



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:22 AM UTC

PDB ID : 6Q23 / pdb_00006q23
Title : Crystal structure of human 1G01 Fab in complex with influenza virus neuraminidase from A/California/04/2009 (H1N1)
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2019-08-06
Resolution : 3.27 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

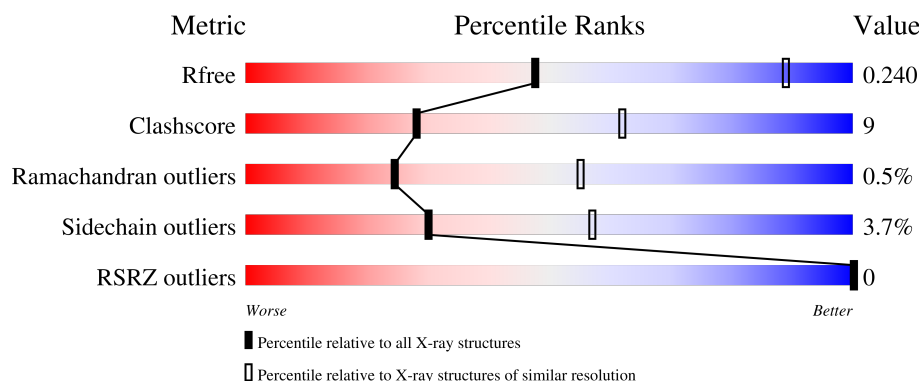
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 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	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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

Mol	Chain	Length	Quality of chain
1	A	391	
1	B	391	
1	C	391	
1	D	391	
2	E	240	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	240	 69%22%5%
2	H	240	 75%18%5%
2	J	240	 72%20%5%
3	F	216	 74%25%
3	I	216	 74%24%5%
3	K	216	 79%19%5%
3	L	216	 76%23%5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25541 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 Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	384	Total	C	N	O	S	0	0	0
			2968	1863	513	571	21			
1	B	384	Total	C	N	O	S	0	0	0
			2968	1863	513	571	21			
1	A	384	Total	C	N	O	S	0	0	0
			2968	1863	513	571	21			
1	D	384	Total	C	N	O	S	0	0	0
			2968	1863	513	571	21			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	77	GLY	-	expression tag	UNP C5MQL2
C	78	SER	-	expression tag	UNP C5MQL2
C	79	PRO	-	expression tag	UNP C5MQL2
C	80	SER	-	expression tag	UNP C5MQL2
C	81	ARG	-	expression tag	UNP C5MQL2
B	77	GLY	-	expression tag	UNP C5MQL2
B	78	SER	-	expression tag	UNP C5MQL2
B	79	PRO	-	expression tag	UNP C5MQL2
B	80	SER	-	expression tag	UNP C5MQL2
B	81	ARG	-	expression tag	UNP C5MQL2
A	77	GLY	-	expression tag	UNP C5MQL2
A	78	SER	-	expression tag	UNP C5MQL2
A	79	PRO	-	expression tag	UNP C5MQL2
A	80	SER	-	expression tag	UNP C5MQL2
A	81	ARG	-	expression tag	UNP C5MQL2
D	77	GLY	-	expression tag	UNP C5MQL2
D	78	SER	-	expression tag	UNP C5MQL2
D	79	PRO	-	expression tag	UNP C5MQL2
D	80	SER	-	expression tag	UNP C5MQL2
D	81	ARG	-	expression tag	UNP C5MQL2

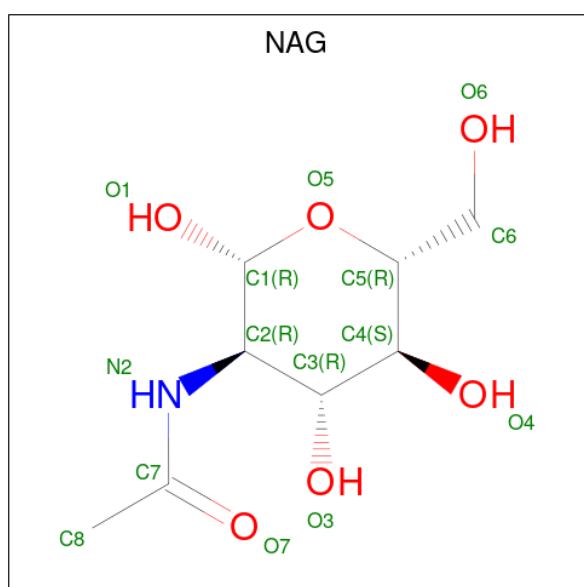
- Molecule 2 is a protein called 1G01 Fab IgG1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	227	Total	C	N	O	S	0	0	0
			1728	1096	295	332	5			
2	E	227	Total	C	N	O	S	0	0	0
			1728	1096	295	332	5			
2	G	227	Total	C	N	O	S	0	0	0
			1728	1096	295	332	5			
2	J	227	Total	C	N	O	S	0	0	0
			1728	1096	295	332	5			

- Molecule 3 is a protein called 1G01 Fab kappa light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	0	0
			1659	1047	275	332	5			
3	F	215	Total	C	N	O	S	0	0	0
			1659	1047	275	332	5			
3	I	215	Total	C	N	O	S	0	0	0
			1659	1047	275	332	5			
3	K	215	Total	C	N	O	S	0	0	0
			1659	1047	275	332	5			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

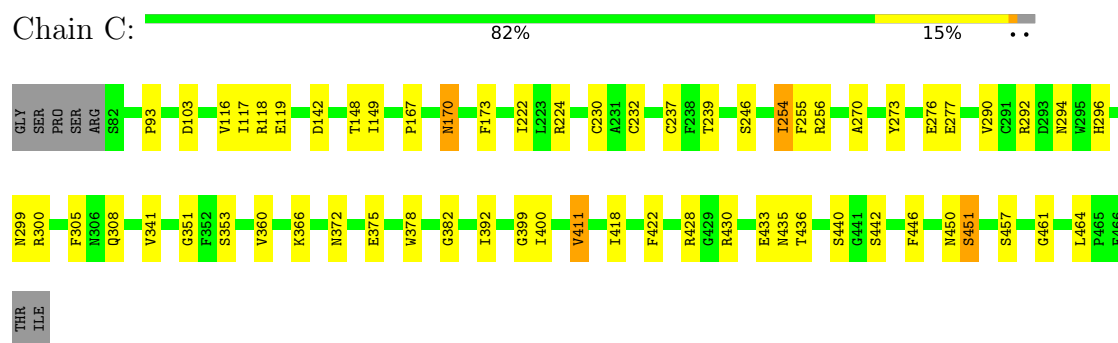
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	2	Total Ca 2 2	0	0
5	B	2	Total Ca 2 2	0	0
5	A	2	Total Ca 2 2	0	0
5	D	3	Total Ca 3 3	0	0

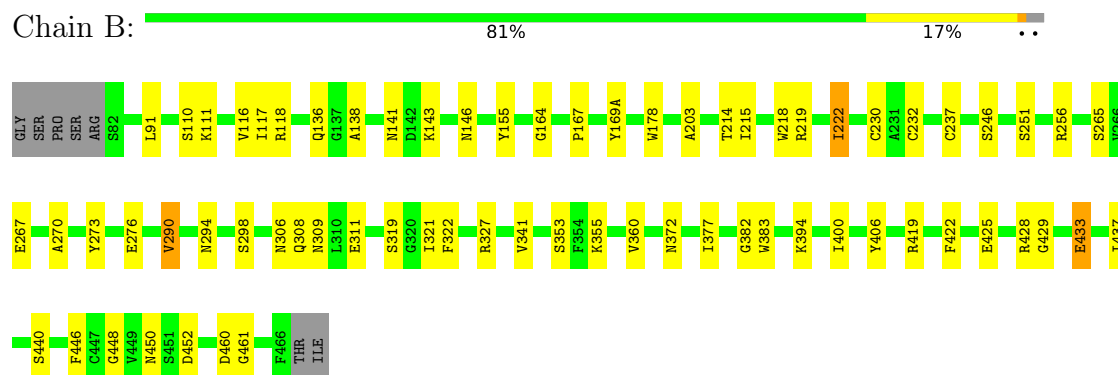
3 Residue-property plots

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.

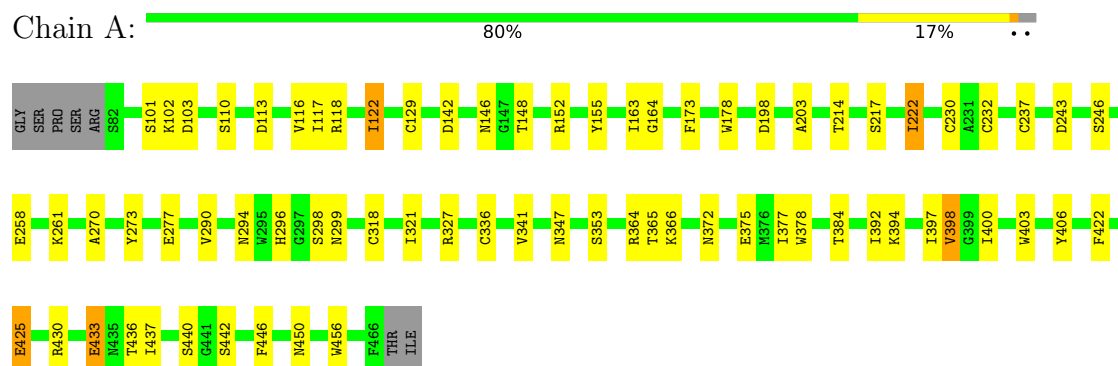
• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase

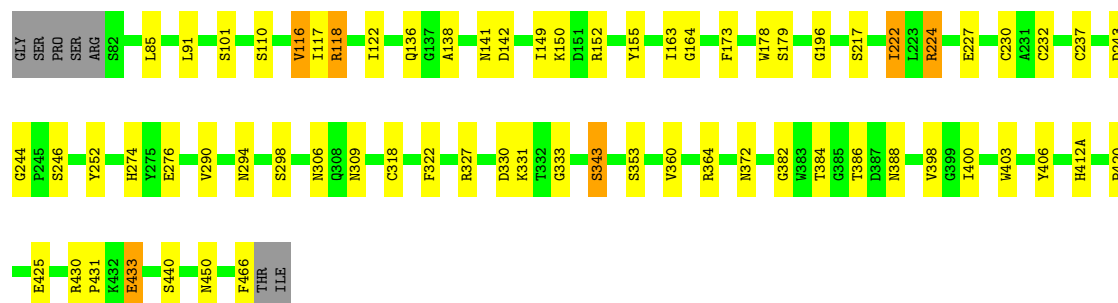


• Molecule 1: Neuraminidase



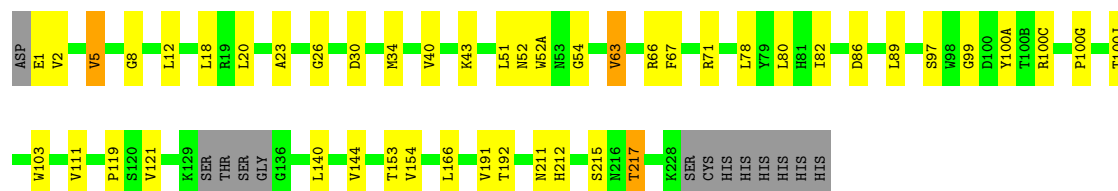
- Molecule 1: Neuraminidase

Chain D:  81% 16% . .



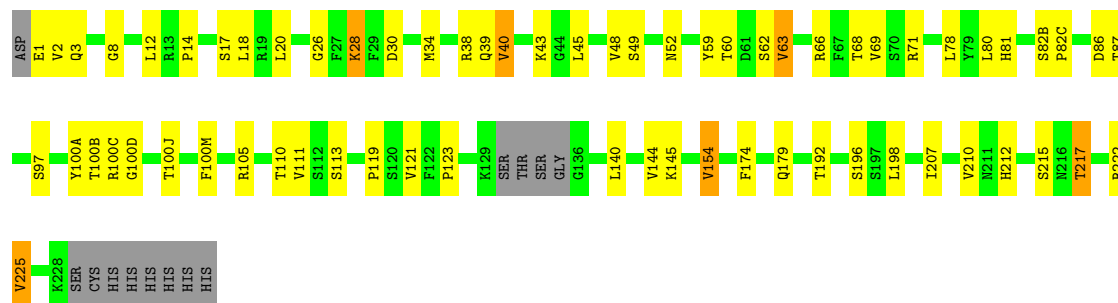
- Molecule 2: 1G01 Fab IgG1 heavy chain

Chain H:  75% 18% . 5%



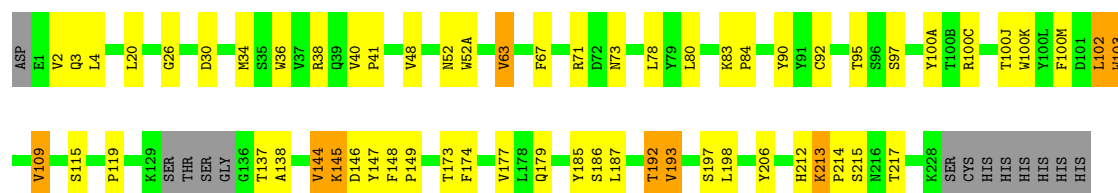
- Molecule 2: 1G01 Fab IgG1 heavy chain

Chain E:  67% 25% . 5%



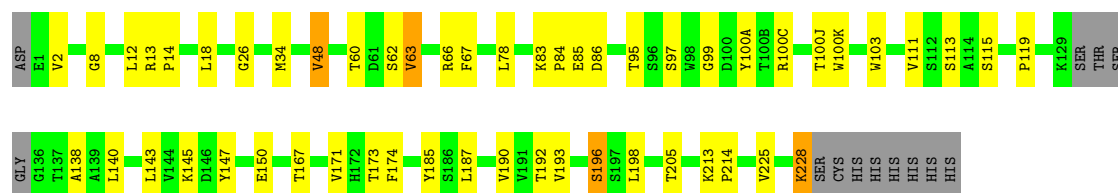
- Molecule 2: 1G01 Fab IgG1 heavy chain

Chain G:  69% 22% . 5%



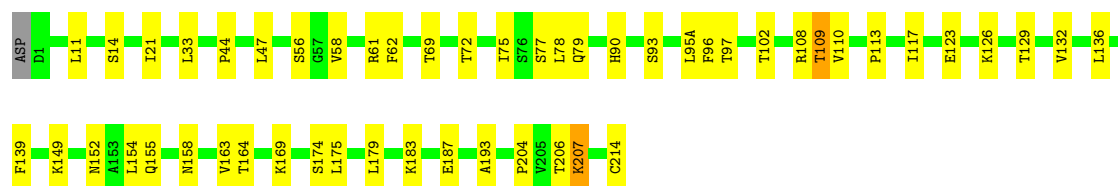
- Molecule 2: 1G01 Fab IgG1 heavy chain

Chain J:  72% 20% 5%



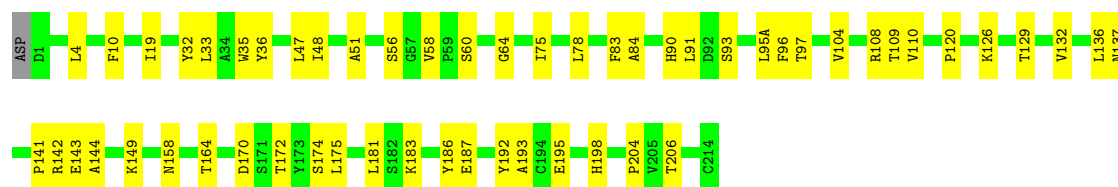
• Molecule 3: 1G01 Fab kappa light chain

Chain L:  76% 23% 1%



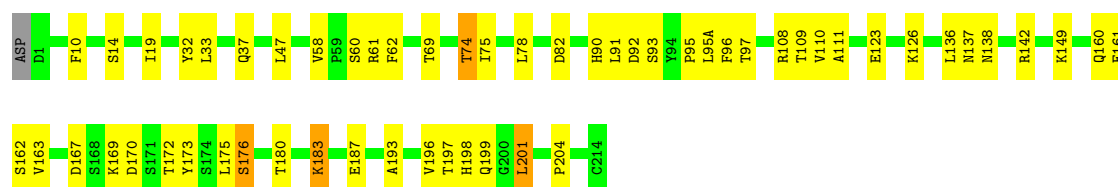
• Molecule 3: 1G01 Fab kappa light chain

Chain F:  74% 25% 1%



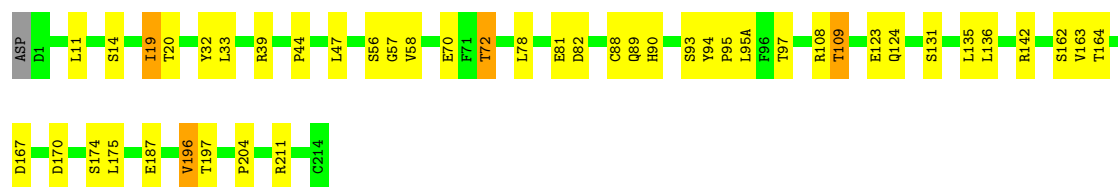
• Molecule 3: 1G01 Fab kappa light chain

Chain I:  74% 24% 1%



• Molecule 3: 1G01 Fab kappa light chain

Chain K:  79% 19% 1%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.59Å 234.99Å 106.28Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	43.30 – 3.27 43.30 – 3.27	Depositor EDS
% Data completeness (in resolution range)	90.4 (43.30-3.27) 90.5 (43.30-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.196 , 0.241 0.199 , 0.240	Depositor DCC
R_{free} test set	3351 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	60.6	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 24.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.329 for l,-k,h	Xtriage
Reported twinning fraction	0.661 for H, K, L 0.339 for -L, -K, -H	Depositor
Outliers	0 of 70197 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25541	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.96% 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.00	0/3050	1.15	2/4145 (0.0%)
1	B	1.00	1/3050 (0.0%)	1.13	0/4145
1	C	0.98	0/3050	1.12	0/4145
1	D	1.00	0/3050	1.12	2/4145 (0.0%)
2	E	0.97	0/1774	1.12	0/2417
2	G	0.98	0/1774	1.11	0/2417
2	H	1.01	0/1774	1.14	0/2417
2	J	0.97	0/1774	1.14	0/2417
3	F	1.00	0/1698	1.17	1/2309 (0.0%)
3	I	1.01	0/1698	1.17	0/2309
3	K	1.00	0/1698	1.15	0/2309
3	L	0.99	0/1698	1.18	0/2309
All	All	0.99	1/26088 (0.0%)	1.14	5/35484 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	429	GLY	C-O	5.30	1.29	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	143	GLU	CB-CG-CD	5.39	121.76	112.60
1	D	398	VAL	CA-C-N	5.16	124.87	119.92
1	D	398	VAL	C-N-CA	5.16	124.87	119.92
1	A	398	VAL	CA-C-N	5.02	124.74	119.92
1	A	398	VAL	C-N-CA	5.02	124.74	119.92

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2968	0	2797	59	0
1	B	2968	0	2798	52	0
1	C	2968	0	2798	46	0
1	D	2968	0	2799	48	0
2	E	1728	0	1692	43	0
2	G	1728	0	1692	38	0
2	H	1728	0	1692	34	0
2	J	1728	0	1692	41	0
3	F	1659	0	1607	31	0
3	I	1659	0	1607	38	0
3	K	1659	0	1607	32	0
3	L	1659	0	1607	31	0
4	A	42	0	39	1	0
4	B	28	0	26	0	0
4	C	28	0	26	0	0
4	D	14	0	13	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	3	0	0	0	0
All	All	25541	0	24492	444	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (444) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:HD3	1:A:436:THR:O	1.64	0.97
3:I:167:ASP:HB3	3:I:170:ASP:OD1	1.70	0.91
3:L:117:ILE:HG22	3:L:207:LYS:HD3	1.53	0.90
1:A:375:GLU:OE1	1:A:394:LYS:HE2	1.72	0.90
3:K:108:ARG:NH1	3:K:109:THR:O	2.04	0.90
1:D:403:TRP:CE2	1:D:433:GLU:OE1	2.27	0.88
1:A:318:CYS:SG	1:A:384:THR:HA	2.14	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:136:LEU:HD11	3:I:196:VAL:HG21	1.55	0.87
3:L:163:VAL:HG22	3:L:175:LEU:HD23	1.59	0.84
1:C:118:ARG:HH21	2:E:100(C):ARG:HB3	1.50	0.78
1:B:116:VAL:HG23	1:B:136:GLN:HB2	1.66	0.78
1:D:318:CYS:SG	1:D:384:THR:HA	2.25	0.76
3:K:33:LEU:HD11	3:K:88:CYS:HB2	1.68	0.75
3:K:167:ASP:HB3	3:K:170:ASP:OD1	1.85	0.74
1:A:403:TRP:NE1	1:A:433:GLU:OE2	2.20	0.74
3:I:149:LYS:HD2	3:I:193:ALA:HB3	1.73	0.71
2:J:48:VAL:HG23	2:J:63:VAL:HG21	1.73	0.71
2:G:213:LYS:HG2	2:G:214:PRO:HD3	1.71	0.70
1:A:122:ILE:HD11	1:A:129:CYS:HB3	1.73	0.70
3:L:123:GLU:OE2	3:L:123:GLU:N	2.25	0.70
2:E:192:THR:HG21	3:F:137:ASN:ND2	2.06	0.69
1:D:246:SER:HB2	1:D:294:ASN:HD22	1.59	0.68
2:E:154:VAL:HG12	2:E:210:VAL:HG22	1.76	0.67
2:E:100(B):THR:HG22	2:E:100(D):GLY:H	1.60	0.67
3:L:21:ILE:HD12	3:L:102:THR:HG21	1.77	0.67
1:B:298:SER:OG	1:B:341:VAL:HG23	1.94	0.66
2:H:153:THR:HG22	2:H:211:ASN:HB3	1.77	0.66
1:D:122:ILE:CD1	1:D:163:ILE:HD12	2.26	0.66
3:L:61:ARG:NH1	3:L:79:GLN:OE1	2.29	0.65
1:C:378:TRP:HB3	1:C:392:ILE:CG2	2.27	0.65
1:D:122:ILE:HD11	1:D:163:ILE:HD12	1.78	0.65
1:A:116:VAL:HG11	1:A:148:THR:HG21	1.79	0.64
2:E:52:ASN:O	2:E:71:ARG:NH1	2.30	0.64
2:J:83:LYS:O	2:J:111:VAL:HG21	1.98	0.64
3:F:108:ARG:NH1	3:F:170:ASP:O	2.31	0.63
2:E:49:SER:HB2	2:E:69:VAL:HG21	1.80	0.63
3:K:47:LEU:HA	3:K:58:VAL:HG21	1.78	0.63
1:B:306:ASN:HD21	1:B:311:GLU:HB2	1.63	0.63
2:G:63:VAL:HG13	2:G:67:PHE:CG	2.34	0.63
1:B:306:ASN:ND2	1:B:311:GLU:HB2	2.13	0.63
2:H:166:LEU:HD21	2:H:191:VAL:HG21	1.81	0.63
3:I:90:HIS:NE2	3:I:92:ASP:OD1	2.32	0.63
1:B:246:SER:HB2	1:B:294:ASN:HD22	1.64	0.62
3:F:47:LEU:HA	3:F:58:VAL:HG21	1.79	0.62
3:I:47:LEU:HA	3:I:58:VAL:HG21	1.80	0.62
2:G:119:PRO:HD2	2:G:217:THR:HG21	1.81	0.62
1:D:403:TRP:NE1	1:D:433:GLU:OE1	2.32	0.62
2:E:66:ARG:NH2	2:E:86:ASP:OD2	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TYR:H	1:A:425:GLU:HG2	1.65	0.62
2:J:63:VAL:HG13	2:J:67:PHE:CG	2.35	0.62
1:C:428:ARG:NE	1:C:433:GLU:OE2	2.31	0.62
2:H:121:VAL:HG12	2:H:144:VAL:HG22	1.82	0.62
1:C:451:SER:HB2	1:B:214:THR:OG1	1.99	0.61
1:D:178:TRP:O	2:G:100(C):ARG:NH2	2.29	0.61
2:J:14:PRO:HD2	2:J:113:SER:HB3	1.81	0.61
3:I:136:LEU:HB2	3:I:175:LEU:HB3	1.82	0.61
2:H:103:TRP:CZ3	3:L:44:PRO:HG2	2.36	0.61
3:K:187:GLU:OE2	3:K:211:ARG:NH1	2.34	0.60
1:A:406:TYR:OH	2:H:100(C):ARG:HG3	2.02	0.60
3:L:47:LEU:HA	3:L:58:VAL:HG21	1.84	0.59
1:B:306:ASN:OD1	1:B:309:ASN:N	2.35	0.59
1:A:298:SER:OG	1:A:341:VAL:HB	2.01	0.59
3:I:62:PHE:CD1	3:I:75:ILE:HD12	2.38	0.59
2:J:174:PHE:O	2:J:187:LEU:CD1	2.50	0.59
3:K:123:GLU:N	3:K:123:GLU:OE1	2.35	0.59
2:J:174:PHE:HB3	3:K:162:SER:OG	2.02	0.59
2:H:63:VAL:HG13	2:H:67:PHE:CG	2.38	0.58
2:G:2:VAL:HA	2:G:26:GLY:HA3	1.85	0.58
2:G:52(A):TRP:O	2:G:73:ASN:ND2	2.36	0.58
2:G:144:VAL:HG22	2:G:187:LEU:HB3	1.85	0.58
1:A:217:SER:OG	1:A:243:ASP:OD2	2.20	0.58
2:E:119:PRO:HD2	2:E:217:THR:HG21	1.84	0.58
1:B:461:GLY:HA3	1:A:155:TYR:CE1	2.39	0.58
1:B:146:ASN:HB3	1:B:437:ILE:HD12	1.85	0.58
2:E:121:VAL:HG22	2:E:144:VAL:HG22	1.86	0.58
3:F:158:ASN:HD22	3:F:181:LEU:HD21	1.67	0.58
3:I:199:GLN:H	3:I:199:GLN:CD	2.12	0.58
3:L:132:VAL:HG23	3:L:179:LEU:HB3	1.86	0.57
1:D:298:SER:OG	1:D:343:SER:O	2.21	0.57
2:E:82(B):SER:N	2:E:82(C):PRO:HD3	2.19	0.57
2:J:34:MET:HB3	2:J:78:LEU:HD22	1.86	0.57
1:A:122:ILE:CD1	1:A:163:ILE:HD12	2.35	0.57
3:F:35:TRP:HD1	3:F:48:ILE:HD11	1.70	0.57
1:A:118:ARG:NH2	1:A:425:GLU:OE1	2.38	0.57
3:L:136:LEU:HB2	3:L:175:LEU:HB3	1.87	0.57
3:I:136:LEU:HD11	3:I:196:VAL:HG11	1.86	0.56
1:C:170:ASN:HD21	1:B:169(A):TYR:HA	1.70	0.56
3:I:137:ASN:OD1	3:I:138:ASN:ND2	2.27	0.56
2:G:100(M):PHE:HB2	2:G:103:TRP:CH2	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:ARG:NH1	1:C:308:GLN:O	2.38	0.56
3:K:136:LEU:HD11	3:K:196:VAL:HG11	1.87	0.56
1:B:428:ARG:NH2	1:B:433:GLU:OE2	2.39	0.56
2:H:153:THR:CG2	2:H:211:ASN:HB3	2.36	0.56
2:E:59:TYR:HE1	2:E:69:VAL:HG23	1.70	0.56
3:K:136:LEU:HB2	3:K:175:LEU:HB3	1.88	0.56
2:H:2:VAL:HA	2:H:26:GLY:HA3	1.88	0.56
2:E:20:LEU:HD13	2:E:80:LEU:HD23	1.87	0.55
2:H:34:MET:HB3	2:H:78:LEU:HD22	1.88	0.55
2:J:63:VAL:HG13	2:J:67:PHE:HB2	1.88	0.55
3:F:48:ILE:HD13	3:F:64:GLY:HA3	1.88	0.55
3:L:123:GLU:O	3:L:126:LYS:HG2	2.07	0.55
3:I:198:HIS:H	3:I:201:LEU:HD11	1.70	0.55
1:D:116:VAL:HG13	1:D:136:GLN:HB2	1.88	0.55
1:A:246:SER:HB2	1:A:294:ASN:HD22	1.72	0.55
1:D:217:SER:OG	1:D:243:ASP:OD2	2.20	0.55
3:L:164:THR:HG22	3:L:174:SER:H	1.71	0.54
2:J:103:TRP:CZ3	3:K:44:PRO:HG2	2.41	0.54
1:D:224:ARG:NH2	1:D:244:GLY:O	2.39	0.54
2:E:140:LEU:HD11	2:E:225:VAL:CG2	2.37	0.54
1:C:93:PRO:O	1:C:450:ASN:ND2	2.40	0.54
2:E:34:MET:HB3	2:E:78:LEU:HD22	1.88	0.54
1:C:461:GLY:HA3	1:B:155:TYR:CE1	2.42	0.54
1:A:164:GLY:HA3	1:D:173:PHE:CG	2.43	0.54
1:A:364:ARG:HD3	1:A:377:ILE:HD12	1.90	0.54
2:G:34:MET:HB3	2:G:78:LEU:HD22	1.89	0.54
3:L:136:LEU:HD13	3:L:175:LEU:HD12	1.90	0.53
2:J:167:THR:O	2:J:171:VAL:HG22	2.08	0.53
3:F:164:THR:HG22	3:F:174:SER:H	1.73	0.53
1:B:256:ARG:NH1	1:B:308:GLN:O	2.39	0.53
2:J:138:ALA:HB3	2:J:198:LEU:HD11	1.90	0.53
3:K:124:GLN:NE2	3:K:131:SER:OG	2.36	0.53
1:B:178:TRP:O	2:J:100(C):ARG:NH2	2.41	0.53
3:L:149:LYS:HG2	3:L:154:LEU:HD13	1.90	0.53
2:E:62:SER:O	2:E:66:ARG:NH1	2.41	0.53
3:I:108:ARG:NH2	3:I:111:ALA:HB2	2.23	0.53
1:A:290:VAL:HG21	1:A:353:SER:HB2	1.90	0.53
2:H:119:PRO:HD2	2:H:217:THR:HG21	1.90	0.53
1:A:101:SER:HA	1:D:173:PHE:CZ	2.44	0.53
2:H:52:ASN:O	2:H:71:ARG:NH1	2.41	0.53
1:D:290:VAL:HG21	1:D:353:SER:HB2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:TYR:HB2	1:B:425:GLU:OE2	2.09	0.52
1:C:277:GLU:OE1	1:C:292:ARG:NH1	2.38	0.52
1:C:239:THR:O	1:C:254:ILE:HD12	2.10	0.52
1:D:150:LYS:NZ	1:D:152:ARG:O	2.41	0.52
2:H:40:VAL:HG21	2:H:43:LYS:HD2	1.90	0.52
2:J:2:VAL:HA	2:J:26:GLY:HA3	1.92	0.52
3:F:35:TRP:CD1	3:F:48:ILE:HD11	2.44	0.52
1:D:403:TRP:CZ2	1:D:433:GLU:OE1	2.61	0.52
2:H:215:SER:OG	2:H:217:THR:HG22	2.09	0.52
1:C:254:ILE:HD12	1:C:255:PHE:H	1.74	0.51
3:I:123:GLU:O	3:I:126:LYS:HG2	2.11	0.51
1:C:372:ASN:HB3	1:C:400:ILE:O	2.09	0.51
2:G:179:GLN:CD	2:G:186:SER:HB2	2.36	0.51
1:C:246:SER:HB2	1:C:294:ASN:HD22	1.75	0.51
1:B:116:VAL:CG2	1:B:136:GLN:HB2	2.39	0.51
1:B:298:SER:H	1:B:341:VAL:HG23	1.75	0.51
1:A:146:ASN:CB	1:A:437:ILE:HG13	2.40	0.51
2:E:2:VAL:HA	2:E:26:GLY:HA3	1.92	0.51
3:I:163:VAL:CG1	3:I:175:LEU:HD23	2.41	0.50
2:J:228:LYS:H	2:J:228:LYS:HZ3	1.58	0.50
1:D:318:CYS:SG	1:D:384:THR:CA	2.99	0.50
1:D:430:ARG:HD3	1:D:431:PRO:HA	1.91	0.50
3:L:149:LYS:HB2	3:L:193:ALA:HB3	1.94	0.50
1:C:378:TRP:HB3	1:C:392:ILE:HG23	1.92	0.50
3:L:183:LYS:O	3:L:187:GLU:HG2	2.12	0.50
2:G:90:TYR:CE1	2:G:109:VAL:HG13	2.46	0.50
3:I:183:LYS:O	3:I:187:GLU:HG2	2.11	0.50
2:J:190:VAL:HG21	3:K:135:LEU:HD21	1.93	0.50
1:C:142:ASP:CG	1:D:110:SER:HG	2.20	0.49
1:C:433:GLU:OE2	1:C:464:LEU:HD22	2.11	0.49
1:B:290:VAL:HG11	1:B:353:SER:H	1.77	0.49
1:B:290:VAL:HG11	1:B:353:SER:N	2.27	0.49
1:B:372:ASN:HB3	1:B:400:ILE:O	2.12	0.49
3:I:95:PRO:HD2	3:I:95(A):LEU:HD22	1.92	0.49
1:A:406:TYR:HH	2:H:100(C):ARG:HG3	1.77	0.49
1:B:419:ARG:HD2	1:B:448:GLY:O	2.12	0.49
2:E:174:PHE:HE2	3:F:174:SER:O	1.95	0.49
3:F:110:VAL:HG22	3:F:141:PRO:HD3	1.95	0.49
1:C:277:GLU:OE2	2:E:100(A):TYR:OH	2.22	0.49
1:B:422:PHE:CE1	1:B:446:PHE:HB2	2.48	0.49
2:E:87:THR:HG23	2:E:110:THR:HA	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:193:VAL:HG11	2:G:206:TYR:OH	2.12	0.49
3:I:183:LYS:HE3	3:I:187:GLU:OE1	2.13	0.49
1:C:149:ILE:HD12	1:C:430:ARG:HB3	1.95	0.49
1:B:117:ILE:CD1	1:B:167:PRO:HB2	2.43	0.49
2:E:40:VAL:HG23	2:E:43:LYS:CG	2.43	0.49
1:A:372:ASN:HB3	1:A:400:ILE:O	2.12	0.48
1:A:422:PHE:CE1	1:A:446:PHE:HB2	2.48	0.48
2:H:12:LEU:O	2:H:111:VAL:HA	2.13	0.48
3:F:4:LEU:HD11	3:F:90:HIS:HB2	1.94	0.48
1:D:372:ASN:HB3	1:D:400:ILE:O	2.13	0.48
3:L:61:ARG:HH11	3:L:79:GLN:CD	2.21	0.48
2:G:137:THR:HG23	2:G:192:THR:HG23	1.95	0.48
1:A:102:LYS:NZ	1:D:155:TYR:CD1	2.81	0.48
3:K:33:LEU:HD12	3:K:89:GLN:O	2.13	0.48
1:D:252:TYR:OH	1:D:274:HIS:HA	2.14	0.48
1:B:118:ARG:NH1	1:B:425:GLU:OE1	2.47	0.48
2:E:140:LEU:HD11	2:E:225:VAL:HG21	1.94	0.48
3:I:61:ARG:NE	3:I:82:ASP:OD2	2.33	0.48
2:E:215:SER:OG	2:E:217:THR:HG22	2.14	0.48
2:J:196:SER:O	2:J:196:SER:OG	2.26	0.48
1:D:322:PHE:HB2	1:D:327:ARG:HD2	1.95	0.48
1:B:360:VAL:HG12	1:B:382:GLY:HA3	1.96	0.48
1:A:378:TRP:HB3	1:A:392:ILE:HB	1.96	0.48
3:I:149:LYS:HD2	3:I:193:ALA:CB	2.42	0.48
1:D:118:ARG:HD2	1:D:425:GLU:OE2	2.13	0.47
3:F:149:LYS:HG3	3:F:193:ALA:HB3	1.96	0.47
3:F:183:LYS:O	3:F:187:GLU:HG2	2.14	0.47
3:K:164:THR:HG22	3:K:174:SER:H	1.78	0.47
1:B:117:ILE:O	1:B:440:SER:HA	2.14	0.47
3:I:136:LEU:HD11	3:I:196:VAL:CG2	2.35	0.47
2:E:3:GLN:HG3	2:E:105:ARG:HH22	1.80	0.47
3:K:95:PRO:HD2	3:K:95(A):LEU:HD22	1.95	0.47
2:E:60:THR:O	2:E:63:VAL:HG22	2.14	0.47
1:C:117:ILE:HD13	1:C:167:PRO:HG3	1.97	0.47
2:G:38:ARG:HD3	2:G:48:VAL:HG11	1.95	0.47
1:A:366:LYS:NZ	1:A:375:GLU:OE1	2.41	0.47
2:E:97:SER:HA	2:E:100(J):THR:O	2.14	0.47
3:K:108:ARG:HG3	3:K:109:THR:O	2.15	0.47
2:H:20:LEU:HD12	2:H:80:LEU:HD23	1.96	0.47
3:L:77:SER:O	3:L:79:GLN:NE2	2.48	0.47
1:C:224:ARG:HE	1:C:276:GLU:CD	2.23	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:VAL:HG23	1:D:440:SER:HB2	1.97	0.47
1:C:254:ILE:CD1	1:C:305:PHE:CZ	2.97	0.46
1:A:406:TYR:N	1:A:425:GLU:HG2	2.29	0.46
1:A:102:LYS:HZ3	1:D:155:TYR:HD1	1.64	0.46
2:G:4:LEU:HG	2:G:102:LEU:CD1	2.45	0.46
1:C:451:SER:CB	1:B:214:THR:OG1	2.63	0.46
1:D:333:GLY:O	1:D:386:THR:HB	2.14	0.46
1:D:406:TYR:HB2	1:D:425:GLU:OE1	2.16	0.46
2:H:103:TRP:CE3	3:L:44:PRO:HD2	2.50	0.46
2:J:213:LYS:HD2	2:J:214:PRO:HD3	1.96	0.46
3:I:32:TYR:HB3	3:I:91:LEU:HB2	1.97	0.46
1:C:103:ASP:OD1	1:C:442:SER:HB2	2.16	0.46
1:C:428:ARG:NH2	1:C:433:GLU:OE2	2.47	0.46
1:A:152:ARG:HE	1:A:198:ASP:CG	2.23	0.46
2:G:4:LEU:HD13	2:G:92:CYS:SG	2.56	0.46
2:G:144:VAL:CG2	2:G:187:LEU:HB3	2.45	0.46
2:J:150:GLU:HG3	2:J:185:TYR:CZ	2.51	0.46
1:B:116:VAL:HG22	1:B:138:ALA:O	2.16	0.46
1:D:179:SER:OG	1:D:227:GLU:OE2	2.28	0.46
2:H:97:SER:HA	2:H:100(J):THR:O	2.15	0.46
2:J:8:GLY:O	2:J:18:LEU:HD11	2.16	0.46
3:K:20:THR:HG23	3:K:72:THR:HG23	1.97	0.46
1:A:456:TRP:CE3	1:D:196:GLY:HA2	2.51	0.46
1:D:117:ILE:O	1:D:440:SER:HA	2.16	0.46
3:L:62:PHE:CD1	3:L:75:ILE:HG22	2.51	0.46
2:E:14:PRO:HD2	2:E:113:SER:HB2	1.97	0.46
3:F:48:ILE:HD12	3:F:51:ALA:C	2.41	0.46
2:G:20:LEU:HD12	2:G:80:LEU:HD23	1.97	0.46
3:I:170:ASP:OD2	3:I:172:THR:OG1	2.32	0.46
2:J:174:PHE:O	2:J:187:LEU:HD11	2.16	0.46
1:D:149:ILE:HD12	1:D:430:ARG:HB3	1.98	0.46
2:G:177:VAL:HG21	3:I:160:GLN:HB3	1.97	0.46
3:K:142:ARG:NH2	3:K:163:VAL:HG21	2.31	0.46
1:D:360:VAL:HG12	1:D:382:GLY:HA3	1.97	0.45
3:F:170:ASP:OD2	3:F:172:THR:OG1	2.28	0.45
2:G:138:ALA:HB3	2:G:198:LEU:HD21	1.99	0.45
2:H:212:HIS:ND1	2:H:215:SER:OG	2.45	0.45
2:E:39:GLN:HB2	2:E:45:LEU:HD13	1.98	0.45
1:C:290:VAL:HG21	1:C:353:SER:HB2	1.98	0.45
3:L:75:ILE:O	3:L:75:ILE:HD12	2.16	0.45
1:B:461:GLY:HA3	1:A:155:TYR:CZ	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ARG:NH1	1:D:276:GLU:OE1	2.49	0.45
3:I:163:VAL:HG13	3:I:175:LEU:HD23	1.99	0.45
1:C:430:ARG:NE	1:C:436:THR:O	2.50	0.45
3:L:95(A):LEU:O	3:L:97:THR:N	2.49	0.45
3:I:62:PHE:CE1	3:I:75:ILE:HD12	2.52	0.45
1:C:170:ASN:ND2	1:B:169(A):TYR:HA	2.31	0.45
1:B:110:SER:HG	1:A:142:ASP:CG	2.25	0.45
1:A:366:LYS:HB3	1:A:400:ILE:HD13	1.98	0.45
2:H:12:LEU:HD22	2:H:82:ILE:HD11	1.98	0.45
2:E:68:THR:HB	2:E:81:HIS:HB3	1.98	0.45
2:G:40:VAL:HG12	2:G:41:PRO:HD2	1.97	0.45
1:C:117:ILE:O	1:C:440:SER:HA	2.17	0.45
2:G:30:ASP:O	2:G:52(A):TRP:HB2	2.17	0.45
2:J:97:SER:HA	2:J:100(J):THR:O	2.17	0.45
1:B:203:ALA:HB3	1:B:215:ILE:HG23	1.98	0.45
3:L:90:HIS:ND1	3:L:93:SER:HB3	2.32	0.45
3:K:95(A):LEU:O	3:K:97:THR:N	2.50	0.45
2:E:38:ARG:HD3	2:E:48:VAL:HG11	1.98	0.45
2:E:119:PRO:HB2	2:E:144:VAL:HG13	1.99	0.45
3:I:95(A):LEU:O	3:I:97:THR:N	2.50	0.45
2:J:143:LEU:HD21	2:J:145:LYS:HD2	1.97	0.45
3:F:78:LEU:HD23	3:F:78:LEU:HA	1.81	0.45
3:I:90:HIS:ND1	3:I:93:SER:HB3	2.32	0.45
2:J:66:ARG:NH1	2:J:86:ASP:OD2	2.48	0.45
1:C:299:ASN:CG	1:C:341:VAL:HG23	2.42	0.44
1:A:347:ASN:ND2	2:H:100(G):PRO:HG3	2.32	0.44
2:H:212:HIS:HB3	2:H:217:THR:HG23	1.99	0.44
2:G:97:SER:HA	2:G:100(J):THR:O	2.18	0.44
1:C:422:PHE:CE1	1:C:446:PHE:HB2	2.52	0.44
3:F:149:LYS:NZ	3:F:195:GLU:HB2	2.32	0.44
2:J:198:LEU:N	2:J:198:LEU:HD12	2.32	0.44
3:L:21:ILE:CD1	3:L:102:THR:HG21	2.46	0.44
2:J:190:VAL:HG21	3:K:135:LEU:CD2	2.47	0.44
3:F:83:PHE:HA	3:F:104:VAL:HG23	1.99	0.44
2:G:145:LYS:HG2	2:G:146:ASP:CG	2.43	0.44
1:C:360:VAL:HG12	1:C:382:GLY:HA3	2.00	0.44
3:I:108:ARG:HD2	3:I:170:ASP:O	2.17	0.44
1:B:232:CYS:HA	1:B:237:CYS:HA	2.00	0.44
1:D:91:LEU:HD22	1:D:420:PRO:HG3	1.99	0.44
2:J:13:ARG:HG2	2:J:113:SER:HA	1.98	0.44
1:A:321:ILE:HG21	1:A:377:ILE:HG21	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ARG:HH11	1:A:377:ILE:CD1	2.30	0.44
2:G:90:TYR:CE1	2:G:109:VAL:CG1	3.01	0.44
1:B:118:ARG:NH1	1:B:425:GLU:CD	2.76	0.44
1:A:146:ASN:HA	1:A:437:ILE:HG13	1.99	0.44
1:D:232:CYS:HA	1:D:237:CYS:HA	1.99	0.44
2:G:52:ASN:O	2:G:71:ARG:NH1	2.51	0.44
2:J:119:PRO:HB3	2:J:147:TYR:HB3	2.00	0.44
1:C:299:ASN:ND2	1:C:341:VAL:HG23	2.33	0.43
3:F:108:ARG:HG3	3:F:109:THR:O	2.18	0.43
2:G:63:VAL:HG13	2:G:67:PHE:HB2	1.99	0.43
3:I:136:LEU:CD1	3:I:196:VAL:HG11	2.47	0.43
3:K:56:SER:OG	3:K:57:GLY:N	2.51	0.43
1:C:116:VAL:HG11	1:C:148:THR:HG21	2.00	0.43
1:C:378:TRP:HB3	1:C:392:ILE:HG22	1.98	0.43
1:B:298:SER:OG	1:B:341:VAL:CG2	2.62	0.43
1:D:85:LEU:HD13	1:D:412(A):HIS:ND1	2.33	0.43
2:J:100(A):TYR:OH	2:J:100(C):ARG:NH1	2.51	0.43
3:L:155:GLN:OE1	3:L:158:ASN:ND2	2.51	0.43
2:E:8:GLY:O	2:E:18:LEU:HD11	2.18	0.43
3:F:120:PRO:HD3	3:F:132:VAL:HG22	2.00	0.43
1:A:277:GLU:OE2	2:H:100(A):TYR:OH	2.24	0.43
2:H:30:ASP:O	2:H:52(A):TRP:HB2	2.19	0.43
1:C:173:PHE:CG	1:D:164:GLY:HA3	2.53	0.43
1:C:173:PHE:CZ	1:D:101:SER:HA	2.53	0.43
1:C:276:GLU:O	1:C:292:ARG:HB3	2.18	0.43
1:B:322:PHE:HB2	1:B:327:ARG:HD2	2.00	0.43
1:A:102:LYS:NZ	1:D:155:TYR:HD1	2.16	0.43
3:L:75:ILE:HD11	3:L:78:LEU:HG	1.99	0.43
3:F:19:ILE:HD11	3:F:75:ILE:HD13	2.01	0.43
3:F:95(A):LEU:O	3:F:97:THR:N	2.52	0.43
1:B:319:SER:HB2	1:B:382:GLY:HA2	1.99	0.43
2:E:100(M):PHE:O	3:F:36:TYR:HE2	2.01	0.43
3:F:10:PHE:CE2	3:F:142:ARG:HG2	2.54	0.43
1:A:178:TRP:O	2:H:100(C):ARG:NH2	2.41	0.43
1:A:232:CYS:HA	1:A:237:CYS:HA	2.00	0.43
3:I:37:GLN:HB2	3:I:47:LEU:HD11	2.01	0.43
2:J:99:GLY:O	3:K:32:TYR:OH	2.31	0.43
3:K:39:ARG:HD2	3:K:81:GLU:O	2.19	0.43
2:E:198:LEU:N	2:E:198:LEU:HD12	2.33	0.43
2:J:60:THR:OG1	3:K:95(A):LEU:HD12	2.19	0.43
1:C:366:LYS:NZ	1:C:375:GLU:OE1	2.46	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:ASN:OD1	1:D:309:ASN:N	2.52	0.42
2:J:63:VAL:HG13	2:J:67:PHE:CB	2.48	0.42
1:C:232:CYS:HA	1:C:237:CYS:HA	1.99	0.42
1:A:103:ASP:OD1	1:A:442:SER:HB2	2.19	0.42
2:H:166:LEU:CD2	2:H:191:VAL:HG21	2.47	0.42
3:I:95(A):LEU:O	3:I:97:THR:HG23	2.19	0.42
1:D:330:ASP:CG	1:D:364:ARG:HH12	2.28	0.42
2:J:12:LEU:O	2:J:111:VAL:HA	2.19	0.42
2:J:213:LYS:HG3	2:J:214:PRO:HD3	2.01	0.42
3:K:163:VAL:HG22	3:K:175:LEU:HD12	1.99	0.42
1:A:146:ASN:HB2	1:A:437:ILE:HG13	2.00	0.42
4:A:505:NAG:H83	4:A:505:NAG:H3	1.99	0.42
3:L:62:PHE:CE1	3:L:75:ILE:HG22	2.54	0.42
1:B:251:SER:OG	1:B:267:GLU:OE1	2.35	0.42
1:A:430:ARG:NH1	1:A:436:THR:O	2.47	0.42
2:E:59:TYR:CE1	2:E:69:VAL:HG23	2.52	0.42
1:B:110:SER:O	1:B:141:ASN:ND2	2.52	0.42
1:D:122:ILE:CD1	1:D:163:ILE:CD1	2.95	0.42
3:F:32:TYR:HB3	3:F:91:LEU:HB2	2.01	0.42
3:K:167:ASP:CB	3:K:170:ASP:OD1	2.64	0.42
1:B:319:SER:HB2	1:B:382:GLY:CA	2.50	0.42
1:A:222:ILE:CD1	2:H:99:GLY:HA2	2.49	0.42
2:H:51:LEU:HD12	2:H:54:GLY:HA2	2.02	0.42
2:H:66:ARG:NH1	2:H:86:ASP:OD2	2.47	0.42
3:L:11:LEU:HD13	3:L:21:ILE:HD11	2.00	0.42
2:G:212:HIS:ND1	2:G:215:SER:OG	2.46	0.42
3:K:11:LEU:HD21	3:K:19:ILE:HG23	2.01	0.42
3:L:75:ILE:HD12	3:L:75:ILE:C	2.45	0.42
3:L:108:ARG:HG3	3:L:109:THR:O	2.20	0.42
2:G:90:TYR:CD1	2:G:109:VAL:CG1	3.03	0.42
3:K:78:LEU:HD22	3:K:82:ASP:HB2	2.02	0.42
2:E:12:LEU:HD21	2:E:111:VAL:HG22	2.02	0.42
3:F:90:HIS:ND1	3:F:93:SER:HB3	2.35	0.42
2:G:137:THR:CG2	2:G:192:THR:HG23	2.50	0.42
3:I:78:LEU:HA	3:I:78:LEU:HD23	1.81	0.42
1:B:452:ASP:O	1:A:214:THR:OG1	2.29	0.42
3:I:19:ILE:O	3:I:74:THR:HA	2.20	0.42
3:I:142:ARG:HB2	3:I:173:TYR:CE2	2.55	0.42
3:K:94:TYR:HA	3:K:95:PRO:HA	1.86	0.42
2:H:63:VAL:HG13	2:H:67:PHE:HB2	2.02	0.41
2:E:123:PRO:CB	2:E:225:VAL:HG12	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:TRP:CD1	1:B:219:ARG:HG2	2.55	0.41
1:B:270:ALA:HB1	1:B:273:TYR:HB2	2.02	0.41
1:B:428:ARG:HG3	1:B:460:ASP:OD2	2.20	0.41
1:A:110:SER:OG	1:D:142:ASP:OD1	2.28	0.41
2:E:145:LYS:NZ	2:E:179:GLN:OE1	2.52	0.41
3:I:161:GLU:HA	3:I:176:SER:O	2.20	0.41
2:J:62:SER:HB2	2:J:85:GLU:OE1	2.20	0.41
2:J:213:LYS:HD2	2:J:214:PRO:CD	2.50	0.41
1:A:327:ARG:NH2	1:A:365:THR:OG1	2.53	0.41
2:E:212:HIS:ND1	2:E:215:SER:OG	2.44	0.41
1:B:355:LYS:HE2	1:B:383:TRP:CD1	2.55	0.41
1:A:299:ASN:CG	1:A:341:VAL:HG23	2.46	0.41
1:D:222:ILE:HD12	2:G:100(A):TYR:HB3	2.03	0.41
2:H:140:LEU:HD12	2:H:140:LEU:C	2.45	0.41
2:E:192:THR:HG21	3:F:137:ASN:HD22	1.81	0.41
3:K:11:LEU:CD2	3:K:19:ILE:HG23	2.50	0.41
1:B:222:ILE:HD11	2:J:99:GLY:HA2	2.02	0.41
1:A:117:ILE:O	1:A:440:SER:HA	2.20	0.41
2:G:83:LYS:HB3	2:G:84:PRO:HD2	2.01	0.41
1:A:203:ALA:O	1:A:214:THR:HA	2.21	0.41
2:G:36:TRP:NE1	2:G:80:LEU:HB2	2.35	0.41
1:A:375:GLU:CD	1:A:394:LYS:HE2	2.42	0.41
2:G:147:TYR:CE1	2:G:185:TYR:HB2	2.55	0.41
2:G:198:LEU:H	2:G:198:LEU:HD22	1.86	0.41
1:C:270:ALA:HB1	1:C:273:TYR:HB2	2.03	0.41
1:C:399:GLY:H	1:C:457:SER:HG	1.69	0.41
1:C:411:VAL:CG2	1:C:418:ILE:CG2	2.98	0.41
1:B:118:ARG:HH21	2:J:100(C):ARG:HB3	1.85	0.41
1:B:164:GLY:HA3	1:A:173:PHE:CG	2.56	0.41
1:D:141:ASN:OD1	1:D:466:PHE:HB3	2.21	0.41
2:H:5:VAL:HG13	2:H:23:ALA:HB3	2.02	0.41
2:H:8:GLY:O	2:H:18:LEU:HD11	2.21	0.41
3:L:93:SER:O	3:L:95(A):LEU:N	2.52	0.41
3:L:113:PRO:HB3	3:L:139:PHE:HB3	2.03	0.41
2:E:28:LYS:HD2	2:E:30:ASP:HB3	2.03	0.41
2:E:207:ILE:HG22	2:E:222:ARG:HA	2.02	0.41
3:F:186:TYR:O	3:F:192:TYR:OH	2.37	0.41
2:J:95:THR:HG21	2:J:100(K):TRP:CD2	2.55	0.41
1:A:258:GLU:O	1:A:261:LYS:HG2	2.19	0.41
1:A:270:ALA:HB1	1:A:273:TYR:HB2	2.02	0.41
1:A:397:ILE:HG22	1:A:398:VAL:HG23	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:213:LYS:N	2:J:214:PRO:CD	2.84	0.41
3:K:90:HIS:ND1	3:K:93:SER:HB3	2.36	0.41
1:C:119:GLU:HG2	2:E:100(C):ARG:HE	1.86	0.40
1:C:300:ARG:CZ	1:C:351:GLY:HA3	2.51	0.40
1:B:91:LEU:HD23	1:B:91:LEU:HA	1.91	0.40
1:B:321:ILE:HG21	1:B:377:ILE:HG21	2.03	0.40
3:F:93:SER:O	3:F:95(A):LEU:N	2.52	0.40
2:G:148:PHE:HA	2:G:149:PRO:HA	1.89	0.40
1:A:430:ARG:CD	1:A:436:THR:O	2.53	0.40
2:G:95:THR:HG21	2:G:100(K):TRP:CD2	2.56	0.40
1:D:116:VAL:HG12	1:D:138:ALA:O	2.21	0.40
2:E:212:HIS:HB3	2:E:217:THR:HG23	2.03	0.40
3:F:144:ALA:HB2	3:F:198:HIS:HD2	1.86	0.40
3:I:10:PHE:CE1	3:I:142:ARG:HG2	2.57	0.40
1:C:254:ILE:HD11	1:C:305:PHE:CZ	2.56	0.40
1:C:411:VAL:CG2	1:C:418:ILE:HG22	2.51	0.40
1:B:110:SER:OG	1:A:142:ASP:OD1	2.34	0.40
1:B:111:LYS:HE2	1:A:113:ASP:OD1	2.22	0.40
1:A:437:ILE:HA	1:A:437:ILE:HD12	1.83	0.40
1:D:331:LYS:O	1:D:388:ASN:HB3	2.22	0.40
2:H:89:LEU:HD23	2:H:89:LEU:H	1.85	0.40
3:F:84:ALA:O	3:F:104:VAL:HG22	2.21	0.40
2:G:174:PHE:HB3	3:I:162:SER:OG	2.20	0.40
2:J:84:PRO:HA	2:J:111:VAL:CG2	2.51	0.40
3:I:93:SER:O	3:I:95(A):LEU:N	2.52	0.40
2:J:140:LEU:HD12	2:J:140:LEU:C	2.46	0.40
3:K:93:SER:O	3:K:95(A):LEU:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	382/391 (98%)	365 (96%)	16 (4%)	1 (0%)	36	66
1	B	382/391 (98%)	364 (95%)	17 (4%)	1 (0%)	36	66
1	C	382/391 (98%)	365 (96%)	16 (4%)	1 (0%)	36	66
1	D	382/391 (98%)	365 (96%)	16 (4%)	1 (0%)	36	66
2	E	223/240 (93%)	208 (93%)	14 (6%)	1 (0%)	30	60
2	G	223/240 (93%)	210 (94%)	12 (5%)	1 (0%)	30	60
2	H	223/240 (93%)	208 (93%)	14 (6%)	1 (0%)	30	60
2	J	223/240 (93%)	208 (93%)	14 (6%)	1 (0%)	30	60
3	F	213/216 (99%)	201 (94%)	10 (5%)	2 (1%)	14	43
3	I	213/216 (99%)	198 (93%)	13 (6%)	2 (1%)	14	43
3	K	213/216 (99%)	198 (93%)	14 (7%)	1 (0%)	24	55
3	L	213/216 (99%)	198 (93%)	13 (6%)	2 (1%)	14	43
All	All	3272/3388 (97%)	3088 (94%)	169 (5%)	15 (0%)	24	55

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	96	PHE
3	I	96	PHE
3	F	96	PHE
3	K	204	PRO
3	I	204	PRO
3	L	204	PRO
3	F	204	PRO
2	J	63	VAL
2	H	63	VAL
2	G	63	VAL
1	C	222	ILE
1	B	222	ILE
1	A	222	ILE
1	D	222	ILE
2	E	63	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/337 (98%)	324 (98%)	7 (2%)	47	67
1	B	331/337 (98%)	323 (98%)	8 (2%)	43	65
1	C	331/337 (98%)	324 (98%)	7 (2%)	47	67
1	D	331/337 (98%)	324 (98%)	7 (2%)	47	67
2	E	192/204 (94%)	184 (96%)	8 (4%)	26	54
2	G	192/204 (94%)	180 (94%)	12 (6%)	16	44
2	H	192/204 (94%)	187 (97%)	5 (3%)	40	64
2	J	192/204 (94%)	183 (95%)	9 (5%)	23	52
3	F	187/188 (100%)	179 (96%)	8 (4%)	26	54
3	I	187/188 (100%)	174 (93%)	13 (7%)	14	41
3	K	187/188 (100%)	180 (96%)	7 (4%)	30	57
3	L	187/188 (100%)	174 (93%)	13 (7%)	14	41
All	All	2840/2916 (97%)	2736 (96%)	104 (4%)	30	57

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	170	ASN
1	C	230	CYS
1	C	254	ILE
1	C	296	HIS
1	C	411	VAL
1	C	435	ASN
1	C	451	SER
1	B	143	LYS
1	B	230	CYS
1	B	265	SER
1	B	276	GLU
1	B	290	VAL
1	B	394	LYS
1	B	433	GLU
1	B	450	ASN
1	A	122	ILE
1	A	230	CYS
1	A	296	HIS
1	A	336	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	425	GLU
1	A	433	GLU
1	A	450	ASN
1	D	116	VAL
1	D	118	ARG
1	D	224	ARG
1	D	230	CYS
1	D	343	SER
1	D	433	GLU
1	D	450	ASN
2	H	1	GLU
2	H	5	VAL
2	H	154	VAL
2	H	192	THR
2	H	217	THR
3	L	14	SER
3	L	33	LEU
3	L	56	SER
3	L	69	THR
3	L	72	THR
3	L	109	THR
3	L	110	VAL
3	L	129	THR
3	L	152	ASN
3	L	169	LYS
3	L	206	THR
3	L	207	LYS
3	L	214	CYS
2	E	1	GLU
2	E	17	SER
2	E	28	LYS
2	E	40	VAL
2	E	154	VAL
2	E	196	SER
2	E	217	THR
2	E	225	VAL
3	F	33	LEU
3	F	56	SER
3	F	60	SER
3	F	126	LYS
3	F	129	THR
3	F	136	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	175	LEU
3	F	206	THR
2	G	3	GLN
2	G	102	LEU
2	G	103	TRP
2	G	109	VAL
2	G	115	SER
2	G	144	VAL
2	G	145	LYS
2	G	173	THR
2	G	192	THR
2	G	193	VAL
2	G	197	SER
2	G	213	LYS
3	I	14	SER
3	I	33	LEU
3	I	60	SER
3	I	69	THR
3	I	74	THR
3	I	109	THR
3	I	110	VAL
3	I	169	LYS
3	I	176	SER
3	I	180	THR
3	I	183	LYS
3	I	197	THR
3	I	201	LEU
2	J	48	VAL
2	J	115	SER
2	J	173	THR
2	J	192	THR
2	J	193	VAL
2	J	196	SER
2	J	205	THR
2	J	225	VAL
2	J	228	LYS
3	K	14	SER
3	K	19	ILE
3	K	70	GLU
3	K	72	THR
3	K	109	THR
3	K	196	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	K	197	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	344	ASN
1	B	146	ASN
1	B	208	ASN
1	A	104	ASN
3	L	160	GLN
2	E	39	GLN
2	E	81	HIS
2	E	82(A)	ASN
3	F	38	GLN
2	G	3	GLN
2	G	39	GLN
3	I	37	GLN
3	I	38	GLN
3	I	79	GLN
3	I	147	GLN
2	J	39	GLN
2	J	81	HIS
2	J	82(A)	ASN
2	J	172	HIS
2	J	179	GLN
3	K	38	GLN
3	K	79	GLN
3	K	138	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 for Mogul analysis.

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	C	501	1	14,14,15	0.49	0	17,19,21	1.34	2 (11%)
4	NAG	A	505	1	14,14,15	0.61	0	17,19,21	2.14	5 (29%)
4	NAG	C	504	1	14,14,15	0.39	0	17,19,21	0.95	0
4	NAG	A	501	1	14,14,15	0.70	0	17,19,21	0.97	1 (5%)
4	NAG	A	502	1	14,14,15	0.36	0	17,19,21	1.34	1 (5%)
4	NAG	B	501	1	14,14,15	0.75	0	17,19,21	1.45	2 (11%)
4	NAG	B	504	1	14,14,15	0.35	0	17,19,21	0.94	1 (5%)
4	NAG	D	502	1	14,14,15	0.50	0	17,19,21	1.25	1 (5%)

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	C	501	1	-	0/6/23/26	0/1/1/1
4	NAG	A	505	1	-	5/6/23/26	0/1/1/1
4	NAG	C	504	1	-	2/6/23/26	0/1/1/1
4	NAG	A	501	1	-	1/6/23/26	0/1/1/1
4	NAG	A	502	1	-	2/6/23/26	0/1/1/1
4	NAG	B	501	1	-	2/6/23/26	0/1/1/1
4	NAG	B	504	1	-	2/6/23/26	0/1/1/1
4	NAG	D	502	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	505	NAG	C2-N2-C7	5.65	130.48	122.90
4	D	502	NAG	C1-O5-C5	4.27	117.90	112.19
4	A	502	NAG	C1-O5-C5	4.20	117.82	112.19
4	A	505	NAG	O5-C1-C2	4.04	117.53	111.29
4	B	501	NAG	O5-C5-C6	3.87	115.20	107.66
4	C	501	NAG	C4-C3-C2	3.02	115.45	111.02
4	C	501	NAG	O5-C5-C6	2.94	113.38	107.66
4	A	505	NAG	C8-C7-N2	2.76	120.69	116.12
4	B	501	NAG	C2-N2-C7	2.75	126.58	122.90
4	B	504	NAG	C1-O5-C5	2.49	115.52	112.19
4	A	505	NAG	O5-C5-C4	-2.31	105.22	110.83
4	A	501	NAG	O5-C5-C6	2.17	111.88	107.66
4	A	505	NAG	C1-C2-N2	2.00	113.59	110.43

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	504	NAG	C4-C5-C6-O6
4	A	502	NAG	O5-C5-C6-O6
4	B	501	NAG	O5-C5-C6-O6
4	A	502	NAG	C4-C5-C6-O6
4	C	504	NAG	O5-C5-C6-O6
4	B	501	NAG	C4-C5-C6-O6
4	A	505	NAG	C8-C7-N2-C2
4	A	505	NAG	O7-C7-N2-C2
4	B	504	NAG	O5-C5-C6-O6
4	A	505	NAG	O5-C5-C6-O6
4	A	501	NAG	C3-C2-N2-C7
4	B	504	NAG	C4-C5-C6-O6
4	A	505	NAG	C1-C2-N2-C7
4	A	505	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	505	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	A	384/391 (98%)	-1.47	0 100 100	33, 54, 76, 125	0
1	B	384/391 (98%)	-1.52	0 100 100	30, 53, 76, 118	0
1	C	384/391 (98%)	-1.48	0 100 100	29, 55, 79, 119	0
1	D	384/391 (98%)	-1.51	0 100 100	36, 58, 81, 137	0
2	E	227/240 (94%)	-1.35	0 100 100	42, 75, 111, 133	0
2	G	227/240 (94%)	-1.37	0 100 100	32, 67, 98, 116	0
2	H	227/240 (94%)	-1.43	0 100 100	32, 57, 86, 115	0
2	J	227/240 (94%)	-1.34	0 100 100	44, 72, 111, 144	0
3	F	215/216 (99%)	-1.40	0 100 100	40, 74, 99, 131	0
3	I	215/216 (99%)	-1.42	0 100 100	38, 61, 86, 103	0
3	K	215/216 (99%)	-1.39	0 100 100	37, 66, 91, 113	0
3	L	215/216 (99%)	-1.39	0 100 100	25, 63, 95, 140	0
All	All	3304/3388 (97%)	-1.44	0 100 100	25, 60, 94, 144	0

There are no RSRZ outliers to report.

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

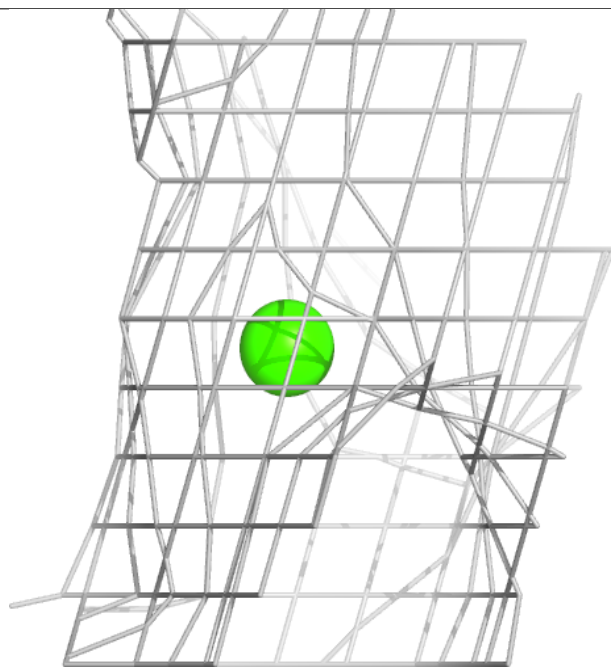
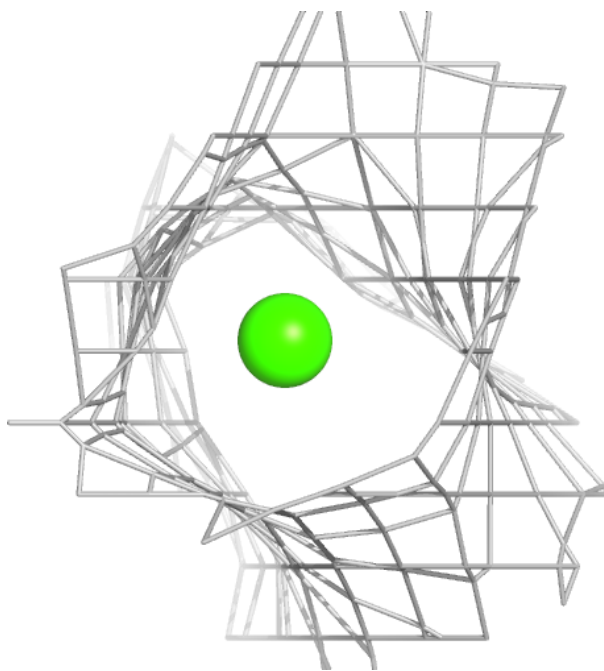
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	505	14/15	0.95	0.06	82,98,113,118	0
4	NAG	B	504	14/15	0.97	0.08	104,122,128,132	0
4	NAG	C	504	14/15	0.97	0.05	88,110,126,130	0
4	NAG	D	502	14/15	0.97	0.06	74,87,95,97	0
4	NAG	A	501	14/15	0.98	0.05	57,64,76,77	0
4	NAG	A	502	14/15	0.98	0.05	70,92,100,101	0
4	NAG	B	501	14/15	0.98	0.04	53,62,66,66	0
4	NAG	C	501	14/15	0.98	0.05	56,62,70,77	0
5	CA	D	504	1/1	0.98	0.04	112,112,112,112	0
5	CA	B	503	1/1	0.99	0.04	300,300,300,300	0
5	CA	A	503	1/1	0.99	0.04	99,99,99,99	0
5	CA	A	504	1/1	0.99	0.06	124,124,124,124	0
5	CA	D	501	1/1	0.99	0.05	68,68,68,68	0
5	CA	D	503	1/1	0.99	0.03	96,96,96,96	0
5	CA	C	503	1/1	0.99	0.07	143,143,143,143	0
5	CA	C	502	1/1	1.00	0.04	68,68,68,68	0
5	CA	B	502	1/1	1.00	0.03	111,111,111,111	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.

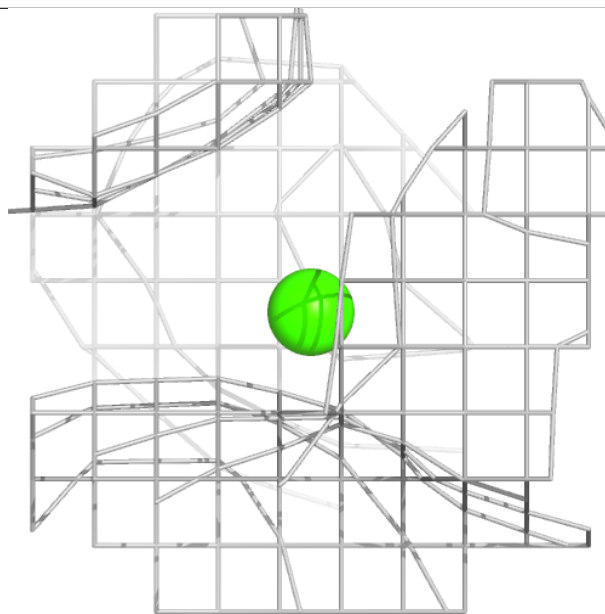
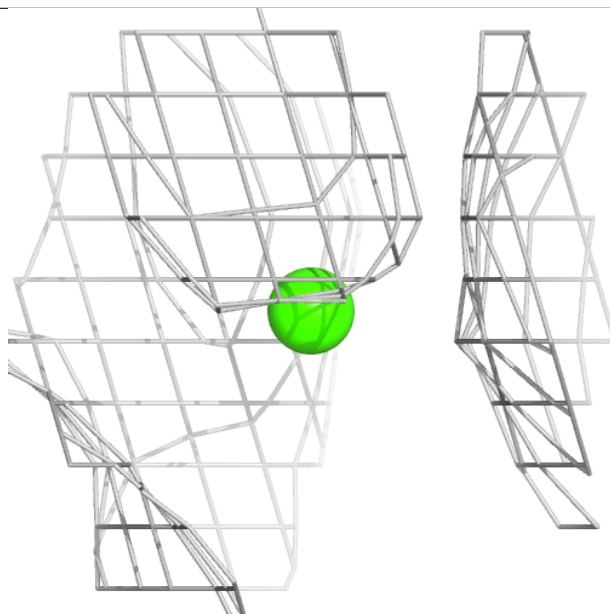
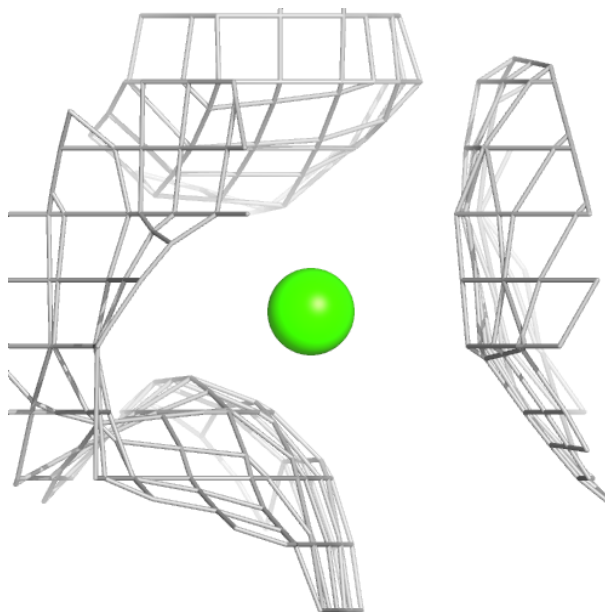
Electron density around CA D 504:

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



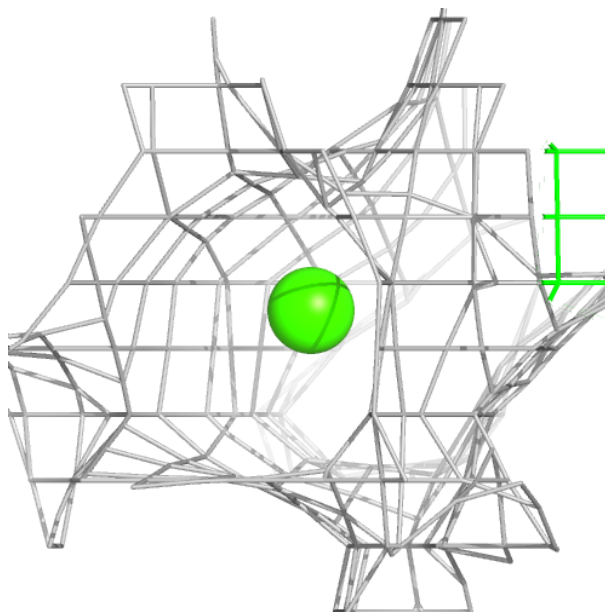
Electron density around CA B 503:

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



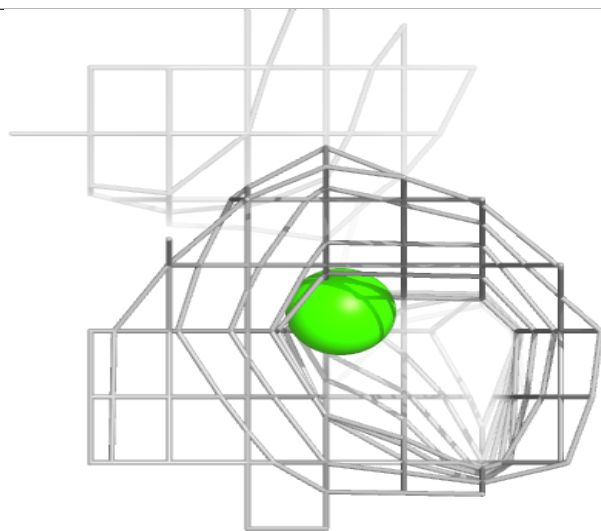
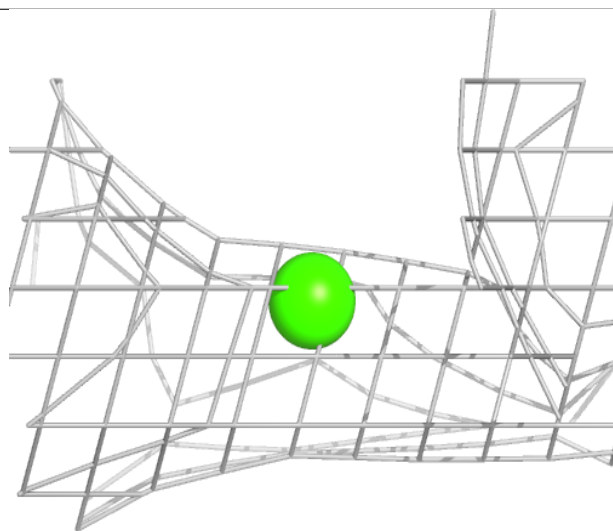
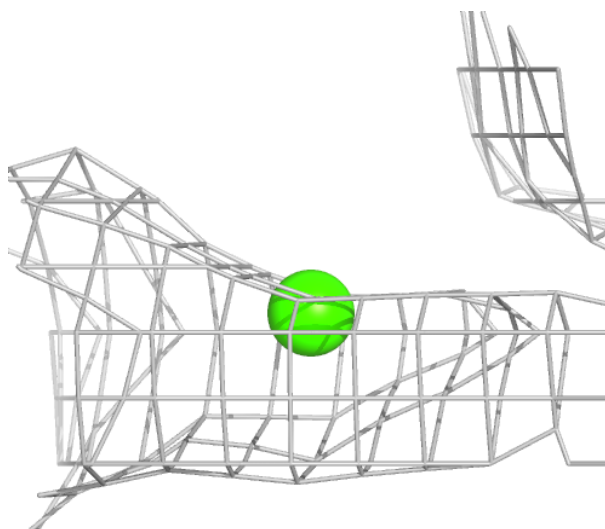
Electron density around CA A 503:

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



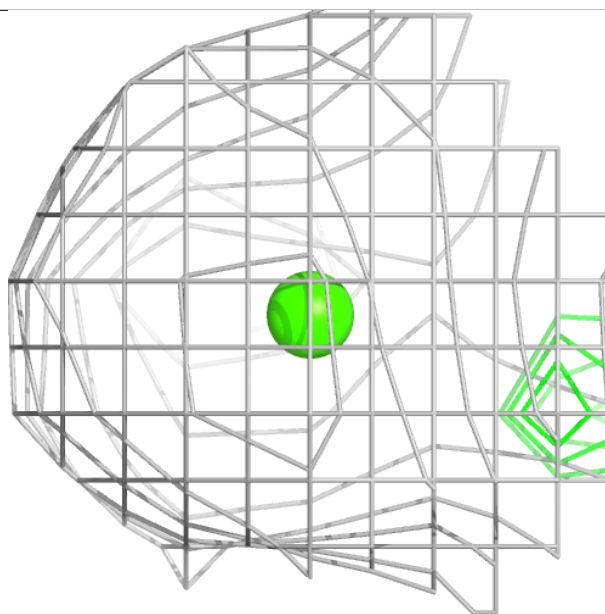
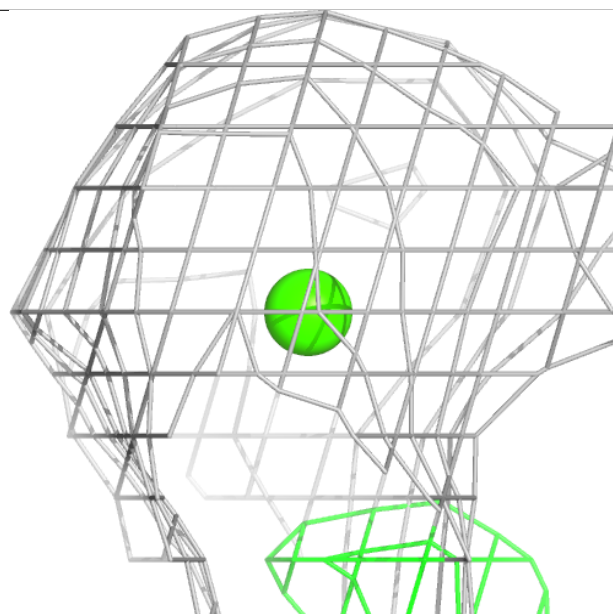
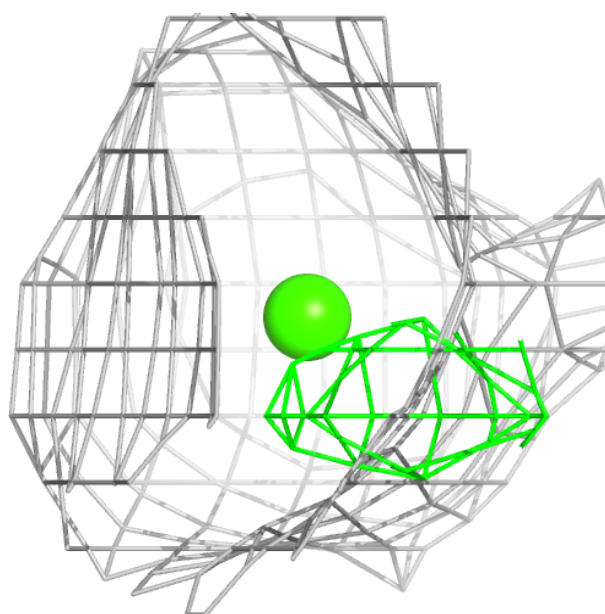
Electron density around CA A 504:

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



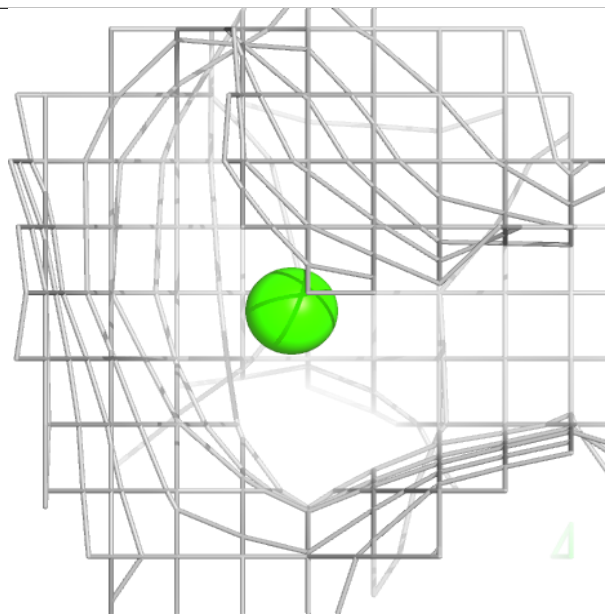
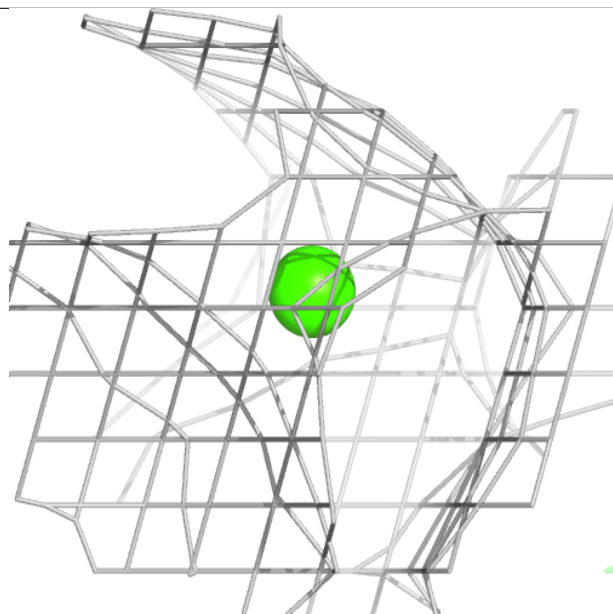
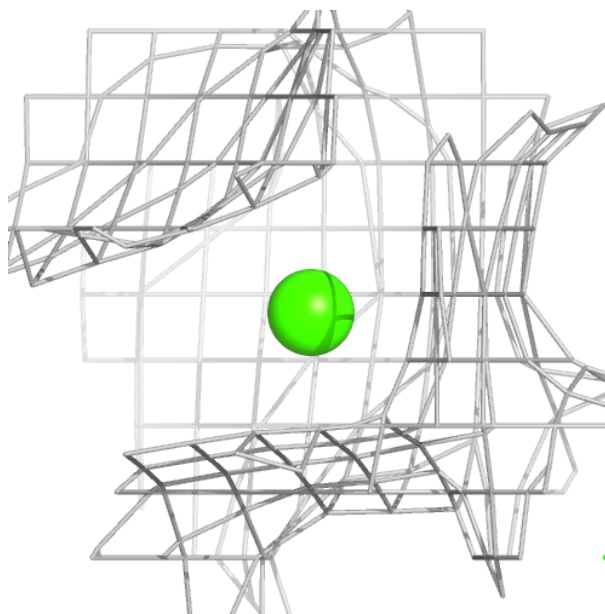
Electron density around CA D 501:

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



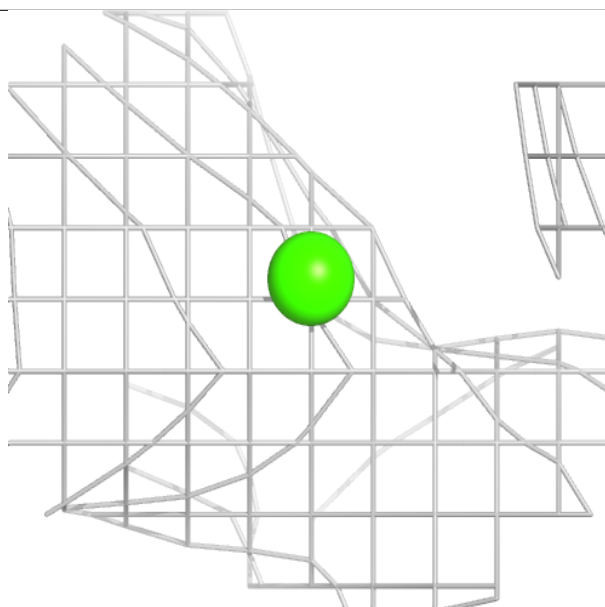
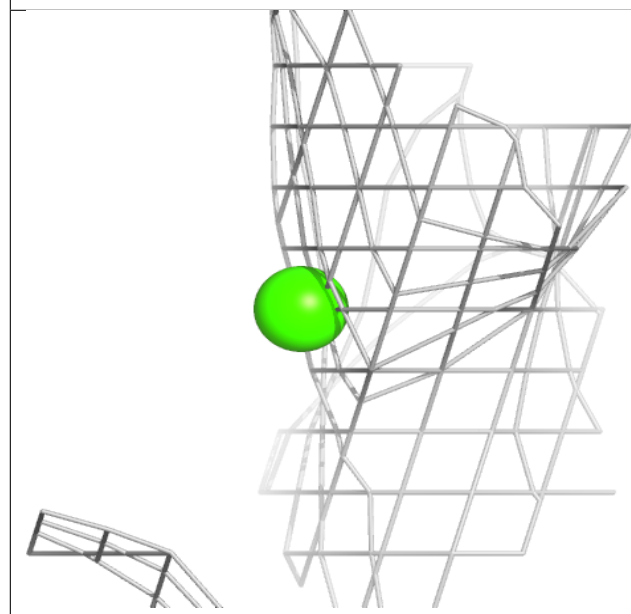
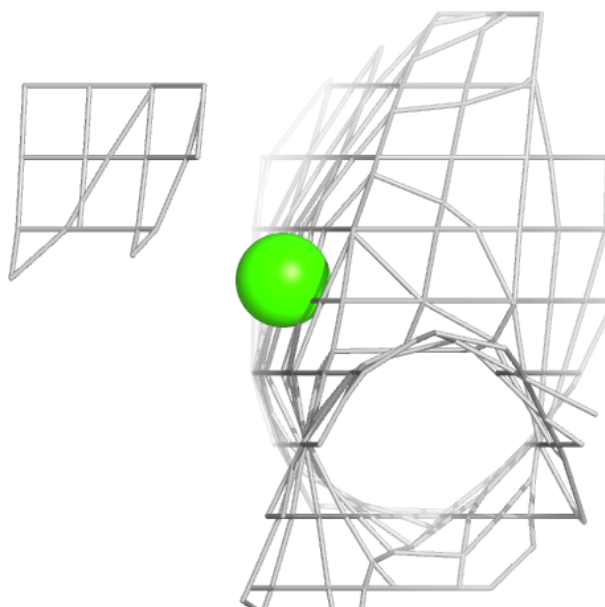
Electron density around CA D 503:

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



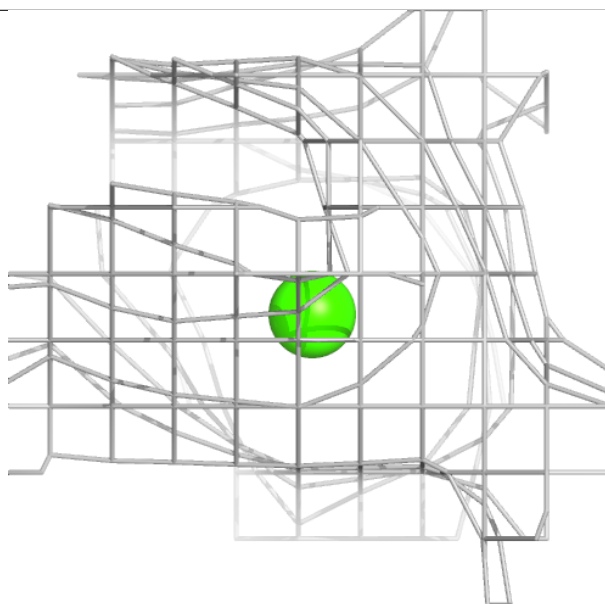
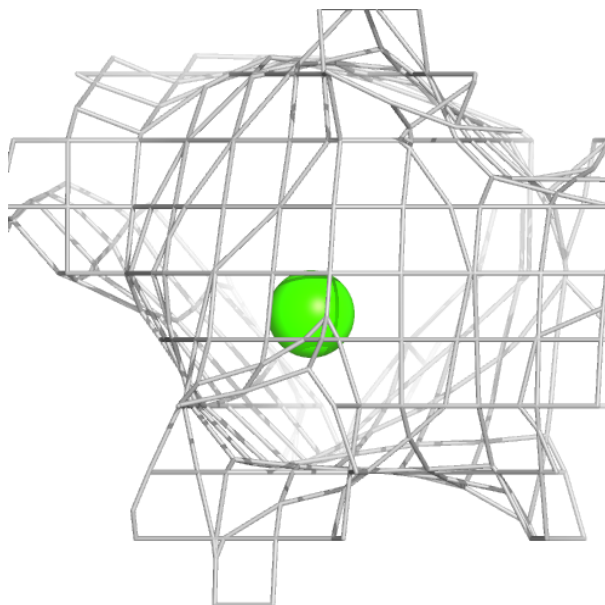
Electron density around CA C 503:

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



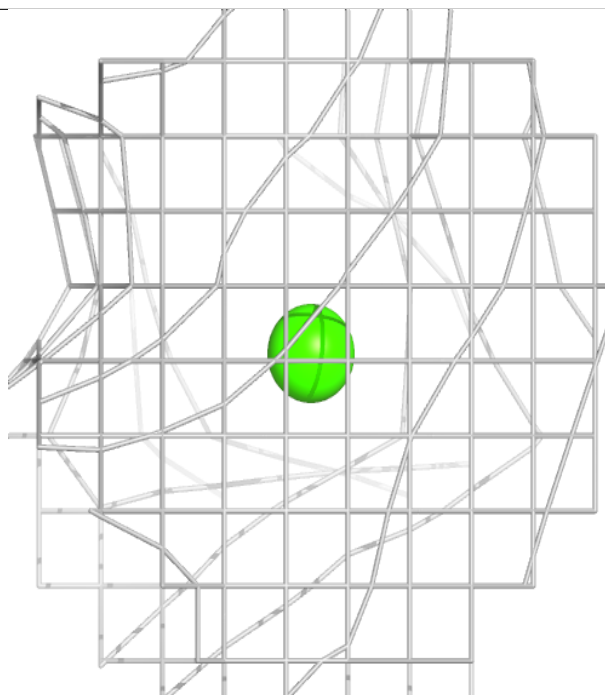
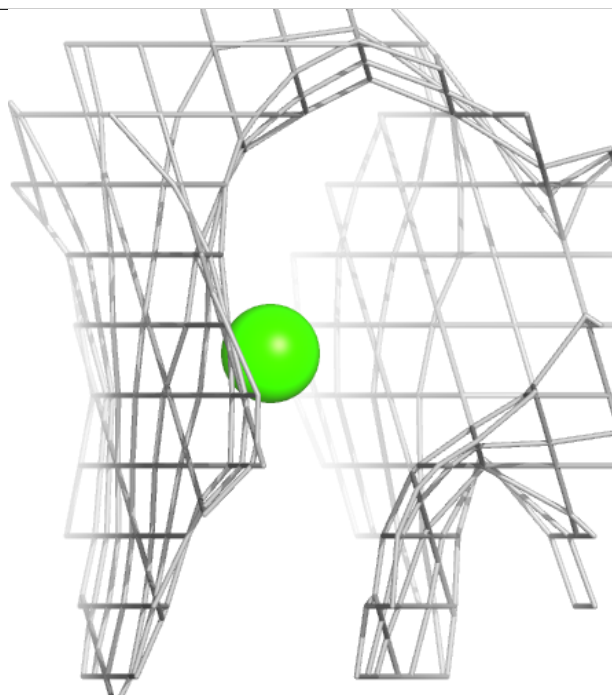
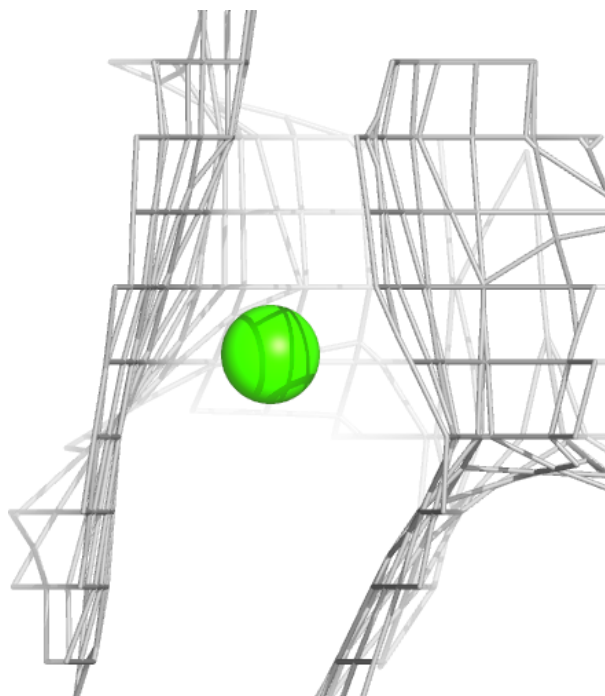
Electron density around CA C 502:

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



Electron density around CA B 502:

$2mF_o - DF_c$ (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.