



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 11:31 PM BST

PDB ID : 6Q23
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 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 : 2.13.1
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) : 2.13.1

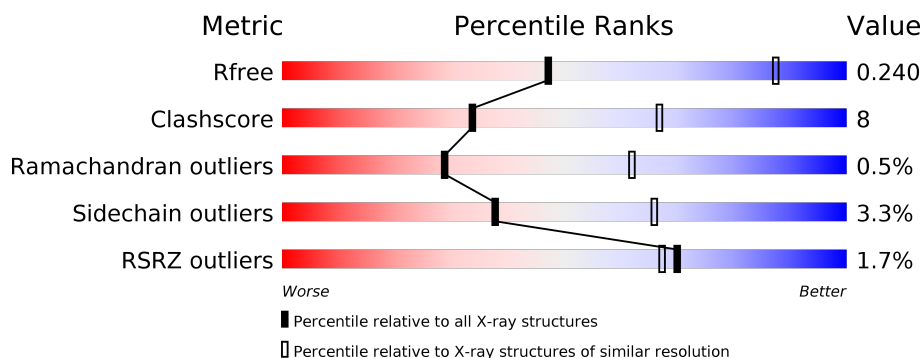
1 Overall quality at a glance

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.






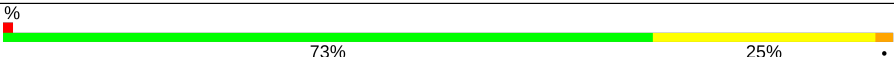
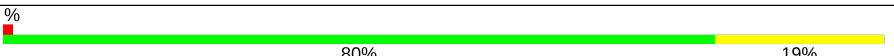
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	<div> <div></div> <div>80% 17% ..</div> </div>
1	B	391	<div> <div></div> <div>82% 16% ..</div> </div>
1	C	391	<div> <div></div> <div>83% 14% ..</div> </div>
1	D	391	<div> <div></div> <div>82% 15% ..</div> </div>
2	E	240	<div> <div>5%</div> <div>67% 25% • 5%</div> </div>
2	G	240	<div> <div>3%</div> <div>70% 23% • 5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	240	
2	J	240	
3	F	216	
3	I	216	
3	K	216	
3	L	216	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	504	-	-	-	X

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

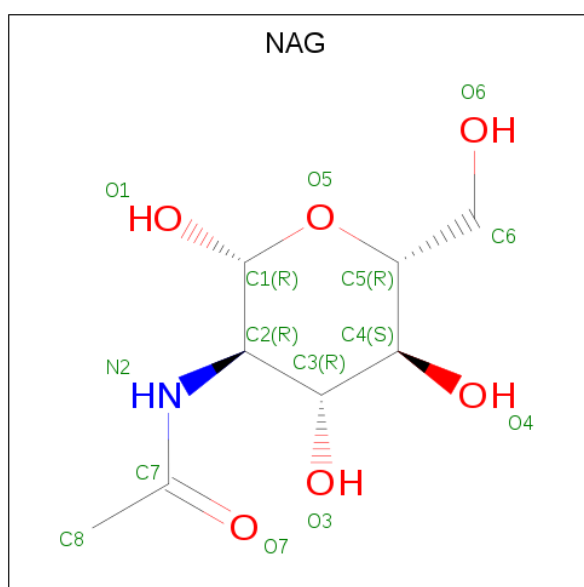
- Molecule 2 is a protein called 1G01 Fab IgG1 heavy chain.

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 (three-letter code: 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

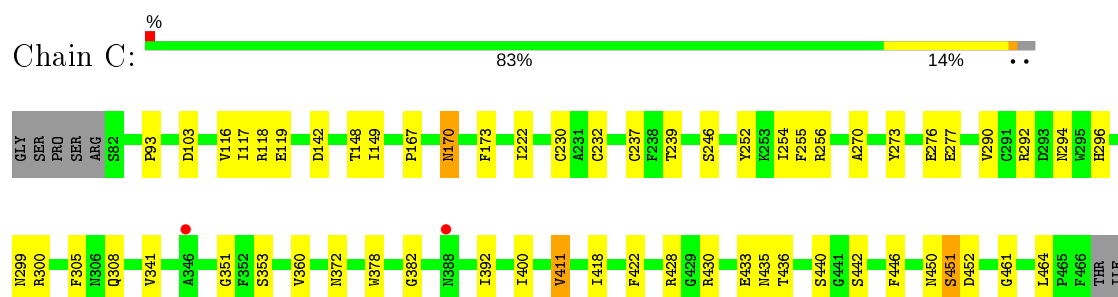
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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
5	C	2	Total Ca 2 2	0	0

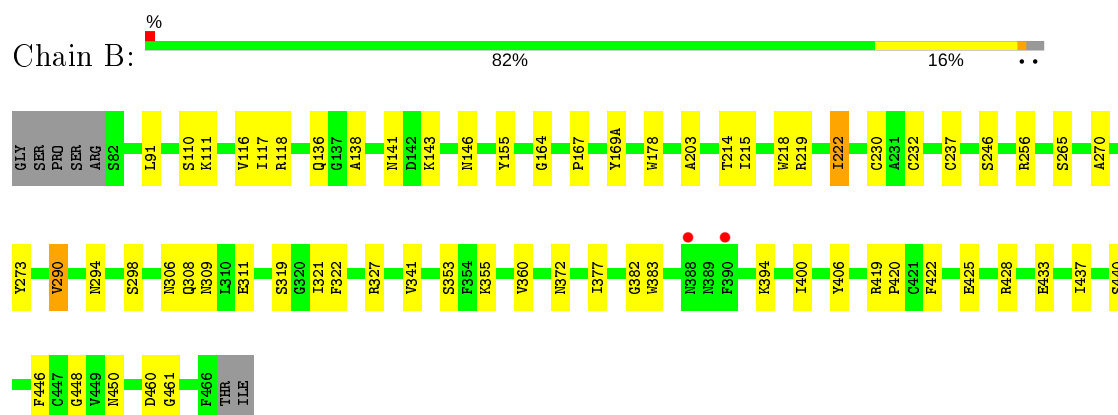
3 Residue-property plots [i](#)

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.

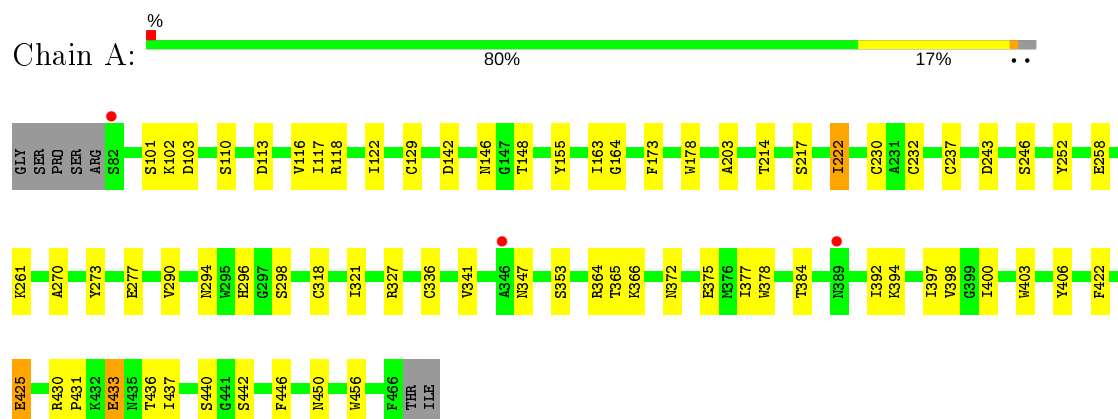
• Molecule 1: Neuraminidase



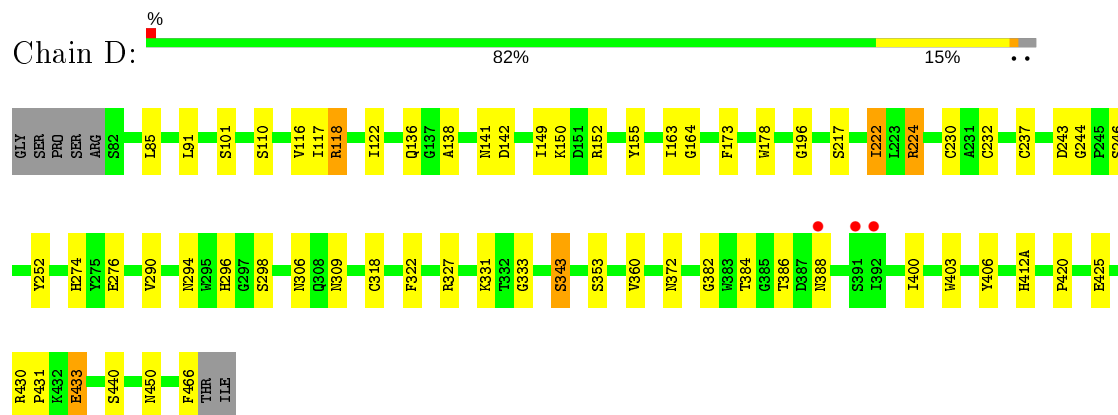
• Molecule 1: Neuraminidase



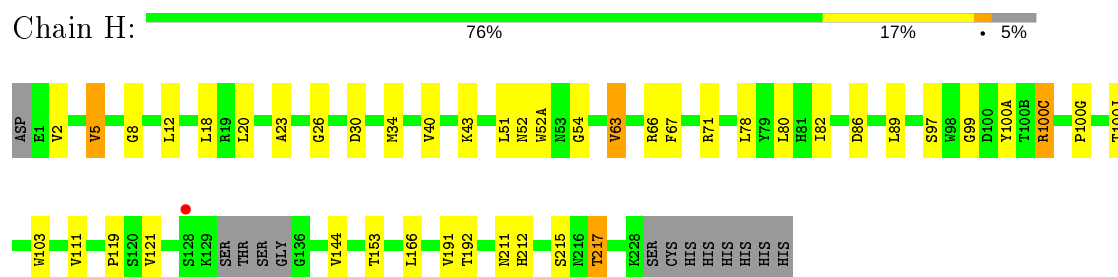
• Molecule 1: Neuraminidase



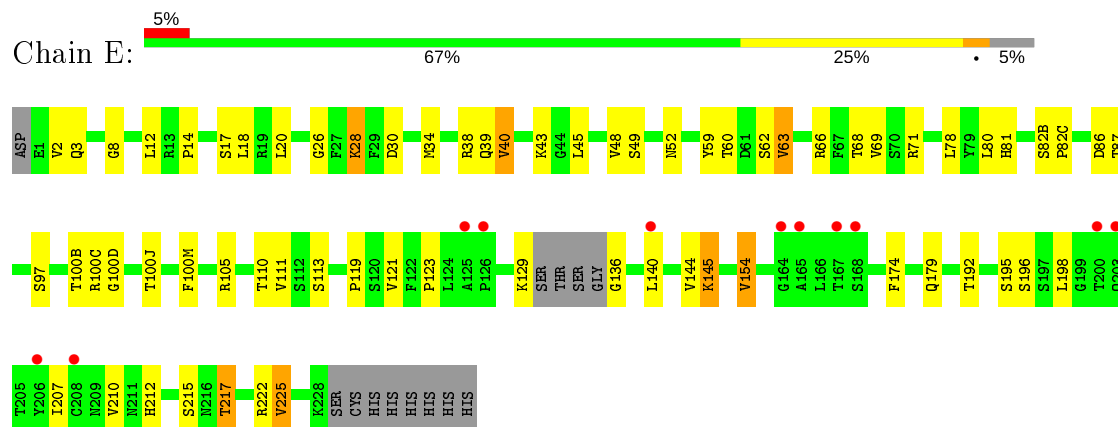
- Molecule 1: Neuraminidase



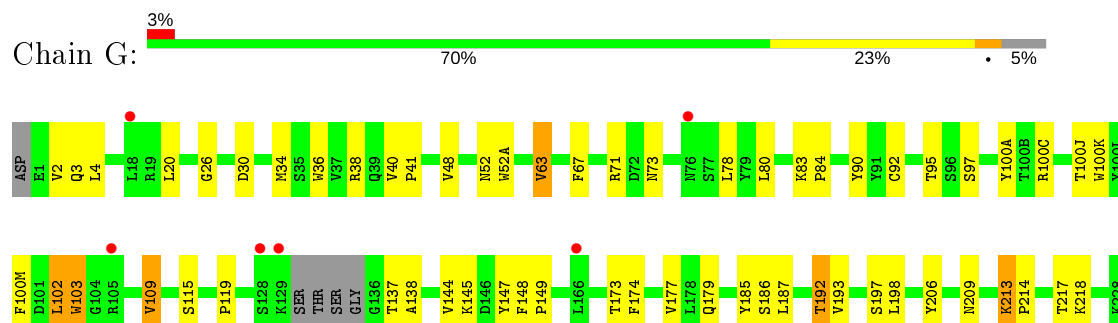
- Molecule 2: 1G01 Fab IgG1 heavy chain



- Molecule 2: 1G01 Fab IgG1 heavy chain



- Molecule 2: 1G01 Fab IgG1 heavy chain



SER
CYS
HIS
HIS
HIS
HIS
HIS

• Molecule 2: 1G01 Fab IgG1 heavy chain

Chain J: 4% 73% 21% 5%

ASP E1 V2 G8 L12 R13 P14 L18 G26 R34 V48 T60 D61 V63 R66 P67 L78 R83 P84 R85 D86 T95 S96 S97 S98 G99 D100 Y100A T100B R100C T100J W100K W103 V111 S112 S113 A114 S115 P119 S128 K129 SER THR

SER GLY G136 T137 A138 L143 V144 K145 Y146 Y147 E150 F151 V152 S156 N157 N162 T167 S168 G169 V171 H172 T173 F174 V190 V191 T192 S196 S197 L198 T205 K213 P214 S215 N216 V219 D220 K221 K228 SER CYS HIS HIS HIS HIS HIS

• Molecule 3: 1G01 Fab kappa light chain

Chain L: % 78% 20% .

ASP D1 L11 L21 L33 P44 L47 S56 G57 V58 R61 P62 T69 T75 S76 S77 L78 Q79 H90 S93 L95A P96 T97 T102 R108 T109 P113 I117 E123 K126 V132 L136 F139 K149 V150 D151 N152 A153

L154 Q155 M158 V163 T164 S174 L175 L179 K183 E187 A193 P204 T205 T206 R207 E213 C214

• Molecule 3: 1G01 Fab kappa light chain

Chain F: 6% 75% 24%

ASP D1 L4 F10 I19 G28 Y32 L33 A34 W35 Y36 L47 I48 A51 S56 G57 V58 F59 S60 G64 I75 L78 F83 A84 H90 L91 D92 S93 L95A F96 T97 V104 R108 T109 V110 V115 P120 S121 D122 K126 S127

Q128 T129 V132 L136 N137 P141 R142 E143 A144 K149 N152 N158 S162 V163 T164 D170 S171 T172 Y173 S174 L175 L181 S182 K183 E187 A193 C194 E195 H198 P204 Y205 T206 E213 C214

• Molecule 3: 1G01 Fab kappa light chain

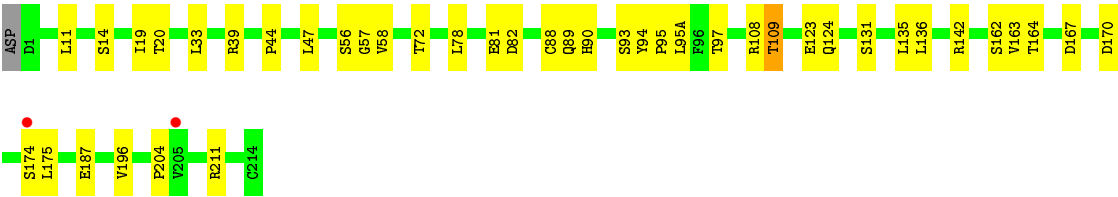
Chain I: % 73% 25% .

ASP D1 F10 S14 T19 Y32 L33 Q37 G41 L47 S56 G57 P59 S60 R61 P62 T69 T74 T75 L78 D82 H90 L91 D92 S93 Y94 P95 L95A F96 T97 R108 A111 E123 K126 L136 N137 N138 R142 K149

Q160 E161 S162 V163 D167 D170 S171 T172 Y173 S174 L175 S176 T180 K183 E187 A193 V196 T197 H198 Q199 G200 L201 P204 K207 C214

• Molecule 3: 1G01 Fab kappa light chain

Chain K: % 80% 19%



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 (4.77%)	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 , 19.7	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	0.89	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.69	0/3050	0.78	0/4145
1	B	0.69	0/3050	0.76	0/4145
1	C	0.68	0/3050	0.76	0/4145
1	D	0.69	0/3050	0.74	0/4145
2	E	0.66	0/1774	0.78	0/2417
2	G	0.67	0/1774	0.79	0/2417
2	H	0.68	0/1774	0.80	0/2417
2	J	0.66	0/1774	0.79	0/2417
3	F	0.68	0/1698	0.77	0/2309
3	I	0.68	0/1698	0.79	0/2309
3	K	0.68	0/1698	0.79	0/2309
3	L	0.67	0/1698	0.79	0/2309
All	All	0.68	0/26088	0.78	0/35484

There are no bond length outliers.

There are no bond angle outliers.

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	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2968	0	2798	49	0
1	C	2968	0	2798	41	0
1	D	2968	0	2799	46	0
2	E	1728	0	1692	42	0
2	G	1728	0	1692	36	0
2	H	1728	0	1692	32	0
2	J	1728	0	1692	39	0
3	F	1659	0	1607	31	0
3	I	1659	0	1607	39	0
3	K	1659	0	1607	31	0
3	L	1659	0	1607	30	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	425	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 8.

All (425) 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
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:B:116:VAL:HG23	1:B:136:GLN:HB2	1.66	0.78
1:C:118:ARG:HH21	2:E:100(C):ARG:HB3	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:298:SER:OG	1:A:341:VAL:HB	2.01	0.59
1:B:306:ASN:OD1	1:B:309:ASN:N	2.35	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:OE1	3:K:123:GLU:N	2.35	0.59
2:J:174:PHE:HB3	3:K:162:SER:OG	2.02	0.59
2:G:2:VAL:HA	2:G:26:GLY:HA3	1.85	0.58
2:H:63:VAL:HG13	2:H:67:PHE:CG	2.38	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
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: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
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:E:59:TYR:HE1	2:E:69:VAL:HG23	1.70	0.56
2:H:153:THR:CG2	2:H:211:ASN:HB3	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:198:HIS:H	3:I:201:LEU:HD11	1.70	0.55
3:L:123:GLU:O	3:L:126:LYS:HG2	2.07	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
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:364:ARG:HD3	1:A:377:ILE:HD12	1.90	0.54
1:A:164:GLY:HA3	1:D:173:PHE:CG	2.43	0.54
2:G:34:MET:HB3	2:G:78:LEU:HD22	1.89	0.54
2:J:167:THR:O	2:J:171:VAL:HG22	2.08	0.53
3:L:136:LEU:HD13	3:L:175:LEU:HD12	1.90	0.53
3:F:164:THR:HG22	3:F:174:SER:H	1.73	0.53
1:A:406:TYR:HH	2:H:100(C):ARG:HG3	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
2:E:62:SER:O	2:E:66:ARG:NH1	2.41	0.53
3:L:149:LYS:HG2	3:L:154:LEU:HD13	1.90	0.53
3:I:199:GLN:H	3:I:199:GLN:CD	2.12	0.53
3:F:171:SER:OG	3:F:171:SER:O	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:116:VAL:CG2	1:B:136:GLN:HB2	2.39	0.51
1:C:246:SER:HB2	1:C:294:ASN:HD22	1.75	0.51
1:A:146:ASN:CB	1:A:437:ILE:HG13	2.40	0.51
1:B:298:SER:H	1:B:341:VAL:HG23	1.75	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
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
2:G:90:TYR:CE1	2:G:109:VAL:HG13	2.46	0.50
3:L:183:LYS:O	3:L:187:GLU:HG2	2.12	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: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: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: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
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:B:117:ILE:CD1	1:B:167:PRO:HB2	2.43	0.49
1:C:149:ILE:HD12	1:C:430:ARG:HB3	1.95	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
3:F:4:LEU:HD11	3:F:90:HIS:HB2	1.94	0.48
2:H:12:LEU:O	2:H:111:VAL:HA	2.13	0.48
1:D:372:ASN:HB3	1:D:400:ILE:O	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:217:SER:OG	1:A:243:ASP:OD2	2.20	0.48
1:A:378:TRP:HB3	1:A:392:ILE:HB	1.96	0.48
1:B:360:VAL:HG12	1:B:382:GLY:HA3	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:183:LYS:O	3:F:187:GLU:HG2	2.14	0.47
3:F:149:LYS:HG3	3:F:193:ALA:HB3	1.96	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
1:A:102:LYS:HZ3	1:D:155:TYR:HD1	1.62	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
3:K:108:ARG:HG3	3:K:109:THR:O	2.15	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
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:D:116:VAL:HG23	1:D:440:SER:HB2	1.97	0.47
1:A:406:TYR:N	1:A:425:GLU:HG2	2.29	0.46
1:C:254:ILE:CD1	1:C:305:PHE:CZ	2.97	0.46
2:G:4:LEU:HG	2:G:102:LEU:CD1	2.45	0.46
2:G:179:GLN:CD	2:G:186:SER:HB2	2.36	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:428:ARG:NH2	1:C:433:GLU:OE2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ASP:OD1	1:C:442:SER:HB2	2.16	0.46
2:G:144:VAL:CG2	2:G:187:LEU:HB3	2.45	0.46
2:G:4:LEU:HD13	2:G:92:CYS:SG	2.56	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
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
2:E:136:GLY:N	2:E:195:SER:HG	2.14	0.46
2:E:14:PRO:HD2	2:E:113:SER:HB2	1.97	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
3:L:62:PHE:CD1	3:L:75:ILE:HG22	2.51	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
2:G:138:ALA:HB3	2:G:198:LEU:HD21	1.99	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
2:J:228:LYS:H	2:J:228:LYS:HZ3	1.63	0.45
3:L:75:ILE:HD12	3:L:75:ILE:O	2.16	0.45
1:B:461:GLY:HA3	1:A:155:TYR:CZ	2.51	0.45
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:I:62:PHE:CE1	3:I:75:ILE:HD12	2.52	0.45
3:L:95(A):LEU:O	3:L:97:THR:N	2.49	0.45
1:A:366:LYS:HB3	1:A:400:ILE:HD13	1.98	0.45
1:C:170:ASN:ND2	1:B:169(A):TYR:HA	2.31	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
2:H:12:LEU:HD22	2:H:82:ILE:HD11	1.98	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
1:C:142:ASP:CG	1:D:110:SER:HG	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:95(A):LEU:O	3:K:97:THR:N	2.50	0.45
3:L:90:HIS:ND1	3:L:93:SER:HB3	2.32	0.45
2:E:119:PRO:HB2	2:E:144:VAL:HG13	1.99	0.45
2:E:38:ARG:HD3	2:E:48:VAL:HG11	1.98	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:HA	3:F:78:LEU:HD23	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
2:G:97:SER:HA	2:G:100(J):THR:O	2.18	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
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:HD12	2:J:198:LEU:N	2.32	0.44
2:J:190:VAL:HG21	3:K:135:LEU:CD2	2.47	0.44
3:L:21:ILE:CD1	3:L:102:THR:HG21	2.46	0.44
1:D:217:SER:OG	1:D:243:ASP:OD2	2.20	0.44
3:F:83:PHE:HA	3:F:104:VAL:HG23	1.99	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
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: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:L:61:ARG:HH11	3:L:79:GLN:CD	2.21	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:B:298:SER:OG	1:B:341:VAL:CG2	2.62	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:D:85:LEU:HD13	1:D:412(A):HIS:ND1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:100(A):TYR:OH	2:J:100(C):ARG:NH1	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
3:L:155:GLN:OE1	3:L:158:ASN:ND2	2.51	0.43
2:H:30:ASP:O	2:H:52(A):TRP:HB2	2.19	0.43
1:A:102:LYS:NZ	1:D:155:TYR:HD1	2.16	0.43
1:B:322:PHE:HB2	1:B:327:ARG:HD2	2.00	0.43
1:C:173:PHE:CG	1:D:164:GLY:HA3	2.53	0.43
1:C:276:GLU:O	1:C:292:ARG:HB3	2.18	0.43
1:C:173:PHE:CZ	1:D:101:SER:HA	2.53	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
3:F:10:PHE:CE2	3:F:142:ARG:HG2	2.54	0.43
2:E:100(M):PHE:O	3:F:36:TYR:HE2	2.01	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
3:K:39:ARG:HD2	3:K:81:GLU:O	2.19	0.43
2:E:198:LEU:HD12	2:E:198:LEU:N	2.33	0.43
2:J:60:THR:OG1	3:K:95(A):LEU:HD12	2.19	0.43
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:A:103:ASP:OD1	1:A:442:SER:HB2	2.19	0.42
1:C:232:CYS:HA	1:C:237:CYS:HA	1.99	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
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:H3	4:A:505:NAG:H83	1.99	0.42
3:L:62:PHE:CE1	3:L:75:ILE:HG22	2.54	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:A:222:ILE:CD1	2:H:99:GLY:HA2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:SER:HB2	1:B:382:GLY:CA	2.50	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:K:11:LEU:HD21	3:K:19:ILE:HG23	2.01	0.42
3:L:11:LEU:HD13	3:L:21:ILE:HD11	2.00	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
3:L:108:ARG:HG3	3:L:109:THR:O	2.20	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:HD23	3:I:78:LEU:HA	1.81	0.42
3:I:142:ARG:HB2	3:I:173:TYR:CE2	2.55	0.42
3:I:19:ILE:O	3:I:74:THR:HA	2.20	0.42
3:K:94:TYR:HA	3:K:95:PRO:HA	1.86	0.42
2:E:123:PRO:CB	2:E:225:VAL:HG12	2.50	0.41
2:H:63:VAL:HG13	2:H:67:PHE:HB2	2.02	0.41
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:213:LYS:HD2	2:J:214:PRO:CD	2.50	0.41
2:J:62:SER:HB2	2:J:85:GLU:OE1	2.20	0.41
1:A:327:ARG:NH2	1:A:365:THR:OG1	2.53	0.41
1:B:355:LYS:HE2	1:B:383:TRP:CD1	2.55	0.41
1:A:277:GLU:OE2	2:H:100(A):TYR:OH	2.24	0.41
1:D:222:ILE:HD12	2:G:100(A):TYR:HB3	2.03	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: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:B:222:ILE:HD11	2:J:99:GLY:HA2	2.02	0.41
1:A:203:ALA:O	1:A:214:THR:HA	2.21	0.41
3:F:48:ILE:HD12	3:F:51:ALA:C	2.41	0.41
2:G:36:TRP:NE1	2:G:80:LEU:HB2	2.35	0.41
2:G:147:TYR:CE1	2:G:185:TYR:HB2	2.55	0.41
2:G:198:LEU:HD22	2:G:198:LEU:H	1.86	0.41
1:C:270:ALA:HB1	1:C:273:TYR:HB2	2.03	0.41
1:C:411:VAL:CG2	1:C:418:ILE:CG2	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:ASN:OD1	1:D:466:PHE:HB3	2.21	0.41
3:F:170:ASP:OD2	3:F:172:THR:OG1	2.28	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
1:B:118:ARG:HH21	2:J:100(C):ARG:HB3	1.85	0.41
3:L:113:PRO:HB3	3:L:139:PHE:HB3	2.03	0.41
3:L:93:SER:O	3:L:95(A):LEU:N	2.52	0.41
1:B:164:GLY:HA3	1:A:173:PHE:CG	2.56	0.41
2:E:207:ILE:HG22	2:E:222:ARG:HA	2.02	0.41
2:E:28:LYS:HD2	2:E:30:ASP:HB3	2.03	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
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:B:321:ILE:HG21	1:B:377:ILE:HG21	2.03	0.40
1:B:91:LEU:HA	1:B:91:LEU:HD23	1.91	0.40
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
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:B:110:SER:HG	1:A:142:ASP:CG	2.25	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
3:I:56:SER:OG	3:I:57:GLY:N	2.55	0.40
1:B:110:SER:OG	1:A:142:ASP:OD1	2.34	0.40
1:A:437:ILE:HA	1:A:437:ILE:HD12	1.83	0.40
1:B:111:LYS:HE2	1:A:113:ASP:OD1	2.22	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:D:331:LYS:O	1:D:388:ASN:HB3	2.22	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:H:89:LEU:HD23	2:H:89:LEU:H	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	41	72
1	B	382/391 (98%)	364 (95%)	17 (4%)	1 (0%)	41	72
1	C	382/391 (98%)	365 (96%)	16 (4%)	1 (0%)	41	72
1	D	382/391 (98%)	365 (96%)	16 (4%)	1 (0%)	41	72
2	E	223/240 (93%)	208 (93%)	14 (6%)	1 (0%)	34	67
2	G	223/240 (93%)	210 (94%)	12 (5%)	1 (0%)	34	67
2	H	223/240 (93%)	208 (93%)	14 (6%)	1 (0%)	34	67
2	J	223/240 (93%)	208 (93%)	14 (6%)	1 (0%)	34	67
3	F	213/216 (99%)	201 (94%)	10 (5%)	2 (1%)	17	50
3	I	213/216 (99%)	198 (93%)	13 (6%)	2 (1%)	17	50
3	K	213/216 (99%)	198 (93%)	14 (7%)	1 (0%)	29	62
3	L	213/216 (99%)	198 (93%)	13 (6%)	2 (1%)	17	50
All	All	3272/3388 (97%)	3088 (94%)	169 (5%)	15 (0%)	29	62

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	96	PHE
3	I	96	PHE
3	F	96	PHE

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Mol	Chain	Res	Type
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%)	323 (98%)	8 (2%)	49	73
1	B	331/337 (98%)	324 (98%)	7 (2%)	53	75
1	C	331/337 (98%)	323 (98%)	8 (2%)	49	73
1	D	331/337 (98%)	324 (98%)	7 (2%)	53	75
2	E	192/204 (94%)	183 (95%)	9 (5%)	26	57
2	G	192/204 (94%)	180 (94%)	12 (6%)	18	47
2	H	192/204 (94%)	188 (98%)	4 (2%)	53	75
2	J	192/204 (94%)	183 (95%)	9 (5%)	26	57
3	F	187/188 (100%)	180 (96%)	7 (4%)	34	62
3	I	187/188 (100%)	175 (94%)	12 (6%)	17	47
3	K	187/188 (100%)	185 (99%)	2 (1%)	73	85
3	L	187/188 (100%)	179 (96%)	8 (4%)	29	59
All	All	2840/2916 (97%)	2747 (97%)	93 (3%)	38	66

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	170	ASN
1	C	230	CYS
1	C	252	TYR
1	C	296	HIS
1	C	411	VAL
1	C	435	ASN
1	C	451	SER
1	C	452	ASP
1	B	143	LYS
1	B	230	CYS
1	B	265	SER
1	B	290	VAL
1	B	394	LYS
1	B	420	PRO
1	B	450	ASN
1	A	230	CYS
1	A	252	TYR
1	A	296	HIS
1	A	336	CYS
1	A	425	GLU
1	A	431	PRO
1	A	433	GLU
1	A	450	ASN
1	D	118	ARG
1	D	224	ARG
1	D	230	CYS
1	D	296	HIS
1	D	343	SER
1	D	433	GLU
1	D	450	ASN
2	H	5	VAL
2	H	100(C)	ARG
2	H	192	THR
2	H	217	THR
3	L	33	LEU
3	L	56	SER
3	L	69	THR
3	L	109	THR
3	L	152	ASN
3	L	206	THR
3	L	207	LYS
3	L	214	CYS
2	E	17	SER

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Mol	Chain	Res	Type
2	E	28	LYS
2	E	40	VAL
2	E	129	LYS
2	E	145	LYS
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	136	LEU
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	145	LYS
2	G	173	THR
2	G	192	THR
2	G	197	SER
2	G	209	ASN
2	G	213	LYS
2	G	218	LYS
3	I	1	ASP
3	I	14	SER
3	I	33	LEU
3	I	60	SER
3	I	69	THR
3	I	74	THR
3	I	95(A)	LEU
3	I	176	SER
3	I	180	THR
3	I	183	LYS
3	I	197	THR
3	I	207	LYS
2	J	115	SER
2	J	129	LYS
2	J	173	THR

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Mol	Chain	Res	Type
2	J	192	THR
2	J	196	SER
2	J	197	SER
2	J	205	THR
2	J	213	LYS
2	J	216	ASN
3	K	14	SER
3	K	109	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	450	ASN
1	B	208	ASN
1	B	272	ASN
3	L	160	GLN
2	G	3	GLN
3	I	37	GLN
2	J	172	HIS
3	K	138	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	504	1	14,14,15	0.35	0	17,19,21	0.93	1 (5%)
4	NAG	A	505	1	14,14,15	0.59	0	17,19,21	2.07	4 (23%)
4	NAG	B	501	1	14,14,15	0.75	0	17,19,21	1.64	2 (11%)
4	NAG	A	501	1	14,14,15	0.68	0	17,19,21	1.08	1 (5%)
4	NAG	C	501	1	14,14,15	0.48	0	17,19,21	1.48	2 (11%)
4	NAG	D	502	1	14,14,15	0.49	0	17,19,21	1.24	1 (5%)
4	NAG	C	504	1	14,14,15	0.39	0	17,19,21	0.95	0
4	NAG	A	502	1	14,14,15	0.36	0	17,19,21	1.37	2 (11%)

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	B	504	1	-	2/6/23/26	0/1/1/1
4	NAG	A	505	1	-	4/6/23/26	0/1/1/1
4	NAG	B	501	1	-	2/6/23/26	0/1/1/1
4	NAG	A	501	1	-	2/6/23/26	0/1/1/1
4	NAG	C	501	1	-	0/6/23/26	0/1/1/1
4	NAG	D	502	1	-	0/6/23/26	0/1/1/1
4	NAG	C	504	1	-	2/6/23/26	0/1/1/1
4	NAG	A	502	1	-	2/6/23/26	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	5.32	130.48	122.90
4	B	501	NAG	O5-C5-C6	5.10	115.20	107.20
4	D	502	NAG	C1-O5-C5	4.22	117.90	112.19
4	A	502	NAG	C1-O5-C5	4.15	117.82	112.19
4	A	505	NAG	O5-C1-C2	3.96	117.53	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	NAG	O5-C5-C6	3.94	113.38	107.20
4	C	501	NAG	C4-C3-C2	3.02	115.45	111.02
4	A	501	NAG	O5-C5-C6	2.99	111.88	107.20
4	A	505	NAG	C8-C7-N2	2.71	120.69	116.10
4	B	501	NAG	C2-N2-C7	2.59	126.58	122.90
4	B	504	NAG	C1-O5-C5	2.45	115.52	112.19
4	A	505	NAG	O5-C5-C4	-2.31	105.22	110.83
4	A	502	NAG	O5-C5-C6	2.09	110.48	107.20

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	C	504	NAG	O5-C5-C6-O6
4	A	502	NAG	C4-C5-C6-O6
4	A	501	NAG	C1-C2-N2-C7
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	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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	384/391 (98%)	0.15	3 (0%) 86 86	33, 54, 76, 125	0
1	B	384/391 (98%)	0.11	2 (0%) 91 91	30, 53, 76, 118	0
1	C	384/391 (98%)	0.13	2 (0%) 91 91	29, 55, 79, 119	0
1	D	384/391 (98%)	0.12	3 (0%) 86 86	36, 58, 81, 137	0
2	E	227/240 (94%)	0.47	11 (4%) 30 29	42, 75, 111, 133	0
2	G	227/240 (94%)	0.35	6 (2%) 56 52	32, 67, 98, 116	0
2	H	227/240 (94%)	0.19	1 (0%) 92 93	32, 57, 86, 115	0
2	J	227/240 (94%)	0.45	9 (3%) 38 36	44, 72, 111, 144	0
3	F	215/216 (99%)	0.46	13 (6%) 21 21	40, 74, 99, 131	0
3	I	215/216 (99%)	0.12	2 (0%) 84 84	38, 61, 86, 103	0
3	K	215/216 (99%)	0.21	2 (0%) 84 84	37, 66, 91, 113	0
3	L	215/216 (99%)	0.19	3 (1%) 75 74	25, 63, 95, 140	0
All	All	3304/3388 (97%)	0.22	57 (1%) 70 67	25, 60, 94, 144	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	128	SER	6.4
2	J	168	SER	5.6
1	D	388	ASN	5.4
2	J	128	SER	4.5
2	J	162	ASN	4.4
2	J	129	LYS	4.4
3	F	213	GLU	4.2
2	E	165	ALA	3.9
1	A	346	ALA	3.8
3	F	214	CYS	3.7
3	I	214	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
2	E	168	SER	3.3
3	F	128	GLY	3.1
3	K	174	SER	3.1
2	J	152	VAL	3.1
2	E	203	GLN	3.0
3	F	144	ALA	2.9
1	C	388	ASN	2.9
1	D	391	SER	2.8
2	H	128	SER	2.7
1	C	346	ALA	2.7
3	L	213	GLU	2.7
1	B	390	PHE	2.6
2	J	169	GLY	2.6
2	E	125	ALA	2.6
1	A	82	SER	2.6
2	E	167	THR	2.6
2	E	164	GLY	2.6
2	G	18	LEU	2.6
3	F	129	THR	2.6
2	J	221	LYS	2.5
3	L	214	CYS	2.5
2	G	129	LYS	2.5
3	F	122	ASP	2.4
3	F	152	ASN	2.4
3	F	162	SER	2.4
3	F	143	GLU	2.3
3	I	41	GLY	2.3
2	E	206	TYR	2.3
1	A	389	ASN	2.3
2	E	200	THR	2.3
2	J	156	SER	2.3
2	E	140	LEU	2.2
2	G	76	ASN	2.2
3	L	151	ASP	2.2
3	F	136	LEU	2.2
3	F	115	VAL	2.2
1	B	388	ASN	2.2
3	F	174	SER	2.1
3	K	205	VAL	2.1
2	E	126	PRO	2.1
3	F	28	GLY	2.1
1	D	392	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	166	LEU	2.1
2	E	208	CYS	2.1
2	J	219	VAL	2.1
2	G	105	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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.

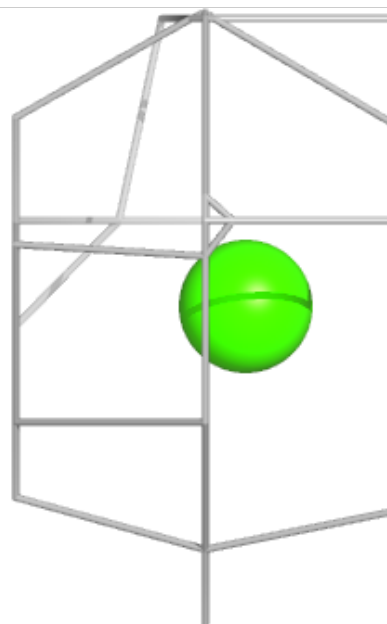
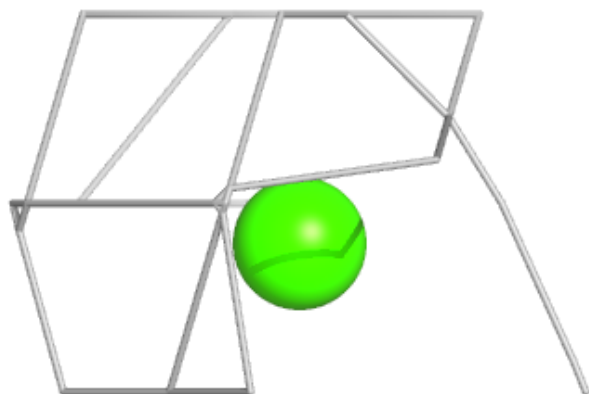
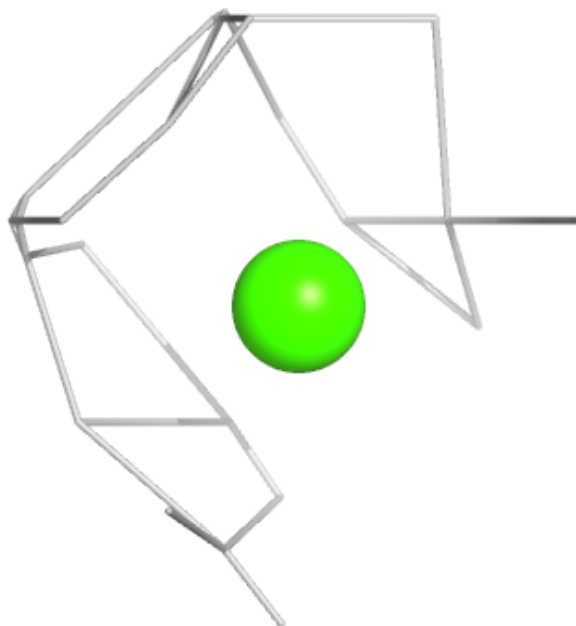
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	B	504	14/15	0.74	0.43	104,122,128,132	0
4	NAG	C	504	14/15	0.78	0.31	88,110,126,130	0
4	NAG	A	502	14/15	0.79	0.22	70,92,100,101	0
4	NAG	A	505	14/15	0.83	0.28	82,98,113,118	0
4	NAG	B	501	14/15	0.86	0.17	53,62,66,66	0
4	NAG	D	502	14/15	0.86	0.22	74,87,95,97	0
4	NAG	C	501	14/15	0.89	0.18	56,62,70,77	0
5	CA	D	504	1/1	0.90	0.20	112,112,112,112	0
5	CA	D	503	1/1	0.91	0.06	96,96,96,96	0
4	NAG	A	501	14/15	0.92	0.21	57,64,76,77	0
5	CA	A	504	1/1	0.94	0.44	124,124,124,124	0
5	CA	D	501	1/1	0.95	0.14	68,68,68,68	0
5	CA	B	503	1/1	0.95	0.70	300,300,300,300	0
5	CA	C	503	1/1	0.95	0.77	143,143,143,143	0
5	CA	C	502	1/1	0.98	0.09	68,68,68,68	0
5	CA	B	502	1/1	0.98	0.07	111,111,111,111	0
5	CA	A	503	1/1	0.99	0.09	99,99,99,99	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.

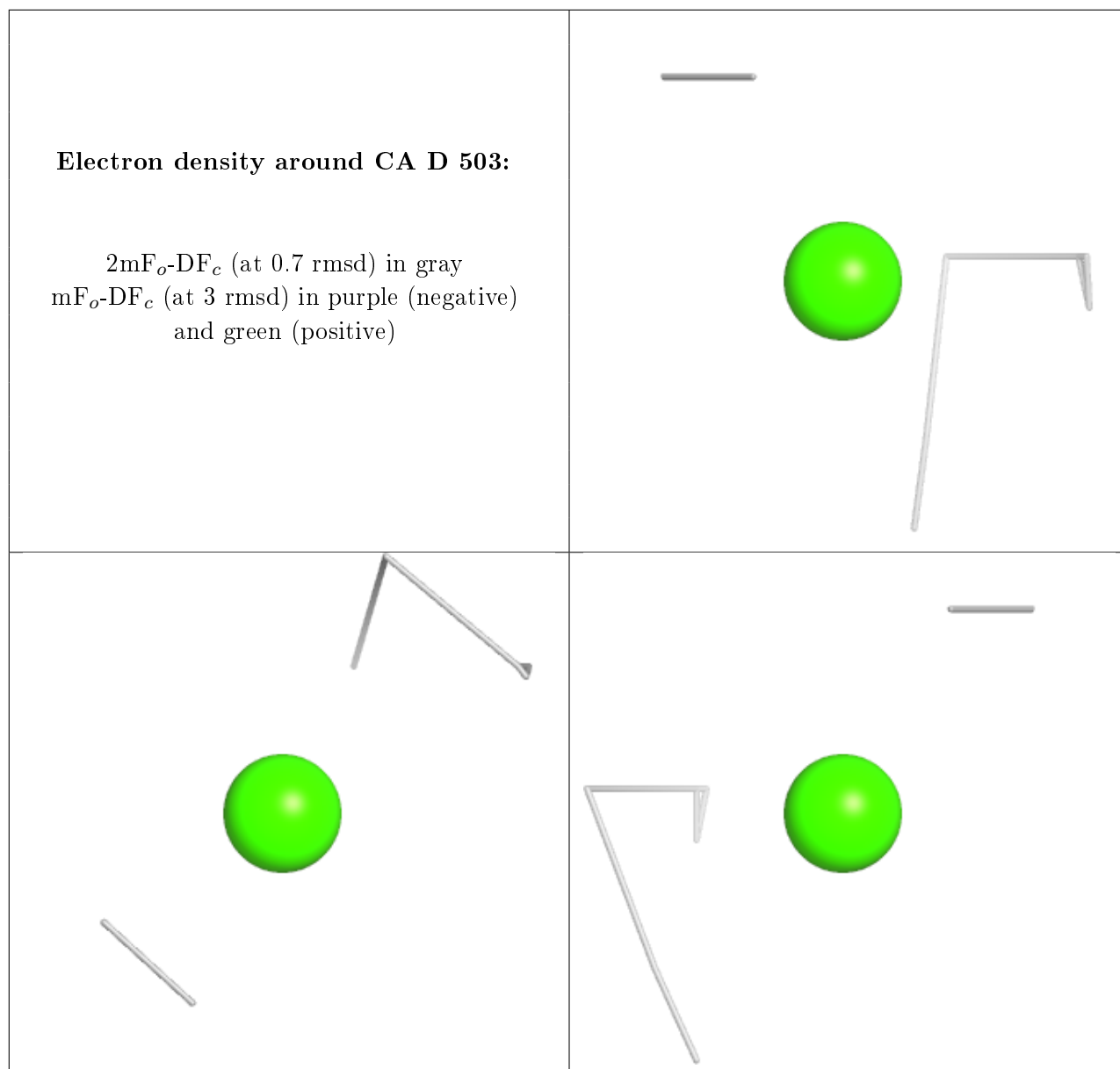
Electron density around CA D 504:

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



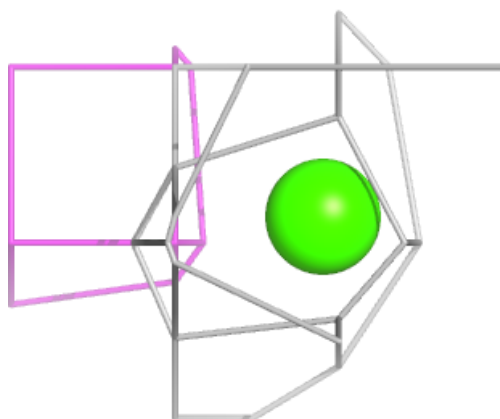
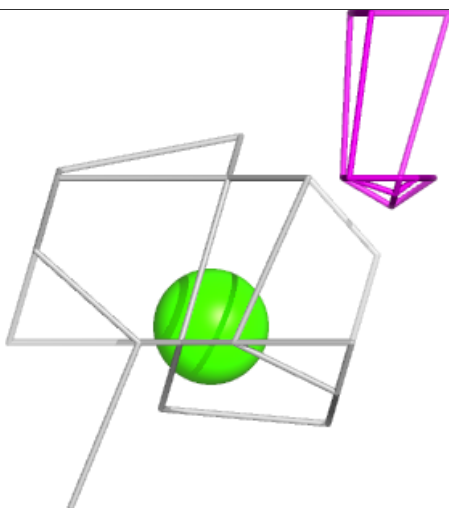
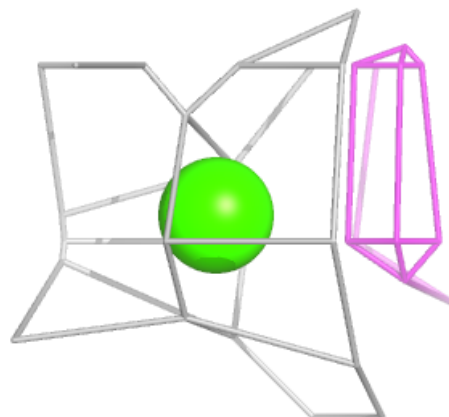
Electron density around CA D 503:

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



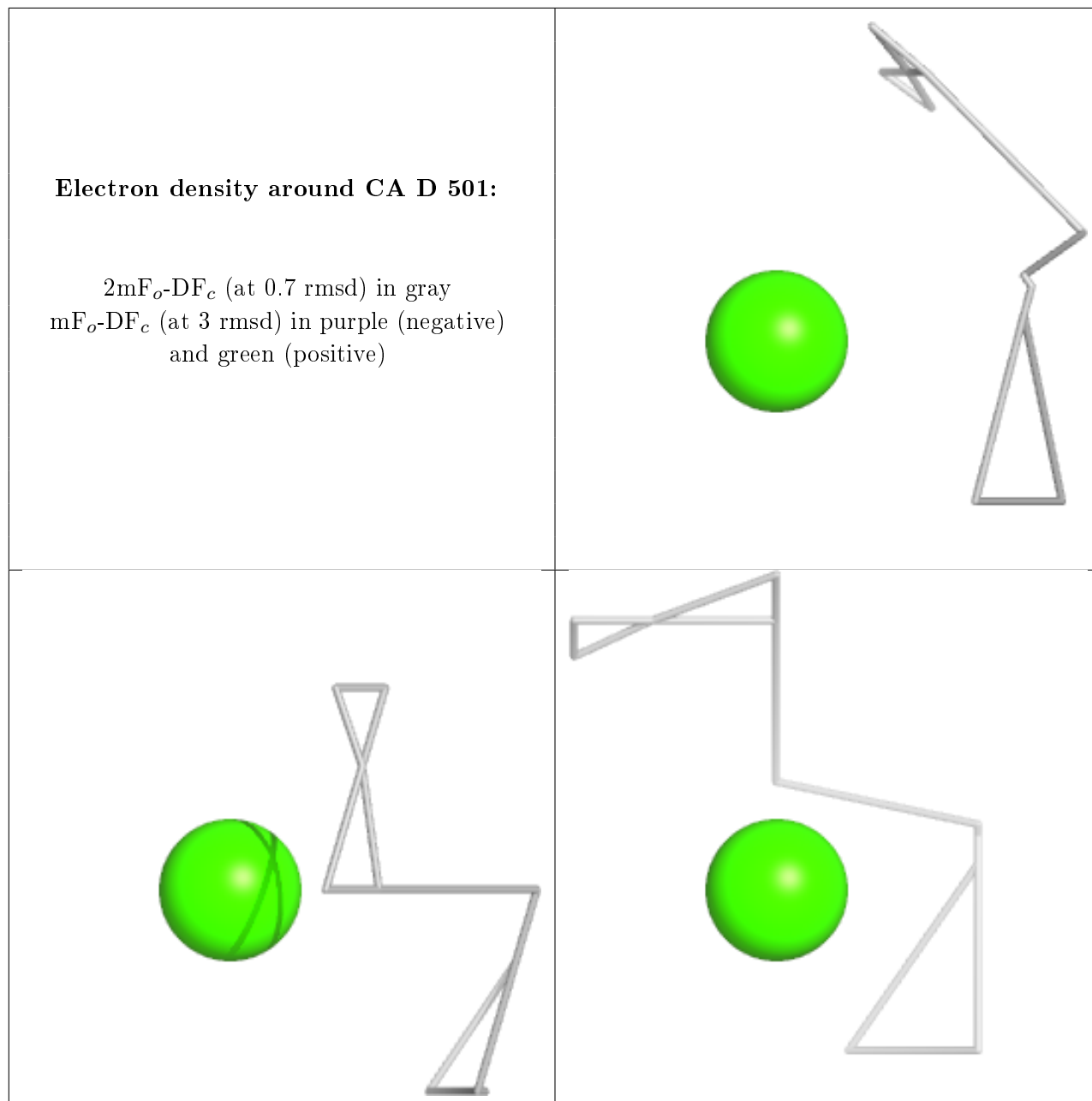
Electron density around CA A 504:

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



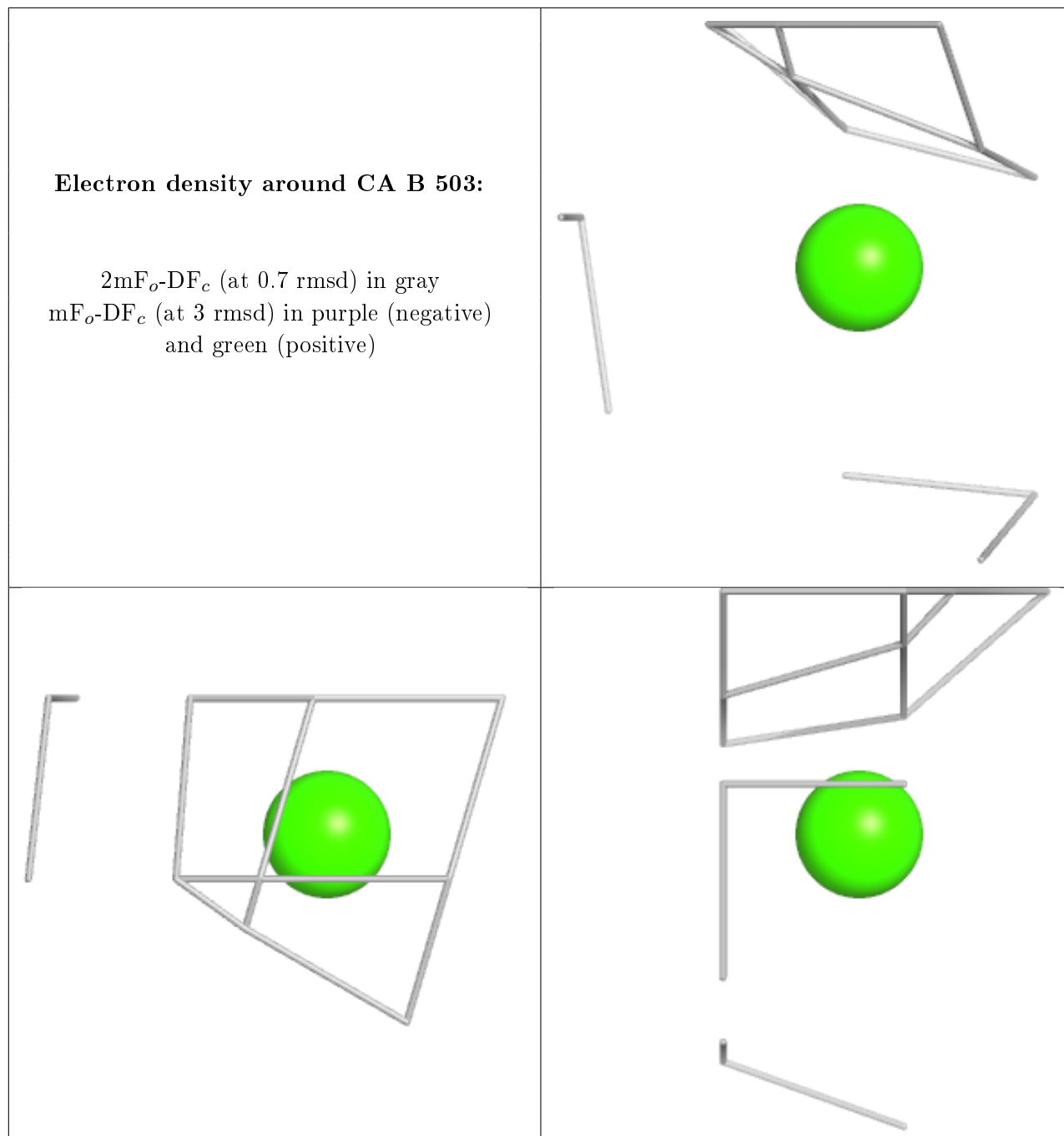
Electron density around CA D 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



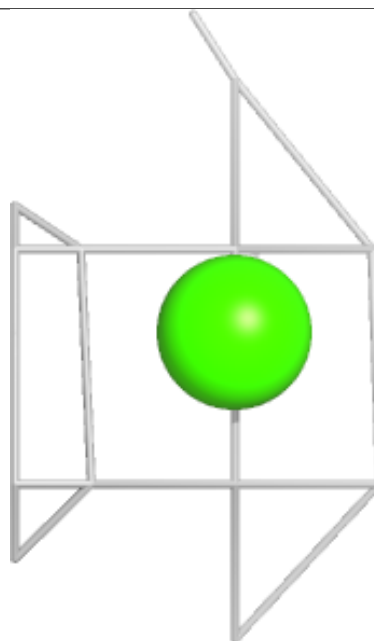
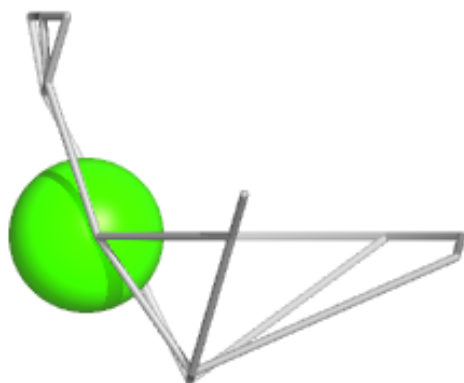
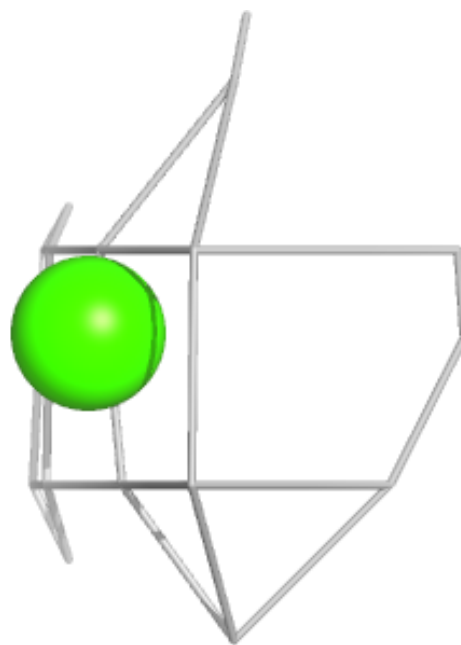
Electron density around CA B 503:

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



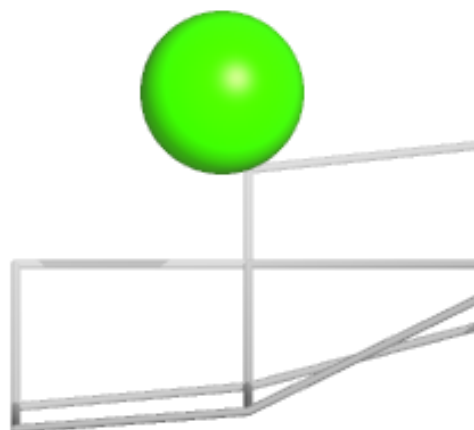
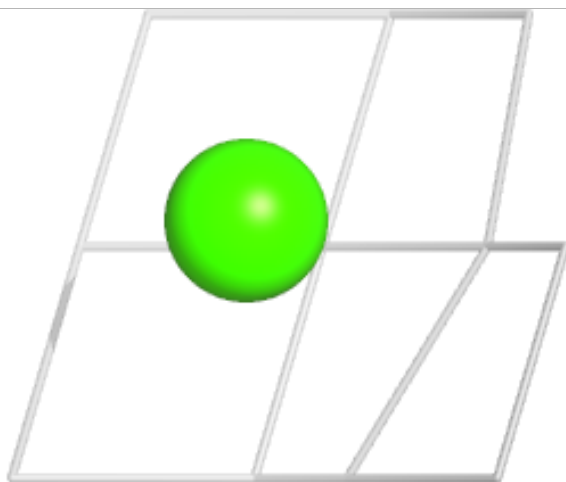
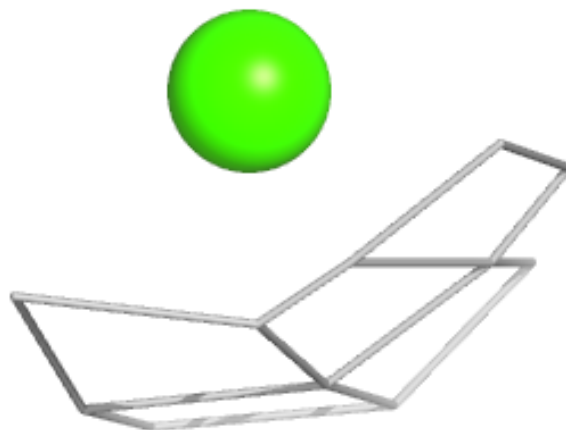
Electron density around CA C 503:

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



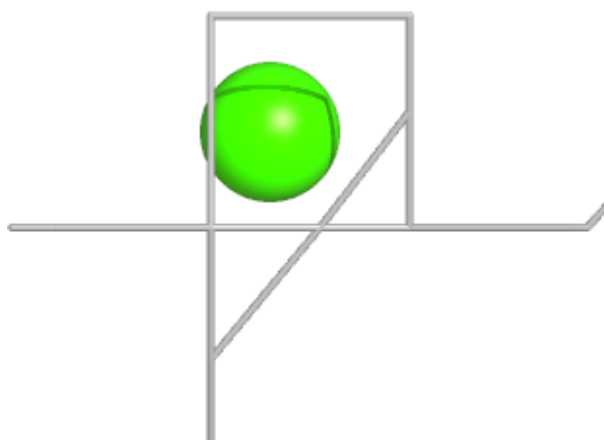
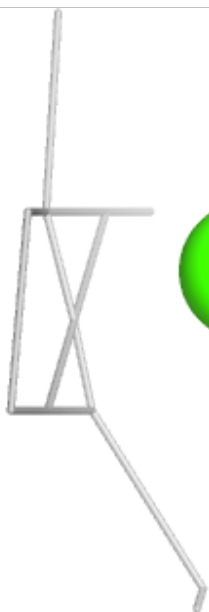
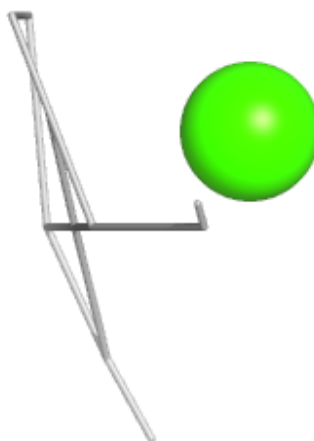
Electron density around CA C 502:

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



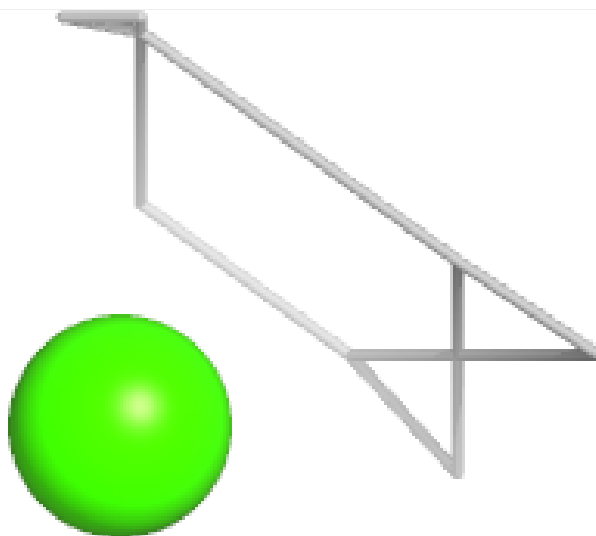
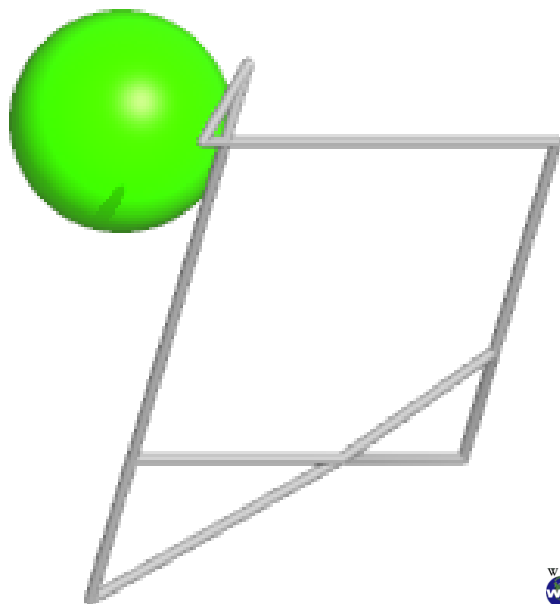
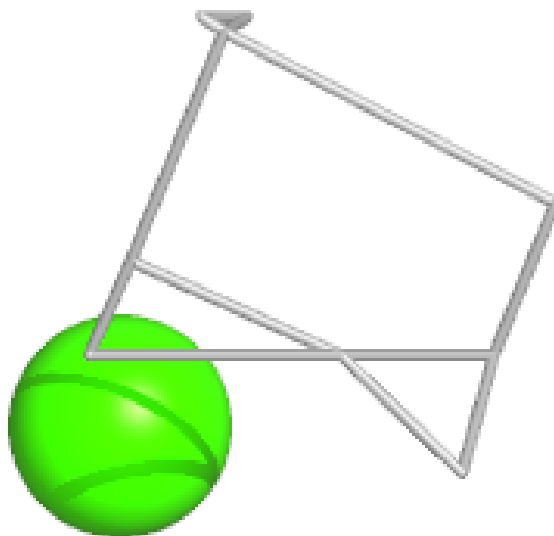
Electron density around CA B 502:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.