:HD21	1:G:176:VAL:HG23	1.85	0.42
1:E:17:TYR:HB2	1:E:320:LEU:HD11	2.02	0.42
1:A:260:MET:HE2	1:A:262:ARG:HG2	2.02	0.42
1:I:46:LYS:N	1:I:297:ILE:HD11	2.35	0.42
2:L:17:MET:SD	2:L:23:GLY:HA3	2.60	0.42
2:B:48:ILE:O	2:B:52:VAL:HG23	2.20	0.42
1:I:155:VAL:HG13	1:I:194:LEU:O	2.20	0.42
1:G:242:LYS:HG2	1:G:243:ILE:N	2.35	0.42
1:G:164:LEU:HD23	1:G:164:LEU:C	2.39	0.41
2:D:27:GLN:O	2:D:27:GLN:HG3	2.20	0.41
1:K:42:LEU:O	1:K:292:LEU:HB3	2.20	0.41
1:A:42:LEU:HD11	1:A:316:LEU:HD22	2.01	0.41
2:L:131:LYS:HZ1	2:L:133:ILE:HG22	1.86	0.41
1:K:195:TYR:O	1:K:196:GLN:HB3	2.20	0.41
1:K:103:ILE:HD12	1:K:103:ILE:N	2.35	0.41
2:F:51:LYS:HE3	2:F:103:GLU:OE2	2.20	0.41
1:I:152:ILE:HG13	1:I:255:ARG:HB2	2.02	0.41
1:K:283:THR:CG2	1:K:285:LYS:H	2.31	0.41
1:I:43:LEU:HB2	1:I:314:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:29:VAL:CG2	2:L:51:LYS:HG3	2.51	0.41
2:D:111:HIS:O	2:D:115:VAL:HG23	2.20	0.41
1:E:83(A):SER:CB	1:E:116:SER:HA	2.50	0.41
1:E:310:LYS:HD3	2:F:89:LEU:HD21	2.03	0.41
1:G:140:PRO:HD2	6:G:431:NAG:H83	2.02	0.41
2:F:5:ALA:HB3	2:F:112:ASP:OD2	2.20	0.41
1:A:222:LYS:HE2	1:A:227:GLU:HG3	2.03	0.41
1:E:116(B):PHE:HE1	1:E:260:MET:HE2	1.86	0.41
1:C:164:LEU:O	1:C:164:LEU:HD12	2.20	0.41
1:G:155:VAL:CG1	1:G:156:LYS:N	2.83	0.41
1:I:215:PRO:HB3	1:I:250:ASN:ND2	2.35	0.41
1:G:17:TYR:HB3	2:H:115:VAL:HG21	2.02	0.41
1:C:211:LYS:HD3	1:C:213:PHE:CZ	2.55	0.41
2:F:142:HIS:HD2	2:F:166:ALA:HB2	1.85	0.41
2:F:167:LYS:HG3	2:F:168:LEU:HD12	2.02	0.41
1:K:47:HIS:HB3	1:K:288:ILE:HG22	2.03	0.41
1:C:202:VAL:HG11	1:C:251:LEU:HD13	2.03	0.41
1:G:58:PRO:HB3	1:G:86:TYR:CZ	2.56	0.41
1:C:222:LYS:NZ	1:C:227:GLU:HG3	2.36	0.41
1:E:97:CYS:HB2	1:E:138:ALA:O	2.21	0.41
2:D:164:GLU:CD	2:D:164:GLU:H	2.24	0.41
1:A:265:GLY:O	1:A:266:SER:CB	2.69	0.41
1:C:48:ASN:ND2	1:C:287:ALA:HB3	2.36	0.41
1:G:26:VAL:O	1:G:32:LYS:O	2.38	0.41
2:J:21:TRP:CE3	2:J:111:HIS:HE1	2.39	0.41
2:D:72:HIS:CD2	2:D:72:HIS:H	2.39	0.41
1:K:310:LYS:O	1:K:310:LYS:HG2	2.21	0.41
2:H:62:GLN:HE21	1:I:310:LYS:NZ	2.14	0.41
1:C:97:CYS:HB2	1:C:138:ALA:O	2.22	0.41
1:I:295:GLN:HE21	1:I:295:GLN:HB3	1.73	0.41
1:A:284:PRO:HG2	1:A:298:HIS:CE1	2.56	0.40
2:D:125:GLN:O	2:D:127:LYS:HD2	2.21	0.40
1:C:316:LEU:HD23	1:C:316:LEU:HA	1.84	0.40
1:G:123:LYS:HB2	1:G:152:ILE:HD11	2.03	0.40
2:L:80:LEU:O	2:L:84:VAL:HG23	2.20	0.40
1:K:134:GLY:HA3	1:K:153:TRP:HB3	2.04	0.40
2:H:3:PHE:CE1	2:H:113:SER:HB2	2.57	0.40
2:L:123:ARG:HB2	2:L:138:PHE:HZ	1.86	0.40
1:A:29:VAL:CG2	2:F:51:LYS:HG3	2.52	0.40
1:C:310:LYS:HB3	1:C:310:LYS:HE2	1.74	0.40
1:A:100:GLY:HA3	1:A:230:MET:O	2.20	0.40
2:L:149:MET:HA	2:L:149:MET:CE	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:90(A):PRO:HD2	1:K:271:ASP:OD1	2.21	0.40
1:K:90:THR:HA	1:K:90(A):PRO:HD3	1.97	0.40
1:I:103:ILE:HD12	1:I:103:ILE:N	2.37	0.40
1:E:298:HIS:CG	1:E:299:PRO:HD2	2.57	0.40
1:A:26:VAL:HG21	1:A:317:ALA:HB2	2.03	0.40
1:C:133(A):LYS:O	3:C:330:SIA:H113	2.21	0.40
1:C:260:MET:CE	1:C:262:ARG:HG2	2.52	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	321/329 (98%)	300 (94%)	18 (6%)	3 (1%)	25	42
1	C	315/329 (96%)	300 (95%)	13 (4%)	2 (1%)	33	55
1	E	321/329 (98%)	294 (92%)	22 (7%)	5 (2%)	14	23
1	G	317/329 (96%)	301 (95%)	16 (5%)	0	100	100
1	I	315/329 (96%)	291 (92%)	21 (7%)	3 (1%)	22	38
1	K	315/329 (96%)	297 (94%)	16 (5%)	2 (1%)	33	55
2	B	172/177 (97%)	167 (97%)	5 (3%)	0	100	100
2	D	169/177 (96%)	156 (92%)	13 (8%)	0	100	100
2	F	168/177 (95%)	157 (94%)	10 (6%)	1 (1%)	33	55
2	H	168/177 (95%)	159 (95%)	9 (5%)	0	100	100
2	J	168/177 (95%)	158 (94%)	8 (5%)	2 (1%)	19	32
2	L	168/177 (95%)	161 (96%)	5 (3%)	2 (1%)	19	32
All	All	2917/3036 (96%)	2741 (94%)	156 (5%)	20 (1%)	30	50

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	60	ASN
1	C	264	ALA
1	E	80	SER
1	I	93	ASP
1	K	265	GLY
1	A	266	SER
1	C	94	ASN
1	E	78	SER
1	E	83	SER
1	E	116(A)	SER
1	I	198	ALA
2	J	5	ALA
1	A	92	SER
1	A	264	ALA
2	F	169	ASN
1	I	324	PRO
1	K	239	PRO
2	L	60	ASN
1	E	81	THR
2	L	59	MET

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	285/290 (98%)	280 (98%)	5 (2%)	71	91
1	C	281/290 (97%)	276 (98%)	5 (2%)	71	91
1	E	285/290 (98%)	279 (98%)	6 (2%)	66	88
1	G	283/290 (98%)	277 (98%)	6 (2%)	66	88
1	I	281/290 (97%)	274 (98%)	7 (2%)	60	85
1	K	281/290 (97%)	275 (98%)	6 (2%)	66	88
2	B	150/152 (99%)	143 (95%)	7 (5%)	36	61
2	D	147/152 (97%)	141 (96%)	6 (4%)	41	67
2	F	146/152 (96%)	142 (97%)	4 (3%)	57	83
2	H	146/152 (96%)	143 (98%)	3 (2%)	66	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	146/152 (96%)	142 (97%)	4 (3%)	57	83
2	L	146/152 (96%)	143 (98%)	3 (2%)	66	88
All	All	2577/2652 (97%)	2515 (98%)	62 (2%)	61	86

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	PHE
1	A	238	GLU
1	A	253	VAL
1	A	315	ARG
1	A	320	LEU
2	B	22	TYR
2	B	26	HIS
2	B	29	GLU
2	B	97	GLU
2	B	161	LYS
2	B	164	GLU
2	B	174	ASP
1	C	77	GLU
1	C	192	GLN
1	C	295	GLN
1	C	316	LEU
1	C	320	LEU
2	D	29	GLU
2	D	66	VAL
2	D	68	LYS
2	D	72	HIS
2	D	102	LEU
2	D	164	GLU
1	E	54	LEU
1	E	79	LEU
1	E	81	THR
1	E	102	PHE
1	E	295	GLN
1	E	320	LEU
2	F	22	TYR
2	F	102	LEU
2	F	150	GLU
2	F	169	ASN
1	G	136	THR

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Mol	Chain	Res	Type
1	G	174	LYS
1	G	203	PHE
1	G	225	ASP
1	G	253	VAL
1	G	261	GLU
2	H	60	ASN
2	H	68	LYS
2	H	164	GLU
1	I	55	ARG
1	I	77	GLU
1	I	102	PHE
1	I	125	SER
1	I	295	GLN
1	I	316	LEU
1	I	320	LEU
2	J	22	TYR
2	J	98	LEU
2	J	102	LEU
2	J	123	ARG
1	K	55	ARG
1	K	97	CYS
1	K	102	PHE
1	K	274	VAL
1	K	283	THR
1	K	295	GLN
2	L	30	GLN
2	L	102	LEU
2	L	149	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
2	B	26	HIS
2	B	43	ASN
2	B	79	ASN
2	B	95	ASN
2	D	72	HIS
2	D	95	ASN
1	E	298	HIS
2	F	30	GLN
2	F	50	ASN

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Mol	Chain	Res	Type
2	H	60	ASN
2	H	62	GLN
1	I	21	ASN
1	I	289	ASN
2	J	30	GLN
2	J	95	ASN
2	J	117	ASN
1	K	196	GLN
2	L	62	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

19 carbohydrates 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$
3	SIA	A	330	3	20,20,21	3.81	1 (5%)	23,28,31	2.23	4 (17%)
3	GAL	A	331	3	10,11,12	0.87	1 (10%)	11,15,17	0.91	1 (9%)
3	NAG	A	332	3	15,15,15	0.45	0	21,21,21	0.55	0
3	SIA	C	330	3	20,20,21	3.85	1 (5%)	23,28,31	2.10	3 (13%)
3	GAL	C	331	3	10,11,12	0.86	1 (10%)	11,15,17	1.17	2 (18%)
3	NAG	C	332	3	15,15,15	0.50	0	21,21,21	0.60	0
3	SIA	E	330	3	20,20,21	3.86	1 (5%)	23,28,31	2.21	4 (17%)
3	GAL	E	331	3	10,11,12	0.82	1 (10%)	11,15,17	1.08	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	332	3	15,15,15	0.47	0	21,21,21	0.72	0
5	SIA	G	401	5	20,20,21	3.85	1 (5%)	23,28,31	2.11	3 (13%)
5	GAL	G	402	5	10,11,12	0.81	1 (10%)	11,15,17	0.79	1 (9%)
6	NAG	G	431	1,6	12,14,15	0.72	1 (8%)	15,19,21	0.96	2 (13%)
6	NAG	G	432	6	12,14,15	0.69	1 (8%)	15,19,21	0.96	1 (6%)
3	SIA	I	501	3	20,20,21	3.91	1 (5%)	23,28,31	2.11	4 (17%)
3	GAL	I	502	3	10,11,12	0.83	1 (10%)	11,15,17	1.01	1 (9%)
3	NAG	I	503	3	15,15,15	0.52	0	21,21,21	0.67	0
3	SIA	K	601	3	20,20,21	3.78	1 (5%)	23,28,31	2.17	4 (17%)
3	GAL	K	602	3	10,11,12	0.84	1 (10%)	11,15,17	1.02	1 (9%)
3	NAG	K	603	3	15,15,15	0.47	0	21,21,21	0.96	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SIA	A	330	3	-	0/15/34/38	0/1/1/1
3	GAL	A	331	3	-	0/2/19/22	0/1/1/1
3	NAG	A	332	3	-	0/6/26/26	0/1/1/1
3	SIA	C	330	3	-	0/15/34/38	0/1/1/1
3	GAL	C	331	3	-	0/2/19/22	0/1/1/1
3	NAG	C	332	3	-	0/6/26/26	0/1/1/1
3	SIA	E	330	3	-	0/15/34/38	0/1/1/1
3	GAL	E	331	3	-	0/2/19/22	0/1/1/1
3	NAG	E	332	3	-	0/6/26/26	0/1/1/1
5	SIA	G	401	5	-	0/15/34/38	0/1/1/1
5	GAL	G	402	5	-	0/2/19/22	0/1/1/1
6	NAG	G	431	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	432	6	-	0/6/23/26	0/1/1/1
3	SIA	I	501	3	-	0/15/34/38	0/1/1/1
3	GAL	I	502	3	-	0/2/19/22	0/1/1/1
3	NAG	I	503	3	-	0/6/26/26	0/1/1/1
3	SIA	K	601	3	-	0/15/34/38	0/1/1/1
3	GAL	K	602	3	-	0/2/19/22	0/1/1/1
3	NAG	K	603	3	-	0/6/26/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	501	SIA	O6-C2	17.22	1.44	1.28
3	E	330	SIA	O6-C2	17.00	1.43	1.28
5	G	401	SIA	O6-C2	16.97	1.43	1.28
3	C	330	SIA	O6-C2	16.95	1.43	1.28
3	A	330	SIA	O6-C2	16.73	1.43	1.28
3	K	601	SIA	O6-C2	16.62	1.43	1.28
3	A	331	GAL	O5-C5	-2.22	1.41	1.45
3	C	331	GAL	O5-C5	-2.18	1.41	1.45
3	K	602	GAL	O5-C5	-2.14	1.41	1.45
3	I	502	GAL	O5-C5	-2.10	1.41	1.45
6	G	432	NAG	O5-C5	-2.10	1.41	1.45
6	G	431	NAG	O5-C5	-2.07	1.41	1.45
3	E	331	GAL	O5-C5	-2.02	1.41	1.45
5	G	402	GAL	O5-C5	-2.00	1.41	1.45

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	330	SIA	O6-C2-C3	-9.21	112.88	124.91
3	K	601	SIA	O6-C2-C3	-8.90	113.28	124.91
5	G	401	SIA	O6-C2-C3	-8.81	113.40	124.91
3	E	330	SIA	O6-C2-C3	-8.81	113.40	124.91
3	C	330	SIA	O6-C2-C3	-8.77	113.45	124.91
3	I	501	SIA	O6-C2-C3	-8.22	114.17	124.91
3	I	501	SIA	C7-C6-C5	-3.34	109.31	114.24
3	E	330	SIA	O6-C6-C5	3.25	114.36	110.29
3	E	330	SIA	C7-C6-C5	-3.17	109.57	114.24
3	E	331	GAL	O5-C5-C6	3.01	110.14	106.98
5	G	401	SIA	O6-C6-C5	2.96	113.99	110.29
3	A	330	SIA	C7-C6-C5	-2.94	109.91	114.24
3	I	501	SIA	O6-C6-C5	2.91	113.93	110.29
3	C	331	GAL	O5-C5-C6	2.84	109.96	106.98
3	K	601	SIA	O6-C6-C5	2.83	113.84	110.29
3	K	602	GAL	O5-C5-C6	2.73	109.84	106.98
6	G	432	NAG	O5-C5-C6	2.67	109.78	106.98
3	K	603	NAG	O5-C1-C2	2.64	112.28	109.61
3	I	502	GAL	O5-C5-C6	2.61	109.72	106.98
3	A	330	SIA	O6-C6-C5	2.41	113.31	110.29
3	C	330	SIA	C7-C6-C5	-2.33	110.81	114.24
6	G	431	NAG	O5-C5-C6	2.30	109.39	106.98
3	K	601	SIA	C7-C6-C5	-2.27	110.89	114.24
5	G	402	GAL	O5-C5-C6	2.22	109.31	106.98
3	I	501	SIA	C3-C2-C1	-2.20	108.80	121.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	601	SIA	C3-C2-C1	-2.17	108.96	121.08
3	E	330	SIA	C3-C2-C1	-2.16	108.98	121.08
3	A	330	SIA	C3-C2-C1	-2.09	109.37	121.08
3	C	330	SIA	C3-C2-C1	-2.07	109.51	121.08
6	G	431	NAG	C3-C2-N2	-2.06	108.63	111.76
5	G	401	SIA	C3-C2-C1	-2.04	109.66	121.08
3	C	331	GAL	O5-C5-C4	-2.02	108.09	110.65
3	A	331	GAL	O5-C5-C6	2.01	109.09	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry

9 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
4	NAG	A	333	1	12,14,15	0.70	1 (8%)	15,19,21	1.31	2 (13%)
4	NAG	A	334	1	12,14,15	0.65	0	15,19,21	0.70	0
4	NAG	A	335	1	12,14,15	0.66	0	15,19,21	0.85	1 (6%)
4	NAG	A	336	1	12,14,15	0.66	0	15,19,21	1.07	1 (6%)
4	NAG	C	333	1	12,14,15	0.66	0	15,19,21	0.82	0
4	NAG	C	334	1	12,14,15	0.66	1 (8%)	15,19,21	0.96	1 (6%)
4	NAG	E	333	1	12,14,15	0.69	1 (8%)	15,19,21	0.79	0
4	NAG	J	561	2	12,14,15	0.67	1 (8%)	15,19,21	0.76	1 (6%)
4	NAG	K	641	1	12,14,15	0.66	0	15,19,21	0.95	1 (6%)

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
4	NAG	A	333	1	-	0/6/23/26	0/1/1/1
4	NAG	A	334	1	-	0/6/23/26	0/1/1/1
4	NAG	A	335	1	-	0/6/23/26	0/1/1/1
4	NAG	A	336	1	-	0/6/23/26	0/1/1/1
4	NAG	C	333	1	-	0/6/23/26	0/1/1/1
4	NAG	C	334	1	-	0/6/23/26	0/1/1/1
4	NAG	E	333	1	-	0/6/23/26	0/1/1/1
4	NAG	J	561	2	-	0/6/23/26	0/1/1/1
4	NAG	K	641	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	333	NAG	O5-C5	-2.13	1.41	1.45
4	A	333	NAG	O5-C5	-2.08	1.41	1.45
4	C	334	NAG	O5-C5	-2.05	1.41	1.45
4	J	561	NAG	O5-C5	-2.01	1.41	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	333	NAG	O5-C5-C6	4.03	111.20	106.98
4	C	334	NAG	O5-C5-C6	2.75	109.86	106.98
4	K	641	NAG	O5-C5-C6	2.28	109.37	106.98
4	A	336	NAG	O5-C5-C4	2.22	113.47	110.65
4	A	333	NAG	C3-C2-N2	-2.21	108.39	111.76
4	J	561	NAG	O5-C5-C6	2.20	109.29	106.98
4	A	335	NAG	O5-C5-C6	2.13	109.22	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	323/329 (98%)	0.03	2 (0%) 86 88	30, 44, 60, 79	0
1	C	319/329 (96%)	-0.19	4 (1%) 74 76	30, 41, 60, 85	0
1	E	323/329 (98%)	0.01	4 (1%) 75 77	35, 49, 67, 88	0
1	G	321/329 (97%)	-0.07	2 (0%) 86 88	28, 41, 61, 83	0
1	I	319/329 (96%)	-0.03	10 (3%) 47 48	32, 46, 62, 81	0
1	K	319/329 (96%)	-0.02	4 (1%) 74 76	28, 42, 60, 85	0
2	B	174/177 (98%)	0.28	10 (5%) 23 23	34, 58, 80, 95	0
2	D	171/177 (96%)	0.50	22 (12%) 4 4	30, 57, 90, 103	0
2	F	170/177 (96%)	0.42	13 (7%) 14 13	32, 55, 94, 105	0
2	H	170/177 (96%)	0.55	19 (11%) 6 5	31, 51, 88, 99	0
2	J	170/177 (96%)	0.09	2 (1%) 75 77	31, 49, 69, 81	0
2	L	170/177 (96%)	-0.01	0 100 100	30, 46, 62, 69	0
All	All	2949/3036 (97%)	0.08	92 (3%) 47 48	28, 46, 79, 105	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	168	LEU	5.5
1	K	94	ASN	4.4
2	H	144	CYS	4.4
2	D	16	GLY	4.3
2	D	147	THR	4.0
2	D	168	LEU	3.9
2	H	143	LYS	3.8
2	D	138	PHE	3.7
2	B	173	ILE	3.4
2	F	29	GLU	3.4
2	B	33	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
2	J	143	LYS	3.3
2	J	133	ILE	3.3
1	I	264	ALA	3.3
2	D	160	PRO	3.3
2	D	144	CYS	3.3
2	F	164	GLU	3.1
2	D	128	ASN	3.1
1	C	12	THR	3.1
2	D	157	TYR	3.1
2	D	162	TYR	3.1
2	H	29	GLU	3.1
1	G	13	LEU	3.0
2	D	19	ASP	3.0
2	D	27	GLN	2.9
2	H	164	GLU	2.9
2	B	138	PHE	2.9
2	F	161	LYS	2.9
1	K	93	ASP	2.9
2	D	141	TYR	2.8
2	B	140	PHE	2.8
2	H	140	PHE	2.8
2	D	129	ASN	2.8
2	F	160	PRO	2.7
1	I	54	LEU	2.7
1	E	198	ALA	2.7
1	C	264	ALA	2.7
2	B	168	LEU	2.7
2	F	158	ASP	2.7
2	F	140	PHE	2.6
2	H	18	VAL	2.6
1	G	12	THR	2.6
2	F	38	LEU	2.6
2	D	140	PHE	2.5
2	H	157	TYR	2.5
2	H	141	TYR	2.5
2	B	133	ILE	2.5
1	E	13	LEU	2.5
2	F	162	TYR	2.5
2	H	167	LYS	2.5
2	H	42	GLN	2.5
1	I	55	ARG	2.5
2	D	143	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	325	SER	2.5
2	D	156	THR	2.5
1	C	90(A)	PRO	2.4
2	F	166	ALA	2.4
2	B	174	ASP	2.4
2	H	23	GLY	2.4
1	A	290	THR	2.4
2	H	33	GLY	2.4
2	H	160	PRO	2.3
1	I	208	ARG	2.3
2	D	152	VAL	2.3
2	D	142	HIS	2.3
2	H	156	THR	2.3
2	D	133	ILE	2.3
2	D	18	VAL	2.3
1	I	288	ILE	2.3
1	I	290	THR	2.3
1	I	94	ASN	2.2
2	H	65	ALA	2.2
2	H	38	LEU	2.2
2	H	32	SER	2.2
1	E	161	TYR	2.2
2	D	159	TYR	2.2
2	H	27	GLN	2.2
2	B	171	GLU	2.2
1	C	78	SER	2.2
1	E	11	ASP	2.2
1	I	95	GLY	2.2
1	I	268	ILE	2.1
2	F	131	LYS	2.1
2	H	152	VAL	2.1
1	K	239	PRO	2.1
2	F	143	LYS	2.1
2	B	160	PRO	2.1
1	K	9	PRO	2.1
2	B	25	HIS	2.1
1	I	198	ALA	2.1
2	D	137	CYS	2.0
2	F	60	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

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
5	GAL	G	402	11/12	0.20	-	55,67,74,76	0
3	NAG	K	603	15/15	0.28	-	58,77,81,85	0
3	GAL	K	602	11/12	0.23	-	64,73,82,85	0
6	NAG	G	431	14/15	0.14	-	38,50,56,56	0
3	SIA	I	501	20/21	0.12	-	31,46,52,52	0
3	NAG	I	503	15/15	0.14	-	45,54,65,66	0
3	GAL	E	331	11/12	0.08	-	51,58,61,61	0
3	SIA	K	601	20/21	0.21	-	47,59,66,68	0
3	SIA	E	330	20/21	0.17	-	49,55,62,66	0
3	SIA	C	330	20/21	0.12	-	33,39,43,47	0
3	SIA	A	330	20/21	0.15	-	36,43,50,52	0
3	NAG	C	332	15/15	0.15	-	47,53,64,65	0
3	NAG	A	332	15/15	0.27	-	57,69,76,78	0
3	GAL	C	331	11/12	0.10	-	44,51,54,58	0
3	GAL	I	502	11/12	0.11	-	48,51,56,58	0
3	NAG	E	332	15/15	0.17	-	55,63,66,68	0
5	SIA	G	401	20/21	0.11	-	35,45,51,52	0
3	GAL	A	331	11/12	0.13	-	49,59,66,73	0
6	NAG	G	432	14/15	0.19	-	48,57,64,68	0

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
4	NAG	C	333	14/15	0.14	-	47,56,67,69	0
4	NAG	K	641	14/15	0.28	-	71,81,89,91	0
4	NAG	A	334	14/15	0.19	-	65,74,89,90	0
4	NAG	A	333	14/15	0.35	-	70,84,86,87	0
4	NAG	C	334	14/15	0.16	-	62,76,83,84	0
4	NAG	A	335	14/15	0.12	-	48,52,58,61	0
4	NAG	J	561	14/15	0.19	-	76,78,83,84	0
4	NAG	A	336	14/15	0.27	-	71,76,80,83	0
4	NAG	E	333	14/15	0.14	-	48,56,60,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.