



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2026 – 04:18 am BST

PDB ID : 30BG / pdb_000030bg
Title : Structure of the Hepatitis C Virus E2 Core from Genotype 6a in Complex with
1-69 Germline-Reverted Variants of the Broadly Neutralizing Antibody U1
Authors : Yechezkel, I.; Tzarum, N.
Deposited on : 2026-04-19
Resolution : 3.31 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

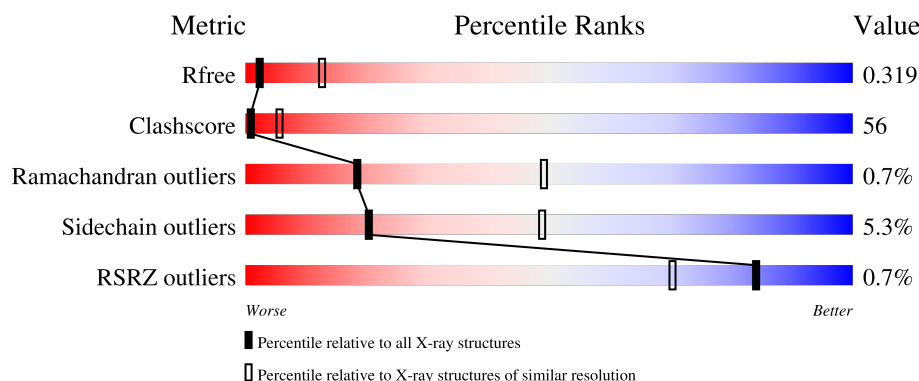
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	189	2% 38% 34% 5% 23%
2	H	230	33% 57% 7%
3	L	214	41% 55%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4405 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 HCV E2 envelope protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	146	Total	C	N	O	S	0	0	0
			1145	736	193	204	12			

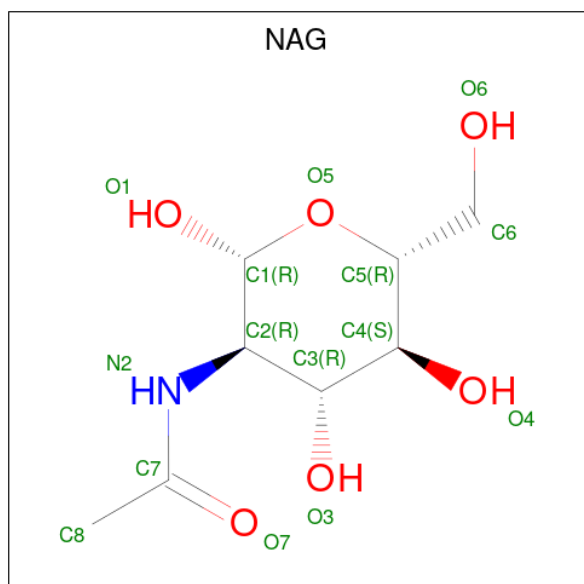
- Molecule 2 is a protein called Fab U1 1-69 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1601	1014	267	313	7			

- Molecule 3 is a protein called Fab U1 1-69 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1616	1012	272	328	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

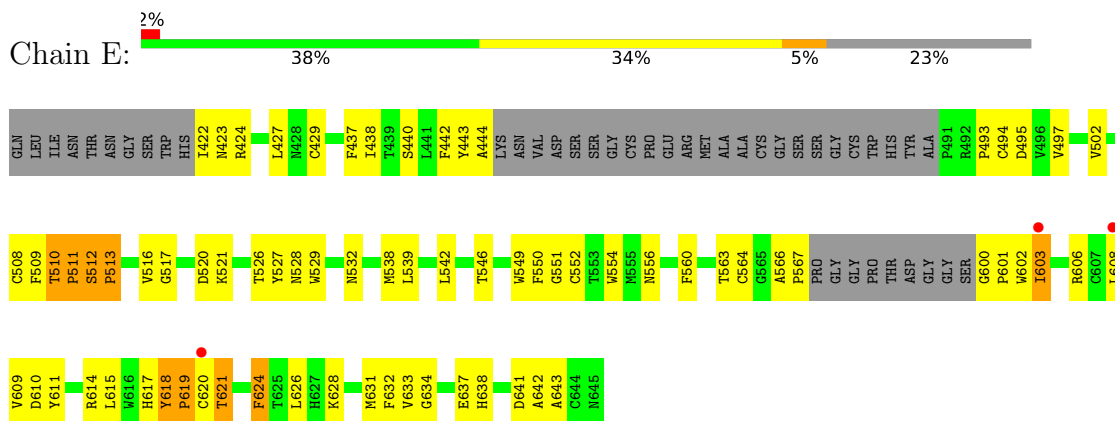
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	5	Total	O	0	0
			5	5		
5	H	7	Total	O	0	0
			7	7		
5	L	3	Total	O	0	0
			3	3		

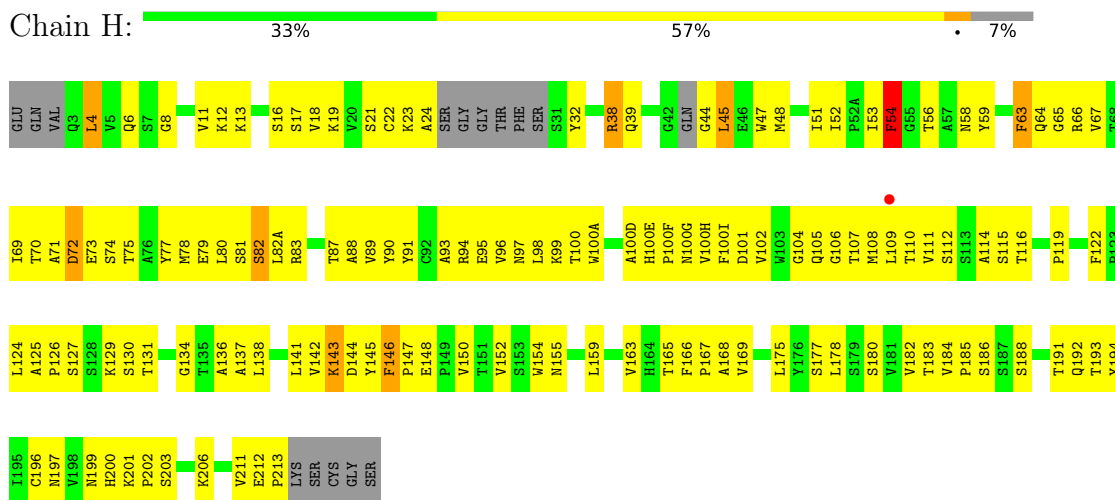
3 Residue-property plots

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

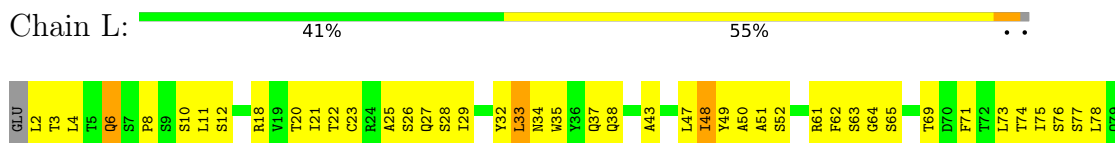
• Molecule 1: HCV E2 envelope protein



• Molecule 2: Fab U1 1-69 heavy chain



• Molecule 3: Fab U1 1-69 light chain



W148	K149	V150	D151	Q155	E161	T164	E165	Q166	D167	S168	K169	D170	S171	T172	Y173	S174	L175	S176	W180	W181	W182	W183	W184	W185	W186	W187	K188	H189	K190	V191	V192	W196	W197	H198	Q199	G200	L201	S202	S203	K207	S208	F209	N210	R211	G212	GLJ	CYS	K145	W146	W147				
W148	K149	V150	D151	Q155	E161	T164	E165	Q166	D167	S168	K169	D170	S171	T172	Y173	S174	L175	S176	W180	W181	W182	W183	W184	W185	W186	W187	K188	H189	K190	V191	V192	W196	W197	H198	Q199	G200	L201	S202	S203	K207	S208	F209	N210	R211	G212	GLJ	CYS	K145	W146	W147				
P80	F83	A84	T85	Y86	Y87	C88	Q89	Q90	Y92	S93	T94	P95	R96	T97	F98	G99	Q100	G101	T102	L106	K107	R108	T109	V110	A111	A112	F118	P119	P120	S121	D122	E123	Q124	L125	K126	S127	G128	T129	S130	S131	S132	V133	C134	L135	L136	M137	H138	F139	Y140	P141	R142	K145	W146	W147

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.85Å 79.07Å 133.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.61 – 3.31 54.61 – 3.31	Depositor EDS
% Data completeness (in resolution range)	87.0 (54.61-3.31) 86.9 (54.61-3.31)	Depositor EDS
R_{merge}	0.68	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.268 , 0.324 0.268 , 0.319	Depositor DCC
R_{free} test set	416 reflections (4.17%)	wwPDB-VP
Wilson B-factor (Å ²)	82.0	Xtriage
Anisotropy	0.756	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4405	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	E	0.93	2/1183 (0.2%)	1.32	6/1618 (0.4%)
2	H	0.76	1/1638 (0.1%)	1.03	1/2232 (0.0%)
3	L	0.70	0/1651	0.95	1/2243 (0.0%)
All	All	0.79	3/4472 (0.1%)	1.09	8/6093 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	619	PRO	N-CA	16.82	1.69	1.47
1	E	618	TYR	C-N	9.52	1.45	1.33
2	H	146	PHE	C-N	8.37	1.50	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	618	TYR	CA-C-N	18.62	138.55	119.56
1	E	618	TYR	C-N-CA	18.62	138.55	119.56
1	E	619	PRO	N-CA-C	-8.42	102.89	113.84
1	E	511	PRO	N-CA-C	-8.41	97.29	110.50
1	E	619	PRO	CA-N-CD	-7.66	101.27	112.00
2	H	54	PHE	CB-CA-C	-7.25	96.57	111.22
3	L	49	TYR	CA-C-O	-5.75	114.61	121.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	511	PRO	CB-CA-C	5.47	117.52	111.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	38	ARG	Sidechain

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	E	1145	0	1084	120	1
2	H	1601	0	1580	209	3
3	L	1616	0	1581	169	3
4	E	28	0	26	0	1
5	E	5	0	0	0	0
5	H	7	0	0	1	0
5	L	3	0	0	0	0
All	All	4405	0	4271	483	4

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 56.

All (483) 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)
3:L:33:LEU:HD23	3:L:71:PHE:CG	1.41	1.53
1:E:619:PRO:N	1:E:619:PRO:CA	1.69	1.37
3:L:33:LEU:CD2	3:L:71:PHE:CD1	2.08	1.37
3:L:33:LEU:HD23	3:L:71:PHE:CD1	1.63	1.34
1:E:510:THR:HG22	1:E:550:PHE:CD1	1.73	1.22
1:E:510:THR:HG22	1:E:550:PHE:CE1	1.82	1.14
2:H:23:LYS:HA	2:H:75:THR:HG22	1.19	1.13
2:H:127:SER:H	2:H:130:SER:HB2	1.10	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:29:ILE:HG23	3:L:92:TYR:CB	1.79	1.11
2:H:23:LYS:HA	2:H:75:THR:CG2	1.82	1.10
3:L:33:LEU:CD2	3:L:71:PHE:CG	2.31	1.10
1:E:509:PHE:HZ	1:E:611:TYR:CG	1.70	1.09
3:L:29:ILE:HG23	3:L:92:TYR:HB3	1.12	1.09
2:H:163:VAL:HG22	2:H:182:VAL:HG12	1.32	1.08
2:H:64:GLN:HG3	2:H:65:GLY:H	1.19	1.06
1:E:510:THR:HB	1:E:511:PRO:CD	1.87	1.05
2:H:97:ASN:HB2	2:H:100(E):HIS:O	1.57	1.03
2:H:22:CYS:O	2:H:75:THR:HB	1.57	1.02
2:H:87:THR:OG1	2:H:110:THR:HA	1.58	1.01
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.04	1.01
2:H:116:THR:HG23	2:H:146:PHE:O	1.59	1.01
2:H:184:VAL:HG11	2:H:194:TYR:CE1	1.95	0.99
1:E:510:THR:CB	1:E:511:PRO:CD	2.41	0.99
3:L:33:LEU:HD22	3:L:71:PHE:CD1	1.97	0.99
1:E:509:PHE:CZ	1:E:611:TYR:CD1	2.51	0.97
2:H:97:ASN:OD1	2:H:100(G):ASN:OD1	1.82	0.97
2:H:23:LYS:HG3	2:H:75:THR:CG2	1.94	0.97
3:L:191:VAL:HG22	3:L:210:ASN:ND2	1.79	0.97
1:E:549:TRP:CZ3	1:E:603:ILE:HG23	2.01	0.96
1:E:556:ASN:OD1	1:E:560:PHE:HB2	1.64	0.96
2:H:163:VAL:HG22	2:H:182:VAL:CG1	1.94	0.96
3:L:29:ILE:CG2	3:L:92:TYR:HB3	1.96	0.96
2:H:119:PRO:CB	2:H:145:TYR:HB3	1.95	0.95
1:E:608:LEU:HD13	1:E:621:THR:HG21	1.47	0.95
2:H:51:ILE:HD11	2:H:71:ALA:HB2	1.46	0.95
1:E:601:PRO:O	1:E:609:VAL:HG23	1.67	0.95
1:E:509:PHE:CZ	1:E:611:TYR:CG	2.55	0.94
2:H:52:ILE:O	2:H:54:PHE:O	1.85	0.94
2:H:53:ILE:HG13	2:H:54:PHE:CD1	2.02	0.94
1:E:510:THR:HB	1:E:511:PRO:HD3	1.50	0.93
2:H:51:ILE:HG21	2:H:69:ILE:HG22	1.48	0.93
2:H:51:ILE:HG23	2:H:69:ILE:HG21	1.50	0.93
1:E:510:THR:HG22	1:E:550:PHE:HD1	1.33	0.93
3:L:175:LEU:HD23	3:L:176:SER:N	1.84	0.93
3:L:28:SER:HA	3:L:69:THR:CG2	1.98	0.92
1:E:510:THR:CG2	1:E:550:PHE:CE1	2.52	0.92
3:L:189:HIS:O	3:L:211:ARG:NH2	2.01	0.92
2:H:97:ASN:HA	2:H:100(G):ASN:OD1	1.69	0.91
2:H:53:ILE:CD1	2:H:54:PHE:CE1	2.53	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:23:LYS:CA	2:H:75:THR:HG22	2.00	0.91
3:L:37:GLN:HG3	3:L:86:TYR:CE1	2.06	0.91
1:E:614:ARG:NH1	1:E:621:THR:OG1	2.04	0.90
2:H:119:PRO:HB3	2:H:145:TYR:CB	1.98	0.90
2:H:95:GLU:HG2	2:H:100(F):PRO:HB2	1.53	0.89
3:L:135:LEU:HD11	3:L:137:ASN:HD22	1.38	0.89
3:L:145:LYS:HB2	3:L:197:THR:HB	1.56	0.88
3:L:37:GLN:HB2	3:L:86:TYR:HE1	1.39	0.88
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.56	0.87
1:E:611:TYR:CZ	1:E:614:ARG:HA	2.09	0.86
2:H:51:ILE:CD1	2:H:71:ALA:HB2	2.05	0.86
2:H:163:VAL:CG2	2:H:182:VAL:HG12	2.06	0.86
3:L:29:ILE:HG22	3:L:29:ILE:O	1.75	0.86
3:L:135:LEU:HD11	3:L:137:ASN:ND2	1.90	0.86
3:L:6:GLN:OE1	3:L:99:GLY:HA3	1.76	0.86
1:E:510:THR:CG2	1:E:550:PHE:HE1	1.89	0.86
3:L:183:LYS:O	3:L:187:GLU:HG2	1.75	0.86
1:E:510:THR:CB	1:E:511:PRO:HD2	2.06	0.85
3:L:33:LEU:HD23	3:L:71:PHE:CD2	2.10	0.85
2:H:134:GLY:O	2:H:186:SER:OG	1.93	0.85
2:H:64:GLN:HG3	2:H:65:GLY:N	1.93	0.84
1:E:510:THR:OG1	1:E:511:PRO:HD2	1.78	0.83
2:H:138:LEU:HD21	2:H:211:VAL:HB	1.57	0.83
2:H:23:LYS:CB	2:H:75:THR:HG21	2.08	0.83
3:L:93:SER:O	3:L:96:ARG:NH1	2.11	0.83
3:L:33:LEU:HD22	3:L:71:PHE:CE1	2.14	0.83
3:L:166:GLN:HE21	3:L:171:SER:HB3	1.42	0.83
2:H:200:HIS:HD1	2:H:203:SER:HG	1.00	0.82
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.61	0.82
2:H:51:ILE:HA	2:H:56:THR:OG1	1.79	0.81
1:E:509:PHE:HZ	1:E:611:TYR:CB	1.93	0.81
1:E:608:LEU:CD1	1:E:621:THR:HG21	2.09	0.81
2:H:163:VAL:HG13	2:H:182:VAL:HG12	1.63	0.81
3:L:28:SER:HA	3:L:69:THR:HG23	1.63	0.81
1:E:549:TRP:CE3	1:E:603:ILE:CG2	2.64	0.81
1:E:549:TRP:CZ3	1:E:603:ILE:CG2	2.64	0.81
2:H:51:ILE:CG2	2:H:69:ILE:CG2	2.59	0.80
2:H:95:GLU:OE2	2:H:100(F):PRO:O	2.00	0.80
2:H:23:LYS:CA	2:H:75:THR:CG2	2.59	0.80
2:H:51:ILE:HG21	2:H:69:ILE:CG2	2.12	0.79
2:H:51:ILE:CG2	2:H:69:ILE:HG21	2.11	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:549:TRP:CE3	1:E:603:ILE:HG22	2.16	0.79
1:E:423:ASN:HB3	1:E:527:TYR:HB3	1.63	0.79
1:E:546:THR:HG21	1:E:634:GLY:HA3	1.63	0.79
3:L:37:GLN:HB2	3:L:86:TYR:CE1	2.18	0.79
3:L:175:LEU:HD23	3:L:175:LEU:C	2.08	0.79
2:H:115:SER:O	2:H:146:PHE:HD2	1.65	0.78
2:H:124:LEU:HB3	3:L:118:PHE:CD2	2.17	0.78
2:H:114:ALA:HB3	2:H:146:PHE:CE2	2.17	0.78
3:L:27:GLN:O	3:L:69:THR:HG22	1.82	0.78
1:E:508:CYS:SG	1:E:550:PHE:CZ	2.76	0.78
2:H:53:ILE:HD12	2:H:54:PHE:HE1	1.48	0.78
2:H:166:PHE:O	2:H:178:LEU:HD11	1.84	0.77
2:H:89:VAL:HA	2:H:107:THR:O	1.85	0.77
3:L:28:SER:HA	3:L:69:THR:HG22	1.65	0.77
3:L:73:LEU:HD12	3:L:74:THR:H	1.50	0.77
2:H:126:PRO:HD3	2:H:138:LEU:HD13	1.65	0.76
2:H:23:LYS:HG3	2:H:75:THR:HG21	1.68	0.75
1:E:520:ASP:O	1:E:538:MET:HE2	1.85	0.75
3:L:6:GLN:CG	3:L:100:GLN:OE1	2.35	0.75
2:H:131:THR:HG22	2:H:136:ALA:CB	2.16	0.74
2:H:53:ILE:HD12	2:H:54:PHE:CE1	2.21	0.74
3:L:140:TYR:CD1	3:L:173:TYR:HE1	2.05	0.74
1:E:509:PHE:HZ	1:E:611:TYR:CD1	1.93	0.74
2:H:95:GLU:HG2	2:H:100(F):PRO:CB	2.18	0.74
2:H:67:VAL:CG2	2:H:80:LEU:HD21	2.18	0.73
2:H:154:TRP:HB3	2:H:159:LEU:HD23	1.69	0.73
3:L:33:LEU:CD2	3:L:71:PHE:CE1	2.67	0.73
2:H:23:LYS:CG	2:H:75:THR:HG21	2.19	0.73
2:H:67:VAL:HG22	2:H:80:LEU:HD21	1.70	0.73
2:H:115:SER:O	2:H:146:PHE:CD2	2.43	0.72
2:H:141:LEU:HD12	2:H:178:LEU:O	1.89	0.72
2:H:47:TRP:CZ3	3:L:95:PRO:HA	2.24	0.72
3:L:6:GLN:HG2	3:L:100:GLN:OE1	1.88	0.72
1:E:424:ARG:NH2	1:E:517:GLY:HA3	2.05	0.72
3:L:6:GLN:HG3	3:L:100:GLN:CD	2.15	0.72
2:H:23:LYS:CG	2:H:75:THR:CG2	2.67	0.71
3:L:28:SER:CA	3:L:69:THR:CG2	2.67	0.71
1:E:508:CYS:SG	1:E:550:PHE:CE1	2.84	0.70
3:L:2:LEU:CD2	3:L:27:GLN:HB3	2.22	0.70
3:L:170:ASP:OD1	3:L:170:ASP:N	2.24	0.70
3:L:112:ALA:HB1	3:L:201:LEU:HD21	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:632:PHE:CE2	1:E:637:GLU:HB2	2.26	0.70
3:L:37:GLN:CB	3:L:86:TYR:HE1	2.05	0.70
1:E:611:TYR:CE1	1:E:614:ARG:HA	2.26	0.69
2:H:23:LYS:CB	2:H:75:THR:CG2	2.71	0.69
3:L:2:LEU:HD21	3:L:27:GLN:OE1	1.93	0.69
1:E:509:PHE:HZ	1:E:611:TYR:HB3	1.56	0.69
1:E:528:ASN:ND2	1:E:532:ASN:ND2	2.41	0.69
2:H:127:SER:N	2:H:130:SER:HB2	1.95	0.69
1:E:556:ASN:OD1	1:E:560:PHE:CB	2.39	0.69
2:H:64:GLN:CG	2:H:65:GLY:H	1.97	0.69
2:H:67:VAL:HG22	2:H:80:LEU:CD2	2.23	0.69
2:H:154:TRP:CD1	2:H:182:VAL:CG1	2.76	0.68
2:H:154:TRP:NE1	2:H:182:VAL:HG13	2.09	0.68
3:L:111:ALA:O	3:L:139:PHE:HA	1.93	0.68
3:L:2:LEU:HD22	3:L:27:GLN:HB3	1.75	0.68
3:L:151:ASP:CG	3:L:189:HIS:HB3	2.19	0.68
1:E:512:SER:HB2	1:E:513:PRO:CD	2.23	0.68
2:H:99:LYS:NZ	3:L:50:ALA:HB1	2.09	0.68
2:H:95:GLU:CG	2:H:100(F):PRO:HB2	2.23	0.67
1:E:509:PHE:CZ	1:E:611:TYR:HB3	2.30	0.67
2:H:87:THR:HB	2:H:111:VAL:H	1.59	0.67
1:E:423:ASN:O	1:E:527:TYR:HA	1.94	0.67
2:H:152:VAL:HA	2:H:197:ASN:O	1.94	0.67
2:H:94:ARG:O	2:H:100(I):PHE:HA	1.95	0.67
3:L:191:VAL:HG22	3:L:210:ASN:HD21	1.58	0.67
1:E:624:PHE:HB3	1:E:643:ALA:HB1	1.77	0.66
1:E:626:LEU:HA	1:E:642:ALA:O	1.96	0.66
2:H:200:HIS:ND1	2:H:203:SER:OG	2.07	0.66
1:E:614:ARG:HH12	1:E:621:THR:HG1	1.43	0.66
3:L:29:ILE:CG2	3:L:29:ILE:O	2.44	0.66
1:E:440:SER:HA	1:E:443:TYR:O	1.95	0.66
2:H:188:SER:HB2	2:H:192:GLN:HG2	1.76	0.66
3:L:191:VAL:HA	3:L:210:ASN:HD22	1.61	0.66
3:L:37:GLN:CG	3:L:86:TYR:CE1	2.78	0.65
1:E:423:ASN:HB2	1:E:527:TYR:HD2	1.60	0.65
1:E:443:TYR:CE2	2:H:73:GLU:HB2	2.31	0.65
2:H:23:LYS:HB2	2:H:75:THR:HG21	1.79	0.65
3:L:181:LEU:HD23	3:L:185:ASP:HB3	1.79	0.65
1:E:510:THR:HB	1:E:511:PRO:HD2	1.68	0.65
1:E:619:PRO:N	1:E:619:PRO:C	2.53	0.65
2:H:154:TRP:CD1	2:H:182:VAL:HG11	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:53:ILE:HD11	2:H:54:PHE:CE1	2.31	0.65
2:H:163:VAL:CG1	2:H:182:VAL:HG12	2.26	0.65
1:E:521:LYS:O	1:E:538:MET:HE3	1.96	0.65
1:E:509:PHE:CD1	1:E:609:VAL:HG11	2.32	0.65
2:H:17:SER:HB3	2:H:81:SER:HA	1.78	0.65
3:L:33:LEU:HD12	3:L:34:ASN:N	2.13	0.64
1:E:422:ILE:O	1:E:529:TRP:CZ3	2.50	0.64
2:H:169:VAL:CG2	2:H:177:SER:OG	2.45	0.64
3:L:184:ALA:O	3:L:188:LYS:HG3	1.97	0.64
2:H:16:SER:O	2:H:82(A):LEU:HD12	1.96	0.64
3:L:21:ILE:HD13	3:L:102:THR:HG21	1.78	0.64
3:L:37:GLN:CB	3:L:86:TYR:CE1	2.81	0.64
2:H:11:VAL:HB	2:H:147:PRO:HG3	1.80	0.64
3:L:6:GLN:HA	3:L:22:THR:O	1.97	0.64
3:L:33:LEU:HD23	3:L:71:PHE:CB	2.22	0.64
2:H:8:GLY:CA	2:H:201:LYS:HD3	2.28	0.64
1:E:429:CYS:HB3	1:E:438:ILE:HD11	1.79	0.63
3:L:29:ILE:CG2	3:L:92:TYR:CB	2.64	0.63
1:E:423:ASN:CB	1:E:527:TYR:HB3	2.28	0.63
2:H:44:GLY:HA2	3:L:87:TYR:HE2	1.63	0.63
2:H:51:ILE:CD1	2:H:71:ALA:CB	2.76	0.63
2:H:98:LEU:HG	2:H:100(H):VAL:HG11	1.81	0.63
3:L:80:PRO:HA	3:L:106:ILE:CD1	2.29	0.62
3:L:61:ARG:HG3	3:L:75:ILE:HG23	1.81	0.62
2:H:13:LYS:HA	2:H:112:SER:O	1.99	0.62
2:H:38:ARG:HB2	2:H:90:TYR:CE2	2.35	0.62
2:H:163:VAL:HG13	2:H:182:VAL:CG1	2.29	0.62
2:H:23:LYS:HG2	2:H:24:ALA:H	1.63	0.62
3:L:73:LEU:HD12	3:L:74:THR:N	2.13	0.62
2:H:4:LEU:HB3	2:H:104:GLY:HA2	1.82	0.62
3:L:6:GLN:HG3	3:L:100:GLN:OE1	2.00	0.62
2:H:126:PRO:HG2	2:H:213:PRO:HB3	1.81	0.62
2:H:12:LYS:HE3	2:H:18:VAL:HB	1.82	0.61
2:H:154:TRP:CG	2:H:182:VAL:HG11	2.35	0.61
1:E:608:LEU:HD22	1:E:614:ARG:HD2	1.83	0.61
3:L:150:VAL:HG13	3:L:192:TYR:CE2	2.35	0.61
2:H:23:LYS:HG2	2:H:24:ALA:N	2.16	0.61
2:H:169:VAL:HG23	2:H:177:SER:OG	2.00	0.61
3:L:2:LEU:HD22	3:L:27:GLN:CB	2.30	0.61
1:E:512:SER:HB2	1:E:513:PRO:HD3	1.83	0.60
3:L:20:THR:HG22	3:L:74:THR:OG1	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:167:PRO:HD3	3:L:164:THR:HA	1.82	0.60
1:E:521:LYS:HA	1:E:538:MET:HE1	1.82	0.60
2:H:48:MET:SD	2:H:63:PHE:CE1	2.95	0.60
3:L:25:ALA:HB3	3:L:69:THR:HB	1.82	0.60
3:L:155:GLN:OE1	3:L:155:GLN:HA	2.02	0.60
1:E:438:ILE:O	1:E:442:PHE:HD2	1.84	0.60
1:E:422:ILE:C	1:E:424:ARG:H	2.08	0.59
1:E:563:THR:HG21	1:E:618:TYR:OH	2.02	0.59
1:E:556:ASN:OD1	1:E:560:PHE:N	2.35	0.59
3:L:27:GLN:C	3:L:69:THR:CG2	2.76	0.59
3:L:28:SER:CA	3:L:69:THR:HG22	2.32	0.59
2:H:18:VAL:HG22	2:H:19:LYS:N	2.18	0.59
2:H:97:ASN:CB	2:H:100(E):HIS:O	2.42	0.59
3:L:61:ARG:HD3	3:L:77:SER:O	2.03	0.58
2:H:142:VAL:O	2:H:178:LEU:N	2.33	0.58
3:L:27:GLN:C	3:L:69:THR:HG22	2.29	0.58
2:H:184:VAL:HG11	2:H:194:TYR:HE1	1.64	0.58
2:H:63:PHE:N	2:H:63:PHE:CD2	2.71	0.58
2:H:91:TYR:CE1	3:L:43:ALA:HB2	2.39	0.58
2:H:51:ILE:HG23	2:H:69:ILE:CG2	2.24	0.57
2:H:165:THR:HG23	2:H:180:SER:HB3	1.85	0.57
1:E:611:TYR:OH	1:E:617:HIS:HB2	2.04	0.57
2:H:154:TRP:CH2	2:H:196:CYS:HB3	2.39	0.57
3:L:124:GLN:HG2	3:L:129:THR:HG23	1.86	0.57
1:E:512:SER:CB	1:E:513:PRO:CD	2.82	0.57
3:L:4:LEU:HD22	3:L:23:CYS:SG	2.44	0.57
3:L:28:SER:N	3:L:69:THR:CG2	2.67	0.57
3:L:37:GLN:CG	3:L:86:TYR:HE1	2.18	0.57
2:H:114:ALA:HB3	2:H:146:PHE:CZ	2.39	0.57
3:L:90:GLN:HE21	3:L:97:THR:H	1.53	0.57
1:E:549:TRP:CH2	1:E:603:ILE:HG23	2.39	0.57
3:L:20:THR:CG2	3:L:74:THR:HG23	2.34	0.57
3:L:33:LEU:O	3:L:51:ALA:N	2.31	0.57
2:H:154:TRP:CZ3	2:H:196:CYS:HB3	2.40	0.56
3:L:12:SER:HB3	3:L:107:LYS:HE3	1.86	0.56
2:H:53:ILE:HG13	2:H:54:PHE:CE1	2.38	0.56
1:E:509:PHE:O	1:E:551:GLY:O	2.23	0.56
1:E:610:ASP:HA	1:E:614:ARG:HD3	1.86	0.56
2:H:166:PHE:HA	3:L:164:THR:OG1	2.06	0.56
3:L:2:LEU:CD2	3:L:27:GLN:CB	2.84	0.55
1:E:615:LEU:H	1:E:615:LEU:HD12	1.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:8:PRO:HG2	3:L:11:LEU:HB2	1.89	0.55
3:L:120:PRO:HD3	3:L:132:VAL:CG2	2.33	0.55
2:H:39:GLN:HB3	2:H:89:VAL:CG2	2.37	0.55
2:H:69:ILE:HG22	2:H:69:ILE:O	2.06	0.55
2:H:150:VAL:HG23	2:H:199:ASN:O	2.07	0.55
1:E:509:PHE:CZ	1:E:611:TYR:CB	2.82	0.55
3:L:20:THR:HG23	3:L:74:THR:HG23	1.89	0.55
3:L:28:SER:CA	3:L:69:THR:HG23	2.32	0.55
3:L:209:PHE:C	3:L:209:PHE:CD2	2.85	0.55
2:H:96:VAL:HG12	2:H:98:LEU:HD23	1.88	0.55
3:L:11:LEU:C	3:L:11:LEU:HD23	2.32	0.55
1:E:494:CYS:HB3	1:E:539:LEU:HB3	1.88	0.55
1:E:546:THR:HG21	1:E:634:GLY:CA	2.35	0.55
2:H:53:ILE:CG1	2:H:54:PHE:CE1	2.90	0.55
3:L:122:ASP:O	3:L:126:LYS:HG3	2.07	0.55
1:E:510:THR:OG1	1:E:511:PRO:CD	2.46	0.54
1:E:424:ARG:HD2	1:E:526:THR:O	2.08	0.54
1:E:521:LYS:HA	1:E:538:MET:CE	2.37	0.54
1:E:556:ASN:CG	1:E:560:PHE:HB2	2.32	0.54
2:H:166:PHE:CD2	3:L:164:THR:OG1	2.55	0.54
3:L:63:SER:OG	3:L:74:THR:HB	2.08	0.54
1:E:516:VAL:HG22	1:E:542:LEU:HD11	1.90	0.53
3:L:111:ALA:O	3:L:139:PHE:CA	2.55	0.53
2:H:90:TYR:N	2:H:107:THR:O	2.40	0.53
1:E:429:CYS:CB	1:E:438:ILE:HD11	2.39	0.53
3:L:112:ALA:HB1	3:L:201:LEU:CD2	2.39	0.53
2:H:116:THR:HG22	2:H:203:SER:HB3	1.90	0.53
1:E:509:PHE:HD1	1:E:609:VAL:HG11	1.71	0.53
2:H:8:GLY:HA3	2:H:201:LYS:HD3	1.91	0.53
2:H:91:TYR:CE1	2:H:106:GLY:CA	2.92	0.53
2:H:131:THR:HG22	2:H:136:ALA:HB1	1.89	0.53
3:L:90:GLN:NE2	3:L:97:THR:H	2.07	0.53
2:H:200:HIS:CE1	2:H:203:SER:HG	2.24	0.52
2:H:122:PHE:CE2	3:L:124:GLN:HG3	2.44	0.52
3:L:37:GLN:CB	3:L:47:LEU:HD11	2.38	0.52
2:H:154:TRP:CE2	2:H:182:VAL:HG13	2.44	0.52
1:E:509:PHE:CE2	1:E:611:TYR:CD1	2.96	0.52
2:H:95:GLU:HA	2:H:100(H):VAL:O	2.10	0.52
2:H:100:THR:O	2:H:100(A):TRP:HB2	2.09	0.52
2:H:98:LEU:HG	2:H:100(H):VAL:CG1	2.39	0.52
2:H:154:TRP:NE1	2:H:182:VAL:CG1	2.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:120:PRO:HB3	3:L:131:SER:H	1.74	0.52
1:E:424:ARG:HG3	1:E:424:ARG:HH11	1.74	0.52
2:H:131:THR:HG22	2:H:136:ALA:HA	1.91	0.51
1:E:422:ILE:C	1:E:424:ARG:N	2.65	0.51
2:H:163:VAL:CB	2:H:182:VAL:HG12	2.40	0.51
1:E:509:PHE:N	1:E:551:GLY:O	2.43	0.51
1:E:423:ASN:HB2	1:E:527:TYR:CD2	2.43	0.51
1:E:509:PHE:CE1	1:E:609:VAL:CG1	2.94	0.51
3:L:191:VAL:HG13	3:L:210:ASN:ND2	2.26	0.51
2:H:17:SER:HA	2:H:80:LEU:O	2.11	0.51
2:H:78:MET:SD	2:H:79:GLU:N	2.84	0.51
2:H:184:VAL:HB	2:H:185:PRO:HD2	1.93	0.51
3:L:33:LEU:HD11	3:L:88:CYS:HB2	1.92	0.51
2:H:16:SER:O	2:H:82(A):LEU:CD1	2.59	0.51
3:L:165:GLU:H	3:L:165:GLU:CD	2.17	0.51
1:E:509:PHE:CD1	1:E:609:VAL:CG1	2.94	0.50
2:H:72:ASP:OD1	2:H:74:SER:N	2.43	0.50
2:H:11:VAL:HG12	2:H:202:PRO:HB3	1.92	0.50
1:E:495:ASP:O	1:E:539:LEU:HB2	2.11	0.50
1:E:552:CYS:O	1:E:600:GLY:HA2	2.11	0.50
3:L:134:CYS:HB2	3:L:148:TRP:CH2	2.47	0.50
1:E:521:LYS:O	1:E:538:MET:CE	2.59	0.50
1:E:552:CYS:HB2	1:E:564:CYS:SG	2.51	0.50
1:E:563:THR:CG2	1:E:618:TYR:OH	2.60	0.50
2:H:32:TYR:CD1	2:H:96:VAL:HG22	2.47	0.50
2:H:126:PRO:HB3	2:H:137:ALA:O	2.12	0.50
3:L:136:LEU:HD11	3:L:146:VAL:CG2	2.41	0.50
2:H:143:LYS:HA	2:H:177:SER:HA	1.94	0.50
2:H:188:SER:O	2:H:191:THR:N	2.35	0.50
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.93	0.49
2:H:70:THR:HG23	2:H:77:TYR:HB2	1.94	0.49
2:H:87:THR:HA	2:H:109:LEU:O	2.12	0.49
3:L:140:TYR:CE1	3:L:173:TYR:HE1	2.30	0.49
3:L:151:ASP:OD2	3:L:189:HIS:HB3	2.12	0.49
1:E:611:TYR:O	1:E:614:ARG:CB	2.60	0.49
3:L:123:GLU:O	3:L:126:LYS:HB2	2.12	0.49
1:E:528:ASN:HD22	1:E:532:ASN:ND2	2.10	0.49
2:H:51:ILE:HD11	2:H:71:ALA:CB	2.30	0.49
3:L:186:TYR:HH	3:L:209:PHE:HZ	1.60	0.49
2:H:99:LYS:CE	3:L:50:ALA:HB1	2.42	0.49
3:L:3:THR:HB	3:L:26:SER:HB3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:18:ARG:HG3	3:L:76:SER:HA	1.95	0.49
2:H:114:ALA:CB	2:H:146:PHE:CE2	2.93	0.49
1:E:497:VAL:HG23	1:E:497:VAL:O	2.11	0.49
3:L:80:PRO:HA	3:L:106:ILE:HD13	1.94	0.49
1:E:429:CYS:CB	1:E:438:ILE:CD1	2.91	0.49
3:L:80:PRO:O	3:L:168:SER:O	2.31	0.49
2:H:67:VAL:CG2	2:H:80:LEU:CD2	2.88	0.49
3:L:132:VAL:HG12	3:L:148:TRP:CH2	2.47	0.49
1:E:509:PHE:CE1	1:E:609:VAL:HG12	2.47	0.48
1:E:556:ASN:OD1	1:E:560:PHE:CA	2.60	0.48
1:E:637:GLU:HG2	1:E:638:HIS:N	2.29	0.48
2:H:81:SER:O	2:H:82:SER:C	2.56	0.48
2:H:11:VAL:CB	2:H:147:PRO:HG3	2.43	0.48
2:H:100(D):ALA:C	2:H:100(F):PRO:HD3	2.38	0.48
2:H:182:VAL:HG23	2:H:182:VAL:O	2.12	0.48
3:L:191:VAL:CG2	3:L:210:ASN:ND2	2.66	0.48
2:H:54:PHE:CD1	2:H:54:PHE:N	2.81	0.48
2:H:51:ILE:HD13	2:H:69:ILE:CG2	2.44	0.47
2:H:131:THR:HG22	2:H:136:ALA:CA	2.43	0.47
3:L:33:LEU:HD12	3:L:34:ASN:H	1.77	0.47
2:H:44:GLY:HA2	3:L:87:TYR:CE2	2.47	0.47
2:H:199:ASN:OD1	2:H:206:LYS:HG3	2.14	0.47
3:L:25:ALA:HB3	3:L:69:THR:CB	2.44	0.47
3:L:62:PHE:CD2	3:L:75:ILE:HG12	2.50	0.47
3:L:110:VAL:HG11	3:L:199:GLN:HG2	1.96	0.47
1:E:619:PRO:N	1:E:620:CYS:N	2.61	0.47
3:L:23:CYS:HB2	3:L:35:TRP:CH2	2.49	0.47
3:L:175:LEU:C	3:L:175:LEU:CD2	2.79	0.47
3:L:110:VAL:HA	3:L:140:TYR:O	2.15	0.47
1:E:429:CYS:HB3	1:E:438:ILE:CD1	2.42	0.47
3:L:37:GLN:HG3	3:L:86:TYR:CZ	2.48	0.47
3:L:183:LYS:O	3:L:187:GLU:CG	2.56	0.47
3:L:186:TYR:CE2	3:L:211:ARG:HD3	2.50	0.47
3:L:140:TYR:CD1	3:L:173:TYR:CE1	2.95	0.47
1:E:566:ALA:HB1	1:E:567:PRO:CD	2.45	0.46
1:E:631:MET:HE2	1:E:633:VAL:HG23	1.97	0.46
2:H:82(A):LEU:C	2:H:83:ARG:HG3	2.40	0.46
3:L:8:PRO:CG	3:L:11:LEU:HB2	2.44	0.46
3:L:110:VAL:HG13	3:L:141:PRO:HD2	1.95	0.46
1:E:601:PRO:HD2	1:E:602:TRP:CD1	2.51	0.46
3:L:120:PRO:HG2	3:L:125:LEU:HD11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:29:ILE:HG23	3:L:92:TYR:CG	2.49	0.46
3:L:100:GLN:HG2	3:L:101:GLY:O	2.15	0.46
2:H:99:LYS:HE3	3:L:50:ALA:CB	2.46	0.46
3:L:207:LYS:HD2	3:L:207:LYS:HA	1.62	0.46
2:H:63:PHE:H	2:H:63:PHE:HD2	1.63	0.46
3:L:32:TYR:HB3	3:L:91:SER:OG	2.16	0.46
2:H:18:VAL:CG2	2:H:19:LYS:N	2.79	0.46
2:H:91:TYR:CE1	2:H:106:GLY:HA3	2.50	0.46
3:L:2:LEU:HD21	3:L:27:GLN:HB3	1.98	0.46
3:L:145:LYS:O	3:L:196:VAL:HA	2.15	0.46
3:L:186:TYR:CE1	3:L:192:TYR:CE1	3.04	0.46
3:L:110:VAL:HG13	3:L:141:PRO:CD	2.46	0.46
1:E:624:PHE:HD1	1:E:624:PHE:HA	1.68	0.45
3:L:52:SER:CB	3:L:64:GLY:O	2.64	0.45
1:E:443:TYR:O	1:E:444:ALA:O	2.33	0.45
3:L:167:ASP:HB3	3:L:170:ASP:OD1	2.17	0.45
3:L:173:TYR:CD1	3:L:173:TYR:N	2.83	0.45
3:L:27:GLN:O	3:L:69:THR:CG2	2.59	0.45
2:H:125:ALA:HB1	2:H:212:GLU:O	2.17	0.45
3:L:38:GLN:O	3:L:84:ALA:HB1	2.17	0.45
1:E:631:MET:HE2	1:E:633:VAL:CG2	2.47	0.45
2:H:100(G):ASN:O	3:L:91:SER:HB3	2.17	0.45
2:H:108:MET:HE1	2:H:148:GLU:O	2.17	0.45
2:H:18:VAL:O	2:H:79:GLU:HG2	2.16	0.44
2:H:87:THR:O	2:H:87:THR:HG23	2.18	0.44
2:H:51:ILE:HD13	2:H:69:ILE:HG22	2.00	0.44
3:L:135:LEU:C	3:L:136:LEU:HD23	2.43	0.44
2:H:39:GLN:O	2:H:89:VAL:HG22	2.17	0.44
2:H:145:TYR:O	2:H:145:TYR:CD2	2.70	0.44
2:H:23:LYS:HA	2:H:75:THR:CB	2.46	0.44
2:H:51:ILE:HD12	2:H:71:ALA:CB	2.46	0.44
3:L:83:PHE:CD2	3:L:83:PHE:O	2.70	0.44
2:H:100(D):ALA:O	2:H:100(F):PRO:HD3	2.17	0.44
3:L:78:LEU:HA	3:L:78:LEU:HD23	1.72	0.44
2:H:108:MET:CE	2:H:148:GLU:O	2.66	0.44
2:H:138:LEU:CD2	2:H:211:VAL:HB	2.39	0.44
2:H:129:LYS:HG3	5:H:304:HOH:O	2.17	0.44
3:L:186:TYR:OH	3:L:209:PHE:HZ	2.00	0.44
2:H:114:ALA:HB3	2:H:146:PHE:HE2	1.77	0.44
2:H:4:LEU:HD13	2:H:4:LEU:HA	1.80	0.44
2:H:147:PRO:HD2	2:H:202:PRO:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:48:ILE:CD1	3:L:64:GLY:N	2.81	0.43
1:E:603:ILE:H	1:E:603:ILE:HG13	1.63	0.43
1:E:549:TRP:CD2	1:E:603:ILE:HG22	2.52	0.43
2:H:11:VAL:CG1	2:H:202:PRO:HB3	2.48	0.43
3:L:89:GLN:NE2	3:L:90:GLN:O	2.51	0.43
2:H:23:LYS:CG	2:H:24:ALA:H	2.31	0.43
2:H:80:LEU:HA	2:H:80:LEU:HD23	1.81	0.43
1:E:424:ARG:HG3	1:E:424:ARG:NH1	2.33	0.43
3:L:33:LEU:HD12	3:L:89:GLN:O	2.19	0.43
3:L:209:PHE:O	3:L:209:PHE:CG	2.70	0.43
2:H:39:GLN:O	2:H:88:ALA:HB1	2.19	0.43
1:E:621:THR:HB	1:E:624:PHE:CD2	2.54	0.43
3:L:186:TYR:O	3:L:192:TYR:OH	2.34	0.43
1:E:422:ILE:HG13	1:E:423:ASN:N	2.33	0.43
1:E:628:LYS:HA	1:E:641:ASP:OD1	2.18	0.43
2:H:93:ALA:HB1	2:H:100(I):PHE:HB3	2.01	0.43
2:H:145:TYR:CZ	2:H:150:VAL:HG12	2.54	0.43
3:L:52:SER:HB2	3:L:64:GLY:O	2.18	0.42
2:H:67:VAL:HG23	2:H:80:LEU:HD21	1.99	0.42
2:H:134:GLY:O	2:H:186:SER:CB	2.66	0.42
3:L:176:SER:O	3:L:176:SER:OG	2.20	0.42
1:E:427:LEU:HD23	1:E:427:LEU:HA	1.59	0.42
1:E:611:TYR:O	1:E:614:ARG:HB2	2.18	0.42
2:H:59:TYR:CD1	2:H:59:TYR:N	2.87	0.42
1:E:615:LEU:O	1:E:618:TYR:C	2.62	0.42
2:H:70:THR:CG2	2:H:77:TYR:HB2	2.49	0.42
2:H:99:LYS:CE	3:L:50:ALA:CB	2.97	0.42
2:H:145:TYR:CD2	2:H:145:TYR:C	2.97	0.42
2:H:101:ASP:OD1	2:H:102:VAL:N	2.53	0.42
2:H:155:ASN:OD1	2:H:194:TYR:HA	2.20	0.42
2:H:6:GLN:HA	2:H:21:SER:O	2.20	0.42
2:H:64:GLN:CG	2:H:65:GLY:N	2.63	0.42
1:E:512:SER:HB2	1:E:513:PRO:HD2	2.01	0.42
2:H:11:VAL:HA	2:H:110:THR:O	2.20	0.42
2:H:206:LYS:HB2	2:H:206:LYS:HE2	1.82	0.42
3:L:91:SER:HA	3:L:96:ARG:CD	2.50	0.42
2:H:23:LYS:CG	2:H:24:ALA:N	2.82	0.41
3:L:6:GLN:O	3:L:100:GLN:NE2	2.38	0.41
1:E:502:VAL:HG22	1:E:554:TRP:CD1	2.55	0.41
3:L:62:PHE:CE2	3:L:75:ILE:HG12	2.54	0.41
1:E:429:CYS:HB2	1:E:438:ILE:CD1	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:19:LYS:HB2	2:H:79:GLU:HG3	2.02	0.41
2:H:143:LYS:CG	2:H:177:SER:HB2	2.50	0.41
3:L:186:TYR:CD1	3:L:192:TYR:CZ	3.09	0.41
1:E:429:CYS:HB2	1:E:438:ILE:HD13	2.03	0.41
1:E:437:PHE:O	1:E:440:SER:OG	2.35	0.41
2:H:87:THR:HG1	2:H:110:THR:HA	1.79	0.41
2:H:108:MET:HE1	2:H:148:GLU:C	2.45	0.41
1:E:422:ILE:C	1:E:529:TRP:CZ3	2.98	0.41
1:E:423:ASN:HB3	1:E:527:TYR:CB	2.42	0.41
2:H:8:GLY:HA2	2:H:201:LYS:HD3	2.03	0.41
2:H:53:ILE:HG13	2:H:54:PHE:N	2.36	0.41
2:H:96:VAL:O	2:H:100(H):VAL:HG12	2.21	0.41
2:H:168:ALA:HA	2:H:178:LEU:HD13	2.02	0.41
3:L:127:SER:OG	3:L:129:THR:HG22	2.20	0.41
2:H:97:ASN:ND2	2:H:100:THR:OG1	2.53	0.41
3:L:124:GLN:HE21	3:L:129:THR:HG23	1.85	0.41
3:L:27:GLN:C	3:L:69:THR:HG21	2.45	0.41
2:H:116:THR:CG2	2:H:203:SER:HB3	2.50	0.40
2:H:143:LYS:HG2	2:H:177:SER:CB	2.51	0.40
3:L:111:ALA:O	3:L:139:PHE:HB2	2.20	0.40
3:L:124:GLN:NE2	3:L:129:THR:HG23	2.36	0.40
1:E:493:PRO:HG2	1:E:493:PRO:O	2.22	0.40
2:H:95:GLU:CD	2:H:100(F):PRO:HB2	2.45	0.40
2:H:144:ASP:HA	2:H:175:LEU:HB3	2.03	0.40

All (4) 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)
2:H:72:ASP:OD1	3:L:65:SER:OG[3_555]	1.47	0.73
2:H:74:SER:N	3:L:65:SER:OG[3_555]	1.99	0.21
2:H:193:THR:OG1	3:L:142:ARG:NH1[4_455]	2.08	0.12
1:E:546:THR:O	4:E:701:NAG:C8[4_456]	2.16	0.04

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	E	140/189 (74%)	126 (90%)	11 (8%)	3 (2%)	5	27
2	H	209/230 (91%)	203 (97%)	5 (2%)	1 (0%)	24	56
3	L	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
All	All	558/633 (88%)	531 (95%)	23 (4%)	4 (1%)	18	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	510	THR
1	E	512	SER
2	H	82	SER
1	E	513	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	127/159 (80%)	123 (97%)	4 (3%)	35	61
2	H	180/192 (94%)	170 (94%)	10 (6%)	19	47
3	L	186/189 (98%)	174 (94%)	12 (6%)	15	43
All	All	493/540 (91%)	467 (95%)	26 (5%)	20	49

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	603	ILE
1	E	606	ARG
1	E	621	THR
1	E	624	PHE
2	H	4	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	45	LEU
2	H	54	PHE
2	H	58	ASN
2	H	63	PHE
2	H	66	ARG
2	H	72	ASP
2	H	105	GLN
2	H	143	LYS
2	H	183	THR
3	L	6	GLN
3	L	10	SER
3	L	33	LEU
3	L	48	ILE
3	L	108	ARG
3	L	137	ASN
3	L	161	GLU
3	L	168	SER
3	L	169	LYS
3	L	170	ASP
3	L	203	SER
3	L	209	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	532	ASN
2	H	39	GLN
2	H	97	ASN
2	H	100(E)	HIS
3	L	79	GLN
3	L	124	GLN
3	L	137	ASN
3	L	166	GLN
3	L	210	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	E	702	1	14,14,15	0.24	0	17,19,21	0.37	0
4	NAG	E	701	1	14,14,15	0.24	0	17,19,21	0.59	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
4	NAG	E	702	1	-	0/6/23/26	0/1/1/1
4	NAG	E	701	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

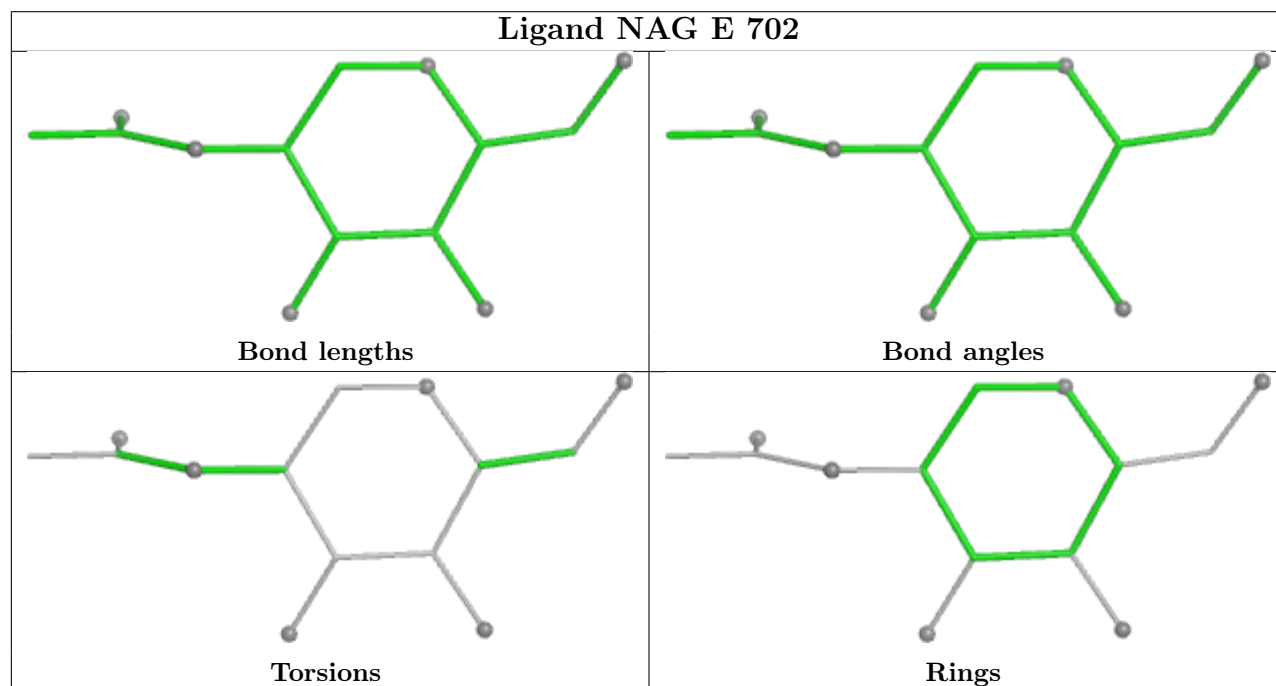
Mol	Chain	Res	Type	Atoms
4	E	701	NAG	C3-C2-N2-C7
4	E	701	NAG	C1-C2-N2-C7

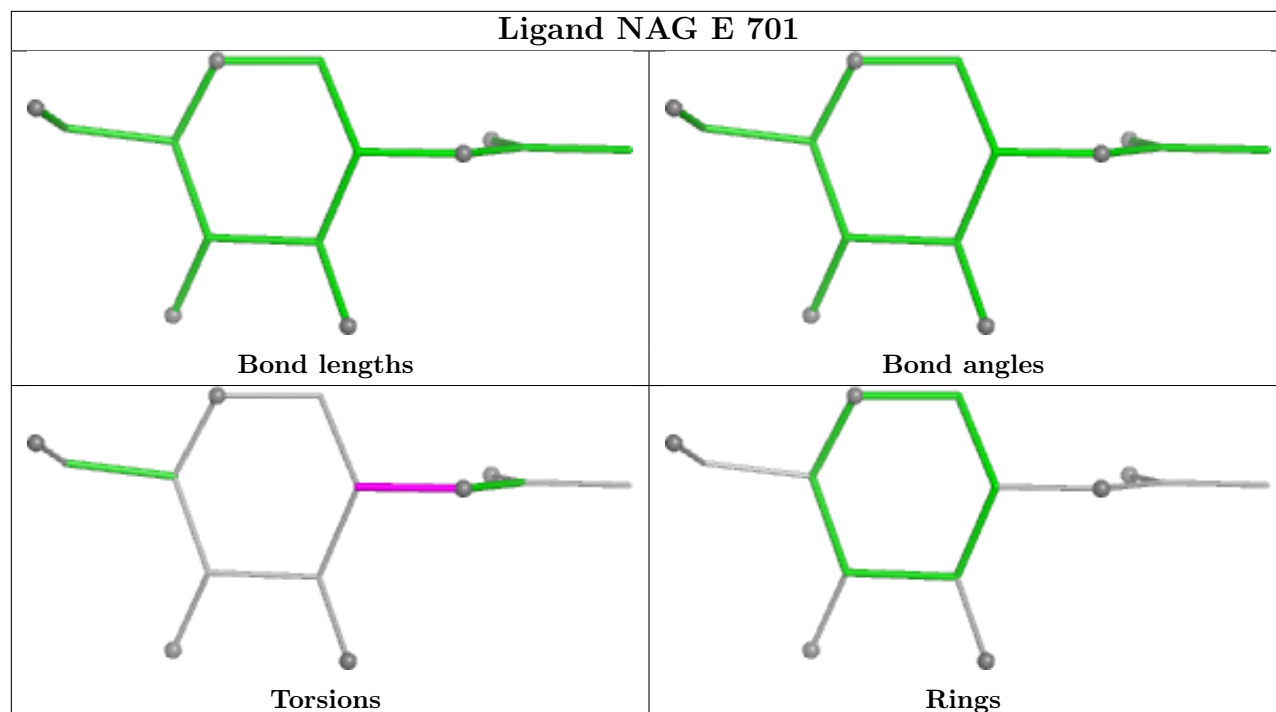
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	701	NAG	0	1

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	E	146/189 (77%)	0.14	3 (2%) 63 44	58, 84, 109, 131	0
2	H	215/230 (93%)	-0.05	1 (0%) 87 76	58, 79, 99, 117	0
3	L	211/214 (98%)	-0.14	0 100 100	59, 81, 96, 108	0
All	All	572/633 (90%)	-0.03	4 (0%) 84 70	58, 80, 102, 131	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	608	LEU	3.7
2	H	109	LEU	2.5
1	E	620	CYS	2.2
1	E	603	ILE	2.2

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

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

6.3 Carbohydrates [i](#)

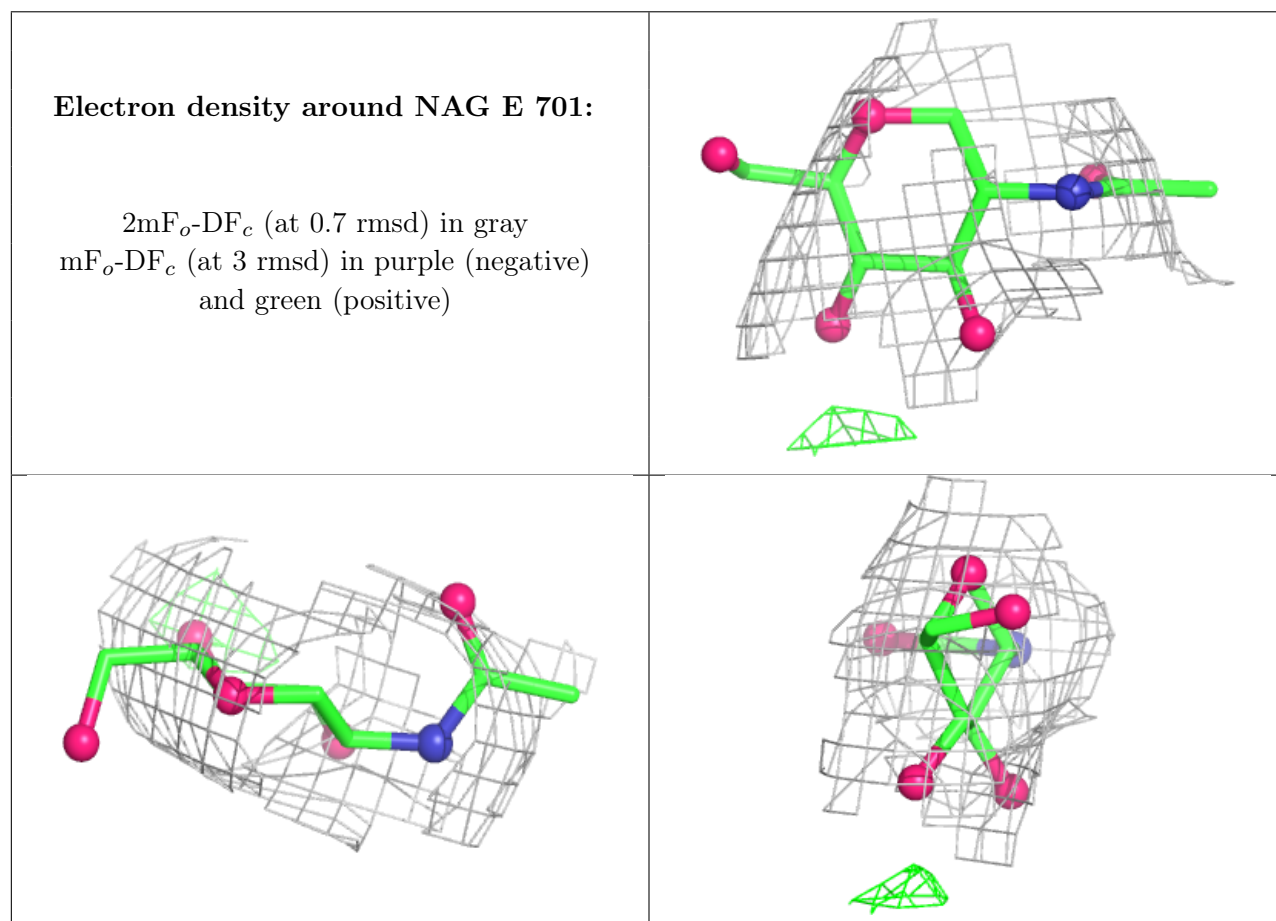
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

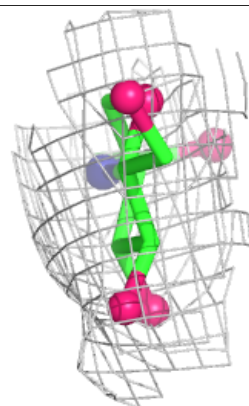
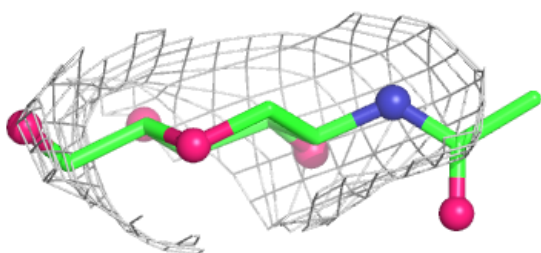
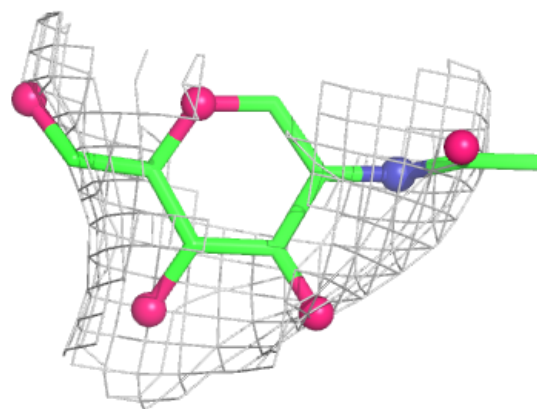
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	E	701	14/15	0.64	0.12	100,106,115,117	0
4	NAG	E	702	14/15	0.81	0.08	104,110,115,116	0

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 E 702:

$2mF_o-DF_c$ (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.