Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:43 AM BST

PDB ID	:	6K73
Title	:	Chaperone-tip adhesin complex is vital for synergistic activation of CFA/I fimbriae biogenesis
Authors	:	Bao, R.; He, L.H.
Deposited on	:	2019-06-05
Resolution	:	2.77 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:

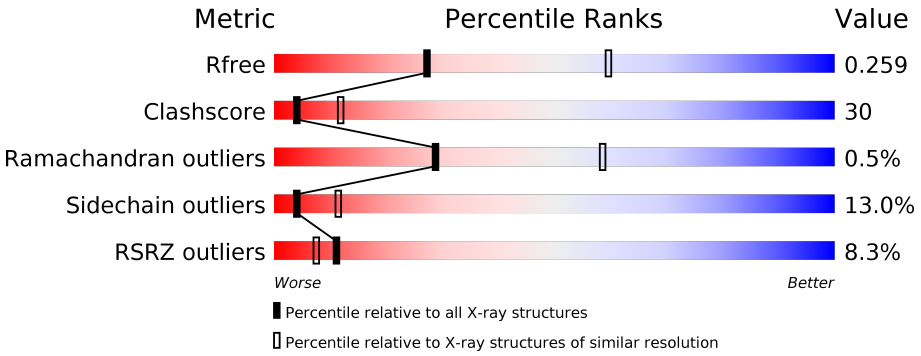
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 <=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	221	8% 41% 39% 12% 8%
1	B	221	7% 48% 42% 6% 5%
2	C	341	9% 52% 36% 5% 6%
2	D	341	8% 65% 26%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8432 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 Colonization factor antigen I chaperone CfaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	0	0
			1642	1062	274	303	3			
1	B	211	Total	C	N	O	S	0	0	0
			1687	1089	281	314	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	ILE	THR	engineered mutation	UNP A0A3Y5Z8F9
A	114	ILE	LEU	engineered mutation	UNP A0A3Y5Z8F9
A	116	ILE	VAL	engineered mutation	UNP A0A3Y5Z8F9
A	220	ALA	-	expression tag	UNP A0A3Y5Z8F9
B	112	ILE	THR	engineered mutation	UNP A0A3Y5Z8F9
B	114	ILE	LEU	engineered mutation	UNP A0A3Y5Z8F9
B	116	ILE	VAL	engineered mutation	UNP A0A3Y5Z8F9
B	220	ALA	-	expression tag	UNP A0A3Y5Z8F9

- Molecule 2 is a protein called CFA/I fimbrial subunit E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	320	Total	C	N	O	S	0	0	0
			2491	1561	438	482	10			
2	D	326	Total	C	N	O	S	0	0	0
			2538	1592	446	490	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	20	HIS	-	expression tag	UNP P25734
C	21	HIS	-	expression tag	UNP P25734
C	22	HIS	-	expression tag	UNP P25734
C	23	HIS	-	expression tag	UNP P25734

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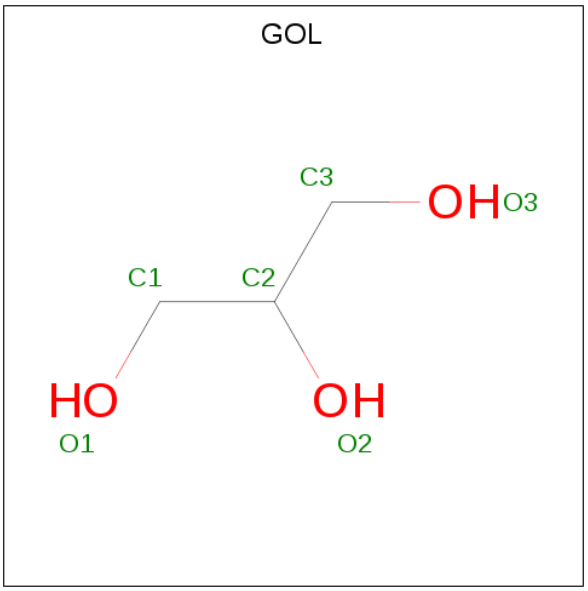
Chain	Residue	Modelled	Actual	Comment	Reference
D	20	HIS	-	expression tag	UNP P25734
D	21	HIS	-	expression tag	UNP P25734
D	22	HIS	-	expression tag	UNP P25734
D	23	HIS	-	expression tag	UNP P25734

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ni 1 1	0	0
4	A	1	Total Ni 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	2	Total Ni 2 2	0	0

- Molecule 5 is water.

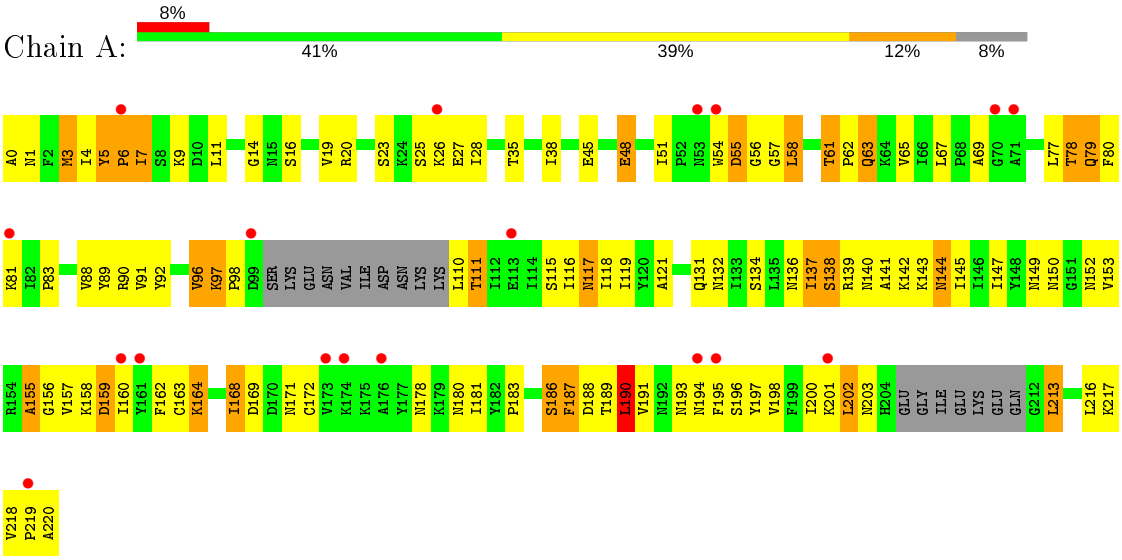
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	7	Total O 7 7	0	0
5	B	14	Total O 14 14	0	0
5	C	14	Total O 14 14	0	0
5	D	11	Total O 11 11	0	0

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.

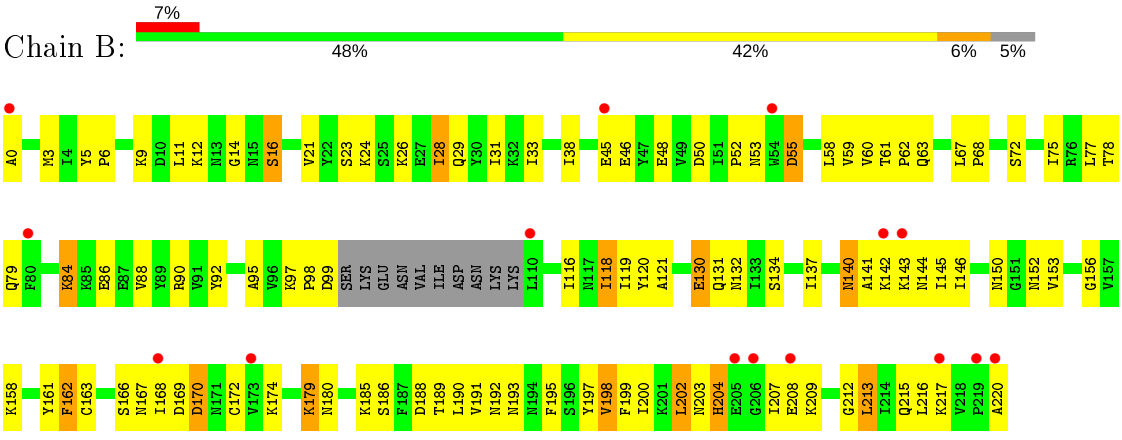
- Molecule 1: Colonization factor antigen I chaperone CfaA

Chain A:



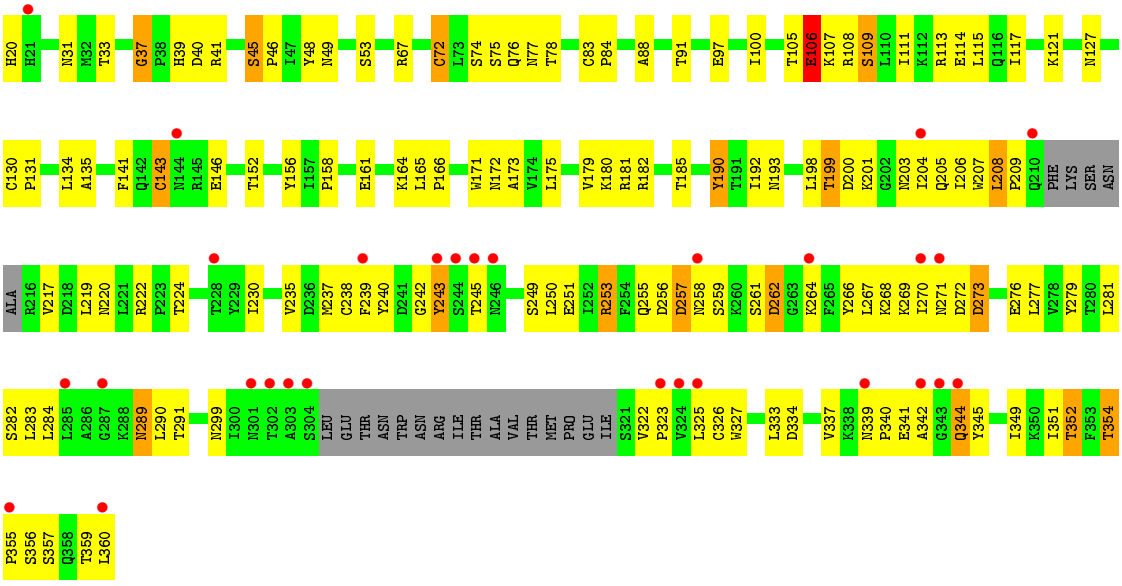
- Molecule 1: Colonization factor antigen I chaperone CfaA

Chain B:



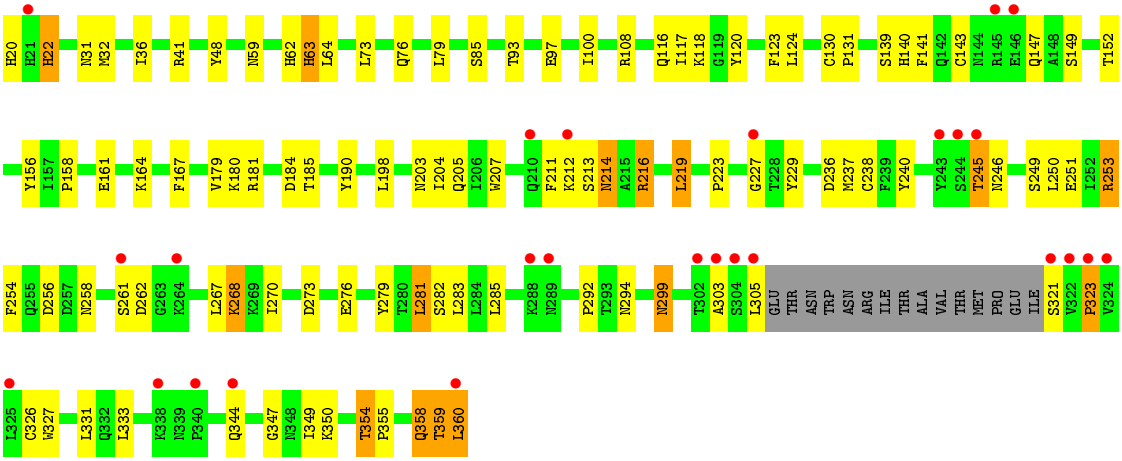
- Molecule 2: CFA/I fimbrial subunit E

Chain C:



- Molecule 2: CFA/I fimbrial subunit E

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	217.16Å 217.16Å 177.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.52 – 2.77 29.52 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.52-2.77) 99.6 (29.52-2.77)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.76Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.225 , 0.260 0.238 , 0.259	Depositor DCC
R_{free} test set	1999 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	52.4	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 56.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8432	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.12	1/1672 (0.1%)	0.94	8/2259 (0.4%)
1	B	0.85	2/1718 (0.1%)	0.71	0/2323
2	C	1.05	4/2542 (0.2%)	0.84	6/3445 (0.2%)
2	D	0.88	0/2591	0.70	2/3512 (0.1%)
All	All	0.98	7/8523 (0.1%)	0.79	16/11539 (0.1%)

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

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	190	TYR	CE1-CZ	-6.61	1.29	1.38
2	C	106	GLU	CD-OE2	-5.62	1.19	1.25
2	C	171	TRP	CE3-CZ3	-5.16	1.29	1.38
2	C	190	TYR	CG-CD1	-5.10	1.32	1.39
1	B	46	GLU	CD-OE2	-5.10	1.20	1.25
1	B	46	GLU	CD-OE1	-5.03	1.20	1.25
1	A	48	GLU	CD-OE1	-5.03	1.20	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	208	LEU	N-CA-C	-9.15	86.30	111.00
1	A	61	THR	C-N-CD	-8.56	101.77	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	6	PRO	CA-N-CD	-8.13	100.12	111.50
1	A	56	GLY	N-CA-C	-7.48	94.39	113.10
2	C	37	GLY	C-N-CD	-6.58	106.13	120.60
2	C	208	LEU	C-N-CD	6.19	141.41	128.40
1	A	155	ALA	N-CA-C	6.12	127.53	111.00
1	A	137	ILE	CG1-CB-CG2	-5.60	99.09	111.40
1	A	190	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	5	TYR	N-CA-C	-5.46	96.27	111.00
2	D	359	THR	CB-CA-C	-5.30	97.30	111.60
2	C	339	ASN	C-N-CD	5.27	139.47	128.40
2	C	284	LEU	N-CA-C	-5.22	96.91	111.00
1	A	58	LEU	CB-CG-CD2	-5.11	102.31	111.00
2	C	208	LEU	CB-CG-CD2	5.00	119.51	111.00
2	D	214	ASN	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	37	GLY	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1642	0	1700	185	0
1	B	1687	0	1733	111	0
2	C	2491	0	2447	191	0
2	D	2538	0	2495	72	0
3	A	6	0	8	0	0
3	C	18	0	24	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	7	0	0	2	0
5	B	14	0	0	7	0
5	C	14	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	11	0	0	3	0
All	All	8432	0	8407	504	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 30.

All (504) 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)
2:C:130:CYS:HB2	2:C:143:CYS:SG	1.52	1.46
1:A:3:MET:CE	2:C:322:VAL:HG21	1.48	1.42
2:C:40:ASP:OD1	2:C:199:THR:CG2	1.66	1.38
1:A:139:ARG:NH1	1:A:194:ASN:HA	1.38	1.36
2:D:238:CYS:HB3	2:D:326:CYS:SG	1.76	1.26
1:B:145:ILE:O	1:B:189:THR:HG22	1.30	1.24
1:A:139:ARG:HD2	1:A:218:VAL:O	1.39	1.21
1:B:197:TYR:O	1:B:217:LYS:HE3	1.42	1.18
2:C:130:CYS:CB	2:C:143:CYS:SG	2.31	1.16
1:A:140:ASN:HB3	1:A:144:ASN:ND2	1.63	1.14
1:A:140:ASN:CB	1:A:144:ASN:ND2	2.13	1.11
1:A:16:SER:HB3	1:A:78:THR:HB	1.19	1.11
2:D:256:ASP:OD1	2:D:294:ASN:ND2	1.83	1.10
2:C:258:ASN:HB3	2:C:268:LYS:NZ	1.64	1.10
1:B:145:ILE:HB	1:B:189:THR:HG21	1.27	1.09
2:D:62:HIS:CE1	2:D:64:LEU:HB2	1.88	1.09
1:A:140:ASN:CB	1:A:144:ASN:HD22	1.66	1.07
1:A:197:TYR:CZ	1:A:216:LEU:CD2	2.37	1.07
1:A:3:MET:HE3	2:C:322:VAL:HG21	1.14	1.07
1:A:162:PHE:O	1:A:172:CYS:HB3	1.53	1.07
1:A:3:MET:SD	2:C:322:VAL:HG11	1.95	1.07
1:A:139:ARG:HH12	1:A:194:ASN:CA	1.69	1.06
2:C:39:HIS:CE1	2:C:46:PRO:HD2	1.91	1.06
2:C:41:ARG:HD3	2:C:200:ASP:CB	1.88	1.04
1:A:3:MET:CE	2:C:322:VAL:CG2	2.36	1.03
2:C:41:ARG:HD3	2:C:200:ASP:HB2	1.07	1.03
1:A:180:ASN:ND2	2:C:359:THR:O	1.93	1.02
1:B:145:ILE:O	1:B:189:THR:CG2	2.07	1.01
2:C:41:ARG:CD	2:C:200:ASP:HB2	1.89	1.01
1:A:197:TYR:CZ	1:A:216:LEU:HD23	1.96	1.00
1:A:97:LYS:HE2	1:A:117:ASN:HD21	1.24	0.99
1:A:138:SER:HA	1:A:218:VAL:HG11	1.43	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LYS:HE2	1:A:117:ASN:ND2	1.78	0.98
2:C:40:ASP:OD1	2:C:199:THR:HG22	0.79	0.96
2:C:39:HIS:CE1	2:C:46:PRO:CD	2.48	0.96
1:A:139:ARG:HH12	1:A:194:ASN:HA	0.85	0.96
1:A:178:ASN:HA	2:C:360:LEU:HD21	1.45	0.96
1:B:197:TYR:C	1:B:217:LYS:HE3	1.87	0.94
1:A:16:SER:CB	1:A:78:THR:HB	1.96	0.94
2:D:63:HIS:CD2	2:D:147:GLN:HB2	2.01	0.94
1:A:140:ASN:ND2	1:A:144:ASN:HD21	1.66	0.93
2:C:258:ASN:CB	2:C:268:LYS:NZ	2.33	0.92
2:C:240:TYR:CE2	2:C:323:PRO:HG3	2.03	0.92
1:B:204:HIS:HB2	1:B:207:ILE:HB	1.51	0.92
2:C:258:ASN:HB3	2:C:268:LYS:CE	2.00	0.92
1:A:3:MET:HE1	2:C:322:VAL:HG21	1.52	0.91
2:C:39:HIS:HE1	2:C:46:PRO:HD3	1.36	0.91
2:D:63:HIS:HD2	2:D:147:GLN:HB2	1.32	0.91
1:A:197:TYR:OH	1:A:216:LEU:HD21	1.69	0.90
2:C:39:HIS:HD1	2:C:48:TYR:HH	0.91	0.90
2:C:256:ASP:OD1	2:C:258:ASN:N	2.04	0.90
2:C:359:THR:C	2:C:360:LEU:HD12	1.93	0.89
1:A:189:THR:O	1:A:190:LEU:HD22	1.71	0.89
1:A:5:TYR:OH	2:C:200:ASP:OD1	1.91	0.89
1:A:189:THR:C	1:A:190:LEU:HD13	1.94	0.88
2:C:258:ASN:HB3	2:C:268:LYS:HZ3	1.33	0.88
1:A:140:ASN:HD22	1:A:144:ASN:ND2	1.71	0.88
1:A:197:TYR:CZ	1:A:216:LEU:HD21	2.06	0.87
2:D:238:CYS:HB3	2:D:326:CYS:HG	1.38	0.87
1:B:158:LYS:NZ	5:B:401:HOH:O	2.06	0.87
1:A:139:ARG:HH21	1:A:219:PRO:HA	1.39	0.86
1:B:189:THR:O	1:B:190:LEU:HB2	1.77	0.85
1:B:212:GLY:CA	5:B:405:HOH:O	2.24	0.85
2:C:39:HIS:HE1	2:C:46:PRO:CD	1.87	0.85
2:C:203:ASN:HD21	2:C:322:VAL:HA	1.39	0.84
1:A:197:TYR:CE1	1:A:216:LEU:HD23	2.12	0.84
1:B:204:HIS:CB	1:B:207:ILE:HB	2.07	0.84
1:B:212:GLY:HA3	5:B:405:HOH:O	1.77	0.84
2:C:268:LYS:HE3	2:C:276:GLU:OE2	1.76	0.83
1:A:0:ALA:HB2	1:A:118:ILE:HB	1.60	0.82
1:A:3:MET:HE1	2:C:322:VAL:CG2	2.06	0.82
1:A:3:MET:HE3	2:C:322:VAL:CG2	2.04	0.82
2:C:78:THR:OG1	2:C:114:GLU:OE1	1.97	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLU:OE1	1:B:130:GLU:HA	1.81	0.81
1:A:140:ASN:HB2	1:A:144:ASN:HD22	1.44	0.81
1:B:197:TYR:O	1:B:217:LYS:CE	2.26	0.81
2:C:207:TRP:HB2	2:C:238:CYS:HB2	1.64	0.80
2:D:62:HIS:ND1	2:D:64:LEU:HB2	1.95	0.80
1:A:197:TYR:CE1	1:A:216:LEU:CD2	2.64	0.80
1:B:84:LYS:H	1:B:84:LYS:HD2	1.47	0.80
1:A:3:MET:HE1	2:C:322:VAL:CB	2.12	0.79
1:A:213:LEU:H	1:A:213:LEU:HD22	1.46	0.79
2:C:224:THR:HG22	5:C:505:HOH:O	1.82	0.79
2:C:205:GLN:OE1	2:C:323:PRO:HD2	1.82	0.79
1:A:3:MET:HE1	2:C:205:GLN:CD	2.03	0.79
1:A:139:ARG:NH1	1:A:194:ASN:CA	2.33	0.79
1:B:24:LYS:NZ	5:B:402:HOH:O	2.15	0.79
2:C:199:THR:HG23	2:C:201:LYS:HG3	1.64	0.79
1:A:140:ASN:ND2	1:A:144:ASN:ND2	2.27	0.78
2:D:251:GLU:OE1	2:D:253:ARG:NH1	2.16	0.78
2:D:97:GLU:OE1	2:D:156:TYR:OH	2.01	0.78
1:B:140:ASN:ND2	1:B:141:ALA:H	1.81	0.78
2:C:172:ASN:ND2	5:C:501:HOH:O	1.98	0.77
2:C:240:TYR:CE2	2:C:323:PRO:CG	2.68	0.77
1:A:3:MET:CE	2:C:205:GLN:CD	2.53	0.77
2:C:130:CYS:CB	2:C:143:CYS:HG	1.97	0.77
1:A:203:ASN:HD22	2:C:360:LEU:HB3	1.49	0.77
1:A:145:ILE:HD13	1:A:217:LYS:HD3	1.67	0.76
1:A:3:MET:CE	2:C:205:GLN:NE2	2.49	0.76
1:B:52:PRO:HG2	1:B:55:ASP:CB	2.16	0.75
1:B:144:ASN:OD1	1:B:191:VAL:C	2.24	0.75
2:D:238:CYS:CB	2:D:326:CYS:SG	2.69	0.75
1:A:7:ILE:HG21	2:C:204:ILE:HD12	1.68	0.75
2:C:209:PRO:HG3	2:C:238:CYS:SG	2.26	0.75
2:C:243:TYR:HE2	2:C:327:TRP:HE1	1.34	0.75
2:C:200:ASP:OD2	2:C:203:ASN:ND2	2.13	0.75
1:A:163:CYS:SG	1:A:168:ILE:HG22	2.27	0.74
2:C:258:ASN:CB	2:C:268:LYS:HZ3	1.97	0.74
1:A:144:ASN:HA	1:A:191:VAL:O	1.88	0.74
1:A:138:SER:HA	1:A:218:VAL:CG1	2.17	0.72
1:B:189:THR:HG23	1:B:191:VAL:H	1.53	0.72
2:C:41:ARG:HH11	2:C:200:ASP:CG	1.93	0.72
2:D:268:LYS:HE2	2:D:276:GLU:HG2	1.70	0.72
2:C:67:ARG:HH22	3:C:403:GOL:H32	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:262:ASP:N	2:C:262:ASP:OD1	2.21	0.71
1:B:161:TYR:CE2	1:B:174:LYS:HD2	2.26	0.71
2:C:251:GLU:OE1	2:C:253:ARG:NH1	2.23	0.71
1:A:3:MET:SD	2:C:322:VAL:HG21	2.31	0.70
2:C:39:HIS:ND1	2:C:48:TYR:OH	2.14	0.70
1:B:52:PRO:HG2	1:B:55:ASP:HB3	1.74	0.70
1:B:208:GLU:HG2	1:B:209:LYS:H	1.56	0.69
1:A:178:ASN:CA	2:C:360:LEU:HD21	2.20	0.68
1:B:162:PHE:CE2	1:B:191:VAL:HG21	2.28	0.68
1:A:3:MET:HE2	2:C:205:GLN:NE2	2.08	0.68
2:D:205:GLN:NE2	2:D:323:PRO:O	2.26	0.68
2:C:239:PHE:H	2:C:326:CYS:HB2	1.58	0.68
2:C:325:LEU:N	2:C:325:LEU:HD12	2.09	0.68
2:C:39:HIS:NE2	2:C:45:SER:HA	2.09	0.68
1:B:212:GLY:N	5:B:405:HOH:O	2.27	0.67
2:C:172:ASN:OD1	2:C:173:ALA:N	2.28	0.67
2:D:167:PHE:HB3	2:D:323:PRO:HB3	1.76	0.67
2:C:269:LYS:HB3	2:C:272:ASP:HB3	1.76	0.67
2:C:325:LEU:H	2:C:325:LEU:HD12	1.60	0.67
1:B:213:LEU:N	1:B:213:LEU:HD23	2.10	0.67
2:C:72:CYS:HB2	2:C:83:CYS:SG	2.35	0.66
2:C:270:ILE:O	2:C:271:ASN:HB2	1.96	0.66
2:C:360:LEU:N	2:C:360:LEU:HD12	2.10	0.66
2:C:220:ASN:ND2	5:C:502:HOH:O	2.29	0.66
2:C:273:ASP:N	2:C:273:ASP:OD1	2.23	0.66
1:A:140:ASN:HB3	1:A:144:ASN:HD22	1.29	0.66
1:A:163:CYS:SG	1:A:168:ILE:CG2	2.84	0.66
2:D:41:ARG:HH22	2:D:321:SER:HA	1.61	0.66
2:C:67:ARG:HH22	3:C:403:GOL:H12	1.61	0.65
1:A:134:SER:HB3	1:A:150:ASN:HB3	1.79	0.65
2:C:243:TYR:HE2	2:C:327:TRP:NE1	1.94	0.65
1:A:110:LEU:HD12	2:C:341:GLU:O	1.97	0.65
2:C:72:CYS:CB	2:C:83:CYS:SG	2.84	0.65
1:A:16:SER:HB3	1:A:78:THR:CB	2.12	0.65
2:C:240:TYR:CD2	2:C:323:PRO:HG2	2.32	0.65
1:A:140:ASN:CG	1:A:144:ASN:HD21	1.99	0.65
2:C:203:ASN:O	2:C:242:GLY:N	2.27	0.65
1:A:48:GLU:OE1	1:A:92:TYR:OH	2.14	0.64
1:A:96:VAL:HG12	1:A:98:PRO:HD2	1.79	0.64
2:C:277:LEU:HD12	2:C:345:TYR:CE2	2.31	0.64
1:A:140:ASN:CB	1:A:144:ASN:HD21	2.07	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:GLY:H	1:B:79:GLN:HE21	1.46	0.64
1:B:170:ASP:OD1	1:B:170:ASP:N	2.18	0.64
1:A:196:SER:C	1:A:197:TYR:HD1	2.00	0.64
1:A:178:ASN:O	2:C:360:LEU:HD11	1.98	0.64
2:D:36:ILE:HD12	2:D:48:TYR:HB3	1.80	0.64
1:B:158:LYS:HE3	1:B:203:ASN:HB3	1.79	0.64
1:B:144:ASN:OD1	1:B:191:VAL:O	2.16	0.64
2:C:109:SER:HB2	2:C:111:ILE:HG12	1.80	0.63
2:C:258:ASN:CB	2:C:268:LYS:HZ2	2.08	0.63
1:A:11:LEU:CD1	1:A:58:LEU:HD11	2.28	0.63
1:B:204:HIS:CD2	1:B:207:ILE:HB	2.34	0.63
1:B:212:GLY:C	1:B:213:LEU:HD23	2.19	0.63
1:A:3:MET:SD	2:C:322:VAL:CG1	2.81	0.63
1:B:208:GLU:HG2	1:B:209:LYS:N	2.13	0.62
1:A:178:ASN:C	2:C:360:LEU:HD11	2.20	0.62
2:C:325:LEU:CD1	2:C:325:LEU:H	2.13	0.62
2:C:39:HIS:CE1	2:C:45:SER:HA	2.35	0.61
1:B:131:GLN:OE1	5:B:403:HOH:O	2.16	0.61
2:C:41:ARG:HG2	2:C:198:LEU:HG	1.81	0.61
1:A:3:MET:HE1	2:C:322:VAL:HB	1.81	0.61
2:C:277:LEU:HD12	2:C:345:TYR:CD2	2.34	0.61
1:B:145:ILE:CB	1:B:189:THR:HG21	2.18	0.61
2:C:205:GLN:OE1	2:C:322:VAL:HB	1.99	0.61
1:B:191:VAL:HG12	1:B:193:ASN:H	1.65	0.61
2:C:277:LEU:HD21	2:C:337:VAL:HG11	1.83	0.61
1:B:204:HIS:HB2	1:B:207:ILE:CB	2.28	0.61
2:C:49:ASN:ND2	5:C:503:HOH:O	2.29	0.61
1:B:130:GLU:O	1:B:152:ASN:ND2	2.30	0.61
1:B:204:HIS:CG	1:B:207:ILE:HB	2.36	0.60
1:A:140:ASN:CG	1:A:144:ASN:ND2	2.53	0.60
2:C:205:GLN:NE2	2:C:207:TRP:CZ2	2.69	0.60
2:C:203:ASN:ND2	2:C:323:PRO:HD3	2.16	0.60
2:C:39:HIS:CG	2:C:48:TYR:HH	2.14	0.60
1:A:51:ILE:O	1:A:51:ILE:HG13	2.00	0.60
2:C:219:LEU:HD21	2:C:333:LEU:HB2	1.82	0.60
1:A:155:ALA:HB3	1:A:181:ILE:HB	1.83	0.60
2:D:167:PHE:CB	2:D:323:PRO:HB3	2.32	0.60
1:A:97:LYS:HE2	1:A:117:ASN:CG	2.22	0.60
2:C:208:LEU:HD23	2:C:237:MET:HB3	1.82	0.60
2:D:85:SER:N	5:D:403:HOH:O	2.26	0.60
2:C:113:ARG:HG3	2:C:166:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:PRO:HG2	1:B:55:ASP:HB2	1.84	0.59
2:C:41:ARG:CG	2:C:198:LEU:HG	2.32	0.59
1:B:53:ASN:HB2	1:B:63:GLN:OE1	2.03	0.59
2:C:158:PRO:HD2	2:C:161:GLU:HG3	1.85	0.59
2:C:20:HIS:ND1	2:C:20:HIS:O	2.36	0.59
2:C:179:VAL:HG21	2:C:190:TYR:CE1	2.38	0.59
1:A:168:ILE:O	1:A:172:CYS:SG	2.54	0.59
1:B:169:ASP:O	1:B:172:CYS:HB2	2.03	0.59
2:C:289:ASN:C	2:C:290:LEU:HG	2.22	0.59
1:A:110:LEU:HD12	2:C:342:ALA:HA	1.85	0.59
1:A:134:SER:CB	1:A:150:ASN:HB3	2.32	0.58
1:A:145:ILE:HD13	1:A:217:LYS:NZ	2.18	0.58
1:A:188:ASP:OD1	1:A:190:LEU:N	2.29	0.58
1:A:139:ARG:HH11	1:A:194:ASN:HA	1.59	0.58
1:B:145:ILE:HD13	1:B:217:LYS:HD3	1.84	0.58
1:B:199:PHE:HA	1:B:213:LEU:O	2.04	0.58
1:B:48:GLU:OE1	1:B:92:TYR:OH	2.22	0.58
2:D:245:THR:OG1	2:D:246:ASN:N	2.36	0.58
1:A:118:ILE:HD13	2:C:351:ILE:HB	1.86	0.58
1:A:57:GLY:HA3	1:A:89:TYR:OH	2.04	0.58
2:C:344:GLN:C	2:C:345:TYR:HD1	2.06	0.58
1:A:189:THR:O	1:A:190:LEU:CD2	2.48	0.58
1:A:144:ASN:H	1:A:144:ASN:ND2	2.02	0.57
1:B:140:ASN:HD22	1:B:141:ALA:H	1.52	0.57
2:C:258:ASN:HB3	2:C:268:LYS:HE2	1.83	0.57
2:C:72:CYS:HG	2:C:83:CYS:HG	0.63	0.57
2:D:227:GLY:N	5:D:402:HOH:O	2.26	0.57
1:B:179:LYS:NZ	5:B:407:HOH:O	2.37	0.57
1:A:189:THR:O	1:A:190:LEU:CB	2.52	0.57
1:B:158:LYS:HE3	1:B:203:ASN:CB	2.34	0.57
2:C:172:ASN:CG	5:C:501:HOH:O	2.38	0.57
2:D:62:HIS:HE1	2:D:64:LEU:HB2	1.62	0.57
1:A:11:LEU:HD12	1:A:58:LEU:HD11	1.86	0.57
1:A:218:VAL:HG22	1:A:220:ALA:H	1.70	0.57
1:A:97:LYS:N	1:A:98:PRO:HD2	2.19	0.57
1:B:161:TYR:CE2	1:B:174:LYS:CD	2.89	0.56
2:C:205:GLN:NE2	2:C:207:TRP:HE1	2.02	0.56
2:C:205:GLN:NE2	2:C:207:TRP:HZ2	2.03	0.56
1:A:145:ILE:HD13	1:A:217:LYS:CD	2.36	0.56
1:B:98:PRO:HG2	1:B:99:ASP:H	1.70	0.56
2:C:106:GLU:OE2	2:C:108:ARG:N	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LEU:HD12	1:B:58:LEU:HD11	1.86	0.56
1:A:55:ASP:N	1:A:55:ASP:OD1	2.37	0.56
2:C:258:ASN:ND2	2:C:268:LYS:HD3	2.20	0.56
1:A:9:LYS:NZ	5:A:401:HOH:O	2.33	0.56
1:B:170:ASP:C	1:B:172:CYS:H	2.08	0.55
2:C:74:SER:OG	3:C:404:GOL:H32	2.05	0.55
1:A:38:ILE:HB	1:A:88:VAL:HG13	1.89	0.55
2:C:269:LYS:HD3	2:C:272:ASP:HB3	1.89	0.55
2:D:211:PHE:CD1	2:D:211:PHE:N	2.75	0.55
1:B:191:VAL:HG13	1:B:193:ASN:OD1	2.06	0.55
2:C:240:TYR:CD2	2:C:323:PRO:CG	2.90	0.54
1:A:5:TYR:O	1:A:20:ARG:N	2.40	0.54
2:C:269:LYS:HD3	2:C:272:ASP:CB	2.38	0.54
2:C:100:ILE:HB	2:C:117:ILE:HB	1.89	0.54
2:C:266:TYR:HB2	2:C:268:LYS:HZ2	1.73	0.54
1:B:198:VAL:HG23	1:B:217:LYS:CE	2.38	0.54
1:A:189:THR:C	1:A:190:LEU:CD1	2.74	0.54
1:A:137:ILE:N	1:A:137:ILE:HD12	2.23	0.54
1:B:163:CYS:O	1:B:195:PHE:HD2	1.90	0.54
1:A:97:LYS:N	1:A:98:PRO:CD	2.71	0.53
2:C:258:ASN:HB2	2:C:268:LYS:NZ	2.22	0.53
2:C:41:ARG:NH1	2:C:200:ASP:CG	2.61	0.53
1:A:140:ASN:O	1:A:143:LYS:N	2.40	0.53
1:A:139:ARG:NH2	1:A:219:PRO:HA	2.18	0.53
1:A:218:VAL:HG21	2:D:31:ASN:HB3	1.89	0.53
2:D:359:THR:OG1	2:D:360:LEU:N	2.40	0.53
1:A:180:ASN:CG	2:C:359:THR:O	2.47	0.53
2:D:93:THR:HG21	2:D:141:PHE:HB3	1.91	0.53
2:C:88:ALA:O	2:C:182:ARG:NH2	2.37	0.53
1:A:193:ASN:HB2	1:A:195:PHE:CE1	2.44	0.52
2:C:130:CYS:HB3	2:C:143:CYS:SG	2.43	0.52
2:C:251:GLU:HB2	2:C:356:SER:HB3	1.91	0.52
1:A:137:ILE:CD1	1:A:137:ILE:N	2.73	0.52
1:B:28:ILE:HB	1:B:68:PRO:HA	1.90	0.52
1:B:207:ILE:CG2	1:B:208:GLU:N	2.73	0.52
2:C:217:VAL:HG11	2:C:235:VAL:HG22	1.91	0.52
1:B:116:ILE:HD13	2:D:349:ILE:HB	1.89	0.52
1:B:90:ARG:NE	2:D:354:THR:HG21	2.24	0.52
2:C:209:PRO:CG	2:C:238:CYS:SG	2.95	0.52
1:B:24:LYS:HG3	2:D:207:TRP:CH2	2.45	0.52
1:A:197:TYR:HD1	1:A:197:TYR:N	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LYS:HA	1:A:69:ALA:HB1	1.91	0.52
1:B:198:VAL:HG23	1:B:217:LYS:HE2	1.92	0.52
2:C:266:TYR:HB2	2:C:268:LYS:NZ	2.25	0.51
2:C:360:LEU:N	2:C:360:LEU:CD1	2.73	0.51
1:A:142:LYS:C	1:A:143:LYS:HG2	2.30	0.51
1:A:0:ALA:HB2	1:A:118:ILE:CB	2.37	0.51
1:A:136:ASN:C	1:A:137:ILE:HD12	2.31	0.51
1:A:158:LYS:HE3	2:C:360:LEU:HD23	1.92	0.51
1:A:23:SER:HB2	1:A:67:LEU:HG	1.93	0.51
1:B:48:GLU:OE2	1:B:90:ARG:NH1	2.41	0.51
2:C:41:ARG:HD3	2:C:200:ASP:CG	2.31	0.51
2:D:62:HIS:C	2:D:63:HIS:ND1	2.64	0.51
2:C:258:ASN:HB2	2:C:268:LYS:HZ2	1.74	0.51
1:B:200:ILE:O	1:B:212:GLY:HA2	2.10	0.51
1:B:118:ILE:HD11	1:B:120:TYR:CE1	2.46	0.50
2:D:59:ASN:O	2:D:149:SER:HB3	2.11	0.50
1:B:38:ILE:HB	1:B:88:VAL:HG13	1.93	0.50
1:A:110:LEU:CD1	2:C:341:GLU:O	2.60	0.50
2:D:240:TYR:CE2	2:D:323:PRO:HG2	2.46	0.50
2:C:172:ASN:OD1	5:C:501:HOH:O	2.19	0.50
1:A:134:SER:OG	1:A:150:ASN:ND2	2.44	0.50
1:A:164:LYS:HD3	1:A:171:ASN:CB	2.42	0.50
1:A:187:PHE:C	1:A:187:PHE:CD1	2.85	0.50
1:A:197:TYR:N	1:A:197:TYR:CD1	2.78	0.50
1:A:6:PRO:N	1:A:19:VAL:HG13	2.26	0.50
1:B:98:PRO:HG2	1:B:99:ASP:N	2.27	0.50
1:B:16:SER:HB2	1:B:78:THR:HB	1.93	0.49
1:A:110:LEU:HB2	2:C:342:ALA:HA	1.94	0.49
1:A:197:TYR:CE2	1:A:216:LEU:HD23	2.43	0.49
1:B:162:PHE:O	1:B:172:CYS:HB3	2.12	0.49
1:B:213:LEU:HB2	1:B:215:GLN:OE1	2.12	0.49
1:A:90:ARG:NH2	2:C:356:SER:HA	2.27	0.49
1:A:152:ASN:OD1	1:A:153:VAL:N	2.45	0.49
1:A:168:ILE:HD12	1:A:168:ILE:N	2.28	0.49
1:A:147:ILE:O	1:A:186:SER:HA	2.13	0.49
2:C:238:CYS:CB	2:C:326:CYS:HG	2.25	0.49
2:D:219:LEU:HD22	2:D:333:LEU:HB2	1.94	0.49
1:B:169:ASP:HB3	1:B:172:CYS:SG	2.53	0.49
1:A:38:ILE:HG12	1:A:48:GLU:HG2	1.94	0.49
1:A:63:GLN:HG2	1:A:63:GLN:O	2.12	0.49
2:D:354:THR:HG22	2:D:355:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:344:GLN:C	2:C:345:TYR:CD1	2.85	0.49
1:A:200:ILE:O	1:A:213:LEU:HD22	2.13	0.48
1:A:213:LEU:N	1:A:213:LEU:HD13	2.28	0.48
1:A:16:SER:HB2	1:A:77:LEU:O	2.13	0.48
1:A:38:ILE:HD11	1:A:90:ARG:HD2	1.94	0.48
2:C:208:LEU:O	2:C:209:PRO:C	2.50	0.48
1:A:6:PRO:HD3	1:A:19:VAL:HA	1.95	0.48
1:A:3:MET:CE	2:C:322:VAL:HG11	2.43	0.48
2:C:267:LEU:HG	2:C:279:TYR:CD1	2.49	0.48
1:A:121:ALA:HB3	2:C:354:THR:HG23	1.96	0.48
1:A:138:SER:CA	1:A:218:VAL:CG1	2.90	0.48
1:A:1:ASN:HB3	1:A:25:SER:HB2	1.95	0.48
2:D:118:LYS:HG2	2:D:158:PRO:HG3	1.96	0.48
1:A:196:SER:C	1:A:197:TYR:CD1	2.83	0.47
1:B:59:VAL:HB	1:B:78:THR:HG23	1.96	0.47
2:C:198:LEU:HA	2:C:198:LEU:HD12	1.73	0.47
2:C:262:ASP:HB2	2:C:264:LYS:HG3	1.96	0.47
1:A:119:ILE:HB	2:C:352:THR:HG23	1.95	0.47
1:B:189:THR:O	1:B:190:LEU:CB	2.54	0.47
2:C:127:ASN:ND2	2:C:146:GLU:OE2	2.42	0.47
1:A:35:THR:HG23	1:A:91:VAL:HG22	1.97	0.47
1:B:23:SER:HB2	1:B:67:LEU:HG	1.97	0.47
2:C:205:GLN:NE2	2:C:207:TRP:NE1	2.62	0.47
2:C:270:ILE:HG23	2:C:270:ILE:O	2.14	0.47
2:D:268:LYS:HE2	2:D:276:GLU:CG	2.41	0.47
1:B:198:VAL:CG2	1:B:217:LYS:HE2	2.45	0.47
1:A:152:ASN:O	1:A:183:PRO:HG3	2.13	0.47
2:C:200:ASP:CG	2:C:203:ASN:HB2	2.35	0.47
2:D:41:ARG:HH12	2:D:321:SER:C	2.17	0.47
2:D:130:CYS:HB2	2:D:143:CYS:SG	2.54	0.47
1:B:162:PHE:HZ	1:B:189:THR:OG1	1.97	0.46
2:C:239:PHE:N	2:C:326:CYS:HB2	2.29	0.46
2:D:250:LEU:HG	2:D:251:GLU:H	1.80	0.46
2:D:279:TYR:HE2	2:D:349:ILE:HD11	1.81	0.46
1:A:138:SER:CA	1:A:218:VAL:HG11	2.32	0.46
1:A:110:LEU:N	5:A:403:HOH:O	2.49	0.46
2:D:212:LYS:HD3	2:D:212:LYS:HA	1.68	0.46
2:D:22:HIS:CD2	2:D:124:LEU:HD13	2.50	0.46
2:D:223:PRO:HA	2:D:229:TYR:HA	1.98	0.46
1:A:164:LYS:H	1:A:164:LYS:HG2	1.45	0.46
1:A:156:GLY:HA2	1:A:180:ASN:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ASN:HA	1:B:191:VAL:O	2.16	0.46
1:B:156:GLY:O	1:B:202:LEU:HA	2.16	0.46
2:C:257:ASP:C	2:C:259:SER:H	2.16	0.46
2:C:240:TYR:CZ	2:C:323:PRO:HG3	2.48	0.46
2:D:205:GLN:OE1	2:D:207:TRP:NE1	2.42	0.46
1:B:188:ASP:OD1	1:B:190:LEU:N	2.49	0.46
2:D:303:ALA:C	2:D:305:LEU:H	2.19	0.46
1:A:163:CYS:O	1:A:195:PHE:HB3	2.16	0.46
1:B:163:CYS:C	1:B:195:PHE:HD2	2.18	0.46
1:A:97:LYS:CE	1:A:117:ASN:OD1	2.64	0.45
1:A:160:ILE:CG2	1:A:198:VAL:HG13	2.46	0.45
2:C:74:SER:HB3	2:C:77:ASN:HB3	1.98	0.45
2:D:120:TYR:HE1	2:D:156:TYR:HE1	1.64	0.45
2:D:281:LEU:N	5:D:401:HOH:O	2.09	0.45
2:C:206:ILE:HD11	2:C:239:PHE:HD1	1.81	0.45
1:A:140:ASN:O	1:A:143:LYS:HA	2.17	0.45
1:A:197:TYR:O	1:A:198:VAL:HG23	2.17	0.45
2:C:39:HIS:CE1	2:C:46:PRO:HD3	2.21	0.45
1:B:119:ILE:HD12	2:D:350:LYS:HG3	1.97	0.45
1:A:164:LYS:HD3	1:A:171:ASN:HB2	1.97	0.45
1:B:170:ASP:C	1:B:172:CYS:N	2.70	0.45
2:C:41:ARG:HG2	2:C:198:LEU:CG	2.47	0.45
2:C:203:ASN:HD21	2:C:323:PRO:HD3	1.79	0.45
2:D:254:PHE:CD1	2:D:292:PRO:HB3	2.52	0.45
1:A:3:MET:HE2	2:C:205:GLN:CD	2.33	0.45
1:B:145:ILE:HB	1:B:189:THR:CG2	2.20	0.45
2:C:41:ARG:NH1	2:C:200:ASP:OD2	2.50	0.45
1:A:190:LEU:N	1:A:190:LEU:HD13	2.30	0.45
1:B:167:ASN:OD1	1:B:167:ASN:N	2.50	0.45
1:B:5:TYR:HA	1:B:6:PRO:HA	1.81	0.45
1:B:53:ASN:HD21	1:B:60:VAL:H	1.64	0.44
2:C:257:ASP:N	2:C:257:ASP:OD1	2.48	0.44
1:A:90:ARG:NH2	2:C:355:PRO:O	2.45	0.44
2:C:106:GLU:OE2	2:C:107:LYS:N	2.50	0.44
1:A:141:ALA:C	1:A:143:LYS:N	2.70	0.44
1:A:159:ASP:N	1:A:159:ASP:OD1	2.50	0.44
1:B:207:ILE:HD13	1:B:207:ILE:HA	1.79	0.44
2:D:360:LEU:HD22	2:D:360:LEU:HA	1.75	0.44
1:A:14:GLY:HA2	1:A:79:GLN:HG3	2.00	0.44
2:C:249:SER:HB3	2:C:359:THR:HG22	2.00	0.44
2:C:251:GLU:HG2	2:C:253:ARG:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:0:ALA:HA	2:D:213:SER:O	2.17	0.44
1:B:179:LYS:HG3	1:B:180:ASN:N	2.32	0.44
1:B:28:ILE:HG12	1:B:29:GLN:N	2.32	0.44
1:B:33:ILE:HD13	1:B:75:ILE:HG12	1.99	0.44
2:D:181:ARG:HB3	2:D:184:ASP:HB3	1.99	0.44
1:A:140:ASN:C	1:A:143:LYS:H	2.21	0.44
1:A:188:ASP:O	1:A:190:LEU:HD13	2.17	0.44
1:A:5:TYR:HA	1:A:6:PRO:HA	1.47	0.44
2:C:67:ARG:NH2	3:C:403:GOL:H12	2.31	0.44
1:A:155:ALA:N	1:A:181:ILE:O	2.36	0.44
1:A:26:LYS:HG2	1:A:26:LYS:O	2.18	0.44
2:D:223:PRO:HB3	2:D:229:TYR:CZ	2.52	0.44
1:A:141:ALA:C	1:A:143:LYS:H	2.17	0.44
1:A:4:ILE:HD11	1:A:7:ILE:HD12	2.00	0.44
2:C:20:HIS:CG	2:C:20:HIS:O	2.68	0.43
2:D:20:HIS:O	2:D:22:HIS:ND1	2.51	0.43
2:D:180:LYS:HE2	2:D:181:ARG:O	2.18	0.43
1:A:190:LEU:N	1:A:190:LEU:CD1	2.81	0.43
1:B:97:LYS:HB3	1:B:98:PRO:HD2	2.01	0.43
2:C:257:ASP:O	2:C:259:SER:N	2.39	0.43
2:D:123:PHE:HE2	2:D:140:HIS:HA	1.84	0.43
2:C:121:LYS:HE2	2:C:135:ALA:O	2.18	0.43
1:A:189:THR:O	1:A:190:LEU:CG	2.67	0.43
1:B:180:ASN:OD1	2:D:359:THR:O	2.36	0.43
2:D:267:LEU:HD23	2:D:347:GLY:HA3	2.00	0.43
1:A:121:ALA:O	2:C:354:THR:HG23	2.19	0.43
2:D:283:LEU:HD12	2:D:331:LEU:HB2	2.00	0.43
1:A:144:ASN:N	1:A:144:ASN:ND2	2.66	0.43
1:B:145:ILE:CD1	1:B:217:LYS:HD3	2.49	0.43
1:B:21:VAL:O	1:B:72:SER:HA	2.19	0.43
2:D:116:GLN:HB2	2:D:161:GLU:OE2	2.19	0.43
1:B:189:THR:HG23	1:B:190:LEU:N	2.33	0.42
1:A:116:ILE:HD13	2:C:349:ILE:HB	2.00	0.42
1:A:188:ASP:O	1:A:190:LEU:CD1	2.67	0.42
1:B:134:SER:O	1:B:150:ASN:N	2.44	0.42
2:C:269:LYS:HG2	2:C:270:ILE:N	2.34	0.42
1:A:3:MET:CE	2:C:205:GLN:CG	2.97	0.42
1:B:140:ASN:ND2	1:B:141:ALA:N	2.58	0.42
2:C:277:LEU:HD21	2:C:337:VAL:CG1	2.49	0.42
1:A:178:ASN:CB	2:C:360:LEU:HD21	2.50	0.42
1:A:142:LYS:O	1:A:143:LYS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:VAL:HG13	1:A:200:ILE:CG2	2.50	0.42
2:C:33:THR:HA	2:C:193:ASN:HB2	2.00	0.42
2:C:97:GLU:OE2	2:C:156:TYR:OH	2.20	0.42
1:A:134:SER:O	1:A:150:ASN:HB3	2.20	0.42
1:A:140:ASN:O	1:A:143:LYS:CA	2.68	0.42
1:B:146:ILE:HD13	1:B:188:ASP:HA	2.02	0.42
2:C:203:ASN:OD1	2:C:322:VAL:HG12	2.20	0.42
2:C:268:LYS:HG3	2:C:276:GLU:CG	2.50	0.42
1:B:90:ARG:HE	2:D:354:THR:HG21	1.83	0.42
1:A:111:THR:O	2:C:344:GLN:HA	2.20	0.42
2:D:358:GLN:HG2	2:D:358:GLN:H	1.40	0.42
1:B:131:GLN:HB3	1:B:153:VAL:HG21	2.01	0.42
2:C:165:LEU:HD12	2:C:198:LEU:HD22	2.02	0.42
1:A:131:GLN:HG2	1:A:153:VAL:HG21	2.02	0.41
1:A:197:TYR:C	1:A:198:VAL:HG23	2.40	0.41
1:A:28:ILE:HG23	1:A:28:ILE:O	2.19	0.41
1:A:97:LYS:HE3	1:A:117:ASN:OD1	2.20	0.41
2:C:238:CYS:HB3	2:C:326:CYS:HG	1.85	0.41
2:C:115:LEU:HD11	2:C:165:LEU:HD21	2.01	0.41
2:C:243:TYR:C	2:C:245:THR:H	2.24	0.41
1:B:26:LYS:HB2	2:D:212:LYS:HG3	2.01	0.41
1:A:116:ILE:HA	1:A:116:ILE:HD13	1.95	0.41
1:B:31:ILE:HD13	1:B:95:ALA:HA	2.01	0.41
2:D:108:ARG:HA	2:D:108:ARG:HD3	1.82	0.41
2:D:100:ILE:HB	2:D:117:ILE:HB	2.01	0.41
1:A:142:LYS:O	1:A:143:LYS:CB	2.67	0.41
1:A:195:PHE:CD1	1:A:195:PHE:N	2.88	0.41
1:B:26:LYS:HG2	2:D:212:LYS:HD2	2.01	0.41
2:D:249:SER:OG	2:D:299:ASN:OD1	2.37	0.41
2:D:41:ARG:HG3	2:D:198:LEU:HG	2.02	0.41
1:A:140:ASN:HB3	1:A:144:ASN:H	1.86	0.41
1:A:157:VAL:HG13	1:A:200:ILE:HG23	2.02	0.41
1:B:207:ILE:HG23	1:B:208:GLU:H	1.85	0.41
1:B:9:LYS:HD2	1:B:9:LYS:HA	1.97	0.41
2:C:175:LEU:HD23	2:C:192:ILE:HD12	2.02	0.41
1:A:110:LEU:CD1	2:C:342:ALA:HA	2.49	0.41
1:A:61:THR:HG22	1:A:62:PRO:HD3	2.03	0.41
2:C:180:LYS:HG2	2:C:181:ARG:O	2.21	0.41
2:C:200:ASP:OD1	2:C:203:ASN:HB2	2.21	0.41
1:B:121:ALA:HB3	2:D:354:THR:HG23	2.03	0.41
1:B:142:LYS:HE2	1:B:142:LYS:HB3	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:LEU:HD23	1:B:190:LEU:HA	1.79	0.41
1:B:216:LEU:HB3	2:C:33:THR:HG21	2.02	0.41
1:A:168:ILE:HD12	1:A:168:ILE:H	1.86	0.41
1:A:1:ASN:HB3	1:A:25:SER:CB	2.51	0.41
2:C:257:ASP:C	2:C:259:SER:N	2.73	0.41
2:D:214:ASN:HB3	2:D:216:ARG:HD2	2.02	0.41
1:A:97:LYS:H	1:A:98:PRO:CD	2.34	0.41
1:B:137:ILE:CD1	1:B:215:GLN:HE21	2.33	0.41
1:B:61:THR:HA	1:B:62:PRO:HA	1.92	0.41
2:D:73:LEU:HA	2:D:73:LEU:HD23	1.90	0.41
1:B:143:LYS:HD3	1:B:220:ALA:HB1	2.02	0.40
2:C:277:LEU:CD2	2:C:337:VAL:HG11	2.49	0.40
1:A:90:ARG:HH22	2:C:356:SER:HA	1.85	0.40
2:D:179:VAL:HG21	2:D:190:TYR:CE1	2.57	0.40
2:C:219:LEU:HD21	2:C:333:LEU:CB	2.48	0.40
1:A:201:LYS:O	1:A:202:LEU:CD1	2.70	0.40
2:C:134:LEU:HD11	2:C:141:PHE:HE1	1.86	0.40
2:C:250:LEU:O	2:C:299:ASN:HA	2.22	0.40
2:C:251:GLU:N	2:C:354:THR:O	2.48	0.40
2:D:180:LYS:HE3	2:D:180:LYS:HB2	1.86	0.40
2:D:184:ASP:OD1	2:D:185:THR:HG22	2.21	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	198/221 (90%)	190 (96%)	7 (4%)	1 (0%)	29	58
1	B	207/221 (94%)	200 (97%)	7 (3%)	0	100	100
2	C	314/341 (92%)	297 (95%)	15 (5%)	2 (1%)	25	54
2	D	322/341 (94%)	308 (96%)	12 (4%)	2 (1%)	25	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1041/1124 (93%)	995 (96%)	41 (4%)	5 (0%)	29 58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	323	PRO
2	C	340	PRO
1	A	97	LYS
2	C	131	PRO
2	D	131	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	186/202 (92%)	156 (84%)	30 (16%)	2 6
1	B	189/202 (94%)	163 (86%)	26 (14%)	3 10
2	C	278/298 (93%)	243 (87%)	35 (13%)	4 12
2	D	283/298 (95%)	252 (89%)	31 (11%)	6 17
All	All	936/1000 (94%)	814 (87%)	122 (13%)	4 11

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	7	ILE
1	A	27	GLU
1	A	45	GLU
1	A	54	TRP
1	A	55	ASP
1	A	63	GLN
1	A	65	VAL
1	A	78	THR
1	A	79	GLN

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Mol	Chain	Res	Type
1	A	80	PHE
1	A	81	LYS
1	A	83	PRO
1	A	96	VAL
1	A	111	THR
1	A	115	SER
1	A	117	ASN
1	A	132	ASN
1	A	138	SER
1	A	144	ASN
1	A	149	ASN
1	A	159	ASP
1	A	164	LYS
1	A	168	ILE
1	A	169	ASP
1	A	186	SER
1	A	187	PHE
1	A	190	LEU
1	A	202	LEU
1	A	213	LEU
1	B	3	MET
1	B	12	LYS
1	B	16	SER
1	B	28	ILE
1	B	45	GLU
1	B	50	ASP
1	B	55	ASP
1	B	77	LEU
1	B	84	LYS
1	B	86	GLU
1	B	118	ILE
1	B	130	GLU
1	B	132	ASN
1	B	140	ASN
1	B	162	PHE
1	B	166	SER
1	B	168	ILE
1	B	170	ASP
1	B	179	LYS
1	B	185	LYS
1	B	186	SER
1	B	192	ASN

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Mol	Chain	Res	Type
1	B	198	VAL
1	B	202	LEU
1	B	204	HIS
1	B	213	LEU
2	C	31	ASN
2	C	45	SER
2	C	53	SER
2	C	72	CYS
2	C	75	SER
2	C	76	GLN
2	C	84	PRO
2	C	91	THR
2	C	105	THR
2	C	106	GLU
2	C	109	SER
2	C	143	CYS
2	C	152	THR
2	C	164	LYS
2	C	185	THR
2	C	199	THR
2	C	222	ARG
2	C	230	ILE
2	C	243	TYR
2	C	253	ARG
2	C	255	GLN
2	C	257	ASP
2	C	261	SER
2	C	262	ASP
2	C	273	ASP
2	C	281	LEU
2	C	282	SER
2	C	283	LEU
2	C	289	ASN
2	C	291	THR
2	C	334	ASP
2	C	344	GLN
2	C	352	THR
2	C	354	THR
2	C	357	SER
2	D	22	HIS
2	D	32	MET
2	D	63	HIS

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Mol	Chain	Res	Type
2	D	76	GLN
2	D	79	LEU
2	D	139	SER
2	D	152	THR
2	D	164	LYS
2	D	203	ASN
2	D	204	ILE
2	D	216	ARG
2	D	219	LEU
2	D	236	ASP
2	D	237	MET
2	D	245	THR
2	D	253	ARG
2	D	258	ASN
2	D	261	SER
2	D	262	ASP
2	D	268	LYS
2	D	270	ILE
2	D	273	ASP
2	D	281	LEU
2	D	282	SER
2	D	285	LEU
2	D	299	ASN
2	D	327	TRP
2	D	344	GLN
2	D	354	THR
2	D	358	GLN
2	D	360	LEU

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

Mol	Chain	Res	Type
1	A	13	ASN
1	A	144	ASN
1	A	150	ASN
1	A	203	ASN
1	A	204	HIS
1	B	140	ASN
2	C	210	GLN
2	D	103	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	GOL	C	402	-	5,5,5	0.36	0	5,5,5	0.25	0
3	GOL	A	301	-	5,5,5	0.38	0	5,5,5	0.27	0
3	GOL	C	403	-	5,5,5	0.39	0	5,5,5	0.25	0
3	GOL	C	404	-	5,5,5	0.36	0	5,5,5	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	402	-	-	2/4/4/4	-
3	GOL	A	301	-	-	2/4/4/4	-
3	GOL	C	403	-	-	4/4/4/4	-
3	GOL	C	404	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402	GOL	C1-C2-C3-O3
3	C	403	GOL	O1-C1-C2-C3
3	C	403	GOL	C1-C2-C3-O3
3	C	404	GOL	O1-C1-C2-C3
3	C	404	GOL	C1-C2-C3-O3
3	C	404	GOL	O1-C1-C2-O2
3	A	301	GOL	C1-C2-C3-O3
3	C	402	GOL	O2-C2-C3-O3
3	C	403	GOL	O1-C1-C2-O2
3	C	403	GOL	O2-C2-C3-O3
3	C	404	GOL	O2-C2-C3-O3
3	A	301	GOL	O2-C2-C3-O3

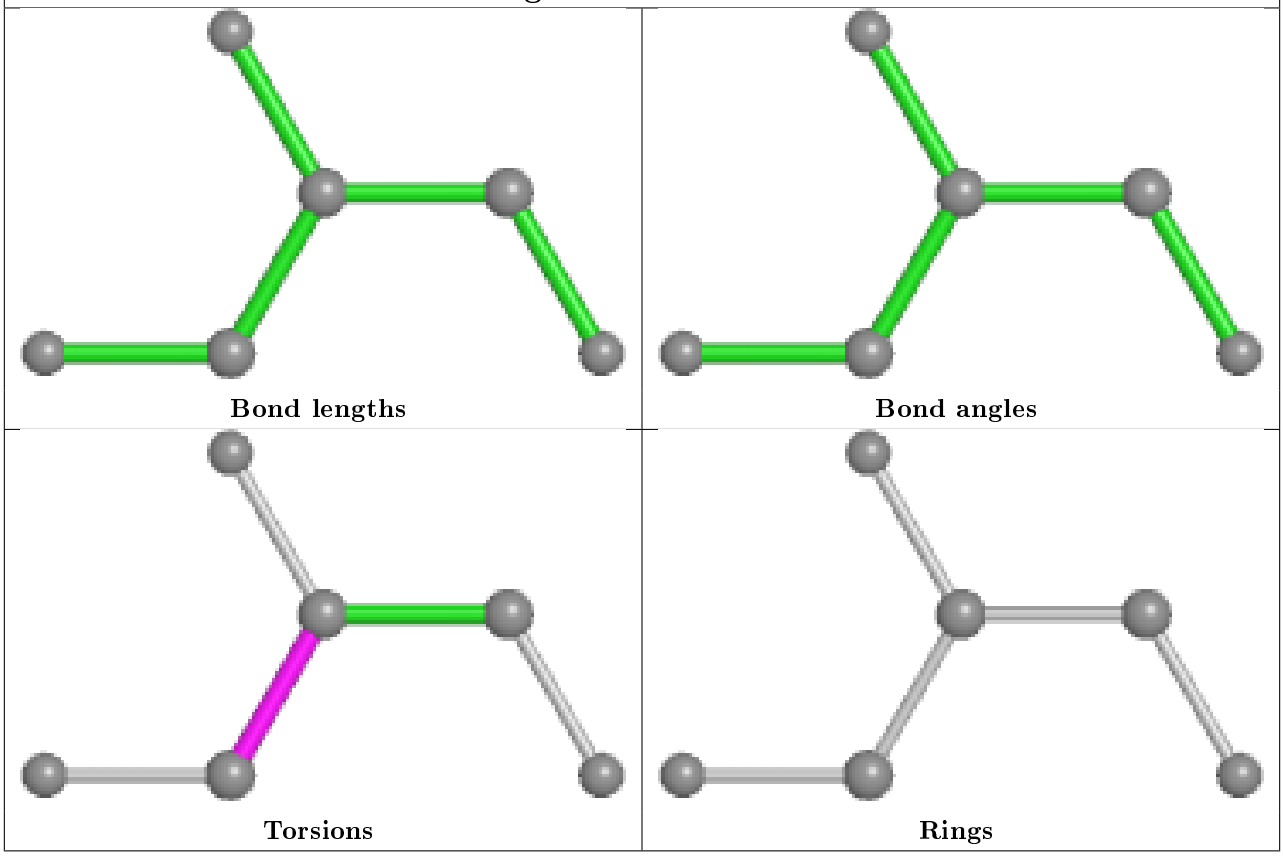
There are no ring outliers.

2 monomers are involved in 4 short contacts:

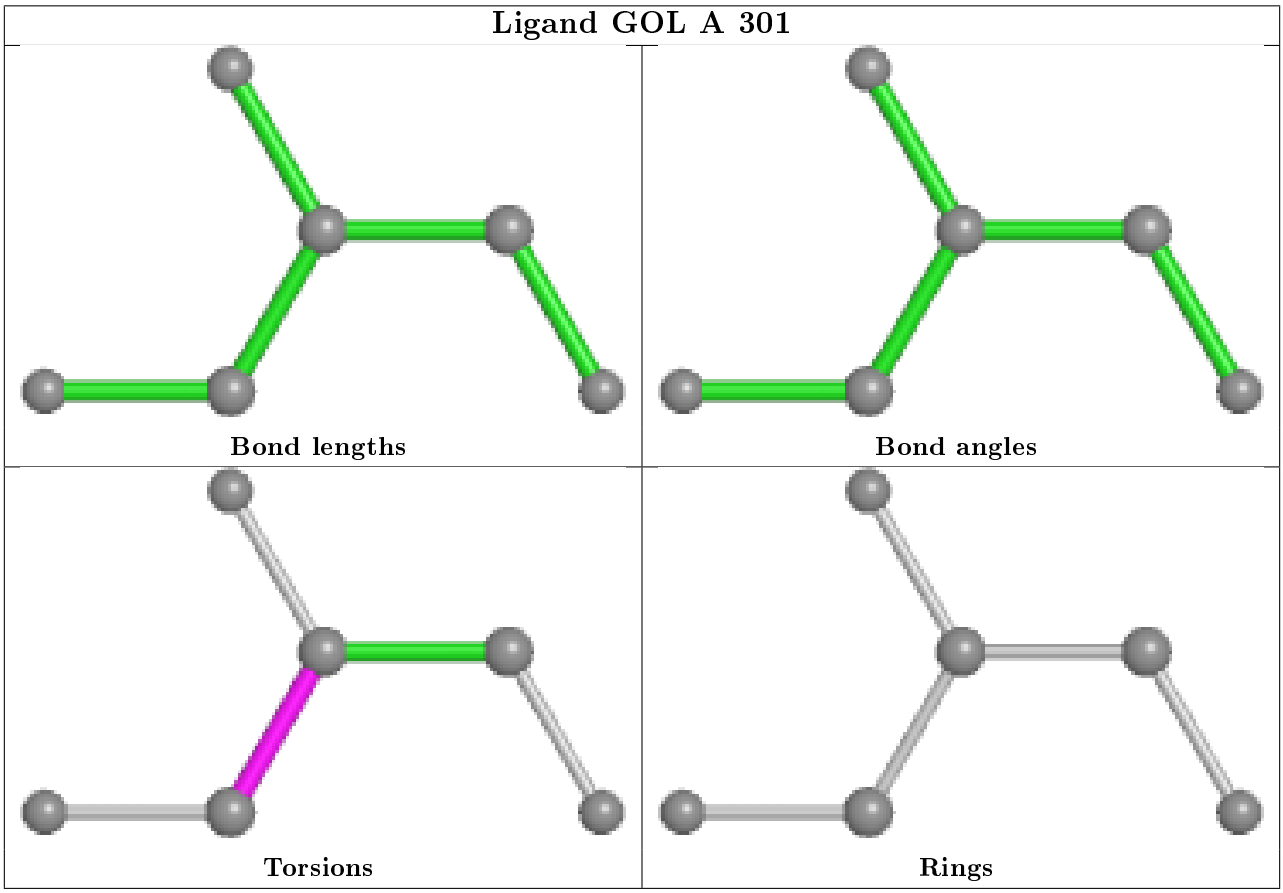
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	403	GOL	3	0
3	C	404	GOL	1	0

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

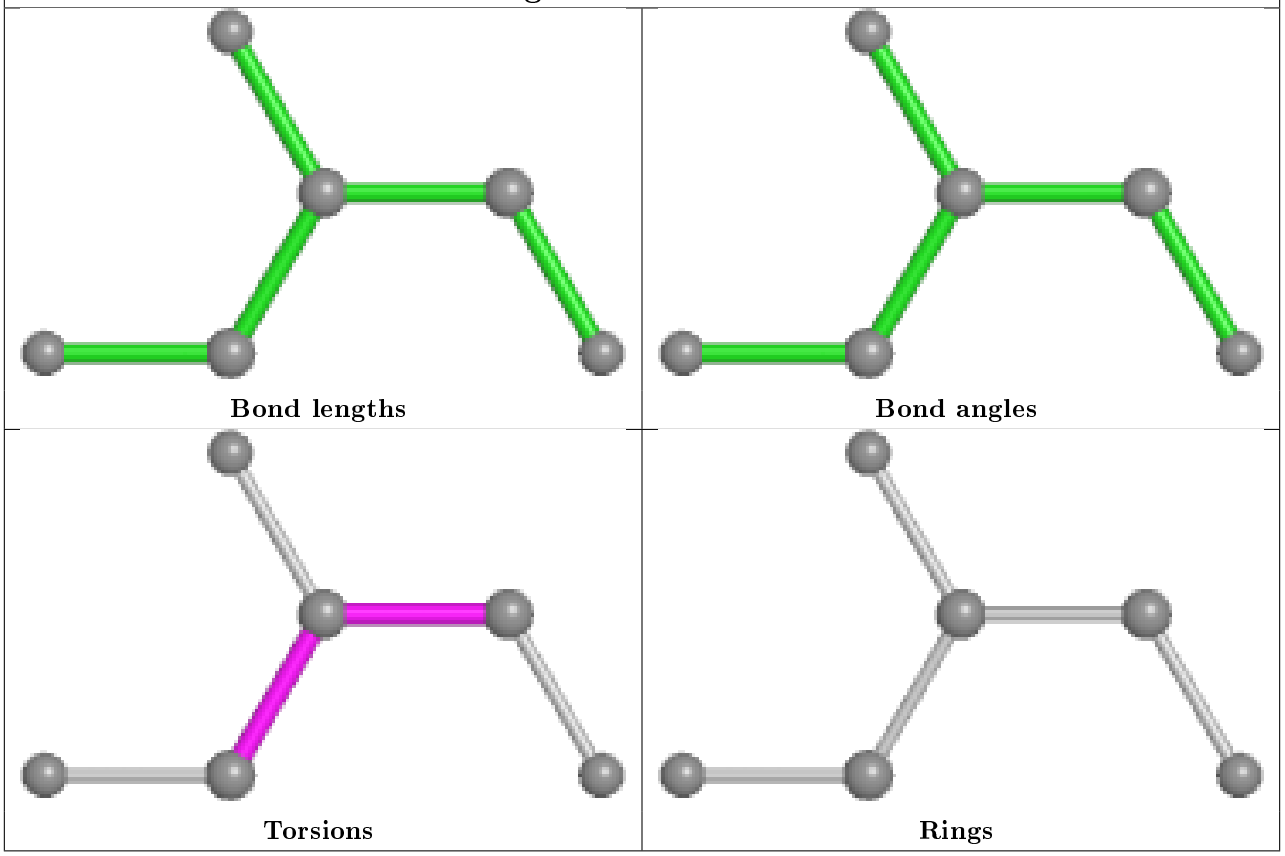
Ligand GOL C 402



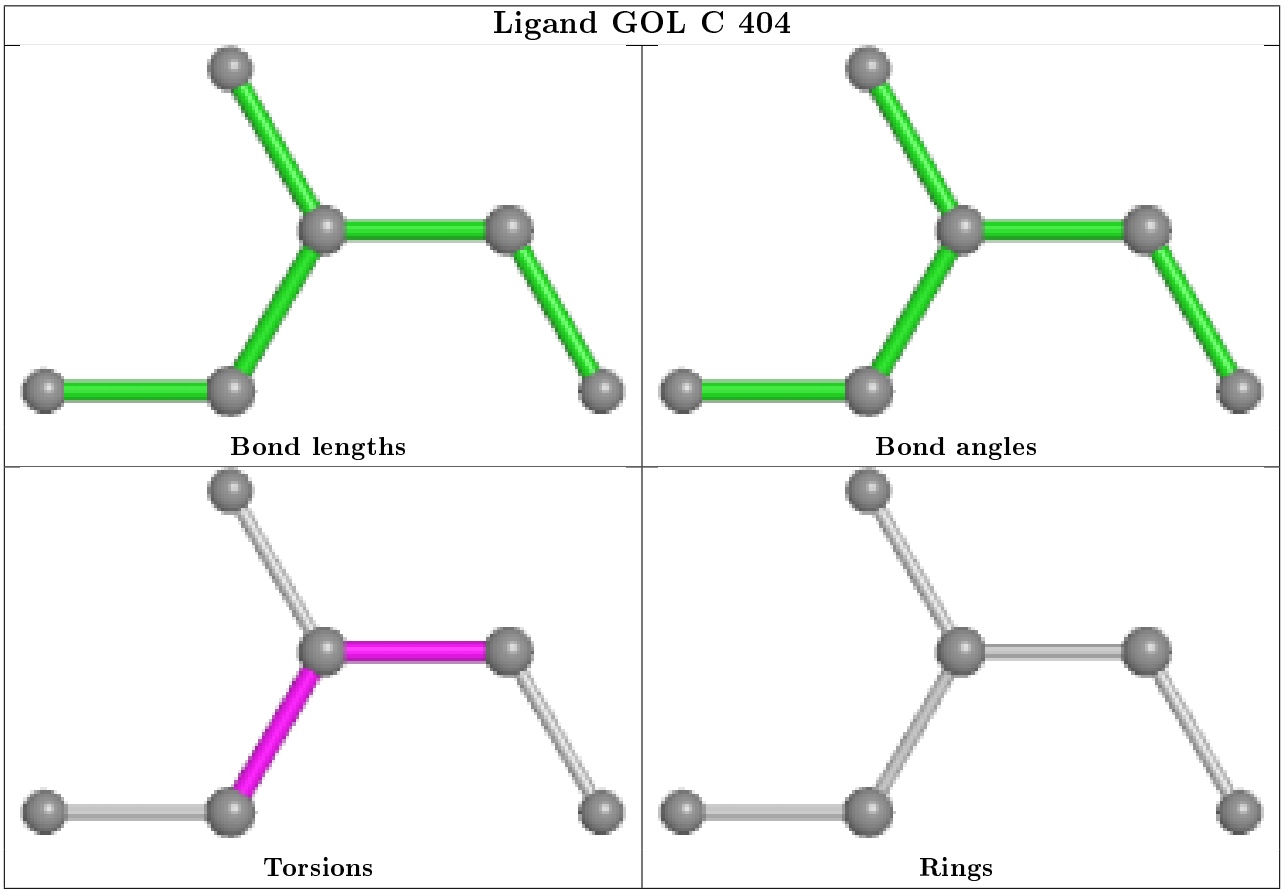
Ligand GOL A 301



Ligand GOL C 403



Ligand GOL C 404



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	204/221 (92%)	0.44	18 (8%) 10 6	31, 61, 108, 141	0
1	B	211/221 (95%)	0.34	15 (7%) 16 11	28, 52, 120, 155	0
2	C	320/341 (93%)	0.56	29 (9%) 9 6	26, 56, 115, 167	0
2	D	326/341 (95%)	0.43	26 (7%) 12 8	30, 53, 93, 117	0
All	All	1061/1124 (94%)	0.45	88 (8%) 11 7	26, 56, 110, 167	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	324	VAL	14.2
2	C	360	LEU	10.4
2	C	244	SER	8.5
1	B	220	ALA	8.1
2	C	246	ASN	6.8
1	B	54	TRP	6.0
2	C	245	THR	5.8
2	D	325	LEU	5.7
2	D	360	LEU	5.6
2	D	303	ALA	5.0
1	B	205	GLU	5.0
2	C	271	ASN	4.8
2	D	210	GLN	4.6
2	D	261	SER	4.5
2	C	228	THR	4.4
1	B	219	PRO	4.4
2	D	244	SER	4.4
2	D	21	HIS	4.3
2	C	325	LEU	4.3
2	C	243	TYR	4.2
1	A	54	TRP	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	161	TYR	3.9
2	D	305	LEU	3.9
1	A	173	VAL	3.9
2	C	285	LEU	3.7
1	A	70	GLY	3.7
2	C	343	GLY	3.7
1	B	206	GLY	3.7
2	C	302	THR	3.6
2	C	204	ILE	3.5
2	D	322	VAL	3.4
2	C	258	ASN	3.4
2	D	338	LYS	3.4
2	C	303	ALA	3.3
2	D	145	ARG	3.3
1	A	201	LYS	3.0
1	A	99	ASP	3.0
1	A	195	PHE	3.0
2	D	324	VAL	2.9
2	D	321	SER	2.9
2	D	340	PRO	2.8
2	D	212	LYS	2.8
2	C	304	SER	2.8
1	A	81	LYS	2.7
1	B	45	GLU	2.7
1	A	219	PRO	2.6
2	C	270	ILE	2.6
1	B	208	GLU	2.6
2	C	344	GLN	2.6
1	B	168	ILE	2.6
2	C	339	ASN	2.6
2	C	210	GLN	2.5
2	D	245	THR	2.5
2	D	288	LYS	2.5
2	D	344	GLN	2.4
1	A	26	LYS	2.4
1	B	110	LEU	2.4
1	B	173	VAL	2.4
2	C	301	ASN	2.4
2	C	323	PRO	2.4
2	D	227	GLY	2.4
1	A	6	PRO	2.4
2	D	264	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	71	ALA	2.3
1	A	194	ASN	2.3
1	A	113	GLU	2.3
1	B	143	LYS	2.3
1	A	53	ASN	2.2
2	C	21	HIS	2.2
1	B	80	PHE	2.2
1	A	174	LYS	2.2
2	C	342	ALA	2.2
1	B	0	ALA	2.2
2	C	264	LYS	2.2
2	D	243	TYR	2.2
2	D	146	GLU	2.2
2	C	287	GLY	2.2
1	B	142	LYS	2.1
2	D	304	SER	2.1
1	A	176	ALA	2.1
2	D	323	PRO	2.1
2	D	289	ASN	2.1
2	C	144	ASN	2.1
1	A	160	ILE	2.0
1	B	217	LYS	2.0
2	C	355	PRO	2.0
2	D	302	THR	2.0
2	C	239	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

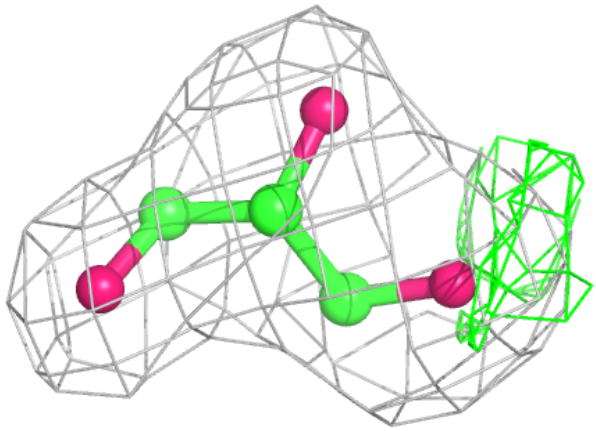
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

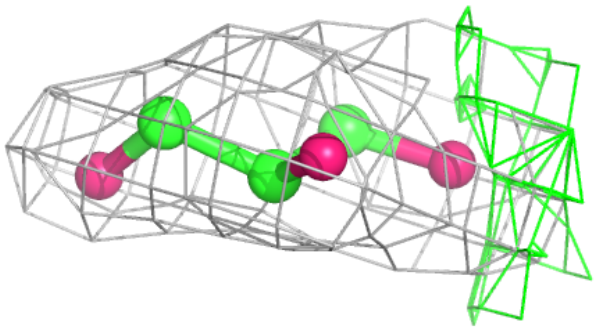
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	301	6/6	0.69	0.18	46,57,66,70	0
4	NI	C	405	1/1	0.77	0.08	131,131,131,131	1
3	GOL	C	402	6/6	0.81	0.17	71,74,84,88	0
4	NI	A	302	1/1	0.83	0.10	85,85,85,85	0
3	GOL	C	403	6/6	0.89	0.18	55,65,67,69	0
3	GOL	C	404	6/6	0.92	0.28	55,62,63,71	0
4	NI	C	401	1/1	0.95	0.07	88,88,88,88	0
4	NI	B	301	1/1	0.97	0.07	93,93,93,93	0

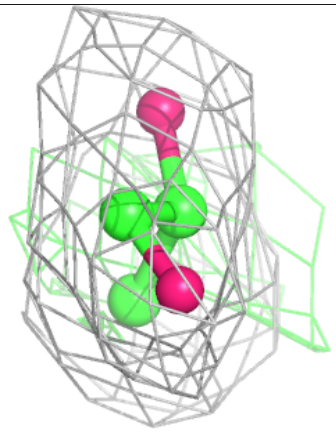
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GOL A 301:

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

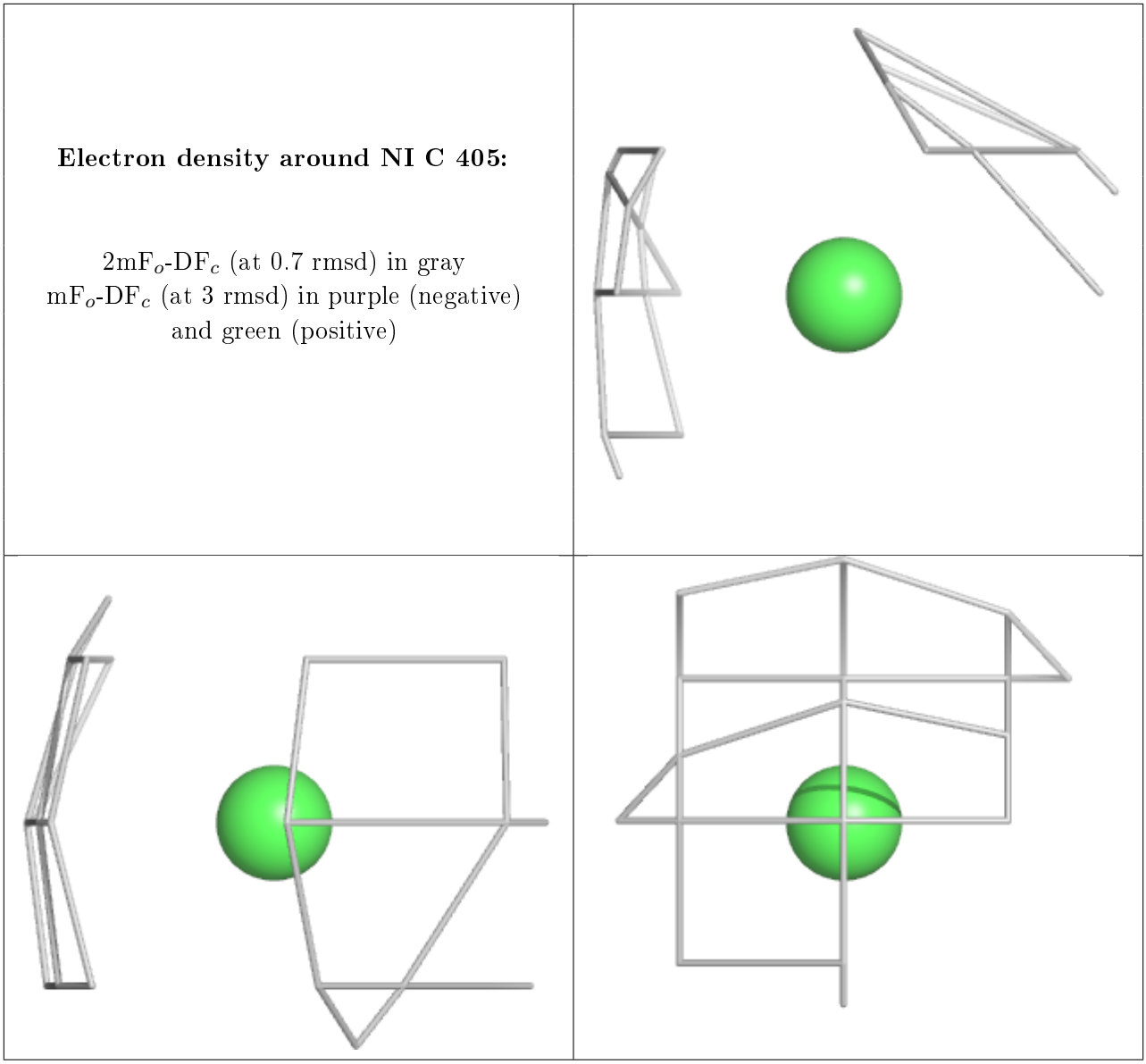






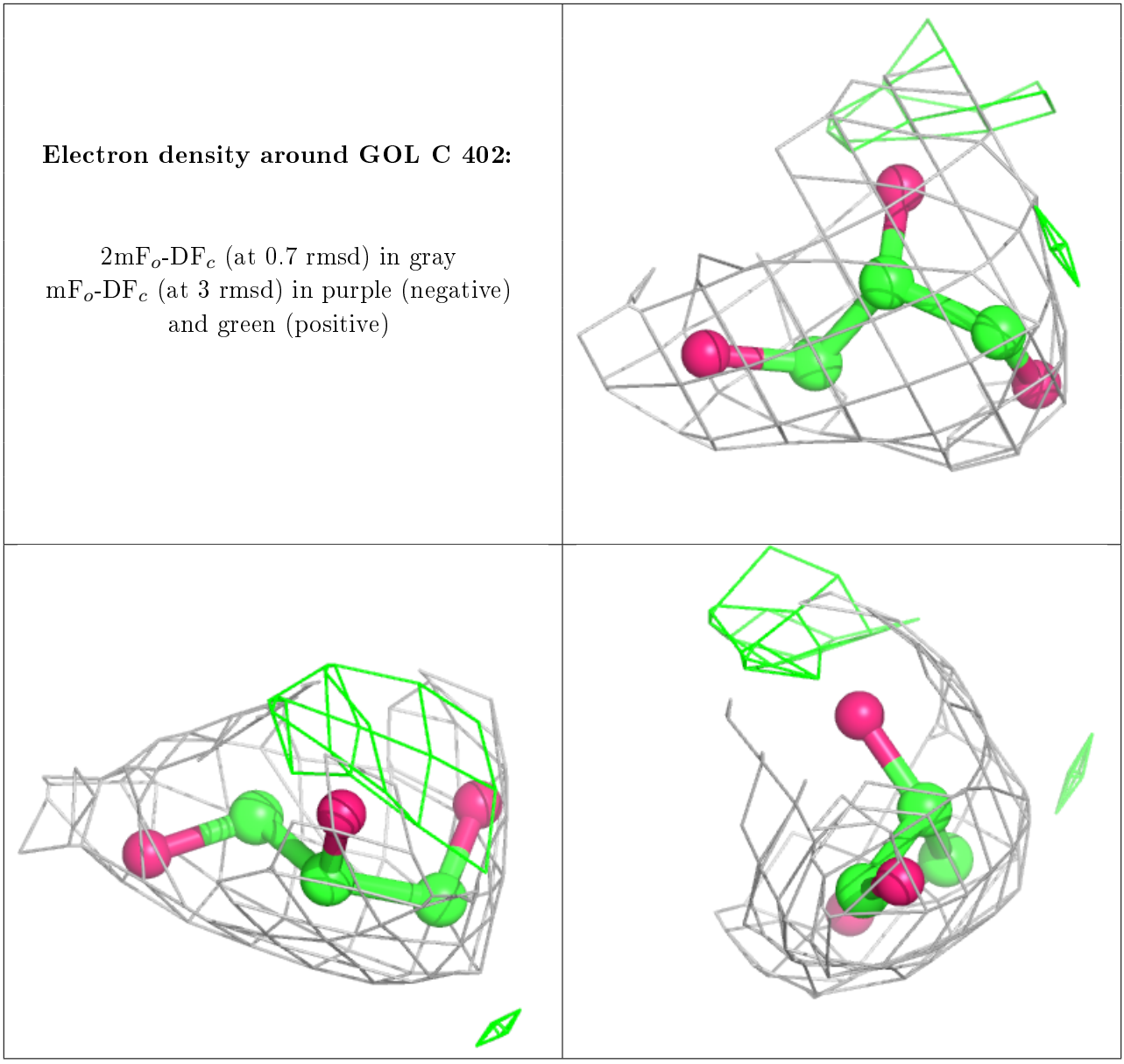
Electron density around NI C 405:

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



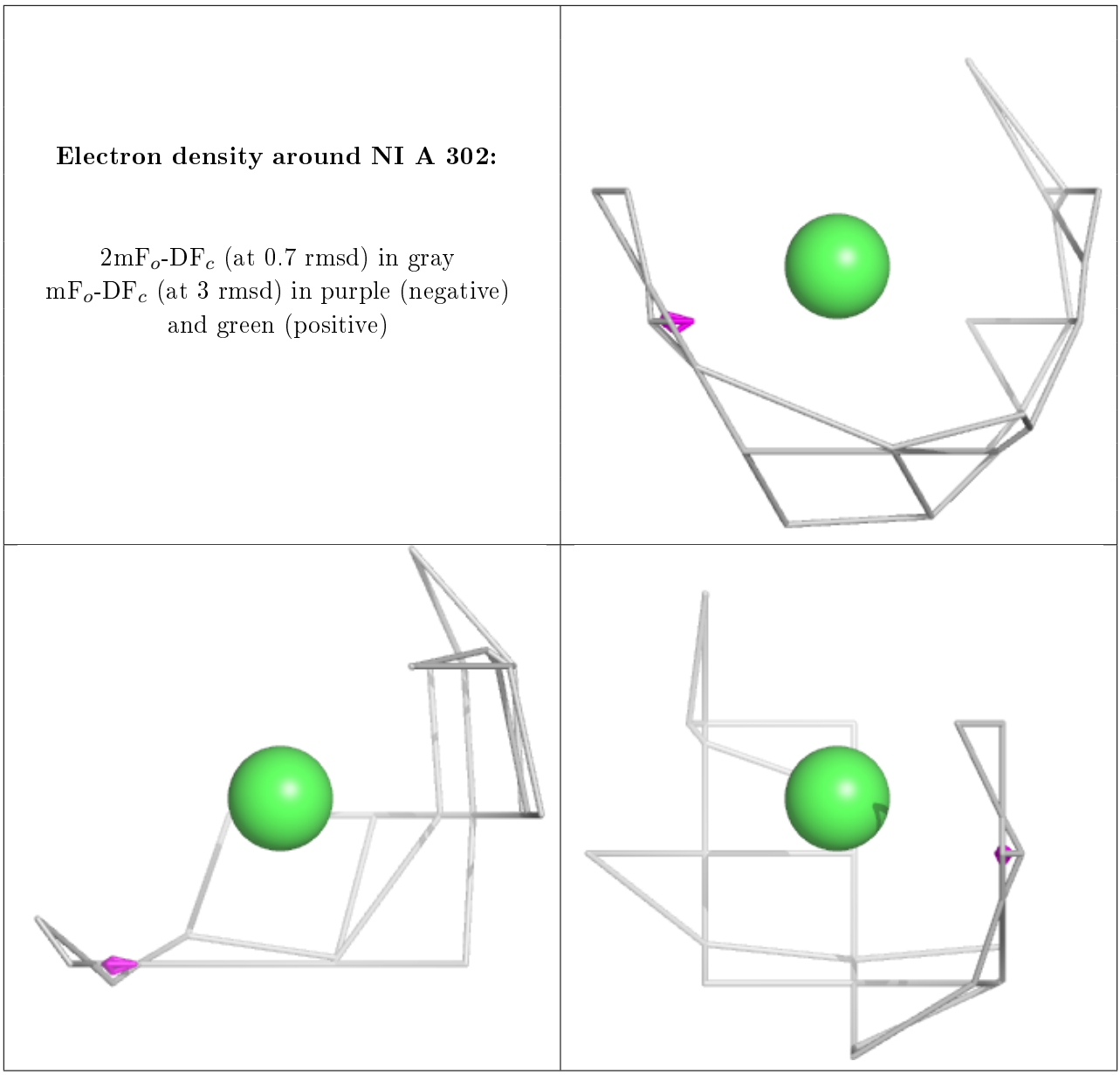
Electron density around GOL C 402:

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



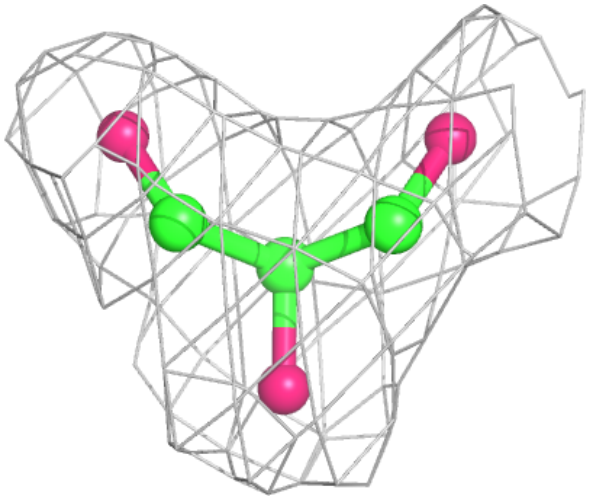
Electron density around NI A 302:

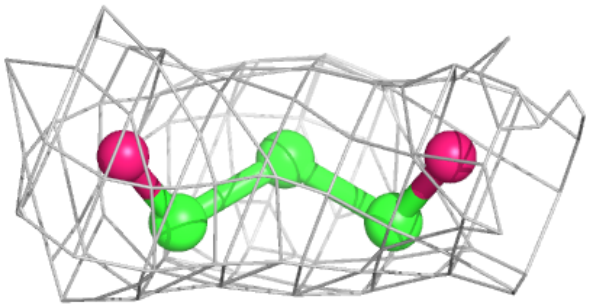
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

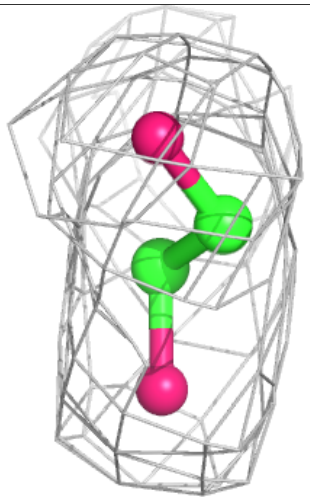


Electron density around GOL C 403:

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

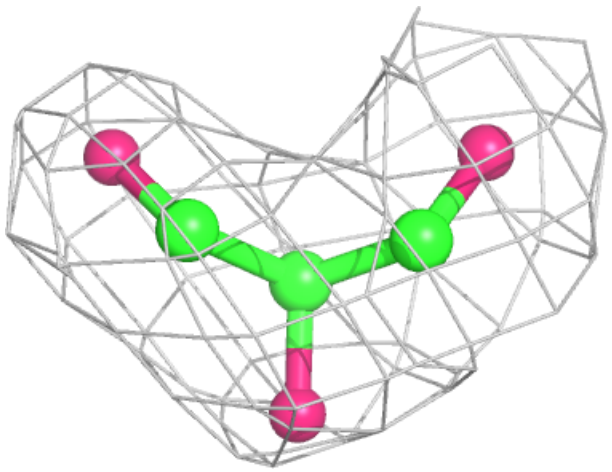


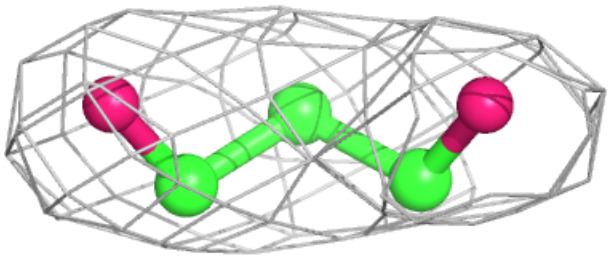


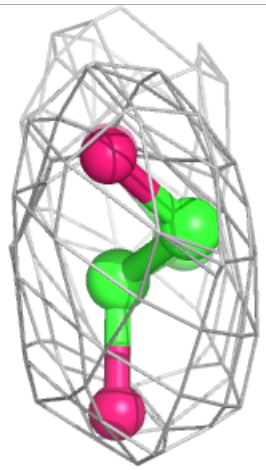


Electron density around GOL C 404:

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

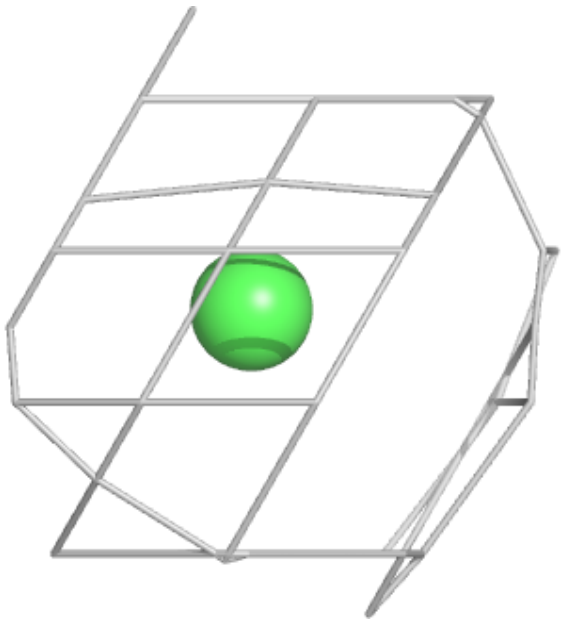


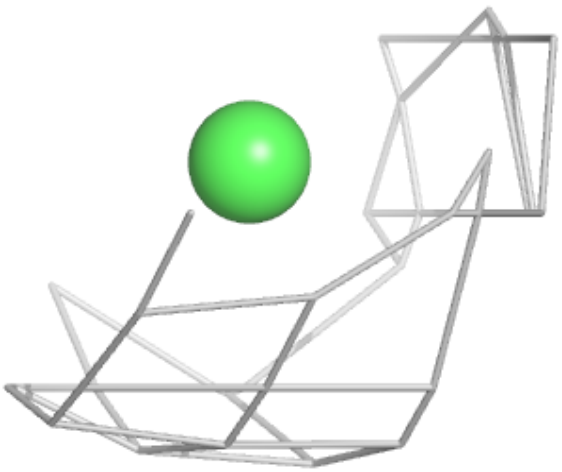


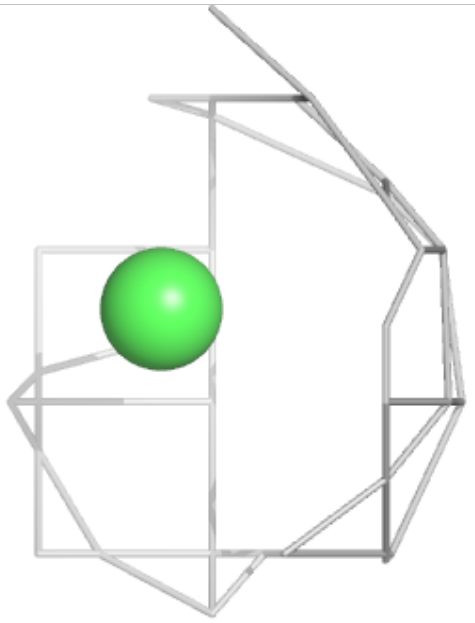


Electron density around NI C 401:

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

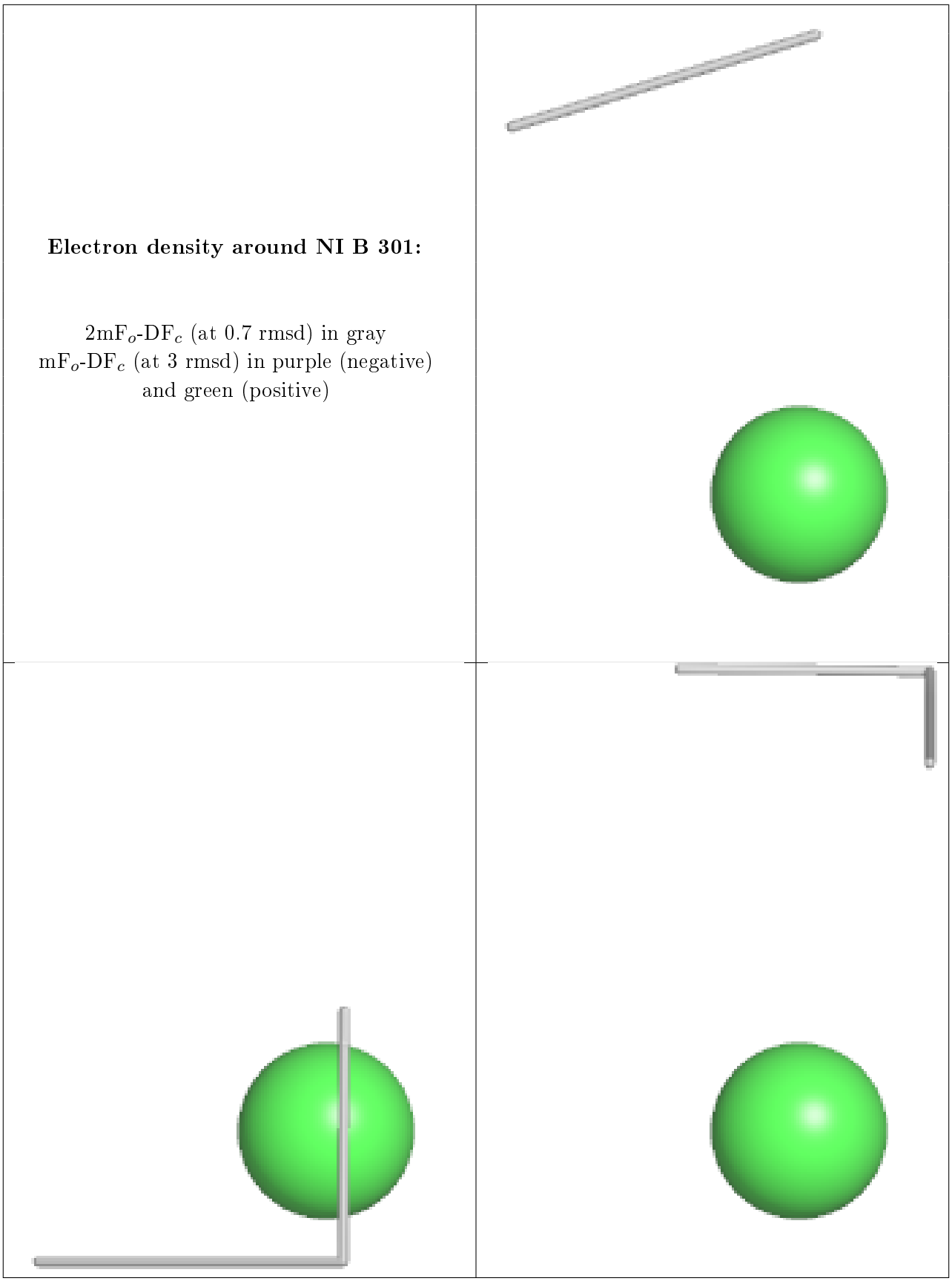






Electron density around NI B 301:

$2mF_o$-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.