Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 02:13 PM JST

PDB ID	:	8HRD
Title	:	Crystal structure of the receptor binding domain of SARS-CoV-2 Delta variant in complex with IMCAS74 Fab and W14 Fab
Authors	:	Zhao, R.C.; Wu, L.L.; Han, P.
Deposited on	:	2022-12-15
Resolution	:	2.86 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:

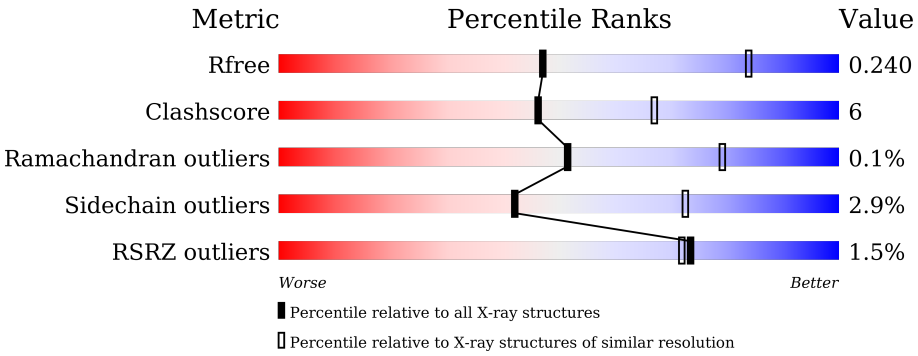
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 <=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	223	70% 17% 13%
1	B	223	76% 12% 13%
1	K	223	75% 13% 13%
1	T	223	3% 71% 16% · 13%
2	C	235	81% 16% ••
2	L	235	% 78% 17% 5%

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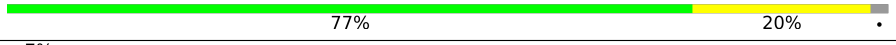
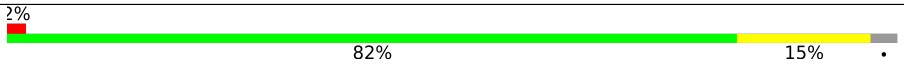
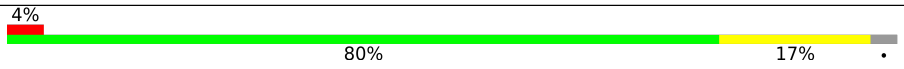
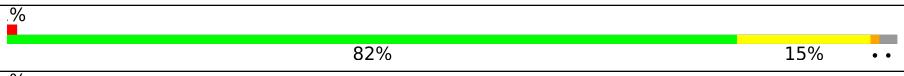
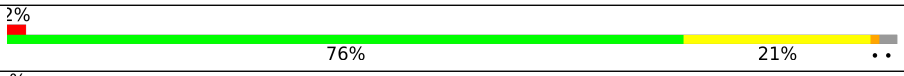
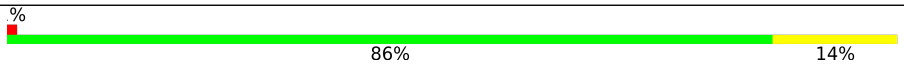
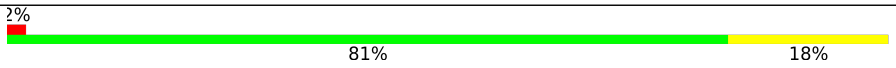
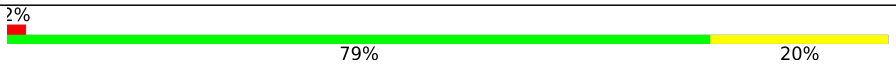
Mol	Chain	Length	Quality of chain
2	O	235	
2	W	235	
3	E	217	
3	M	217	
3	P	217	
3	X	217	
4	D	234	
4	G	234	
4	N	234	
4	Y	234	
5	F	215	
5	H	215	
5	Q	215	
5	Z	215	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 33039 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1548	991	261	288	8			
1	B	195	Total	C	N	O	S	0	0	0
			1548	991	261	288	8			
1	K	195	Total	C	N	O	S	0	0	0
			1548	991	261	288	8			
1	T	195	Total	C	N	O	S	0	0	0
			1548	991	261	288	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	452	ARG	LEU	variant	UNP P0DTC2
A	478	LYS	THR	engineered mutation	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	478	LYS	THR	engineered mutation	UNP P0DTC2
K	452	ARG	LEU	variant	UNP P0DTC2
K	478	LYS	THR	engineered mutation	UNP P0DTC2
T	452	ARG	LEU	variant	UNP P0DTC2
T	478	LYS	THR	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called IMCAS74 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	230	Total	C	N	O	S	0	0	0
			1744	1106	295	335	8			
2	C	230	Total	C	N	O	S	0	0	0
			1744	1106	295	335	8			
2	L	224	Total	C	N	O	S	0	0	0
			1703	1082	287	326	8			
2	W	230	Total	C	N	O	S	0	0	0
			1744	1106	295	335	8			

- Molecule 3 is a protein called IMCAS74 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	213	Total	C	N	O	S	0	0	0
			1566	977	266	319	4			
3	E	213	Total	C	N	O	S	0	0	0
			1566	977	266	319	4			
3	M	210	Total	C	N	O	S	0	0	0
			1547	965	263	315	4			
3	X	210	Total	C	N	O	S	0	0	0
			1547	965	263	315	4			

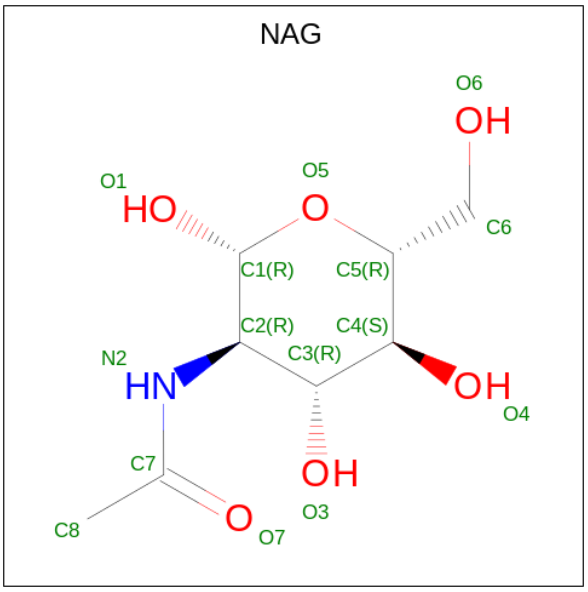
- Molecule 4 is a protein called W14 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	229	Total	C	N	O	S	0	0	0
			1732	1102	284	342	4			
4	G	229	Total	C	N	O	S	0	0	0
			1732	1102	284	342	4			
4	N	229	Total	C	N	O	S	0	0	0
			1732	1102	284	342	4			
4	Y	229	Total	C	N	O	S	0	0	0
			1732	1102	284	342	4			

- Molecule 5 is a protein called W14 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	215	Total	C	N	O	S	3	1	0
			1650	1033	273	338	6			
5	H	215	Total	C	N	O	S	3	1	0
			1650	1033	273	338	6			
5	Q	215	Total	C	N	O	S	0	0	0
			1647	1031	273	338	5			
5	Z	215	Total	C	N	O	S	3	2	0
			1654	1037	273	338	6			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	K	1	Total C N O 14 8 1 5	0	0
6	T	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 1 1	0	0
7	O	6	Total O 6 6	0	0
7	P	9	Total O 9 9	0	0
7	D	6	Total O 6 6	0	0
7	F	3	Total O 3 3	0	0
7	B	5	Total O 5 5	0	0
7	C	2	Total O 2 2	0	0
7	E	2	Total O 2 2	0	0

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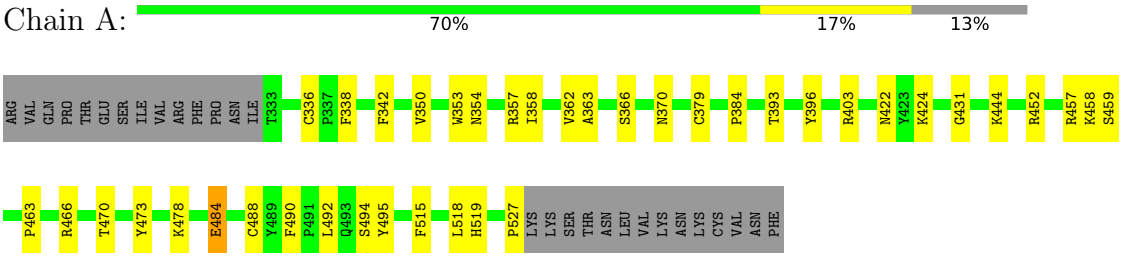
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	4	Total O 4 4	0	0
7	H	4	Total O 4 4	0	0
7	K	8	Total O 8 8	0	0
7	L	8	Total O 8 8	0	0
7	M	8	Total O 8 8	0	0
7	N	19	Total O 19 19	0	0
7	Q	9	Total O 9 9	0	0
7	W	2	Total O 2 2	0	0
7	Y	3	Total O 3 3	0	0
7	Z	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

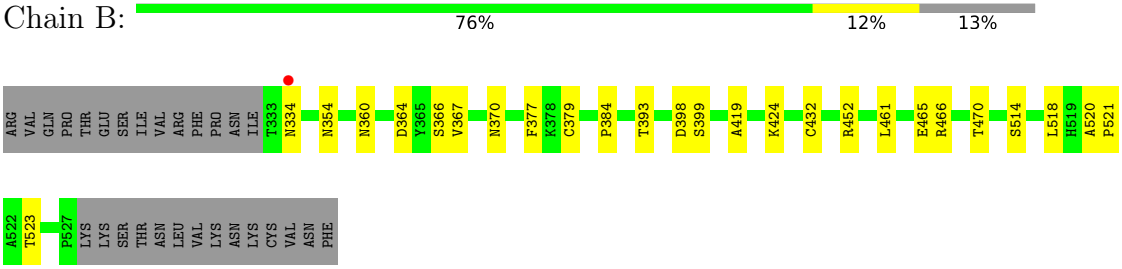
• Molecule 1: Spike protein S1

Chain A:



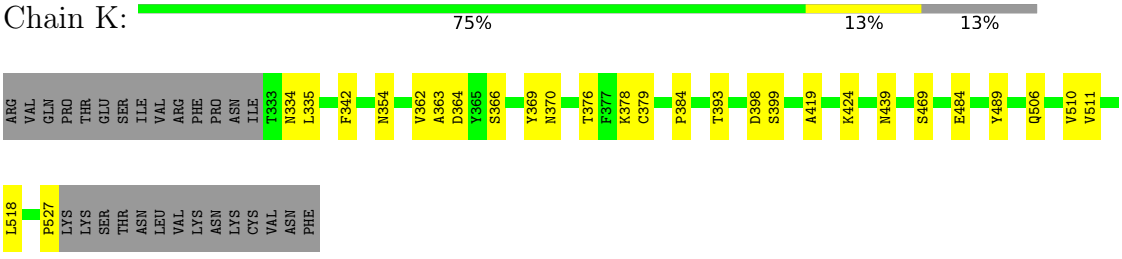
• Molecule 1: Spike protein S1

Chain B:



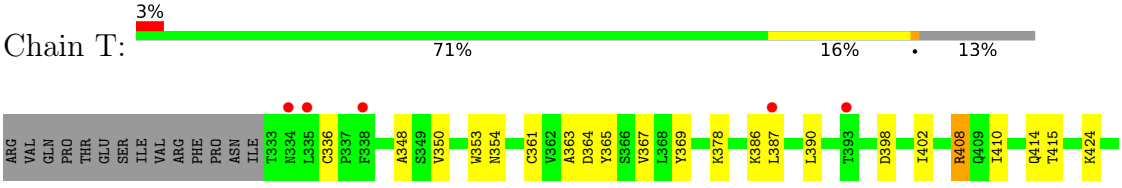
• Molecule 1: Spike protein S1

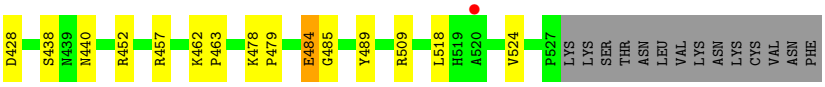
Chain K:



• Molecule 1: Spike protein S1

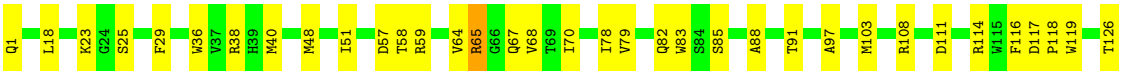
Chain T:





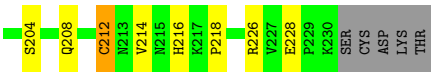
• Molecule 2: IMCAS74 Fab heavy chain

Chain O:



• Molecule 2: IMCAS74 Fab heavy chain

Chain C:

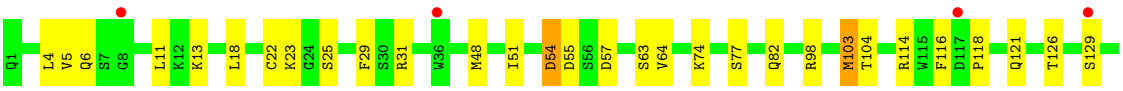


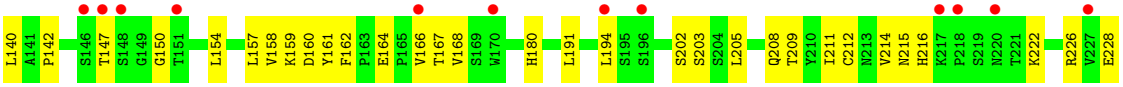
• Molecule 2: IMCAS74 Fab heavy chain

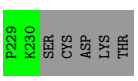
Chain L:

• Molecule 2: IMCAS74 Fab heavy chain

Chain W:

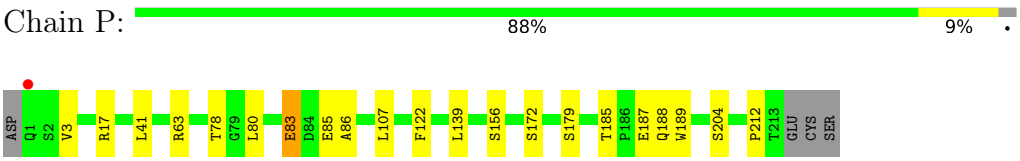






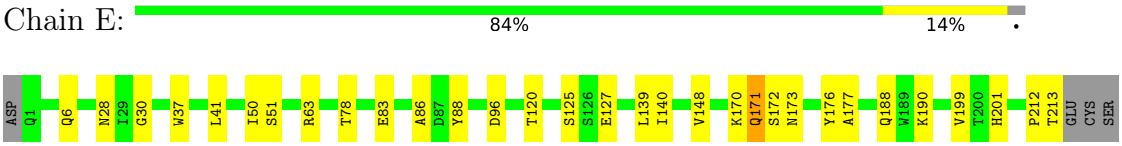
• Molecule 3: IMCAS74 Fab light chain

Chain P:



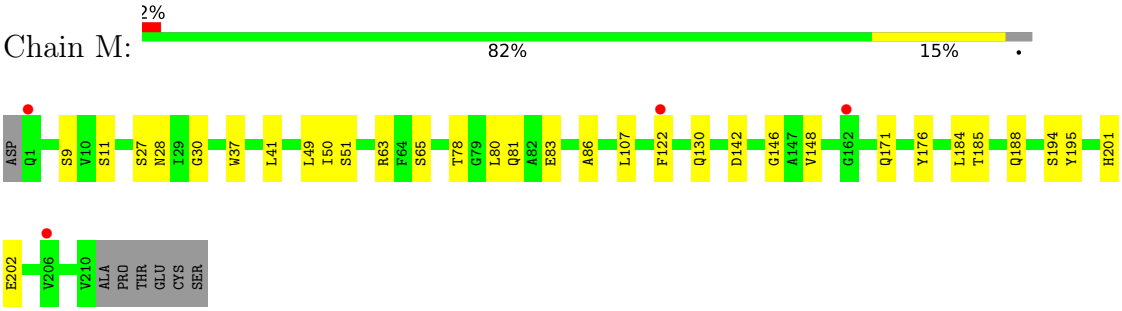
• Molecule 3: IMCAS74 Fab light chain

Chain E:



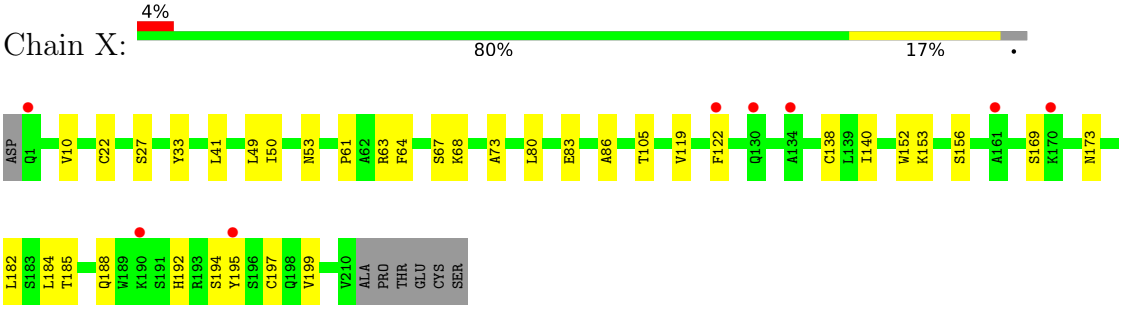
• Molecule 3: IMCAS74 Fab light chain

Chain M:



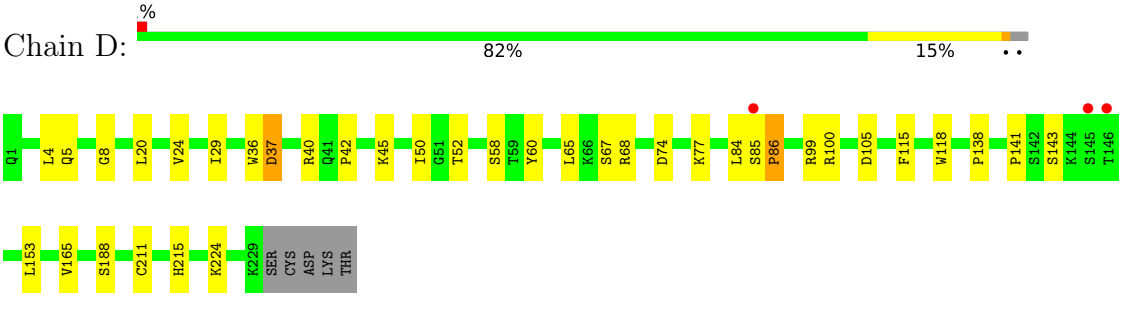
• Molecule 3: IMCAS74 Fab light chain

Chain X:



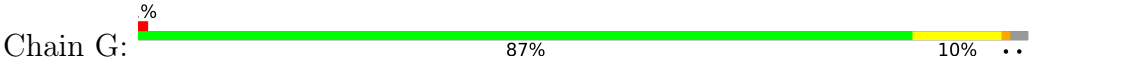
• Molecule 4: W14 Fab heavy chain

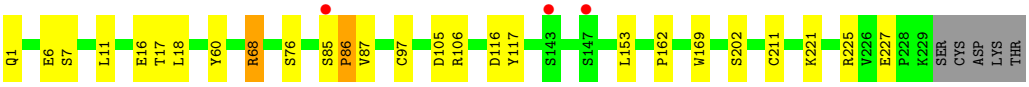
Chain D:



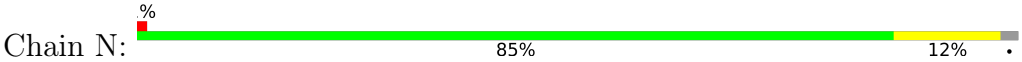
• Molecule 4: W14 Fab heavy chain

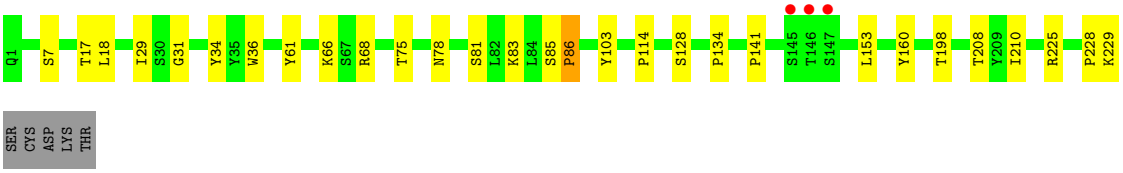
Chain G:



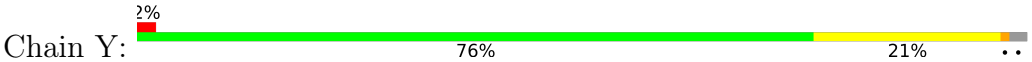


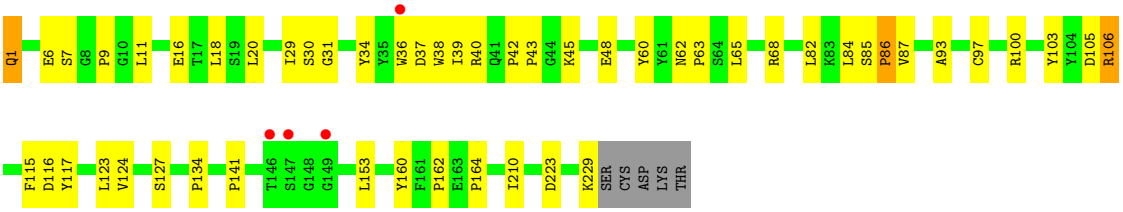
• Molecule 4: W14 Fab heavy chain



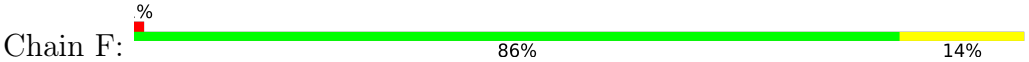


• Molecule 4: W14 Fab heavy chain

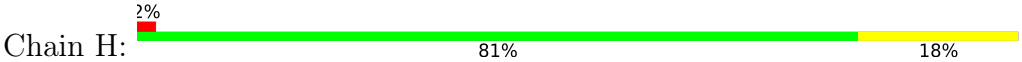


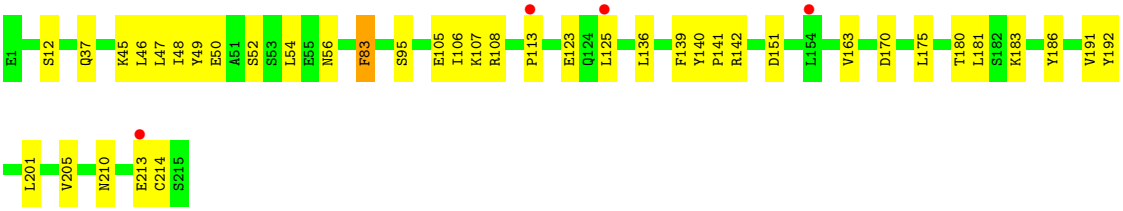


• Molecule 5: W14 Fab light chain

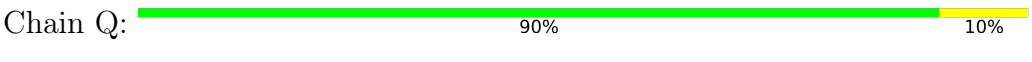


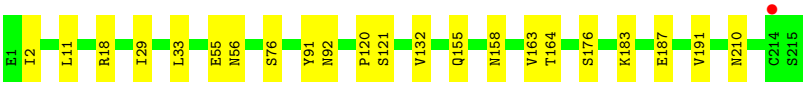
• Molecule 5: W14 Fab light chain





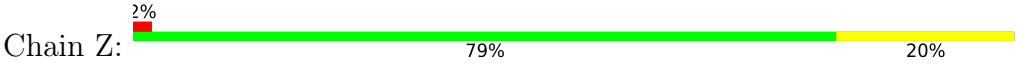
• Molecule 5: W14 Fab light chain

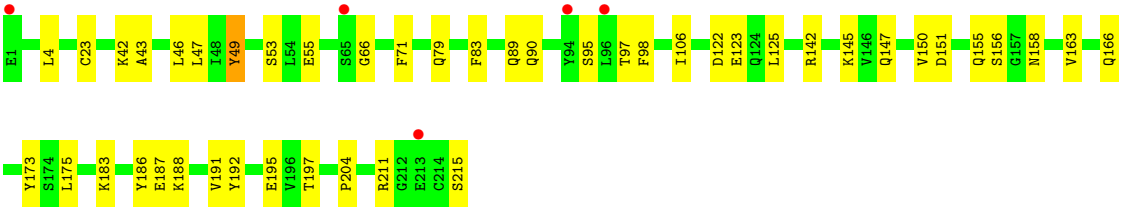




• Molecule 5: W14 Fab light chain

Chain Z:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	196.66Å 270.05Å 118.16Å 90.00° 107.85° 90.00°	Depositor
Resolution (Å)	63.06 – 2.86 93.60 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.5 (63.06-2.86) 93.6 (93.60-2.86)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.86Å)	Xtriage
Refinement program	PHENIX dev_4382, PHENIX dev_4382	Depositor
R, R_{free}	0.212 , 0.244 0.209 , 0.240	Depositor DCC
R_{free} test set	1995 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å^2)	53.2	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	33039	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.28	0/1592	0.50	0/2165
1	B	0.28	0/1592	0.51	0/2165
1	K	0.27	0/1592	0.51	0/2165
1	T	0.28	0/1592	0.52	0/2165
2	C	0.27	0/1791	0.53	0/2438
2	L	0.28	0/1749	0.55	0/2382
2	O	0.27	0/1791	0.53	0/2438
2	W	0.27	0/1791	0.56	0/2438
3	E	0.29	0/1604	0.49	0/2191
3	M	0.26	0/1584	0.49	0/2162
3	P	0.28	0/1604	0.48	0/2191
3	X	0.27	0/1584	0.48	0/2162
4	D	0.28	0/1779	0.52	0/2432
4	G	0.27	0/1779	0.53	0/2432
4	N	0.27	0/1779	0.54	0/2432
4	Y	0.27	0/1779	0.52	0/2432
5	F	0.28	0/1688	0.53	0/2292
5	H	0.28	0/1688	0.56	1/2292 (0.0%)
5	Q	0.29	0/1682	0.53	0/2284
5	Z	0.27	0/1695	0.55	0/2302
All	All	0.28	0/33735	0.52	1/45960 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	170	ASP	CB-CG-OD2	6.30	123.97	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1548	0	1467	25	0
1	B	1548	0	1467	14	0
1	K	1548	0	1467	18	0
1	T	1548	0	1467	33	0
2	C	1744	0	1718	22	0
2	L	1703	0	1671	22	0
2	O	1744	0	1718	30	0
2	W	1744	0	1718	40	0
3	E	1566	0	1520	16	0
3	M	1547	0	1501	20	0
3	P	1566	0	1520	12	1
3	X	1547	0	1501	21	0
4	D	1732	0	1705	20	0
4	G	1732	0	1705	14	0
4	N	1732	0	1705	15	1
4	Y	1732	0	1705	34	0
5	F	1650	0	1603	18	0
5	H	1650	0	1603	21	0
5	Q	1647	0	1596	10	0
5	Z	1654	0	1612	34	0
6	A	14	0	13	1	0
6	B	14	0	13	0	0
6	K	14	0	13	1	0
6	T	14	0	13	0	0
7	A	1	0	0	0	0
7	B	5	0	0	0	0
7	C	2	0	0	0	0
7	D	6	0	0	1	0
7	E	2	0	0	0	0
7	F	3	0	0	0	0
7	G	4	0	0	1	0
7	H	4	0	0	0	0
7	K	8	0	0	0	0
7	L	8	0	0	0	0
7	M	8	0	0	0	0
7	N	19	0	0	0	0
7	O	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P	9	0	0	0	0
7	Q	9	0	0	0	0
7	W	2	0	0	0	0
7	Y	3	0	0	1	0
7	Z	2	0	0	0	0
All	All	33039	0	32021	406	1

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 6.

All (406) 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)
4:N:134:PRO:HB3	4:N:160:TYR:HB3	1.53	0.90
1:T:415:THR:HG21	4:Y:1:GLN:HE21	1.44	0.82
4:Y:210:ILE:HD11	4:Y:223:ASP:HB3	1.63	0.78
2:C:48:MET:HG2	2:C:64:VAL:HG11	1.67	0.76
4:N:85:SER:HB3	4:N:86:PRO:HD3	1.67	0.75
2:W:11:LEU:HD12	2:W:126:THR:HB	1.67	0.75
4:D:85:SER:HB3	4:D:86:PRO:HD3	1.70	0.73
4:Y:65:LEU:HD23	4:Y:68:ARG:HH21	1.52	0.73
2:L:34:ILE:HG21	2:L:79:VAL:HG21	1.71	0.72
5:Z:46:LEU:HG	5:Z:55:GLU:HG3	1.70	0.71
2:O:65:ARG:HE	2:O:65:ARG:HA	1.54	0.71
5:Z:123:GLU:N	5:Z:123:GLU:OE2	2.22	0.71
4:N:29:ILE:HD11	4:N:75:THR:HA	1.71	0.71
3:X:33:TYR:O	3:X:68:LYS:NZ	2.24	0.70
2:C:201:PRO:HG2	2:C:204:SER:HB3	1.74	0.69
2:C:98:ARG:HB3	2:C:118:PRO:HD2	1.75	0.68
5:F:132:VAL:HG22	5:F:179:LEU:HB3	1.75	0.68
4:Y:85:SER:HB2	4:Y:86:PRO:HD3	1.74	0.68
2:O:51:ILE:HD12	2:O:58:THR:HB	1.73	0.68
5:H:140:TYR:CD1	5:H:141:PRO:HA	2.28	0.68
2:W:209:THR:HG22	2:W:211:ILE:HD11	1.75	0.68
4:Y:105:ASP:OD1	4:Y:106:ARG:N	2.27	0.67
2:O:48:MET:HG2	2:O:64:VAL:HG11	1.77	0.66
2:W:211:ILE:HG13	2:W:226:ARG:HB2	1.78	0.66
4:Y:1:GLN:N	7:Y:301:HOH:O	2.28	0.66
2:L:140:LEU:HD12	3:M:122:PHE:HB3	1.78	0.66
3:M:81:GLN:NE2	3:M:83:GLU:OE1	2.30	0.65
5:Q:183:LYS:O	5:Q:187:GLU:HG2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:225:ARG:HG2	4:G:227:GLU:HG3	1.79	0.64
2:C:76:THR:HG23	2:C:78:ILE:HG22	1.79	0.64
1:A:379:CYS:SG	1:A:384:PRO:HG3	2.38	0.64
4:N:17:THR:HG22	4:N:85:SER:HA	1.77	0.64
5:Z:211:ARG:HG2	5:Z:211:ARG:HH11	1.62	0.64
5:F:123:GLU:N	5:F:123:GLU:OE2	2.28	0.64
2:C:117:ASP:HB3	2:C:118:PRO:HD3	1.80	0.63
5:Z:142:ARG:HG2	5:Z:142:ARG:HH11	1.64	0.63
1:K:518:LEU:HA	2:L:103:MET:HE1	1.81	0.63
4:Y:40:ARG:NE	4:Y:48:GLU:OE2	2.30	0.63
4:G:105:ASP:OD1	4:G:106:ARG:N	2.32	0.63
1:B:360:ASN:HA	1:B:523:THR:HB	1.81	0.62
3:E:188:GLN:HE22	3:M:130:GLN:NE2	1.97	0.62
4:N:61:TYR:HB2	4:N:66:LYS:HG3	1.81	0.62
5:F:150:VAL:HB	5:F:155:GLN:NE2	2.14	0.62
4:Y:42:PRO:HG2	4:Y:45:LYS:HB2	1.82	0.62
3:X:192:HIS:HB2	3:X:195:TYR:CE2	2.35	0.62
2:C:168:VAL:HG13	2:C:214:VAL:HG22	1.80	0.62
2:C:55:ASP:O	2:C:57:ASP:N	2.29	0.61
1:A:362:VAL:HB	1:A:527:PRO:HD3	1.82	0.61
3:E:188:GLN:HE22	3:M:130:GLN:HE21	1.49	0.61
4:D:60:TYR:CE2	5:F:94:TYR:HB3	2.36	0.61
4:Y:105:ASP:OD1	4:Y:106:ARG:NE	2.27	0.61
3:M:142:ASP:H	3:M:171:GLN:HE22	1.49	0.60
1:B:419:ALA:O	1:B:424:LYS:HD2	2.00	0.60
4:N:228:PRO:O	4:N:229:LYS:HB2	2.01	0.60
1:K:419:ALA:O	1:K:424:LYS:HD2	2.01	0.60
2:L:179:VAL:HG22	2:L:198:VAL:HG12	1.82	0.60
5:Z:151:ASP:HA	5:Z:191:VAL:HG22	1.84	0.60
3:X:41:LEU:HD23	3:X:86:ALA:HB2	1.84	0.60
5:H:163:VAL:HG22	5:H:175:LEU:HD23	1.83	0.59
3:X:49:LEU:O	3:X:50:ILE:HD13	2.01	0.59
4:G:85:SER:HB3	4:G:86:PRO:HD3	1.84	0.59
1:T:365:TYR:CD2	1:T:387:LEU:HB3	2.38	0.59
2:W:140:LEU:HD21	2:W:157:LEU:HB2	1.83	0.59
2:O:91:THR:HG23	2:O:126:THR:HA	1.85	0.59
5:Q:155:GLN:HB3	5:Q:158:ASN:HD21	1.67	0.59
5:Z:122:ASP:HA	5:Z:125:LEU:HD12	1.84	0.59
5:Z:155:GLN:HE21	5:Z:158:ASN:HD21	1.51	0.58
3:M:184:LEU:HB3	3:M:188:GLN:HB2	1.85	0.58
4:Y:123:LEU:HD23	4:Y:164:PRO:HD3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:141:PRO:HG3	4:D:153:LEU:HB3	1.84	0.58
2:C:6:GLN:O	2:C:121:GLN:NE2	2.37	0.58
4:N:29:ILE:HA	4:N:36:TRP:CZ2	2.39	0.58
2:O:29:PHE:HZ	2:O:79:VAL:HG23	1.69	0.57
5:Z:83:PHE:HB2	5:Z:106:ILE:HD13	1.85	0.57
3:E:148:VAL:HG12	3:E:201:HIS:HB2	1.86	0.57
2:C:21:SER:HB2	2:C:78:ILE:HD11	1.87	0.57
1:K:364:ASP:OD1	1:K:366:SER:OG	2.21	0.57
4:Y:62:ASN:HD22	4:Y:63:PRO:HD2	1.68	0.57
4:D:8:GLY:HA3	4:D:20:LEU:HD23	1.87	0.57
5:F:32:TRP:HB2	5:F:92:ASN:HB2	1.87	0.57
5:H:108:ARG:HG3	5:H:140:TYR:CD2	2.40	0.56
2:W:6:GLN:O	2:W:121:GLN:NE2	2.37	0.56
4:G:16:GLU:O	4:G:87:VAL:HG22	2.05	0.56
5:Z:163[B]:VAL:HG22	5:Z:175:LEU:HD12	1.87	0.56
1:A:452:ARG:HE	1:A:494:SER:HB3	1.70	0.56
5:F:189:HIS:O	5:F:211:ARG:HD3	2.06	0.56
1:B:379:CYS:SG	1:B:384:PRO:HG3	2.45	0.56
5:Z:49:TYR:CE1	5:Z:53:SER:HB2	2.40	0.56
3:M:41:LEU:HD23	3:M:86:ALA:HB2	1.88	0.56
1:A:393:THR:HG21	1:A:518:LEU:HD12	1.87	0.55
3:M:185:THR:OG1	3:M:188:GLN:HG3	2.05	0.55
5:Z:183:LYS:O	5:Z:187:GLU:HG3	2.07	0.55
1:B:470:THR:HG21	1:K:484:GLU:HB3	1.88	0.55
5:H:37:GLN:HB2	5:H:47:LEU:HD11	1.87	0.55
3:M:148:VAL:HG12	3:M:201:HIS:HB2	1.89	0.55
1:T:438:SER:HB3	1:T:509:ARG:HG3	1.89	0.55
2:W:167:THR:OG1	2:W:215:ASN:HB3	2.07	0.55
5:Z:163[A]:VAL:HG22	5:Z:175:LEU:HD12	1.88	0.55
3:M:184:LEU:HD11	3:M:195:TYR:CZ	2.41	0.55
2:W:129:SER:HB3	2:W:162:PHE:CE1	2.42	0.55
1:T:350:VAL:O	1:T:353:TRP:HD1	1.91	0.54
2:W:114:ARG:HH11	2:W:114:ARG:HG2	1.71	0.54
2:W:168:VAL:HG22	2:W:214:VAL:HG22	1.88	0.54
3:P:83:GLU:OE1	3:P:83:GLU:N	2.41	0.54
3:X:185:THR:OG1	3:X:188:GLN:HG3	2.07	0.54
1:K:379:CYS:SG	1:K:384:PRO:HG3	2.48	0.54
1:T:424:LYS:HG2	1:T:463:PRO:HA	1.90	0.54
4:Y:11:LEU:HD11	4:Y:127:SER:HB3	1.89	0.54
1:B:366:SER:O	1:B:370:ASN:HB2	2.08	0.54
1:A:366:SER:O	1:A:370:ASN:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:41:LEU:HD23	3:E:86:ALA:HB2	1.89	0.53
2:L:168:VAL:HG22	2:L:214:VAL:HG22	1.88	0.53
1:T:408:ARG:HD3	5:Z:49:TYR:CE2	2.43	0.53
2:O:111:ASP:OD1	2:O:114:ARG:NH1	2.41	0.53
2:O:155:GLY:HA2	2:O:170:TRP:CH2	2.44	0.53
3:M:37:TRP:HB2	3:M:50:ILE:HB	1.91	0.53
1:A:457:ARG:NH1	1:A:459:SER:O	2.37	0.53
1:K:376:THR:HG23	1:K:378:LYS:HG3	1.90	0.53
4:Y:29:ILE:HA	4:Y:36:TRP:CZ2	2.45	0.52
4:N:68:ARG:HD2	4:N:86:PRO:HD2	1.91	0.52
2:O:208:GLN:OE1	2:O:209:THR:N	2.42	0.52
5:Z:89:GLN:HB2	5:Z:98:PHE:CD1	2.44	0.52
2:L:202:SER:HA	2:L:205:LEU:HD13	1.91	0.52
4:Y:115:PHE:HE1	5:Z:89:GLN:HE22	1.58	0.52
1:K:439:ASN:OD1	1:K:506:GLN:HG2	2.10	0.52
1:T:408:ARG:HD3	5:Z:49:TYR:HE2	1.75	0.52
2:W:4:LEU:HD22	2:W:22:CYS:SG	2.50	0.52
2:W:160:ASP:HB3	2:W:191:LEU:HD23	1.92	0.52
4:Y:39:ILE:HD11	4:Y:115:PHE:CE2	2.44	0.52
3:P:41:LEU:HD23	3:P:86:ALA:HB2	1.91	0.52
5:H:136:LEU:HB2	5:H:175:LEU:HB3	1.92	0.52
1:T:518:LEU:HA	2:W:103:MET:HE1	1.92	0.52
2:O:170:TRP:CH2	2:O:212:CYS:HB3	2.45	0.51
2:W:142:PRO:HG3	2:W:154:LEU:HD12	1.92	0.51
4:D:100:ARG:HD2	4:D:115:PHE:CE1	2.45	0.51
1:A:519:HIS:H	2:O:103:MET:HE1	1.75	0.51
5:Z:147:GLN:NE2	5:Z:195:GLU:OE1	2.38	0.51
4:D:74:ASP:OD2	4:D:77:LYS:HG3	2.11	0.51
2:W:147:THR:HG23	2:W:203:SER:HA	1.92	0.51
3:X:153:LYS:HE2	3:X:156:SER:HA	1.92	0.51
5:F:120:PRO:HD3	5:F:132:VAL:HG12	1.93	0.51
5:F:150:VAL:HG22	5:F:192:TYR:CD2	2.45	0.51
4:G:11:LEU:HB2	4:G:162:PRO:HG3	1.93	0.51
1:T:408:ARG:HG3	1:T:414:GLN:NE2	2.25	0.51
2:C:6:GLN:H	2:C:121:GLN:HE21	1.59	0.50
2:L:171:ASN:ND2	2:L:211:ILE:H	2.08	0.50
3:P:187:GLU:OE1	3:P:187:GLU:N	2.33	0.50
2:L:154:LEU:HB2	2:L:227:VAL:HG11	1.93	0.50
4:D:68:ARG:HG3	4:D:68:ARG:HH11	1.77	0.50
4:G:18:LEU:HB2	4:G:87:VAL:HG11	1.92	0.50
2:O:29:PHE:CZ	2:O:79:VAL:HG23	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:1:GLN:N	7:G:301:HOH:O	2.43	0.50
2:L:13:LYS:N	2:L:13:LYS:HD2	2.25	0.50
2:W:13:LYS:HD2	2:W:13:LYS:N	2.25	0.50
4:D:37:ASP:OD2	4:D:52:THR:OG1	2.30	0.50
3:X:22:CYS:HB3	3:X:73:ALA:HB3	1.94	0.50
1:B:452:ARG:HD2	1:K:489:TYR:CD1	2.46	0.50
4:G:1:GLN:HG2	4:G:117:TYR:HE2	1.77	0.50
5:H:186:TYR:HA	5:H:192:TYR:OH	2.12	0.50
3:X:182:LEU:HG	3:X:184:LEU:HD21	1.94	0.50
1:A:470:THR:HG21	1:T:484:GLU:HB3	1.95	0.49
5:H:125:LEU:O	5:H:183:LYS:HD2	2.12	0.49
1:T:350:VAL:HG21	1:T:402:ILE:HG23	1.94	0.49
3:P:189:TRP:CZ2	3:P:212:PRO:HA	2.47	0.49
1:B:393:THR:HG21	1:B:518:LEU:HD12	1.93	0.49
2:W:140:LEU:HD12	3:X:122:PHE:CG	2.47	0.49
2:W:166:VAL:HG23	2:W:216:HIS:HD2	1.76	0.49
1:T:440:ASN:N	1:T:440:ASN:OD1	2.46	0.49
1:A:484:GLU:HG2	1:A:488:CYS:O	2.13	0.49
3:E:212:PRO:HD2	3:E:213:THR:HG23	1.95	0.49
5:H:49:TYR:CD2	5:H:50:GLU:HG2	2.47	0.49
2:C:170:TRP:CH2	2:C:212:CYS:HB2	2.47	0.49
1:K:363:ALA:O	1:K:527:PRO:HD3	2.11	0.49
4:D:65:LEU:HD23	4:D:68:ARG:NH2	2.28	0.49
2:C:91:THR:HG23	2:C:126:THR:HA	1.94	0.49
2:W:98:ARG:HB3	2:W:118:PRO:HD2	1.95	0.49
3:P:83:GLU:CD	3:P:83:GLU:H	2.16	0.49
1:T:518:LEU:HD23	2:W:103:MET:HE2	1.94	0.49
1:K:334:ASN:OD1	1:K:334:ASN:N	2.42	0.48
5:Q:191:VAL:HG22	5:Q:210:ASN:OD1	2.13	0.48
5:H:123:GLU:H	5:H:123:GLU:CD	2.15	0.48
1:T:354:ASN:O	1:T:398:ASP:HA	2.13	0.48
5:Z:95:SER:HB2	5:Z:97:THR:HG23	1.95	0.48
4:G:68:ARG:CB	4:G:86:PRO:HD2	2.43	0.48
1:K:378:LYS:HD3	4:N:103:TYR:CZ	2.49	0.48
5:Z:4:LEU:HD22	5:Z:23:CYS:SG	2.54	0.48
2:O:97:ALA:HB1	2:O:116:PHE:HB3	1.95	0.48
2:O:65:ARG:HE	2:O:65:ARG:CA	2.26	0.48
1:A:458:LYS:HD3	1:A:473:TYR:CE1	2.49	0.48
4:N:29:ILE:HG12	4:N:78:ASN:HA	1.96	0.48
4:Y:11:LEU:HD13	4:Y:162:PRO:HG3	1.96	0.48
4:N:210:ILE:CD1	4:N:225:ARG:HG3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:117:ASP:HB3	2:L:118:PRO:HD3	1.96	0.47
4:Y:16:GLU:O	4:Y:87:VAL:HG23	2.14	0.47
2:C:97:ALA:HB1	2:C:116:PHE:HB3	1.96	0.47
2:C:175:LEU:HD21	2:C:198:VAL:HG11	1.96	0.47
3:E:170:LYS:HD3	3:E:176:TYR:CZ	2.49	0.47
5:F:132:VAL:CG2	5:F:179:LEU:HB3	2.43	0.47
2:W:54:ASP:HA	2:W:74:LYS:NZ	2.29	0.47
4:D:68:ARG:HG3	4:D:68:ARG:NH1	2.29	0.47
3:X:138:CYS:HB2	3:X:152:TRP:CH2	2.50	0.47
5:Q:2:ILE:HD12	5:Q:2:ILE:H	1.79	0.47
3:X:119:VAL:HG22	3:X:140:ILE:HG23	1.96	0.47
5:Z:42:LYS:HD2	5:Z:43:ALA:H	1.79	0.47
5:Z:66:GLY:HA3	5:Z:71:PHE:CD2	2.49	0.47
1:A:424:LYS:HG2	1:A:463:PRO:HA	1.97	0.47
2:O:138:PHE:HE2	2:O:159:LYS:HE2	1.80	0.47
2:O:36:TRP:CD1	2:O:70:ILE:HG12	2.50	0.47
5:F:35:TRP:CG	5:F:73:LEU:HD13	2.50	0.47
1:B:466:ARG:NH2	3:E:96:ASP:OD1	2.48	0.47
2:C:226:ARG:HD2	2:C:228:GLU:OE2	2.15	0.47
1:T:348:ALA:HB2	1:T:354:ASN:HD22	1.78	0.47
5:Z:166:GLN:HG3	5:Z:173:TYR:CZ	2.50	0.47
1:T:478:LYS:HG3	1:T:479:PRO:HD2	1.95	0.46
5:Z:90:GLN:HE21	5:Z:97:THR:H	1.63	0.46
5:F:132:VAL:HG23	5:F:148:TRP:CH2	2.51	0.46
3:E:6:GLN:NE2	3:E:88:TYR:O	2.44	0.46
2:W:31:ARG:NH1	2:W:104:THR:HB	2.30	0.46
2:W:202:SER:HA	2:W:205:LEU:HD12	1.96	0.46
4:G:6:GLU:HG3	4:G:97:CYS:SG	2.55	0.46
1:T:364:ASP:O	1:T:367:VAL:HG12	2.16	0.46
2:L:67:GLN:HG3	2:L:68:VAL:HG13	1.97	0.46
1:T:378:LYS:HD3	4:Y:103:TYR:CZ	2.51	0.46
4:Y:62:ASN:ND2	4:Y:63:PRO:HD2	2.30	0.46
4:Y:134:PRO:HB3	4:Y:160:TYR:HB3	1.98	0.46
1:A:353:TRP:NE1	1:A:466:ARG:HG3	2.30	0.46
2:O:23:LYS:HG2	2:O:78:ILE:HG12	1.98	0.46
1:B:354:ASN:O	1:B:398:ASP:HA	2.16	0.46
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.50	0.46
5:H:83:PHE:HB2	5:H:106:ILE:HD13	1.96	0.46
5:H:105:GLU:HG2	5:H:106:ILE:N	2.30	0.46
5:Z:211:ARG:HG2	5:Z:211:ARG:NH1	2.31	0.46
2:O:88:ALA:HA	2:O:127:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:37:TRP:HB2	3:E:50:ILE:HB	1.98	0.46
5:H:45:LYS:HE3	5:H:46:LEU:O	2.16	0.46
5:H:201:LEU:CD1	5:H:205:VAL:HG12	2.46	0.46
2:W:158:VAL:HB	2:W:194:LEU:HG	1.98	0.45
2:W:161:TYR:HE1	2:W:164:GLU:HG2	1.80	0.45
3:P:17:ARG:HG3	3:P:78:THR:HG22	1.97	0.45
2:L:98:ARG:HB3	2:L:118:PRO:HD2	1.97	0.45
5:H:210:ASN:ND2	5:H:213:GLU:OE1	2.37	0.45
3:M:80:LEU:HD11	3:M:107:LEU:HD21	1.98	0.45
2:W:150:GLY:HA2	2:W:202:SER:H	1.81	0.45
4:D:40:ARG:HD3	4:D:50:ILE:HD11	1.99	0.45
4:D:68:ARG:HB3	4:D:86:PRO:HD2	1.98	0.45
4:D:99:ARG:NH1	7:D:301:HOH:O	2.48	0.45
5:H:151:ASP:OD2	5:H:191:VAL:HG12	2.17	0.45
3:M:28:ASN:O	3:M:30:GLY:N	2.46	0.45
1:T:386:LYS:HE2	1:T:386:LYS:HB3	1.58	0.45
3:X:140:ILE:HG21	3:X:199:VAL:HG11	1.99	0.45
1:A:403:ARG:HG3	1:A:495:TYR:CE1	2.52	0.45
5:F:113:PRO:HD2	5:F:201:LEU:HD21	1.98	0.45
3:E:28:ASN:O	3:E:30:GLY:N	2.44	0.45
5:H:48:ILE:CD1	5:H:54:LEU:HD12	2.46	0.45
2:W:161:TYR:CE1	2:W:164:GLU:HG2	2.52	0.45
1:A:452:ARG:HD2	1:T:489:TYR:CD1	2.52	0.45
2:L:225:LYS:HE2	2:L:225:LYS:HB2	1.86	0.45
3:X:83:GLU:H	3:X:83:GLU:CD	2.20	0.45
4:Y:37:ASP:OD2	4:Y:100:ARG:NH1	2.50	0.45
3:P:185:THR:OG1	3:P:188:GLN:HG3	2.17	0.45
3:E:63:ARG:HB3	3:E:78:THR:O	2.17	0.45
4:G:17:THR:HG23	4:G:85:SER:HA	1.98	0.45
3:M:142:ASP:H	3:M:171:GLN:NE2	2.14	0.45
2:O:57:ASP:OD2	2:O:59:ARG:NH1	2.51	0.45
2:O:117:ASP:HB3	2:O:118:PRO:HD3	1.99	0.45
1:B:461:LEU:HD22	1:B:465:GLU:HB3	1.98	0.45
3:E:127:GLU:OE2	3:E:127:GLU:N	2.22	0.45
1:T:390:LEU:HD12	1:T:390:LEU:HA	1.87	0.45
1:T:402:ILE:HD13	1:T:410:ILE:HD11	1.98	0.44
3:M:201:HIS:CE1	3:M:202:GLU:HG2	2.51	0.44
5:Q:18:ARG:HG3	5:Q:76:SER:HA	1.99	0.44
2:W:48:MET:HE3	2:W:64:VAL:HG11	2.00	0.44
2:O:1:GLN:HA	2:O:1:GLN:HE21	1.81	0.44
1:B:364:ASP:O	1:B:367:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:342:PHE:HB2	6:K:601:NAG:H82	1.98	0.44
2:O:68:VAL:HG12	2:O:83:TRP:CD1	2.53	0.44
4:D:4:LEU:HD22	4:D:24:VAL:HG22	2.00	0.44
4:D:29:ILE:HA	4:D:36:TRP:CZ2	2.53	0.44
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.99	0.44
2:C:98:ARG:O	2:C:116:PHE:HA	2.18	0.44
2:L:166:VAL:HG23	2:L:216:HIS:HD2	1.82	0.44
4:Y:38:TRP:CD1	4:Y:82:LEU:HB2	2.52	0.44
1:A:357:ARG:HG3	1:A:396:TYR:CE1	2.53	0.44
5:Q:55:GLU:HG3	5:Q:56:ASN:N	2.32	0.44
2:O:111:ASP:HA	2:O:114:ARG:NH1	2.32	0.43
5:F:150:VAL:HB	5:F:155:GLN:HE21	1.83	0.43
2:C:6:GLN:N	2:C:121:GLN:HE21	2.16	0.43
3:E:140:ILE:HG12	3:E:199:VAL:HG21	1.99	0.43
5:F:145:LYS:HB3	5:F:145:LYS:HE2	1.74	0.43
5:Q:163:VAL:HG12	5:Q:164:THR:O	2.17	0.43
5:Q:120:PRO:HG3	5:Q:132:VAL:HG22	1.99	0.43
3:P:122:PHE:HE2	3:P:139:LEU:HD12	1.84	0.43
4:D:42:PRO:HG2	4:D:45:LYS:HB2	2.01	0.43
1:T:369:TYR:O	4:Y:106:ARG:HB2	2.17	0.43
3:X:138:CYS:HB2	3:X:152:TRP:CZ2	2.53	0.43
1:A:336:CYS:SG	1:A:363:ALA:HB2	2.59	0.43
1:A:338:PHE:CE1	1:A:358:ILE:HD13	2.54	0.43
2:C:137:VAL:HA	2:C:157:LEU:O	2.18	0.43
2:O:38:ARG:HB2	2:O:40:MET:HE3	2.01	0.43
2:O:178:GLY:O	2:O:198:VAL:HA	2.18	0.43
2:L:171:ASN:HD21	2:L:210:TYR:HA	1.83	0.43
4:N:18:LEU:O	4:N:83:LYS:HA	2.18	0.43
1:T:378:LYS:HD3	4:Y:103:TYR:CE1	2.53	0.43
4:Y:9:PRO:O	4:Y:124:VAL:HG22	2.18	0.43
2:W:98:ARG:O	2:W:116:PHE:HA	2.19	0.43
4:Y:18:LEU:HB3	4:Y:84:LEU:HB2	2.01	0.43
5:Z:42:LYS:HG3	5:Z:43:ALA:O	2.19	0.43
5:H:180:THR:O	5:H:181:LEU:HD23	2.19	0.43
1:K:354:ASN:O	1:K:398:ASP:HA	2.19	0.43
4:N:141:PRO:HD3	4:N:153:LEU:HB3	2.01	0.43
2:O:38:ARG:HB3	2:O:48:MET:SD	2.59	0.43
3:E:171:GLN:HE21	3:E:177:ALA:HB2	1.83	0.43
3:X:192:HIS:HB2	3:X:195:TYR:HE2	1.82	0.43
1:B:379:CYS:HA	1:B:432:CYS:HA	2.00	0.42
2:C:38:ARG:NH2	2:C:46:GLU:OE2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:6:GLU:HG3	4:Y:97:CYS:SG	2.59	0.42
1:A:452:ARG:HD2	1:T:489:TYR:HD1	1.84	0.42
2:O:18:LEU:O	2:O:82:GLN:HA	2.19	0.42
3:P:63:ARG:HB3	3:P:78:THR:O	2.19	0.42
3:E:120:THR:HG23	3:E:139:LEU:HB2	2.00	0.42
1:B:514:SER:HB3	2:C:106:MET:CE	2.49	0.42
3:M:171:GLN:HE21	3:M:176:TYR:C	2.23	0.42
1:T:361:CYS:O	1:T:524:VAL:HA	2.19	0.42
2:W:54:ASP:OD1	2:W:74:LYS:NZ	2.52	0.42
3:X:61:PRO:HB2	3:X:63:ARG:HG3	2.02	0.42
5:Z:150:VAL:HB	5:Z:155:GLN:OE1	2.19	0.42
3:P:80:LEU:HD21	3:P:107:LEU:HD21	2.01	0.42
4:D:165:VAL:HG12	4:D:215:HIS:HB2	2.00	0.42
2:L:13:LYS:HD3	2:L:16:GLU:OE2	2.20	0.42
2:L:140:LEU:HB3	3:M:122:PHE:CD1	2.55	0.42
4:Y:43:PRO:HD3	4:Y:93:ALA:HA	2.01	0.42
2:L:97:ALA:HB1	2:L:116:PHE:HB3	2.01	0.42
4:N:31:GLY:HA3	4:N:34:TYR:CD2	2.54	0.42
4:Y:141:PRO:HG3	4:Y:153:LEU:HB3	2.02	0.42
1:K:393:THR:HG21	1:K:518:LEU:HD12	2.01	0.42
4:G:68:ARG:HB2	4:G:86:PRO:HD2	2.02	0.42
1:A:478:LYS:HA	1:A:478:LYS:HD3	1.79	0.42
2:W:5:VAL:HG12	2:W:23:LYS:HB2	2.02	0.42
1:B:520:ALA:HB1	1:B:521:PRO:HD2	2.00	0.42
3:E:190:LYS:HE2	3:E:190:LYS:HB2	1.76	0.42
4:Y:31:GLY:HA3	4:Y:34:TYR:CD2	2.54	0.42
4:G:68:ARG:HB3	4:G:86:PRO:HD2	2.00	0.42
5:H:12:SER:OG	5:H:107:LYS:HG3	2.20	0.42
5:H:113:PRO:HA	5:H:139:PHE:HB3	2.02	0.42
1:T:408:ARG:HG3	1:T:408:ARG:O	2.20	0.42
2:W:140:LEU:HD12	3:X:122:PHE:CB	2.49	0.42
2:L:138:PHE:CE2	2:L:159:LYS:HD3	2.54	0.41
1:T:336:CYS:SG	1:T:363:ALA:HB2	2.60	0.41
1:T:365:TYR:CE2	1:T:387:LEU:HB3	2.55	0.41
5:Z:89:GLN:HG2	5:Z:90:GLN:N	2.35	0.41
5:Z:186:TYR:HA	5:Z:192:TYR:OH	2.19	0.41
4:D:68:ARG:O	4:D:84:LEU:HA	2.20	0.41
4:D:138:PRO:HG3	4:D:224:LYS:HE3	2.02	0.41
2:L:150:GLY:N	2:L:202:SER:HG	2.19	0.41
1:T:484:GLU:HG3	1:T:485:GLY:N	2.35	0.41
4:Y:18:LEU:HD21	4:Y:20:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:51:ILE:HA	2:W:57:ASP:O	2.20	0.41
3:X:53:ASN:HD21	3:X:68:LYS:HD2	1.85	0.41
2:O:67:GLN:OE1	2:O:67:GLN:N	2.52	0.41
5:F:39:LYS:HG2	5:F:84:ALA:HB2	2.02	0.41
1:K:398:ASP:O	1:K:511:VAL:HA	2.20	0.41
1:T:518:LEU:HA	2:W:103:MET:CE	2.50	0.41
2:O:36:TRP:HD1	2:O:70:ILE:HG12	1.84	0.41
2:O:211:ILE:HG12	2:O:226:ARG:HG3	2.02	0.41
4:G:169:TRP:CZ3	4:G:211:CYS:HB3	2.56	0.41
1:K:366:SER:O	1:K:370:ASN:HB2	2.21	0.41
2:L:19:LYS:HB2	2:L:82:GLN:HG3	2.03	0.41
3:P:187:GLU:H	3:P:187:GLU:CD	2.19	0.41
5:Q:29:ILE:HD11	5:Q:33:LEU:HB2	2.02	0.41
5:Z:187:GLU:HA	5:Z:211:ARG:NE	2.36	0.41
4:D:118:TRP:CE3	5:F:44:PRO:HD2	2.56	0.41
5:H:125:LEU:HD22	5:H:183:LYS:HG3	2.03	0.41
1:K:335:LEU:HD12	1:K:362:VAL:CG1	2.51	0.41
3:M:146:GLY:HA3	3:M:176:TYR:CG	2.56	0.41
3:X:61:PRO:HD2	3:X:64:PHE:CE2	2.56	0.41
5:Z:197:THR:HG22	5:Z:204:PRO:HG3	2.03	0.41
1:A:342:PHE:HB2	6:A:601:NAG:H82	2.03	0.41
1:A:444:LYS:HB3	1:A:444:LYS:HE3	1.83	0.41
3:P:85:GLU:HG3	3:P:107:LEU:O	2.21	0.41
5:H:136:LEU:HD13	5:H:175:LEU:HD12	2.03	0.41
1:K:399:SER:HA	1:K:510:VAL:O	2.20	0.41
2:W:18:LEU:O	2:W:82:GLN:HA	2.20	0.41
2:W:29:PHE:CD2	2:W:77:SER:HA	2.56	0.41
2:W:211:ILE:HA	2:W:226:ARG:HA	2.03	0.41
5:Z:186:TYR:CZ	5:Z:211:ARG:HG3	2.56	0.41
2:O:111:ASP:HA	2:O:114:ARG:HH11	1.86	0.41
2:W:222:LYS:HE3	2:W:222:LYS:HB3	1.69	0.41
2:W:98:ARG:NE	2:W:118:PRO:HG2	2.36	0.40
4:Y:229:LYS:HE2	5:Z:215:SER:O	2.20	0.40
1:T:462:LYS:NZ	2:W:57:ASP:OD1	2.40	0.40
1:A:484:GLU:OE1	1:T:452:ARG:NH1	2.54	0.40
1:A:490:PHE:HE2	1:A:492:LEU:HB2	1.86	0.40
2:C:23:LYS:HB2	2:C:78:ILE:HD12	2.03	0.40
2:L:135:PRO:HB2	2:L:158:VAL:HG13	2.03	0.40
3:X:10:VAL:HG12	3:X:105:THR:HG22	2.03	0.40
3:X:152:TRP:CZ3	3:X:197:CYS:HB2	2.57	0.40
5:F:83:PHE:O	5:F:83:PHE:CG	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:167:ASP:HB3	5:F:170:ASP:OD1	2.20	0.40
3:M:49:LEU:O	3:M:50:ILE:HD13	2.21	0.40
4:N:114:PRO:HD3	5:Q:91:TYR:CE1	2.57	0.40
2:C:216:HIS:CD2	2:C:218:PRO:HD2	2.56	0.40
3:M:63:ARG:HB3	3:M:78:THR:O	2.22	0.40
2:W:226:ARG:HD3	2:W:228:GLU:OE2	2.22	0.40
4:Y:1:GLN:HG2	4:Y:117:TYR:HE2	1.86	0.40
4:Y:115:PHE:HE1	5:Z:89:GLN:NE2	2.19	0.40
5:Z:46:LEU:HD12	5:Z:47:LEU:N	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:156:SER:OG	4:N:208:THR:OG1[4_545]	2.18	0.02

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	193/223 (86%)	182 (94%)	11 (6%)	0	100	100
1	B	193/223 (86%)	186 (96%)	7 (4%)	0	100	100
1	K	193/223 (86%)	188 (97%)	5 (3%)	0	100	100
1	T	193/223 (86%)	186 (96%)	7 (4%)	0	100	100
2	C	228/235 (97%)	218 (96%)	9 (4%)	1 (0%)	34	62
2	L	220/235 (94%)	215 (98%)	4 (2%)	1 (0%)	29	57
2	O	228/235 (97%)	223 (98%)	5 (2%)	0	100	100
2	W	228/235 (97%)	220 (96%)	8 (4%)	0	100	100
3	E	211/217 (97%)	206 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	208/217 (96%)	202 (97%)	6 (3%)	0	100	100
3	P	211/217 (97%)	204 (97%)	7 (3%)	0	100	100
3	X	208/217 (96%)	200 (96%)	8 (4%)	0	100	100
4	D	227/234 (97%)	221 (97%)	5 (2%)	1 (0%)	34	62
4	G	227/234 (97%)	221 (97%)	5 (2%)	1 (0%)	34	62
4	N	227/234 (97%)	219 (96%)	7 (3%)	1 (0%)	34	62
4	Y	227/234 (97%)	218 (96%)	8 (4%)	1 (0%)	34	62
5	F	214/215 (100%)	207 (97%)	7 (3%)	0	100	100
5	H	214/215 (100%)	206 (96%)	8 (4%)	0	100	100
5	Q	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
5	Z	215/215 (100%)	209 (97%)	6 (3%)	0	100	100
All	All	4278/4496 (95%)	4135 (97%)	137 (3%)	6 (0%)	51	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	Y	86	PRO
2	C	56	SER
4	N	86	PRO
4	G	86	PRO
2	L	117	ASP
4	D	86	PRO

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	168/196 (86%)	166 (99%)	2 (1%)	71	89
1	B	168/196 (86%)	165 (98%)	3 (2%)	59	82
1	K	168/196 (86%)	166 (99%)	2 (1%)	71	89
1	T	168/196 (86%)	164 (98%)	4 (2%)	49	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	196/201 (98%)	190 (97%)	6 (3%)	40	71
2	L	191/201 (95%)	185 (97%)	6 (3%)	40	71
2	O	196/201 (98%)	190 (97%)	6 (3%)	40	71
2	W	196/201 (98%)	187 (95%)	9 (5%)	27	56
3	E	174/178 (98%)	168 (97%)	6 (3%)	37	67
3	M	172/178 (97%)	166 (96%)	6 (4%)	36	67
3	P	174/178 (98%)	169 (97%)	5 (3%)	42	72
3	X	172/178 (97%)	166 (96%)	6 (4%)	36	67
4	D	199/204 (98%)	191 (96%)	8 (4%)	31	62
4	G	199/204 (98%)	191 (96%)	8 (4%)	31	62
4	N	199/204 (98%)	195 (98%)	4 (2%)	55	80
4	Y	199/204 (98%)	193 (97%)	6 (3%)	41	72
5	F	190/189 (100%)	184 (97%)	6 (3%)	39	69
5	H	190/189 (100%)	184 (97%)	6 (3%)	39	69
5	Q	189/189 (100%)	185 (98%)	4 (2%)	53	79
5	Z	191/189 (101%)	186 (97%)	5 (3%)	46	75
All	All	3699/3872 (96%)	3591 (97%)	108 (3%)	42	72

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	354	ASN
1	A	484	GLU
2	O	25	SER
2	O	65	ARG
2	O	85	SER
2	O	108	ARG
2	O	119	TRP
2	O	147	THR
3	P	3	VAL
3	P	83	GLU
3	P	172	SER
3	P	179	SER
3	P	204	SER
4	D	5	GLN
4	D	37	ASP

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Mol	Chain	Res	Type
4	D	58	SER
4	D	67	SER
4	D	105	ASP
4	D	143	SER
4	D	188	SER
4	D	211	CYS
5	F	7	SER
5	F	122	ASP
5	F	154	LEU
5	F	175	LEU
5	F	176	SER
5	F	195	GLU
1	B	334	ASN
1	B	377	PHE
1	B	399	SER
2	C	61	SER
2	C	121	GLN
2	C	129	SER
2	C	188	SER
2	C	208	GLN
2	C	212	CYS
3	E	51	SER
3	E	83	GLU
3	E	125	SER
3	E	171	GLN
3	E	172	SER
3	E	173	ASN
4	G	7	SER
4	G	60	TYR
4	G	68	ARG
4	G	76	SER
4	G	116	ASP
4	G	153	LEU
4	G	202	SER
4	G	221	LYS
5	H	52	SER
5	H	56	ASN
5	H	83	PHE
5	H	95	SER
5	H	142	ARG
5	H	214	CYS
1	K	369	TYR

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Mol	Chain	Res	Type
1	K	469	SER
2	L	25	SER
2	L	61	SER
2	L	63	SER
2	L	191	LEU
2	L	203	SER
2	L	213	ASN
3	M	9	SER
3	M	11	SER
3	M	27	SER
3	M	51	SER
3	M	65	SER
3	M	194	SER
4	N	7	SER
4	N	81	SER
4	N	128	SER
4	N	198	THR
5	Q	11	LEU
5	Q	92	ASN
5	Q	121	SER
5	Q	176	SER
1	T	408	ARG
1	T	428	ASP
1	T	457	ARG
1	T	484	GLU
2	W	25	SER
2	W	54	ASP
2	W	55	ASP
2	W	63	SER
2	W	103	MET
2	W	159	LYS
2	W	180	HIS
2	W	208	GLN
2	W	212	CYS
3	X	27	SER
3	X	67	SER
3	X	80	LEU
3	X	169	SER
3	X	173	ASN
3	X	194	SER
4	Y	1	GLN
4	Y	7	SER

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Mol	Chain	Res	Type
4	Y	30	SER
4	Y	60	TYR
4	Y	106	ARG
4	Y	116	ASP
5	Z	49	TYR
5	Z	79	GLN
5	Z	145	LYS
5	Z	156	SER
5	Z	188	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	ASN
2	O	1	GLN
2	O	215	ASN
3	P	28	ASN
3	P	188	GLN
4	D	5	GLN
4	D	214	ASN
5	F	137	ASN
5	F	147	GLN
2	C	121	GLN
3	E	171	GLN
3	E	173	ASN
4	G	3	GLN
4	G	5	GLN
2	L	171	ASN
2	L	215	ASN
3	M	130	GLN
3	M	132	ASN
3	M	171	GLN
1	T	354	ASN
2	W	82	GLN
4	Y	1	GLN
4	Y	62	ASN
5	Z	155	GLN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
6	NAG	T	601	1	14,14,15	0.28	0	17,19,21	0.48	0
6	NAG	A	601	1	14,14,15	0.52	0	17,19,21	0.51	0
6	NAG	B	601	1	14,14,15	0.37	0	17,19,21	0.44	0
6	NAG	K	601	1	14,14,15	0.37	0	17,19,21	0.54	0

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
6	NAG	T	601	1	-	0/6/23/26	0/1/1/1
6	NAG	A	601	1	-	2/6/23/26	0/1/1/1
6	NAG	B	601	1	-	0/6/23/26	0/1/1/1
6	NAG	K	601	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	601	NAG	O5-C5-C6-O6
6	A	601	NAG	C4-C5-C6-O6
6	K	601	NAG	O5-C5-C6-O6

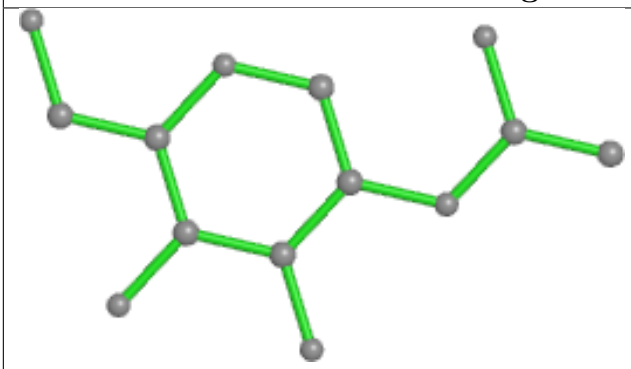
There are no ring outliers.

2 monomers are involved in 2 short contacts:

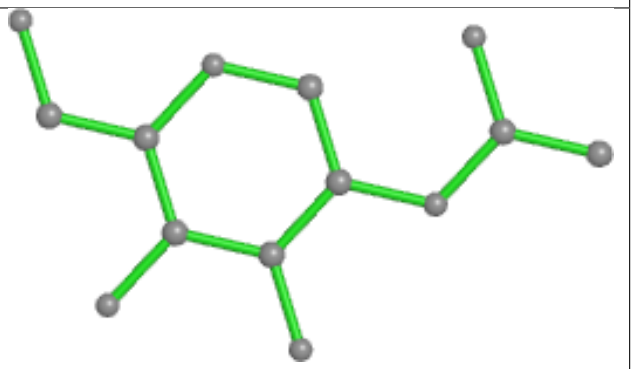
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	601	NAG	1	0
6	K	601	NAG	1	0

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 then 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.

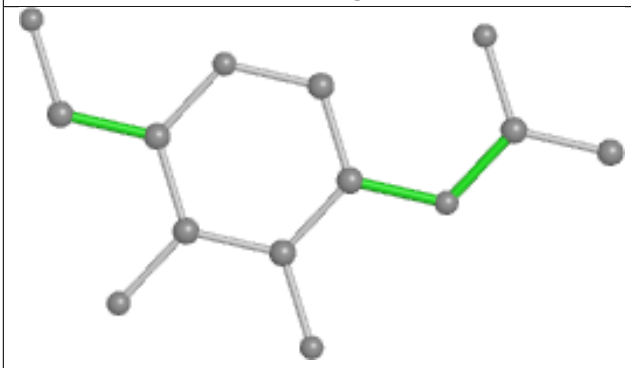
Ligand NAG T 601



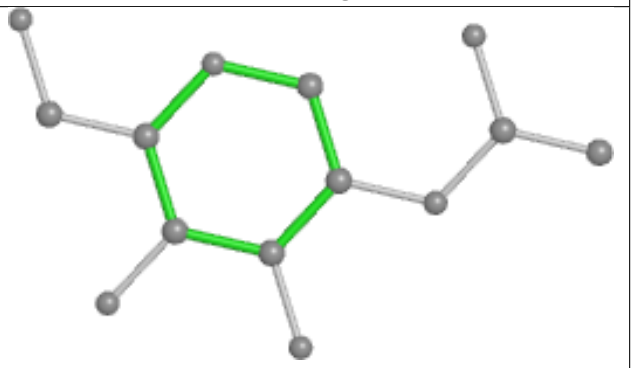
Bond lengths



Bond angles

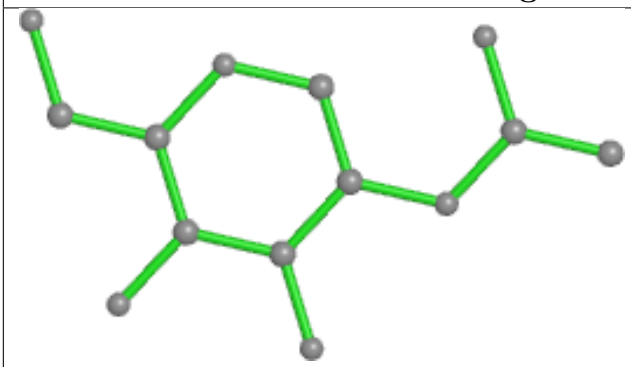


Torsions

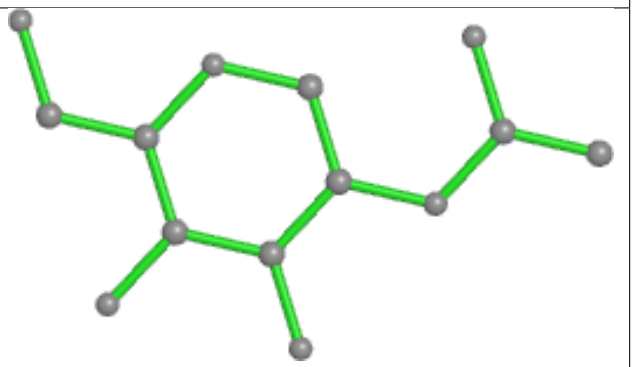


Rings

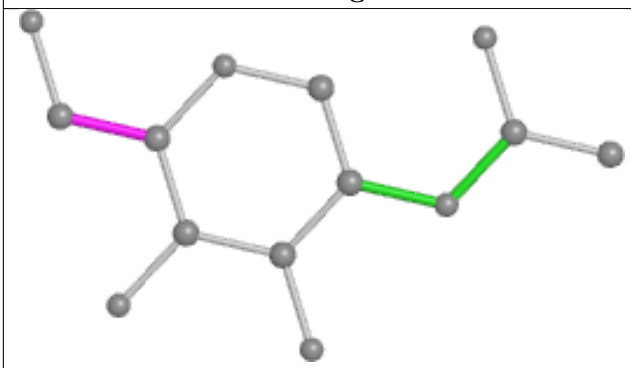
Ligand NAG A 601



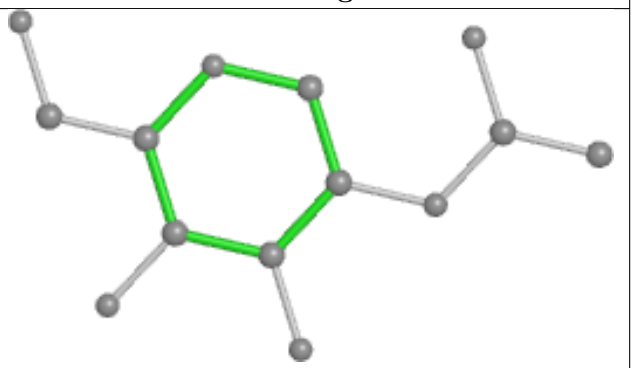
Bond lengths



Bond angles

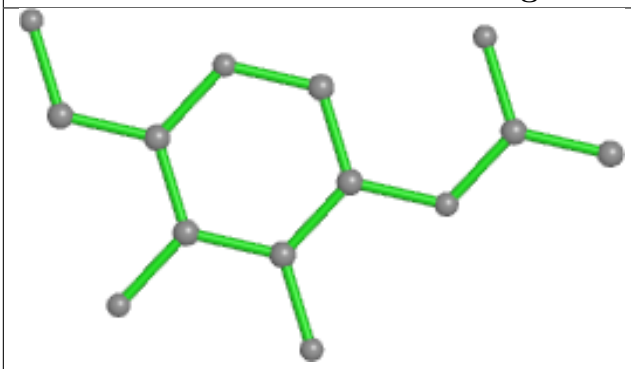


Torsions

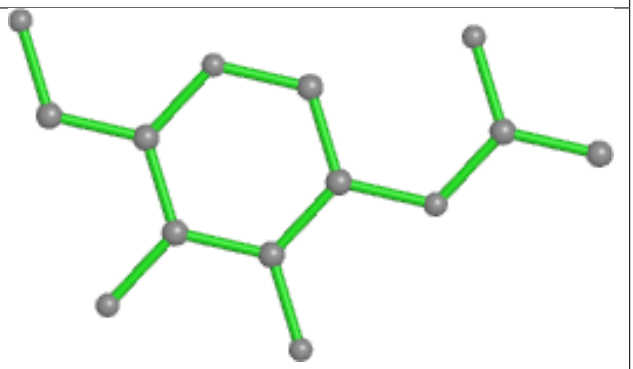


Rings

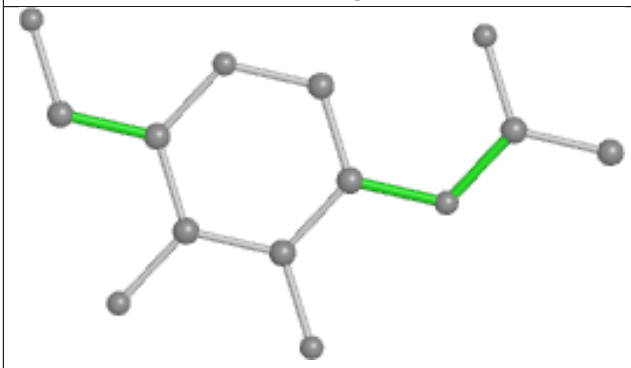
Ligand NAG B 601



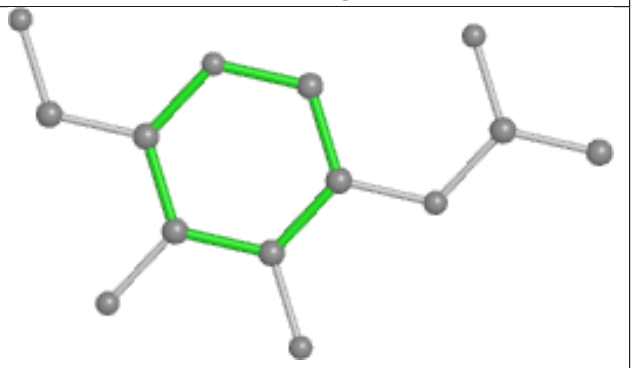
Bond lengths



Bond angles

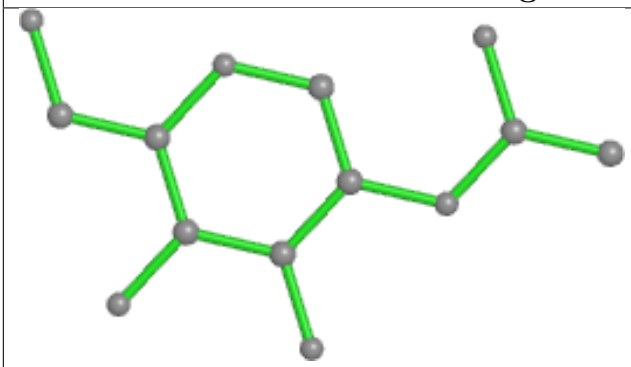


Torsions

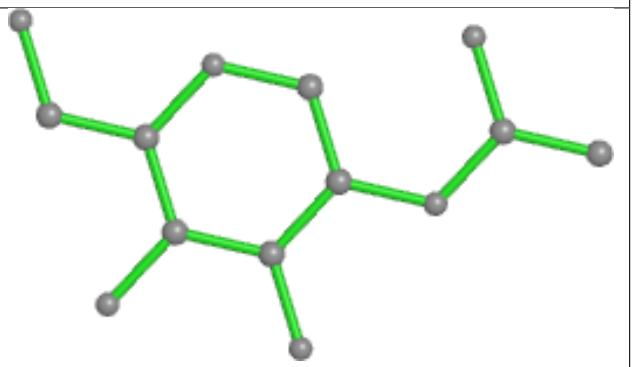


Rings

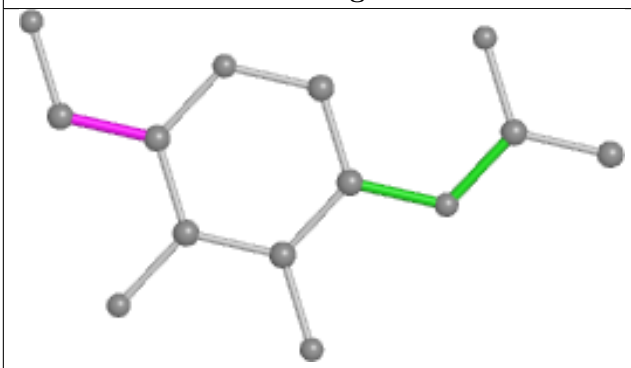
Ligand NAG K 601



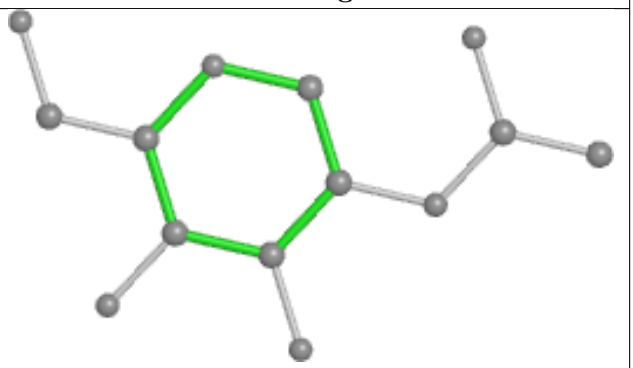
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	195/223 (87%)	-0.02	0 100 100	35, 55, 77, 93	0
1	B	195/223 (87%)	-0.01	1 (0%) 91 90	28, 46, 70, 97	0
1	K	195/223 (87%)	-0.07	0 100 100	30, 52, 69, 80	0
1	T	195/223 (87%)	0.26	6 (3%) 49 44	43, 71, 110, 126	0
2	C	230/235 (97%)	0.18	1 (0%) 92 92	38, 70, 96, 103	0
2	L	224/235 (95%)	0.16	2 (0%) 84 84	34, 67, 110, 128	0
2	O	230/235 (97%)	-0.06	0 100 100	44, 62, 80, 92	0
2	W	230/235 (97%)	0.64	16 (6%) 16 12	62, 88, 118, 134	0
3	E	213/217 (98%)	0.03	0 100 100	39, 58, 88, 104	0
3	M	210/217 (96%)	0.11	4 (1%) 66 64	39, 57, 113, 125	0
3	P	213/217 (98%)	-0.03	1 (0%) 91 90	37, 53, 82, 95	0
3	X	210/217 (96%)	0.34	8 (3%) 40 35	59, 76, 110, 128	0
4	D	229/234 (97%)	-0.03	3 (1%) 77 76	42, 53, 74, 126	0
4	G	229/234 (97%)	0.10	3 (1%) 77 76	39, 51, 73, 108	0
4	N	229/234 (97%)	0.07	3 (1%) 77 76	34, 48, 70, 110	0
4	Y	229/234 (97%)	0.21	4 (1%) 70 68	48, 74, 95, 118	0
5	F	215/215 (100%)	0.02	2 (0%) 84 84	42, 64, 104, 111	0
5	H	215/215 (100%)	0.25	4 (1%) 66 64	41, 68, 95, 109	0
5	Q	215/215 (100%)	0.16	1 (0%) 91 90	33, 58, 79, 109	0
5	Z	215/215 (100%)	0.24	5 (2%) 60 57	50, 72, 96, 133	0
All	All	4316/4496 (95%)	0.13	64 (1%) 73 72	28, 61, 101, 134	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	N	146	THR	7.8
2	W	146	SER	5.3
4	D	145	SER	4.8
3	X	130	GLN	4.6
4	Y	146	THR	4.6
5	Q	214	CYS	4.6
4	N	145	SER	4.2
4	D	146	THR	3.6
4	Y	147	SER	3.5
5	F	94	TYR	3.4
2	W	8	GLY	3.4
2	W	220	ASN	3.2
4	N	147	SER	3.2
1	T	387	LEU	3.1
3	X	122	PHE	3.0
2	W	151	THR	3.0
5	H	154	LEU	2.9
5	H	113	PRO	2.8
2	W	218	PRO	2.8
2	W	170	TRP	2.7
2	L	207	THR	2.7
2	W	217	LYS	2.6
4	G	85	SER	2.6
2	W	147	THR	2.6
3	P	1	GLN	2.5
2	W	166	VAL	2.5
5	Z	1	GLU	2.5
3	M	122	PHE	2.4
5	F	92	ASN	2.4
2	C	10	GLN	2.4
2	W	129	SER	2.4
4	G	147	SER	2.3
1	T	335	LEU	2.3
3	X	134	ALA	2.3
2	W	194	LEU	2.3
1	T	334	ASN	2.3
2	W	148	SER	2.3
1	T	338	PHE	2.3
2	W	227	VAL	2.2
2	W	196	SER	2.2
2	L	227	VAL	2.2
4	Y	149	GLY	2.2
3	X	1	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
4	G	143	SER	2.2
4	D	85	SER	2.2
3	M	1	GLN	2.2
2	W	117	ASP	2.1
1	B	334	ASN	2.1
5	Z	65	SER	2.1
5	Z	213	GLU	2.1
1	T	393	THR	2.1
3	M	162	GLY	2.1
5	Z	94	TYR	2.1
5	Z	96	LEU	2.1
5	H	213	GLU	2.1
2	W	36	TRP	2.1
3	X	170	LYS	2.1
5	H	125	LEU	2.1
3	X	195	TYR	2.1
1	T	520	ALA	2.1
3	M	206	VAL	2.1
3	X	161	ALA	2.1
4	Y	36	TRP	2.0
3	X	190	LYS	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 monosaccharides 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, 95^{th} 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
6	NAG	T	601	14/15	0.67	0.24	93,101,107,108	0
6	NAG	A	601	14/15	0.81	0.17	67,77,91,92	0

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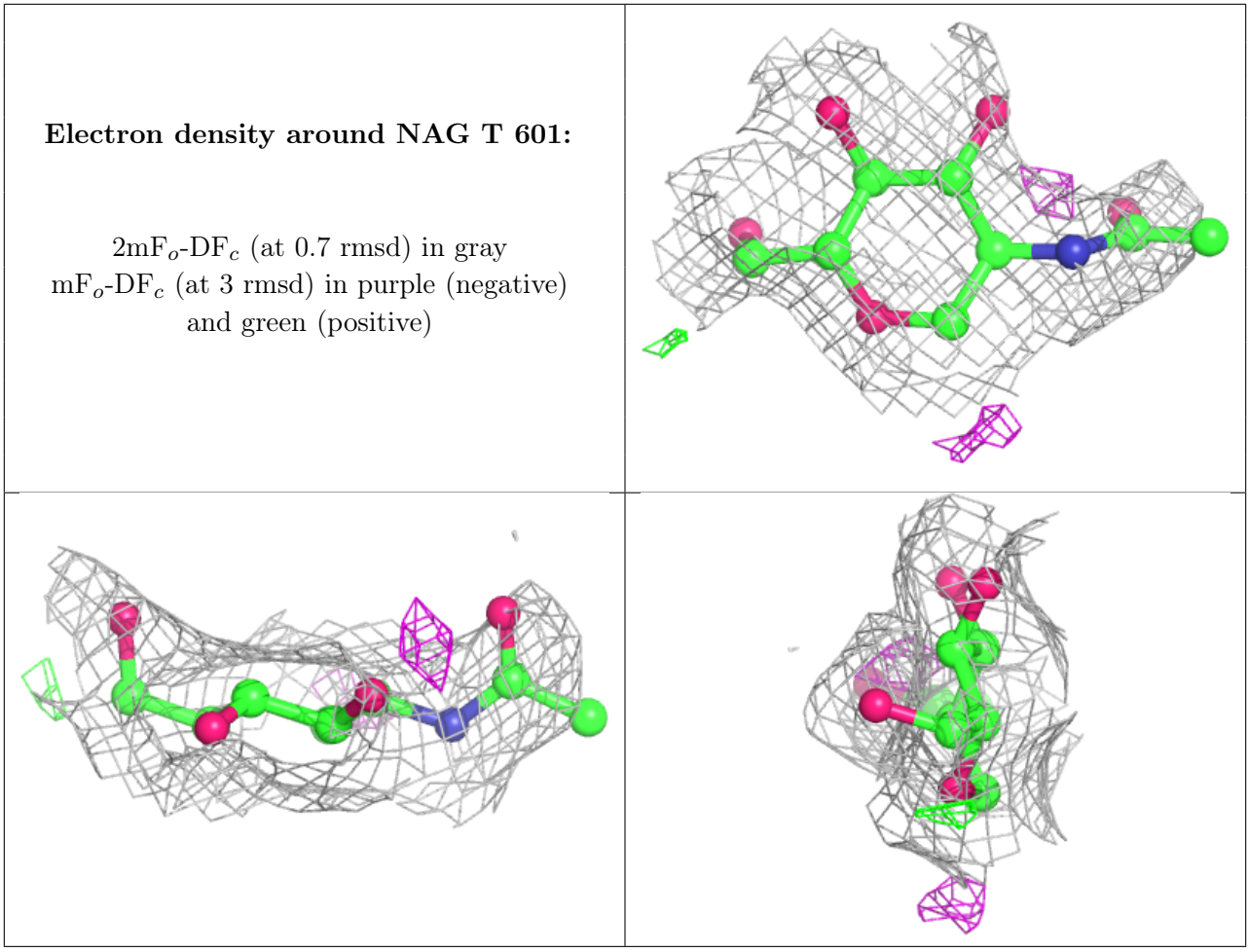
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	K	601	14/15	0.85	0.19	64,90,109,109	0
6	NAG	B	601	14/15	0.87	0.18	50,77,90,94	0

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.

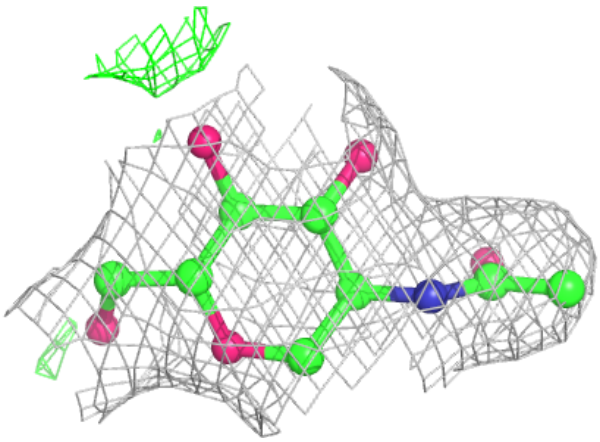
Electron density around NAG T 601:

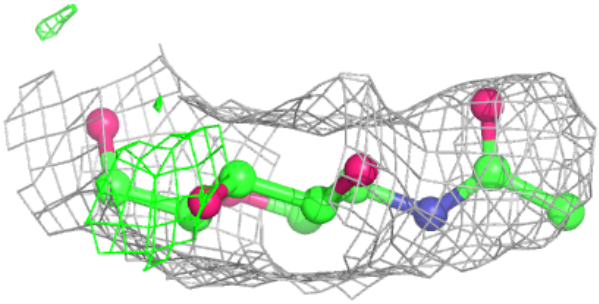
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

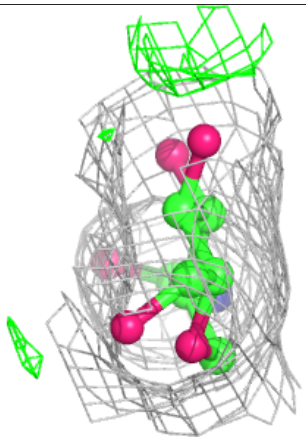


Electron density around NAG A 601:

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

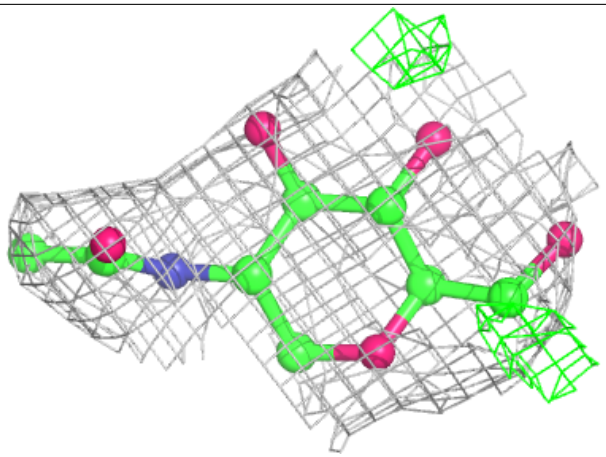


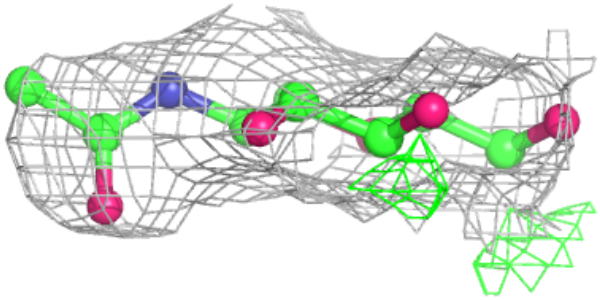


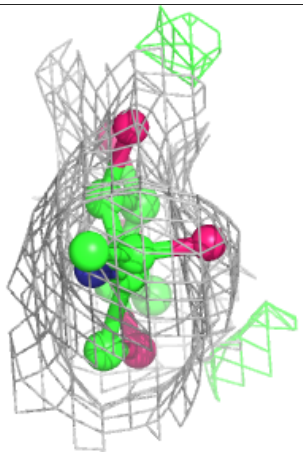


Electron density around NAG K 601:

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

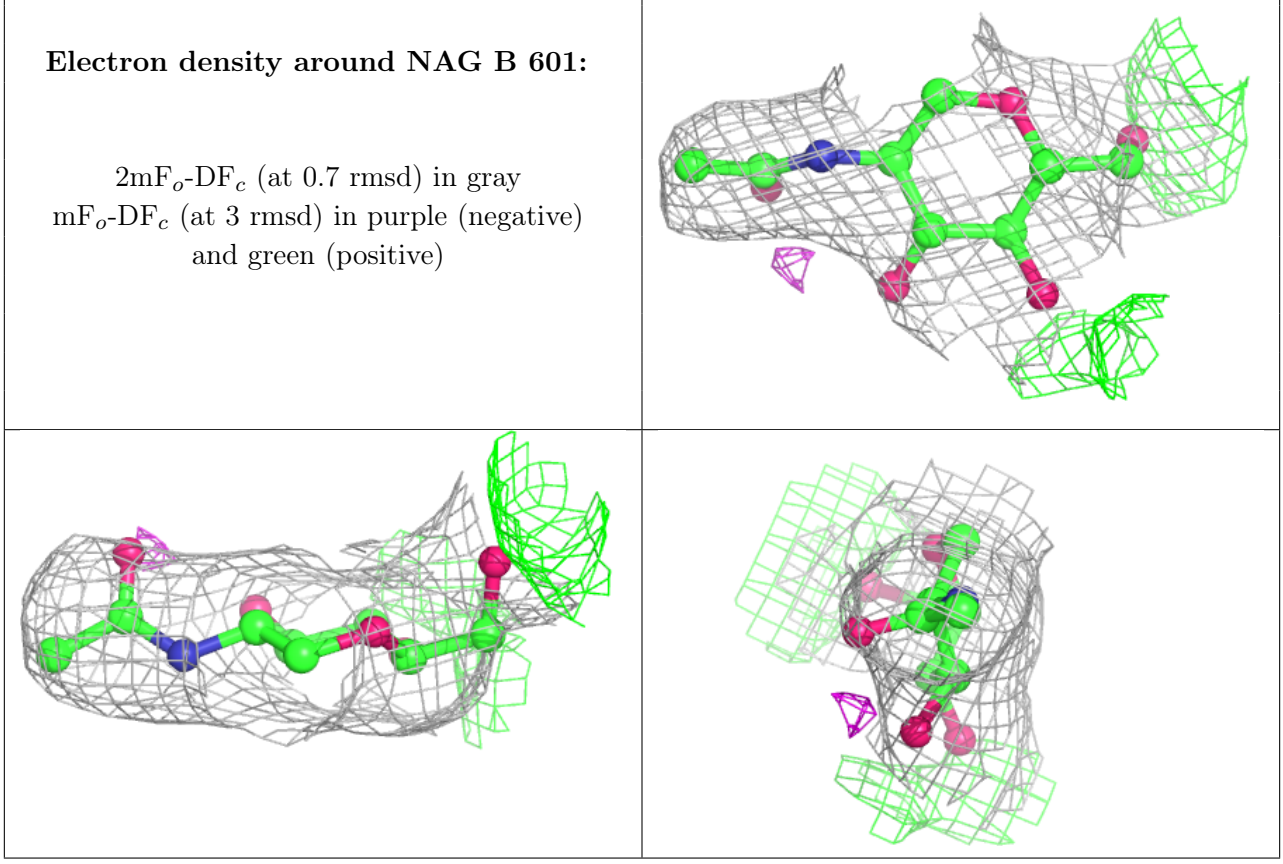






Electron density around NAG B 601:

$2mF_o$-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.