Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 12:43 AM JST

PDB ID	:	7E9R
Title	:	Crystal structure of Sesquisabinene B Synthase 1 mutant T313S
Authors	:	Singh, S.; Thulasiram, H.V.; Kulkarni, K.A.
Deposited on	:	2021-03-04
Resolution	:	3.41 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

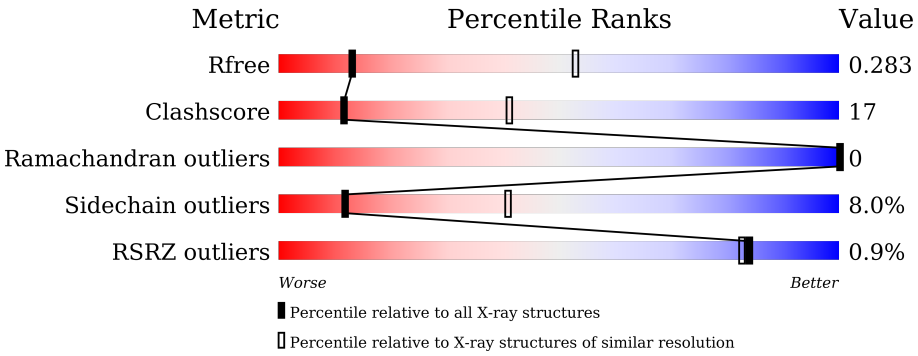
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.41 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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

Mol	Chain	Length	Quality of chain
1	A	555	65% 24% • 8%
1	B	555	% 63% 27% • 9%
1	C	555	% 59% 27% 5% 9%
1	D	555	% 57% 30% • 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16432 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 Sesquisabinene B synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			4129	2665	687	760	17			
1	B	506	Total	C	N	O	S	0	0	0
			4105	2652	682	754	17			
1	C	506	Total	C	N	O	S	0	0	0
			4108	2653	683	755	17			
1	D	504	Total	C	N	O	S	0	0	0
			4082	2635	679	752	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	-	expression tag	UNP A0A0A0RDR2
A	13	GLU	-	expression tag	UNP A0A0A0RDR2
A	14	CYS	-	expression tag	UNP A0A0A0RDR2
A	15	GLY	-	expression tag	UNP A0A0A0RDR2
A	16	ASP	-	expression tag	UNP A0A0A0RDR2
A	17	MET	-	expression tag	UNP A0A0A0RDR2
A	196	LYS	GLY	cloning artifact	UNP A0A0A0RDR2
A	313	SER	THR	engineered mutation	UNP A0A0A0RDR2
B	12	GLY	-	expression tag	UNP A0A0A0RDR2
B	13	GLU	-	expression tag	UNP A0A0A0RDR2
B	14	CYS	-	expression tag	UNP A0A0A0RDR2
B	15	GLY	-	expression tag	UNP A0A0A0RDR2
B	16	ASP	-	expression tag	UNP A0A0A0RDR2
B	17	MET	-	expression tag	UNP A0A0A0RDR2
B	196	LYS	GLY	cloning artifact	UNP A0A0A0RDR2
B	313	SER	THR	engineered mutation	UNP A0A0A0RDR2
C	12	GLY	-	expression tag	UNP A0A0A0RDR2
C	13	GLU	-	expression tag	UNP A0A0A0RDR2
C	14	CYS	-	expression tag	UNP A0A0A0RDR2
C	15	GLY	-	expression tag	UNP A0A0A0RDR2
C	16	ASP	-	expression tag	UNP A0A0A0RDR2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	17	MET	-	expression tag	UNP A0A0A0RDR2
C	196	LYS	GLY	cloning artifact	UNP A0A0A0RDR2
C	313	SER	THR	engineered mutation	UNP A0A0A0RDR2
D	12	GLY	-	expression tag	UNP A0A0A0RDR2
D	13	GLU	-	expression tag	UNP A0A0A0RDR2
D	14	CYS	-	expression tag	UNP A0A0A0RDR2
D	15	GLY	-	expression tag	UNP A0A0A0RDR2
D	16	ASP	-	expression tag	UNP A0A0A0RDR2
D	17	MET	-	expression tag	UNP A0A0A0RDR2
D	196	LYS	GLY	cloning artifact	UNP A0A0A0RDR2
D	313	SER	THR	engineered mutation	UNP A0A0A0RDR2

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

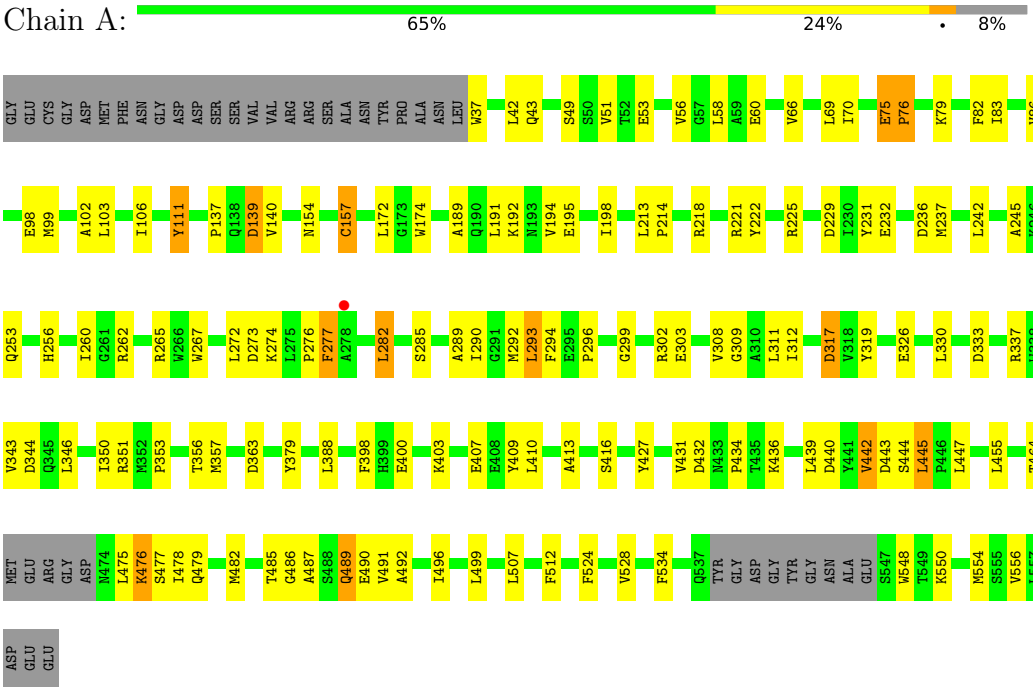
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0

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.

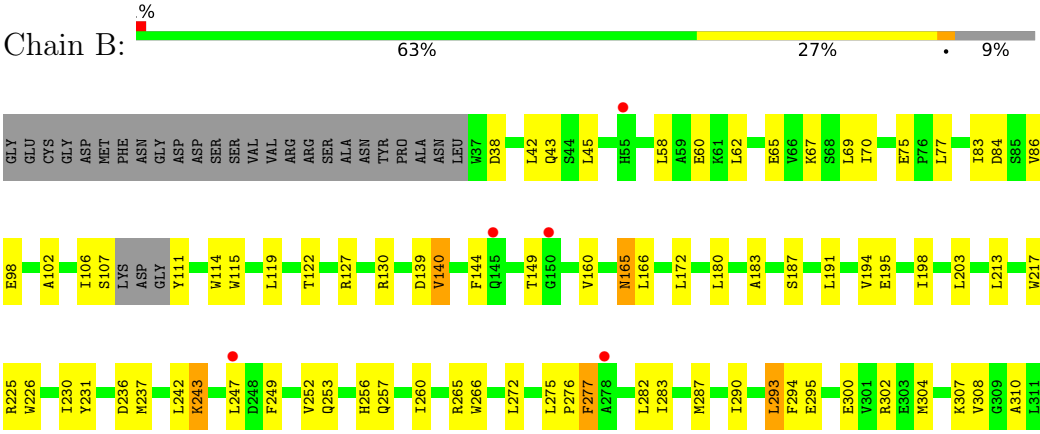
• Molecule 1: Sesquisabinene B synthase 1

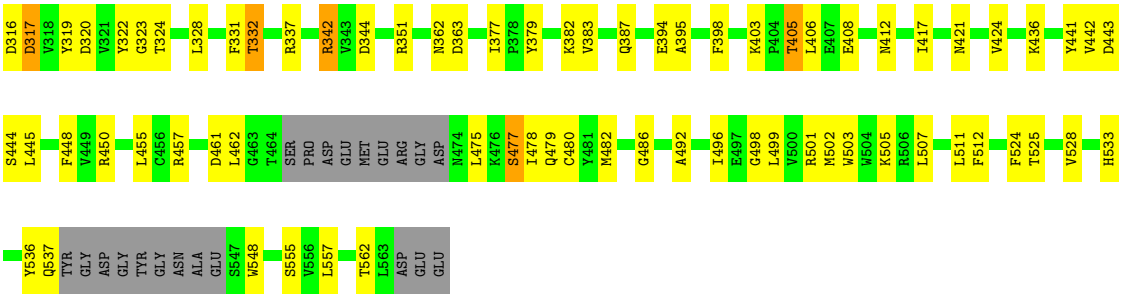
Chain A:



• Molecule 1: Sesquisabinene B synthase 1

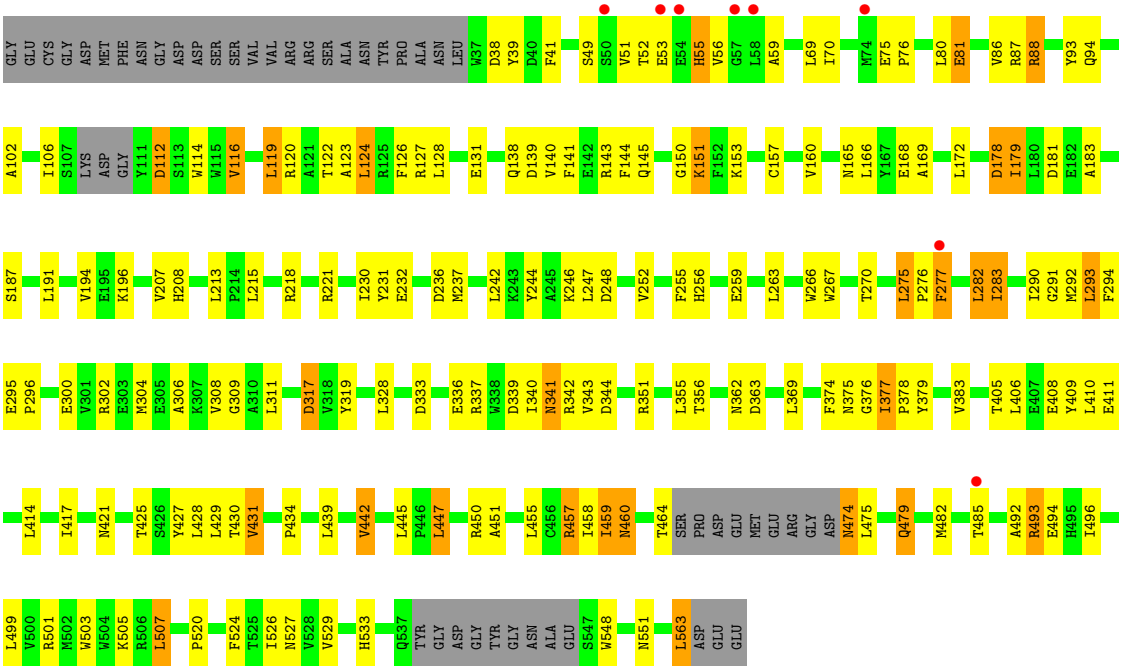
Chain B:





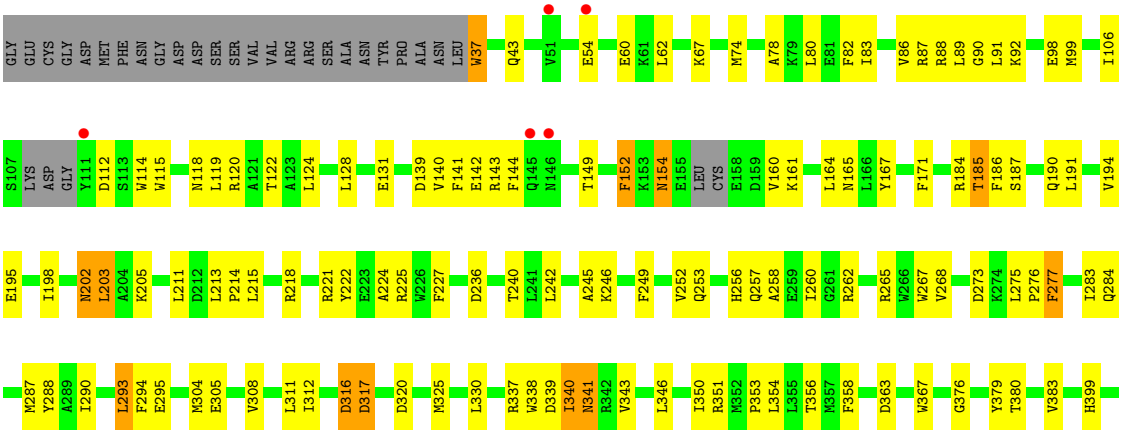
• Molecule 1: Sesquisabinene B synthase 1

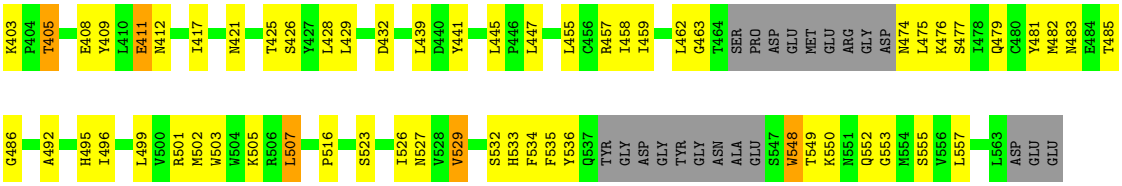
Chain C:



• Molecule 1: Sesquisabinene B synthase 1

Chain D:




K403 P404 T405 E408 Y409 L410 E411 N412 I417 N421 T425 S426 Y427 L428 L429 D432 L439 D440 Y441 L445 P446 L447 L455 C456 R457 I458 I459 L462 G463 T464 SER PRO ASP GLU MET GLU ARG GLY ASP N474 L475 K476 S477 I478 Q479 C480 Y481 M482 N483 E484 T485
G486 A492 H495 I496 L499 V500 R501 M502 W503 W504 K505 R506 L507 P516 S523 I526 N527 V528 V529 S532 H533 F534 F535 Y536 Q537 TYR GLY ASP GLY TYR GLY ASN ALA GLU S547 W548 T549 K550 N551 Q552 G553 M554 S555 V556 L557 L563 ASP GLU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	81.88Å 82.06Å 136.83Å 99.77° 91.55° 119.78°	Depositor
Resolution (Å)	45.62 – 3.41 45.62 – 3.41	Depositor EDS
% Data completeness (in resolution range)	98.4 (45.62-3.41) 98.4 (45.62-3.41)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.219 , 0.283 0.219 , 0.283	Depositor DCC
R_{free} test set	2163 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.084 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	16432	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: MG

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	0.55	0/4232	0.69	0/5739
1	B	0.55	0/4207	0.69	0/5705
1	C	0.54	0/4210	0.72	0/5709
1	D	0.58	0/4182	0.71	0/5672
All	All	0.55	0/16831	0.70	0/22825

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	4129	0	4028	100	0
1	B	4105	0	4003	110	0
1	C	4108	0	4007	198	0
1	D	4082	0	3970	161	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
All	All	16432	0	16008	567	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 17.

All (567) 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:C:255:PHE:CD2	1:C:296:PRO:HB3	1.52	1.42
1:C:255:PHE:CE2	1:C:296:PRO:HB3	1.70	1.25
1:C:417:ILE:HD13	1:C:457:ARG:HH21	1.09	1.15
1:D:288:TYR:CE2	1:D:535:PHE:CE2	2.35	1.13
1:D:305:GLU:OE2	1:D:426:SER:HB3	1.48	1.13
1:B:312:ILE:HG12	1:B:387:GLN:HE22	1.10	1.08
1:C:112:ASP:HB3	1:C:114:TRP:NE1	1.70	1.04
1:C:362:ASN:HA	1:C:377:ILE:HD13	1.39	1.02
1:C:417:ILE:CD1	1:C:457:ARG:HH21	1.74	1.01
1:C:124:LEU:CD1	1:C:128:LEU:CD1	2.37	1.01
1:C:124:LEU:HD11	1:C:128:LEU:HD11	1.43	1.00
1:D:288:TYR:CE2	1:D:535:PHE:CD2	2.51	0.99
1:C:417:ILE:HD13	1:C:457:ARG:NH2	1.80	0.97
1:C:255:PHE:CD2	1:C:296:PRO:CB	2.47	0.96
1:D:119:LEU:HB2	1:D:144:PHE:CD1	2.00	0.96
1:C:124:LEU:HD11	1:C:128:LEU:CD1	1.97	0.94
1:C:417:ILE:HD13	1:C:457:ARG:HD3	1.48	0.94
1:B:221:ARG:CZ	1:B:249:PHE:HE2	1.79	0.94
1:C:255:PHE:HD2	1:C:296:PRO:HB3	1.17	0.93
1:C:383:VAL:CG1	1:C:421:ASN:HA	1.98	0.93
1:A:292:MET:HG3	1:A:528:VAL:HG12	1.48	0.93
1:C:124:LEU:HD12	1:C:128:LEU:CD1	2.00	0.92
1:C:112:ASP:CB	1:C:114:TRP:HE1	1.80	0.92
1:B:293:LEU:H	1:B:293:LEU:HD12	1.33	0.92
1:B:221:ARG:CZ	1:B:249:PHE:CE2	2.52	0.91
1:C:255:PHE:CE2	1:C:296:PRO:CB	2.52	0.91
1:C:88:ARG:HH11	1:C:88:ARG:HB3	1.36	0.91
1:C:124:LEU:HD12	1:C:128:LEU:HD13	1.53	0.90
1:C:112:ASP:CB	1:C:114:TRP:NE1	2.35	0.89
1:C:124:LEU:CD1	1:C:128:LEU:HD13	2.03	0.88
1:B:319:TYR:OH	1:B:332:THR:HG22	1.74	0.88
1:D:160:VAL:HG11	1:D:203:LEU:HD23	1.56	0.88
1:C:383:VAL:HG13	1:C:421:ASN:HA	1.55	0.87
1:C:496:ILE:HA	1:C:499:LEU:HD12	1.57	0.86
1:C:417:ILE:CD1	1:C:457:ARG:NH2	2.37	0.85
1:C:112:ASP:OD1	1:C:114:TRP:CD1	2.29	0.85
1:C:119:LEU:HB3	1:C:144:PHE:CD1	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:TRP:HE1	1:A:42:LEU:HD21	1.42	0.84
1:C:116:VAL:HG23	1:C:143:ARG:CZ	2.07	0.84
1:C:283:ILE:HD12	1:C:283:ILE:O	1.78	0.83
1:B:277:PHE:HE2	1:B:322:TYR:CD1	1.96	0.83
1:C:119:LEU:CB	1:C:144:PHE:CE1	2.62	0.83
1:D:288:TYR:CZ	1:D:535:PHE:CD2	2.67	0.83
1:A:256:HIS:CE1	1:A:290:ILE:CD1	2.64	0.81
1:D:447:LEU:HD12	1:D:447:LEU:O	1.81	0.81
1:A:293:LEU:HD12	1:A:293:LEU:H	1.44	0.81
1:D:154:ASN:O	1:D:154:ASN:ND2	2.12	0.81
1:C:116:VAL:HG23	1:C:143:ARG:NE	1.97	0.80
1:C:52:THR:H	1:C:55:HIS:CD2	1.99	0.80
1:D:119:LEU:N	1:D:144:PHE:HE1	1.80	0.80
1:C:116:VAL:HG23	1:C:143:ARG:NH1	1.97	0.79
1:C:166:LEU:HD23	1:C:187:SER:HB3	1.63	0.79
1:D:441:TYR:HE2	1:D:516:PRO:HG3	1.48	0.79
1:B:243:LYS:HE2	1:B:243:LYS:HA	1.63	0.79
1:C:362:ASN:HA	1:C:377:ILE:CD1	2.11	0.79
1:A:447:LEU:O	1:A:447:LEU:HD12	1.81	0.78
1:D:293:LEU:N	1:D:293:LEU:HD12	1.99	0.78
1:D:496:ILE:HA	1:D:499:LEU:HD12	1.66	0.77
1:C:119:LEU:HB3	1:C:144:PHE:CE1	2.18	0.77
1:A:256:HIS:ND1	1:A:290:ILE:CD1	2.47	0.76
1:D:305:GLU:OE2	1:D:426:SER:CB	2.31	0.76
1:C:112:ASP:HB3	1:C:114:TRP:CD1	2.19	0.76
1:D:288:TYR:CD2	1:D:535:PHE:CE2	2.74	0.75
1:C:459:ILE:HD13	1:C:533:HIS:CE1	2.21	0.75
1:D:459:ILE:HD13	1:D:533:HIS:CE1	2.21	0.75
1:D:479:GLN:N	1:D:479:GLN:OE1	2.19	0.75
1:A:292:MET:HG3	1:A:528:VAL:CG1	2.18	0.74
1:C:112:ASP:CG	1:C:114:TRP:HE1	1.90	0.74
1:B:221:ARG:NH2	1:B:249:PHE:CE2	2.56	0.74
1:C:124:LEU:CD1	1:C:128:LEU:HD11	2.12	0.74
1:C:232:GLU:HG2	1:C:242:LEU:HD21	1.69	0.73
1:B:312:ILE:HG12	1:B:387:GLN:NE2	1.96	0.72
1:C:344:ASP:OD1	1:C:351:ARG:NH2	2.23	0.71
1:A:311:LEU:HD21	1:A:356:THR:HG22	1.73	0.71
1:C:126:PHE:HD2	1:C:169:ALA:HB1	1.55	0.71
1:C:255:PHE:HD2	1:C:296:PRO:CB	1.94	0.71
1:C:479:GLN:N	1:C:479:GLN:OE1	2.24	0.70
1:D:256:HIS:CE1	1:D:290:ILE:HD12	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:PHE:HE2	1:C:296:PRO:CB	2.05	0.70
1:C:383:VAL:CG1	1:C:421:ASN:CG	2.60	0.70
1:A:66:VAL:HA	1:A:69:LEU:HD12	1.72	0.70
1:C:383:VAL:HG11	1:C:421:ASN:HA	1.72	0.70
1:C:119:LEU:CB	1:C:144:PHE:CD1	2.74	0.70
1:C:427:TYR:CD2	1:C:442:VAL:HG21	2.27	0.70
1:D:277:PHE:HB3	1:D:317:ASP:HB3	1.74	0.69
1:C:127:ARG:HG2	1:C:172:LEU:HD23	1.74	0.69
1:A:256:HIS:ND1	1:A:290:ILE:HD11	2.08	0.69
1:C:383:VAL:HG13	1:C:421:ASN:CA	2.22	0.69
1:D:119:LEU:N	1:D:144:PHE:CE1	2.61	0.68
1:B:293:LEU:HD12	1:B:293:LEU:N	2.00	0.68
1:C:383:VAL:HG11	1:C:421:ASN:OD1	1.94	0.67
1:B:424:VAL:HG22	1:B:442:VAL:HG13	1.75	0.67
1:D:160:VAL:HG11	1:D:203:LEU:CD2	2.23	0.67
1:C:417:ILE:HD13	1:C:457:ARG:CD	2.24	0.67
1:D:283:ILE:O	1:D:287:MET:HG3	1.95	0.67
1:B:293:LEU:O	1:B:302:ARG:NH1	2.26	0.67
1:B:457:ARG:NH2	1:B:461:ASP:OD1	2.22	0.67
1:C:341:ASN:OD1	1:C:341:ASN:N	2.29	0.66
1:A:326:GLU:HB2	1:C:196:LYS:HB3	1.77	0.66
1:D:293:LEU:HD12	1:D:293:LEU:H	1.60	0.66
1:A:262:ARG:NH1	1:A:303:GLU:OE2	2.27	0.66
1:C:116:VAL:CG2	1:C:143:ARG:CZ	2.74	0.66
1:C:383:VAL:CG1	1:C:421:ASN:CA	2.73	0.66
1:A:400:GLU:HG3	1:C:208:HIS:NE2	2.10	0.66
1:C:116:VAL:CG2	1:C:143:ARG:NE	2.59	0.66
1:D:459:ILE:CD1	1:D:533:HIS:CE1	2.78	0.66
1:C:246:LYS:HB3	1:C:563:LEU:HD11	1.77	0.65
1:A:427:TYR:CD2	1:A:442:VAL:HG21	2.31	0.65
1:B:119:LEU:HA	1:B:122:THR:HB	1.77	0.65
1:B:127:ARG:HG3	1:B:172:LEU:HD23	1.79	0.65
1:D:534:PHE:CE2	1:D:548:TRP:HH2	2.15	0.65
1:C:213:LEU:HB2	1:C:218:ARG:CZ	2.27	0.64
1:C:259:GLU:OE2	1:C:302:ARG:NH2	2.24	0.64
1:C:459:ILE:CD1	1:C:533:HIS:CE1	2.80	0.64
1:C:275:LEU:N	1:C:275:LEU:HD23	2.12	0.64
1:D:293:LEU:HD13	1:D:293:LEU:O	1.97	0.64
1:D:119:LEU:HB2	1:D:144:PHE:CE1	2.33	0.64
1:D:441:TYR:CE2	1:D:516:PRO:HG3	2.31	0.64
1:D:119:LEU:CA	1:D:144:PHE:CE1	2.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:481:TYR:O	1:D:485:THR:HG22	1.99	0.63
1:B:225:ARG:HD3	1:B:249:PHE:CE1	2.34	0.62
1:B:496:ILE:HA	1:B:499:LEU:HD12	1.82	0.62
1:A:285:SER:OG	1:A:309:GLY:C	2.37	0.62
1:D:312:ILE:O	1:D:316:ASP:HB2	1.99	0.62
1:C:526:ILE:O	1:C:529:VAL:HG22	1.98	0.62
1:C:126:PHE:CD2	1:C:169:ALA:HB1	2.34	0.62
1:B:304:MET:O	1:B:308:VAL:HG23	1.99	0.62
1:D:379:TYR:CE1	1:D:439:LEU:HB3	2.35	0.61
1:B:195:GLU:HA	1:B:198:ILE:HD12	1.82	0.61
1:C:405:THR:HG23	1:C:408:GLU:H	1.64	0.61
1:C:295:GLU:N	1:C:295:GLU:OE1	2.31	0.61
1:A:476:LYS:HD2	1:A:479:GLN:HG3	1.83	0.61
1:B:243:LYS:HA	1:B:243:LYS:CE	2.25	0.61
1:A:482:MET:O	1:A:486:GLY:N	2.28	0.61
1:D:202:ASN:OD1	1:D:202:ASN:N	2.18	0.61
1:A:407:GLU:OE1	1:A:407:GLU:N	2.32	0.61
1:D:83:ILE:HG23	1:D:99:MET:HE3	1.81	0.61
1:D:195:GLU:HA	1:D:198:ILE:HD12	1.81	0.60
1:A:253:GLN:NE2	1:A:556:VAL:O	2.32	0.60
1:C:119:LEU:C	1:C:119:LEU:HD23	2.22	0.60
1:D:455:LEU:O	1:D:459:ILE:HG13	2.01	0.60
1:B:455:LEU:HD21	1:B:503:TRP:HB2	1.84	0.60
1:D:325:MET:SD	1:D:399:HIS:NE2	2.75	0.59
1:A:256:HIS:CE1	1:A:290:ILE:HD12	2.37	0.59
1:B:166:LEU:HD23	1:B:187:SER:HB3	1.84	0.59
1:B:405:THR:HG23	1:B:408:GLU:HB2	1.84	0.59
1:C:38:ASP:OD1	1:C:39:TYR:N	2.35	0.59
1:B:107:SER:O	1:B:111:TYR:OH	2.20	0.59
1:A:232:GLU:HG2	1:A:242:LEU:HD21	1.85	0.59
1:A:267:TRP:HB2	1:A:282:LEU:HD13	1.84	0.59
1:C:383:VAL:CG1	1:C:421:ASN:OD1	2.50	0.59
1:D:242:LEU:HD11	1:D:246:LYS:HE3	1.84	0.58
1:C:455:LEU:O	1:C:459:ILE:HG13	2.02	0.58
1:C:474:ASN:O	1:C:479:GLN:HG2	2.04	0.58
1:C:112:ASP:OD1	1:C:114:TRP:HD1	1.83	0.58
1:D:87:ARG:NH1	1:D:131:GLU:OE2	2.36	0.58
1:D:152:PHE:CD1	1:D:186:PHE:CD1	2.92	0.58
1:B:394:GLU:HG3	1:B:412:ASN:ND2	2.19	0.58
1:B:482:MET:O	1:B:486:GLY:N	2.32	0.58
1:D:284:GLN:O	1:D:288:TYR:CD2	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ARG:CZ	1:B:249:PHE:CD2	2.86	0.58
1:B:323:GLY:HA3	1:B:328:LEU:HD21	1.84	0.58
1:D:139:ASP:O	1:D:142:GLU:HB2	2.03	0.58
1:D:275:LEU:HB3	1:D:276:PRO:HD2	1.86	0.58
1:D:144:PHE:CD2	1:D:144:PHE:N	2.72	0.58
1:D:459:ILE:HD13	1:D:533:HIS:ND1	2.19	0.58
1:A:252:VAL:HG23	1:A:296:PRO:HG3	1.86	0.57
1:C:116:VAL:HG23	1:C:143:ARG:HE	1.68	0.57
1:C:145:GLN:HG2	1:C:151:LYS:O	2.04	0.57
1:C:263:LEU:O	1:C:266:TRP:HB3	2.04	0.57
1:B:479:GLN:N	1:B:479:GLN:OE1	2.36	0.57
1:D:288:TYR:HE2	1:D:535:PHE:CE2	2.14	0.57
1:D:288:TYR:CE2	1:D:535:PHE:HE2	2.14	0.57
1:B:344:ASP:OD1	1:B:351:ARG:NH2	2.38	0.57
1:C:232:GLU:HG2	1:C:242:LEU:CD2	2.32	0.57
1:A:231:TYR:O	1:A:237:MET:HG3	2.05	0.56
1:A:293:LEU:HD13	1:A:302:ARG:HB2	1.87	0.56
1:C:337:ARG:HD2	1:C:342:ARG:HH12	1.70	0.56
1:D:455:LEU:HD21	1:D:503:TRP:HB2	1.86	0.56
1:D:340:ILE:HD13	1:D:358:PHE:CE2	2.39	0.56
1:B:58:LEU:HG	1:B:247:LEU:HD11	1.87	0.56
1:C:122:THR:HG21	1:C:144:PHE:CE2	2.40	0.56
1:C:430:THR:HG21	1:C:524:PHE:HE2	1.69	0.56
1:D:463:GLY:HA3	1:D:536:TYR:HB3	1.86	0.56
1:A:75:GLU:HG2	1:A:76:PRO:HD2	1.87	0.56
1:C:231:TYR:CE2	1:C:237:MET:HG2	2.41	0.56
1:C:374:PHE:CZ	1:C:379:TYR:HE2	2.24	0.56
1:A:43:GLN:HG2	1:A:265:ARG:HG2	1.88	0.56
1:D:311:LEU:HD21	1:D:356:THR:HG22	1.87	0.56
1:B:445:LEU:HB3	1:B:450:ARG:HB2	1.87	0.56
1:A:191:LEU:HA	1:A:194:VAL:HG12	1.88	0.55
1:C:383:VAL:HG13	1:C:421:ASN:CB	2.36	0.55
1:A:496:ILE:HA	1:A:499:LEU:HD12	1.89	0.55
1:B:256:HIS:CE1	1:B:290:ILE:HD12	2.42	0.55
1:D:441:TYR:HE2	1:D:516:PRO:CG	2.17	0.55
1:D:144:PHE:H	1:D:144:PHE:HD2	1.55	0.55
1:C:112:ASP:OD1	1:C:114:TRP:NE1	2.40	0.55
1:D:475:LEU:N	1:D:475:LEU:HD12	2.21	0.55
1:C:166:LEU:HD11	1:C:183:ALA:HB1	1.88	0.55
1:B:122:THR:HG23	1:B:140:VAL:HG23	1.89	0.55
1:A:256:HIS:ND1	1:A:290:ILE:HD12	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:VAL:HB	1:B:421:ASN:HA	1.89	0.55
1:D:67:LYS:HE3	1:D:98:GLU:OE1	2.07	0.55
1:B:75:GLU:OE2	1:B:77:LEU:HB3	2.06	0.55
1:C:119:LEU:HA	1:C:122:THR:HB	1.89	0.55
1:C:383:VAL:CG1	1:C:421:ASN:CB	2.85	0.55
1:A:189:ALA:HA	1:A:192:LYS:HD2	1.89	0.54
1:B:221:ARG:NE	1:B:249:PHE:HE2	2.05	0.54
1:C:112:ASP:CG	1:C:114:TRP:NE1	2.57	0.54
1:A:69:LEU:O	1:A:79:LYS:HE3	2.07	0.54
1:B:382:LYS:NZ	1:B:443:ASP:OD1	2.40	0.54
1:C:116:VAL:HG23	1:C:143:ARG:HH11	1.71	0.54
1:C:221:ARG:HG2	1:C:290:ILE:CG2	2.37	0.54
1:D:253:GLN:O	1:D:257:GLN:HG3	2.08	0.54
1:B:441:TYR:O	1:B:444:SER:OG	2.20	0.54
1:A:53:GLU:HA	1:A:56:VAL:HG22	1.90	0.54
1:C:409:TYR:CD2	1:C:410:LEU:HD23	2.42	0.54
1:C:417:ILE:CD1	1:C:457:ARG:HD3	2.31	0.54
1:D:256:HIS:CE1	1:D:290:ILE:CD1	2.90	0.54
1:D:268:VAL:HA	1:D:273:ASP:OD1	2.08	0.54
1:C:276:PRO:HG2	1:C:277:PHE:CD2	2.43	0.53
1:C:455:LEU:O	1:C:459:ILE:CG1	2.56	0.53
1:A:195:GLU:HA	1:A:198:ILE:HD12	1.90	0.53
1:C:160:VAL:HG22	1:C:194:VAL:HG21	1.90	0.53
1:C:76:PRO:HB2	1:C:114:TRP:CE3	2.44	0.53
1:A:221:ARG:NH2	1:A:252:VAL:HG13	2.24	0.53
1:C:267:TRP:HB2	1:C:282:LEU:HD13	1.90	0.53
1:A:299:GLY:O	1:A:303:GLU:HG3	2.09	0.53
1:B:119:LEU:HB2	1:B:144:PHE:CD1	2.43	0.53
1:A:93:TYR:OH	1:A:248:ASP:OD2	2.20	0.53
1:B:272:LEU:HA	1:B:275:LEU:HG	1.90	0.53
1:B:130:ARG:HA	1:B:512:PHE:HZ	1.74	0.53
1:B:479:GLN:HA	1:B:482:MET:HE2	1.91	0.53
1:A:49:SER:OG	1:A:51:VAL:HG22	2.08	0.53
1:D:462:LEU:HD21	1:D:496:ILE:CG2	2.39	0.53
1:B:114:TRP:CE3	1:B:115:TRP:HB3	2.43	0.52
1:D:350:ILE:C	1:D:353:PRO:HD2	2.29	0.52
1:C:291:GLY:O	1:C:527:ASN:HB3	2.09	0.52
1:C:122:THR:HG23	1:C:140:VAL:HG12	1.90	0.52
1:C:119:LEU:HB2	1:C:144:PHE:CE1	2.43	0.52
1:C:427:TYR:CZ	1:C:431:VAL:CG2	2.93	0.52
1:A:256:HIS:O	1:A:260:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:THR:HG21	1:C:144:PHE:HE2	1.74	0.52
1:D:354:LEU:HD23	1:D:354:LEU:O	2.09	0.52
1:C:292:MET:HG2	1:C:293:LEU:HG	1.91	0.52
1:D:425:THR:O	1:D:429:LEU:HG	2.08	0.52
1:C:191:LEU:HA	1:C:194:VAL:HG12	1.92	0.52
1:D:82:PHE:O	1:D:86:VAL:HG13	2.10	0.52
1:C:141:PHE:HB2	1:C:179:ILE:CD1	2.40	0.51
1:C:417:ILE:HD12	1:C:457:ARG:NH2	2.24	0.51
1:D:83:ILE:O	1:D:86:VAL:HG22	2.10	0.51
1:D:122:THR:HG22	1:D:141:PHE:HE1	1.74	0.51
1:D:288:TYR:CZ	1:D:535:PHE:HD2	2.26	0.51
1:A:277:PHE:HB3	1:A:317:ASP:HB2	1.93	0.51
1:C:362:ASN:O	1:C:377:ILE:HD11	2.09	0.51
1:C:479:GLN:HA	1:C:482:MET:HE2	1.93	0.51
1:D:304:MET:HE1	1:D:367:TRP:CD2	2.45	0.51
1:A:37:TRP:NE1	1:A:42:LEU:HD21	2.19	0.51
1:A:308:VAL:O	1:A:312:ILE:HG13	2.11	0.51
1:C:87:ARG:NH1	1:C:131:GLU:OE2	2.44	0.51
1:A:293:LEU:HD12	1:A:293:LEU:N	2.13	0.51
1:A:341:ASN:N	1:A:341:ASN:OD1	2.43	0.51
1:B:221:ARG:NH1	1:B:249:PHE:CD2	2.79	0.51
1:B:395:ALA:O	1:B:398:PHE:HB3	2.11	0.51
1:D:89:LEU:O	1:D:224:ALA:HB1	2.11	0.51
1:D:167:TYR:HB2	1:D:187:SER:HB2	1.92	0.51
1:B:379:TYR:O	1:B:383:VAL:HG22	2.11	0.51
1:D:376:GLY:HA3	1:D:428:LEU:HD21	1.93	0.51
1:A:294:PHE:CD1	1:A:294:PHE:C	2.85	0.50
1:C:383:VAL:HG12	1:C:421:ASN:CG	2.31	0.50
1:D:186:PHE:CE1	1:D:190:GLN:HG3	2.46	0.50
1:D:379:TYR:O	1:D:383:VAL:HG22	2.11	0.50
1:B:122:THR:HG23	1:B:140:VAL:CG2	2.42	0.50
1:B:282:LEU:HD12	1:B:310:ALA:HB2	1.94	0.50
1:B:194:VAL:O	1:B:198:ILE:HG13	2.11	0.50
1:B:492:ALA:O	1:B:496:ILE:HG12	2.10	0.50
1:D:164:LEU:HD23	1:D:191:LEU:HD13	1.93	0.50
1:D:221:ARG:NH2	1:D:252:VAL:HG12	2.27	0.50
1:D:383:VAL:HB	1:D:421:ASN:HA	1.93	0.50
1:D:89:LEU:HD13	1:D:245:ALA:HB2	1.94	0.50
1:D:534:PHE:CE2	1:D:548:TRP:CH2	2.97	0.50
1:A:333:ASP:OD1	1:A:337:ARG:NH1	2.43	0.50
1:C:80:LEU:HD22	1:C:128:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ALA:O	1:C:106:ILE:HG13	2.12	0.50
1:D:164:LEU:HA	1:D:191:LEU:HD11	1.94	0.50
1:C:294:PHE:C	1:C:294:PHE:CD1	2.85	0.50
1:D:160:VAL:CG1	1:D:203:LEU:CD2	2.89	0.50
1:A:214:PRO:O	1:A:218:ARG:HG3	2.12	0.50
1:B:524:PHE:O	1:B:528:VAL:HG13	2.12	0.50
1:A:137:PRO:HB2	1:A:139:ASP:OD1	2.11	0.49
1:B:236:ASP:OD1	1:B:236:ASP:N	2.45	0.49
1:B:276:PRO:HG2	1:B:277:PHE:CE2	2.47	0.49
1:C:49:SER:OG	1:C:51:VAL:HG22	2.12	0.49
1:D:376:GLY:O	1:D:380:THR:HG23	2.12	0.49
1:D:43:GLN:O	1:D:265:ARG:NH1	2.45	0.49
1:D:119:LEU:HB2	1:D:144:PHE:HD1	1.67	0.49
1:D:341:ASN:OD1	1:D:341:ASN:N	2.44	0.49
1:D:346:LEU:O	1:D:351:ARG:NH1	2.45	0.49
1:C:340:ILE:O	1:C:343:VAL:HG22	2.12	0.49
1:D:405:THR:HG23	1:D:408:GLU:HB2	1.94	0.49
1:A:344:ASP:OD1	1:A:351:ARG:NH2	2.45	0.49
1:D:222:TYR:OH	1:D:287:MET:O	2.26	0.49
1:D:276:PRO:HG2	1:D:277:PHE:CD2	2.48	0.49
1:D:277:PHE:CB	1:D:317:ASP:HB3	2.40	0.49
1:B:43:GLN:HG2	1:B:265:ARG:HG3	1.93	0.49
1:A:82:PHE:O	1:A:86:VAL:HG23	2.13	0.49
1:B:226:TRP:CZ2	1:B:230:ILE:HD12	2.48	0.49
1:B:294:PHE:CD1	1:B:294:PHE:C	2.85	0.49
1:D:277:PHE:CB	1:D:317:ASP:CB	2.91	0.49
1:D:409:TYR:HE2	1:D:477:SER:HG	1.58	0.49
1:B:83:ILE:O	1:B:86:VAL:HG12	2.13	0.49
1:B:293:LEU:O	1:B:293:LEU:HD13	2.12	0.49
1:C:93:TYR:CE1	1:C:94:GLN:HG2	2.48	0.49
1:C:277:PHE:HB3	1:C:317:ASP:CB	2.43	0.49
1:C:451:ALA:HB1	1:C:507:LEU:HD22	1.94	0.49
1:B:362:ASN:HA	1:B:377:ILE:HG12	1.95	0.48
1:C:236:ASP:OD1	1:C:236:ASP:N	2.44	0.48
1:A:319:TYR:CE1	1:A:388:LEU:HD22	2.49	0.48
1:C:266:TRP:O	1:C:270:THR:HG23	2.13	0.48
1:C:300:GLU:O	1:C:304:MET:HE3	2.14	0.48
1:C:319:TYR:HA	1:C:328:LEU:HD13	1.95	0.48
1:C:427:TYR:CE2	1:C:431:VAL:HG21	2.48	0.48
1:C:455:LEU:HD12	1:C:507:LEU:HD23	1.94	0.48
1:D:258:ALA:HB1	1:D:262:ARG:HH22	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:HB2	1:A:218:ARG:NH1	2.29	0.48
1:A:492:ALA:O	1:A:496:ILE:HG12	2.13	0.48
1:B:266:TRP:CD1	1:B:307:LYS:HE2	2.48	0.48
1:A:221:ARG:HH22	1:A:252:VAL:HG13	1.77	0.48
1:A:379:TYR:CE1	1:A:439:LEU:HB3	2.49	0.48
1:B:478:ILE:HD12	1:B:478:ILE:H	1.78	0.48
1:C:119:LEU:CA	1:C:144:PHE:CE1	2.97	0.48
1:C:427:TYR:CZ	1:C:431:VAL:HG21	2.49	0.48
1:C:447:LEU:O	1:C:447:LEU:HG	2.13	0.48
1:D:74:MET:HE1	1:D:78:ALA:O	2.14	0.48
1:B:221:ARG:NH1	1:B:249:PHE:HD2	2.12	0.48
1:C:53:GLU:HA	1:C:56:VAL:HB	1.95	0.48
1:C:70:ILE:HD11	1:C:86:VAL:HG21	1.95	0.48
1:B:45:LEU:HD22	1:B:257:GLN:HB3	1.96	0.48
1:B:93:TYR:CE2	1:B:94:GLN:HG2	2.49	0.48
1:C:377:ILE:N	1:C:378:PRO:CD	2.77	0.48
1:D:83:ILE:CG2	1:D:99:MET:HE3	2.44	0.48
1:D:277:PHE:HB3	1:D:317:ASP:CB	2.43	0.47
1:D:548:TRP:CZ2	1:D:552:GLN:HG3	2.49	0.47
1:A:267:TRP:CZ3	1:A:272:LEU:HD12	2.49	0.47
1:A:477:SER:HB3	1:A:496:ILE:HD12	1.96	0.47
1:C:277:PHE:HB3	1:C:317:ASP:HB3	1.95	0.47
1:C:409:TYR:HD2	1:C:410:LEU:HD23	1.79	0.47
1:C:492:ALA:O	1:C:496:ILE:HG12	2.14	0.47
1:D:37:TRP:CD2	1:D:37:TRP:N	2.82	0.47
1:B:260:ILE:HD11	1:B:557:LEU:HD13	1.97	0.47
1:D:225:ARG:HD3	1:D:249:PHE:CZ	2.50	0.47
1:D:523:SER:O	1:D:527:ASN:ND2	2.48	0.47
1:B:213:LEU:HB2	1:B:218:ARG:NH1	2.30	0.47
1:B:252:VAL:O	1:B:256:HIS:HD2	1.98	0.47
1:C:122:THR:CG2	1:C:140:VAL:HG12	2.45	0.47
1:C:319:TYR:HA	1:C:328:LEU:CD1	2.45	0.47
1:C:376:GLY:HA3	1:C:428:LEU:HD21	1.97	0.47
1:D:88:ARG:HG2	1:D:227:PHE:CD1	2.48	0.47
1:D:89:LEU:HD22	1:D:245:ALA:HB1	1.97	0.47
1:D:526:ILE:O	1:D:529:VAL:HG23	2.15	0.47
1:A:276:PRO:HG2	1:A:277:PHE:CE2	2.49	0.47
1:C:333:ASP:HA	1:C:336:GLU:HB2	1.97	0.47
1:C:293:LEU:HD23	1:C:524:PHE:CZ	2.50	0.47
1:D:260:ILE:HD11	1:D:557:LEU:HD22	1.97	0.47
1:A:427:TYR:CE2	1:A:442:VAL:HG21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ARG:HG2	1:C:290:ILE:HG21	1.96	0.46
1:C:383:VAL:HG11	1:C:421:ASN:CA	2.42	0.46
1:D:350:ILE:O	1:D:353:PRO:HD2	2.14	0.46
1:A:409:TYR:CD2	1:A:410:LEU:HD23	2.50	0.46
1:C:88:ARG:HB3	1:C:88:ARG:NH1	2.18	0.46
1:C:244:TYR:HA	1:C:247:LEU:HD12	1.98	0.46
1:D:479:GLN:HA	1:D:482:MET:HE2	1.97	0.46
1:A:221:ARG:HH12	1:A:252:VAL:HG11	1.80	0.46
1:D:112:ASP:HB2	1:D:115:TRP:NE1	2.31	0.46
1:D:492:ALA:O	1:D:496:ILE:HG12	2.16	0.46
1:B:461:ASP:OD2	1:B:477:SER:HB2	2.16	0.46
1:D:455:LEU:HD13	1:D:529:VAL:HG11	1.98	0.46
1:D:534:PHE:CZ	1:D:548:TRP:CZ2	3.04	0.46
1:C:127:ARG:HD2	1:C:131:GLU:OE2	2.16	0.46
1:C:337:ARG:CD	1:C:342:ARG:HH12	2.27	0.46
1:D:184:ARG:NH2	1:D:185:THR:HG23	2.30	0.46
1:A:344:ASP:HA	1:A:351:ARG:CZ	2.45	0.46
1:B:102:ALA:O	1:B:106:ILE:HG13	2.15	0.46
1:B:114:TRP:CE2	1:B:115:TRP:HD1	2.34	0.46
1:B:293:LEU:HD13	1:B:302:ARG:HB2	1.98	0.46
1:C:374:PHE:HB2	1:C:434:PRO:HG2	1.97	0.46
1:D:330:LEU:HD23	1:D:346:LEU:CD2	2.46	0.46
1:B:277:PHE:HB3	1:B:317:ASP:HB3	1.98	0.46
1:C:344:ASP:HA	1:C:351:ARG:CZ	2.46	0.46
1:A:252:VAL:O	1:A:256:HIS:CD2	2.69	0.46
1:D:482:MET:O	1:D:486:GLY:N	2.40	0.46
1:B:315:ILE:O	1:B:315:ILE:HG22	2.15	0.45
1:D:304:MET:CE	1:D:367:TRP:CD2	2.99	0.45
1:A:213:LEU:HB2	1:A:218:ARG:CZ	2.46	0.45
1:A:311:LEU:HD13	1:A:357:MET:HA	1.98	0.45
1:B:295:GLU:O	1:B:302:ARG:NH2	2.42	0.45
1:A:225:ARG:NH1	1:A:229:ASP:OD2	2.49	0.45
1:B:394:GLU:HG3	1:B:412:ASN:HD21	1.81	0.45
1:C:311:LEU:HD21	1:C:356:THR:HG22	1.98	0.45
1:D:459:ILE:HD11	1:D:533:HIS:CE1	2.50	0.45
1:C:145:GLN:NE2	1:C:150:GLY:O	2.49	0.45
1:D:194:VAL:O	1:D:198:ILE:HG13	2.16	0.45
1:A:58:LEU:HD23	1:A:247:LEU:HD11	1.98	0.45
1:B:62:LEU:HD12	1:B:247:LEU:HD12	1.98	0.45
1:B:294:PHE:CD1	1:B:294:PHE:O	2.70	0.45
1:D:119:LEU:CB	1:D:144:PHE:CE1	2.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:PHE:O	1:D:294:PHE:CD1	2.70	0.45
1:D:262:ARG:HG3	1:D:262:ARG:NH2	2.31	0.45
1:C:88:ARG:CZ	1:C:215:LEU:HD13	2.47	0.45
1:C:119:LEU:HB2	1:C:144:PHE:CD1	2.52	0.45
1:C:248:ASP:O	1:C:252:VAL:HG23	2.17	0.45
1:D:114:TRP:CE2	1:D:115:TRP:HD1	2.35	0.45
1:D:294:PHE:CD1	1:D:294:PHE:C	2.90	0.45
1:D:502:MET:O	1:D:505:LYS:HB2	2.17	0.45
1:A:154:ASN:O	1:A:157:CYS:HB3	2.17	0.45
1:C:119:LEU:HD23	1:C:120:ARG:N	2.32	0.45
1:A:478:ILE:O	1:A:482:MET:HG3	2.17	0.45
1:B:475:LEU:HB3	1:B:480:CYS:SG	2.57	0.45
1:C:460:ASN:C	1:C:460:ASN:ND2	2.71	0.45
1:D:119:LEU:HA	1:D:144:PHE:CE1	2.51	0.45
1:B:498:GLY:HA2	1:B:501:ARG:CZ	2.47	0.44
1:D:213:LEU:HB2	1:D:218:ARG:CZ	2.47	0.44
1:A:294:PHE:CD1	1:A:294:PHE:O	2.70	0.44
1:A:431:VAL:HG13	1:A:434:PRO:HG3	1.98	0.44
1:B:403:LYS:HG2	1:B:475:LEU:HD21	1.99	0.44
1:D:213:LEU:HB2	1:D:218:ARG:NH1	2.32	0.44
1:D:87:ARG:NH2	1:D:215:LEU:HG	2.33	0.44
1:A:174:TRP:HZ2	1:A:512:PHE:CD1	2.36	0.44
1:B:221:ARG:NH2	1:B:249:PHE:CD2	2.85	0.44
1:C:411:GLU:HA	1:C:414:LEU:HD23	1.98	0.44
1:D:120:ARG:NH2	1:D:161:LYS:HD2	2.32	0.44
1:C:127:ARG:HG3	1:C:169:ALA:HA	1.99	0.44
1:C:191:LEU:HD22	1:C:207:VAL:HG13	1.99	0.44
1:D:171:PHE:CE2	1:D:214:PRO:HB3	2.53	0.44
1:A:89:LEU:HD13	1:A:245:ALA:HB2	2.00	0.44
1:A:554:MET:SD	1:A:558:ILE:HD13	2.58	0.44
1:C:493:ARG:O	1:C:493:ARG:HG3	2.18	0.44
1:C:213:LEU:HD23	1:C:213:LEU:HA	1.82	0.44
1:C:427:TYR:CZ	1:C:431:VAL:HG23	2.53	0.44
1:A:37:TRP:HZ3	1:A:550:LYS:HA	1.83	0.44
1:A:256:HIS:CE1	1:A:290:ILE:HD13	2.49	0.44
1:C:304:MET:O	1:C:308:VAL:HG23	2.18	0.44
1:C:457:ARG:HD3	1:C:457:ARG:HA	1.81	0.44
1:D:417:ILE:HD13	1:D:457:ARG:CZ	2.48	0.44
1:B:70:ILE:HD11	1:B:86:VAL:HG21	1.98	0.43
1:B:191:LEU:HA	1:B:194:VAL:HG12	2.00	0.43
1:B:253:GLN:HG2	1:B:257:GLN:HE21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:MET:O	1:B:505:LYS:HB2	2.18	0.43
1:C:116:VAL:CG2	1:C:143:ARG:NH1	2.75	0.43
1:A:70:ILE:O	1:A:79:LYS:HE2	2.18	0.43
1:A:236:ASP:OD1	1:A:236:ASP:N	2.46	0.43
1:C:520:PRO:HB2	1:C:524:PHE:CZ	2.53	0.43
1:D:214:PRO:O	1:D:218:ARG:HG3	2.18	0.43
1:D:284:GLN:O	1:D:288:TYR:HD2	1.99	0.43
1:C:252:VAL:HG12	1:C:256:HIS:CE1	2.53	0.43
1:D:482:MET:HE2	1:D:482:MET:HB2	1.89	0.43
1:A:83:ILE:HD13	1:A:103:LEU:HG	2.00	0.43
1:C:112:ASP:CB	1:C:114:TRP:CD1	2.94	0.43
1:C:277:PHE:HB3	1:C:317:ASP:OD2	2.18	0.43
1:D:403:LYS:HE3	1:D:483:ASN:OD1	2.18	0.43
1:B:293:LEU:N	1:B:293:LEU:CD1	2.72	0.43
1:C:123:ALA:HB3	1:C:165:ASN:HB3	2.01	0.43
1:D:211:LEU:HD23	1:D:211:LEU:HA	1.86	0.43
1:B:448:PHE:CZ	1:B:525:THR:HB	2.53	0.43
1:D:304:MET:O	1:D:308:VAL:HG23	2.19	0.43
1:A:350:ILE:O	1:A:353:PRO:HD2	2.19	0.43
1:D:340:ILE:O	1:D:343:VAL:HG22	2.19	0.43
1:D:501:ARG:O	1:D:505:LYS:HG3	2.18	0.43
1:A:343:VAL:HB	1:A:351:ARG:HG3	2.00	0.43
1:A:455:LEU:HA	1:A:455:LEU:HD23	1.70	0.43
1:B:417:ILE:HD12	1:B:417:ILE:HA	1.86	0.43
1:D:549:THR:O	1:D:553:GLY:N	2.51	0.43
1:A:403:LYS:HG2	1:A:475:LEU:HD22	2.00	0.43
1:B:293:LEU:HB3	1:B:524:PHE:HE1	1.84	0.43
1:B:213:LEU:HB2	1:B:218:ARG:CZ	2.49	0.42
1:C:293:LEU:HD13	1:C:302:ARG:HB2	2.01	0.42
1:A:285:SER:OG	1:A:309:GLY:HA3	2.19	0.42
1:B:217:TRP:HB3	1:B:533:HIS:CD2	2.53	0.42
1:B:287:MET:HG2	1:B:557:LEU:HD11	2.01	0.42
1:A:436:LYS:HG2	1:A:440:ASP:OD2	2.19	0.42
1:C:119:LEU:HB2	1:C:144:PHE:CZ	2.54	0.42
1:C:369:LEU:HB2	1:C:375:ASN:HA	2.02	0.42
1:D:90:GLY:HA3	1:D:224:ALA:CB	2.49	0.42
1:D:106:ILE:HG23	1:D:114:TRP:CZ2	2.55	0.42
1:A:267:TRP:CD1	1:A:273:ASP:HB3	2.55	0.42
1:A:330:LEU:HD23	1:A:346:LEU:HG	2.02	0.42
1:B:300:GLU:O	1:B:304:MET:HE3	2.19	0.42
1:C:38:ASP:HB3	1:C:41:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:TYR:HA	1:B:328:LEU:CD1	2.49	0.42
1:C:374:PHE:CZ	1:C:379:TYR:CE2	3.07	0.42
1:C:501:ARG:O	1:C:505:LYS:HG3	2.19	0.42
1:D:114:TRP:CE3	1:D:115:TRP:HB3	2.55	0.42
1:D:139:ASP:C	1:D:141:PHE:H	2.22	0.42
1:B:406:LEU:HA	1:B:406:LEU:HD12	1.79	0.42
1:D:124:LEU:HB2	1:D:165:ASN:HD22	1.85	0.42
1:A:524:PHE:O	1:A:528:VAL:HG13	2.20	0.42
1:D:118:ASN:C	1:D:144:PHE:HE1	2.22	0.42
1:D:267:TRP:CD1	1:D:273:ASP:HB3	2.55	0.42
1:A:311:LEU:HD21	1:A:356:THR:CG2	2.46	0.42
1:B:84:ASP:CG	1:B:127:ARG:HH22	2.23	0.42
1:C:124:LEU:HB2	1:C:165:ASN:ND2	2.35	0.42
1:C:178:ASP:O	1:C:181:ASP:HB2	2.20	0.42
1:C:306:ALA:O	1:C:309:GLY:N	2.53	0.42
1:D:340:ILE:HG22	1:D:343:VAL:CG1	2.50	0.42
1:D:447:LEU:HD12	1:D:447:LEU:C	2.35	0.42
1:D:507:LEU:HD12	1:D:507:LEU:HA	1.83	0.42
1:C:406:LEU:HD12	1:C:406:LEU:HA	1.82	0.41
1:D:288:TYR:HE2	1:D:535:PHE:HE2	1.60	0.41
1:C:81:GLU:H	1:C:81:GLU:HG2	1.54	0.41
1:B:283:ILE:HD12	1:B:283:ILE:HA	1.85	0.41
1:B:337:ARG:HD2	1:B:342:ARG:NH1	2.35	0.41
1:B:379:TYR:OH	1:B:436:LYS:HG3	2.20	0.41
1:C:493:ARG:HE	1:C:493:ARG:HB2	1.69	0.41
1:D:139:ASP:C	1:D:141:PHE:N	2.73	0.41
1:A:413:ALA:HA	1:A:416:SER:OG	2.21	0.41
1:A:445:LEU:HD12	1:A:445:LEU:HA	1.70	0.41
1:A:487:ALA:HB1	1:A:491:VAL:CG1	2.50	0.41
1:C:59:ALA:HA	1:C:247:LEU:HD13	2.01	0.41
1:C:276:PRO:HG2	1:C:277:PHE:CE2	2.56	0.41
1:D:236:ASP:N	1:D:236:ASP:OD1	2.48	0.41
1:A:83:ILE:HG23	1:A:99:MET:HE2	2.02	0.41
1:C:460:ASN:C	1:C:460:ASN:HD22	2.23	0.41
1:A:252:VAL:HG23	1:A:296:PRO:CG	2.50	0.41
1:B:180:LEU:HA	1:B:183:ALA:HB3	2.03	0.41
1:C:93:TYR:CZ	1:C:94:GLN:HG2	2.56	0.41
1:C:153:LYS:HB3	1:C:153:LYS:HE3	1.85	0.41
1:A:111:TYR:HD2	1:A:111:TYR:HA	1.70	0.41
1:C:355:LEU:HA	1:C:355:LEU:HD23	1.75	0.41
1:A:172:LEU:HD13	1:A:172:LEU:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:GLU:O	1:B:69:LEU:HD13	2.21	0.41
1:B:165:ASN:N	1:B:165:ASN:HD22	2.17	0.41
1:D:91:LEU:HD11	1:D:245:ALA:HB2	2.01	0.41
1:D:115:TRP:HZ3	1:D:140:VAL:CG1	2.33	0.41
1:D:276:PRO:HG2	1:D:277:PHE:CE2	2.56	0.41
1:A:102:ALA:O	1:A:106:ILE:HG13	2.21	0.41
1:A:489:GLN:HG3	1:A:490:GLU:N	2.36	0.41
1:B:42:LEU:HA	1:B:42:LEU:HD23	1.86	0.41
1:C:55:HIS:O	1:C:59:ALA:N	2.51	0.41
1:C:119:LEU:N	1:C:144:PHE:CE1	2.88	0.41
1:C:425:THR:O	1:C:429:LEU:HG	2.21	0.41
1:C:455:LEU:CD1	1:C:507:LEU:HD23	2.51	0.41
1:D:164:LEU:HD23	1:D:191:LEU:CD1	2.51	0.41
1:D:481:TYR:CE1	1:D:495:HIS:CG	3.08	0.41
1:A:222:TYR:CD1	1:A:534:PHE:HE2	2.38	0.41
1:B:536:TYR:CD2	1:B:536:TYR:N	2.89	0.41
1:D:92:LYS:HG3	1:D:99:MET:CE	2.51	0.41
1:B:319:TYR:HA	1:B:328:LEU:HD13	2.03	0.40
1:C:138:GLN:HG3	1:C:139:ASP:N	2.36	0.40
1:C:116:VAL:O	1:C:116:VAL:HG22	2.21	0.40
1:D:340:ILE:CD1	1:D:358:PHE:CE2	3.03	0.40
1:B:231:TYR:O	1:B:237:MET:HG3	2.22	0.40
1:C:80:LEU:HD13	1:C:124:LEU:HG	2.03	0.40
1:C:300:GLU:O	1:C:304:MET:CE	2.69	0.40
1:D:351:ARG:HE	1:D:351:ARG:HB2	1.53	0.40
1:D:411:GLU:HG2	1:D:412:ASN:N	2.35	0.40
1:D:550:LYS:O	1:D:553:GLY:N	2.54	0.40
1:A:289:ALA:O	1:A:293:LEU:HD12	2.22	0.40
1:B:462:LEU:HA	1:B:478:ILE:HD11	2.04	0.40
1:C:141:PHE:HB2	1:C:179:ILE:HD13	2.03	0.40
1:C:246:LYS:HE2	1:C:563:LEU:HD12	2.04	0.40
1:D:80:LEU:HD22	1:D:128:LEU:HD22	2.02	0.40
1:D:118:ASN:C	1:D:144:PHE:CE1	2.95	0.40
1:B:160:VAL:HG11	1:B:203:LEU:HG	2.04	0.40
1:B:231:TYR:CE2	1:B:237:MET:HG2	2.57	0.40
1:C:168:GLU:CD	1:C:215:LEU:H	2.25	0.40
1:C:455:LEU:HD21	1:C:503:TRP:HB2	2.04	0.40
1:D:277:PHE:HB2	1:D:317:ASP:CB	2.51	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	503/555 (91%)	488 (97%)	15 (3%)	0	100	100
1	B	498/555 (90%)	482 (97%)	16 (3%)	0	100	100
1	C	498/555 (90%)	485 (97%)	13 (3%)	0	100	100
1	D	494/555 (89%)	478 (97%)	16 (3%)	0	100	100
All	All	1993/2220 (90%)	1933 (97%)	60 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	441/488 (90%)	411 (93%)	30 (7%)	16	48
1	B	438/488 (90%)	409 (93%)	29 (7%)	16	49
1	C	439/488 (90%)	394 (90%)	45 (10%)	7	30
1	D	435/488 (89%)	398 (92%)	37 (8%)	10	38
All	All	1753/1952 (90%)	1612 (92%)	141 (8%)	12	41

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLU
1	A	75	GLU

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Mol	Chain	Res	Type
1	A	76	PRO
1	A	98	GLU
1	A	111	TYR
1	A	139	ASP
1	A	140	VAL
1	A	157	CYS
1	A	274	LYS
1	A	277	PHE
1	A	282	LEU
1	A	293	LEU
1	A	317	ASP
1	A	339	ASP
1	A	341	ASN
1	A	363	ASP
1	A	398	PHE
1	A	432	ASP
1	A	442	VAL
1	A	443	ASP
1	A	444	SER
1	A	445	LEU
1	A	464	THR
1	A	476	LYS
1	A	485	THR
1	A	489	GLN
1	A	507	LEU
1	A	548	TRP
1	A	558	ILE
1	A	562	THR
1	B	38	ASP
1	B	60	GLU
1	B	67	LYS
1	B	98	GLU
1	B	139	ASP
1	B	140	VAL
1	B	149	THR
1	B	165	ASN
1	B	242	LEU
1	B	243	LYS
1	B	277	PHE
1	B	293	LEU
1	B	313	SER
1	B	316	ASP

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Mol	Chain	Res	Type
1	B	317	ASP
1	B	320	ASP
1	B	324	THR
1	B	331	PHE
1	B	332	THR
1	B	342	ARG
1	B	363	ASP
1	B	405	THR
1	B	477	SER
1	B	507	LEU
1	B	511	LEU
1	B	537	GLN
1	B	548	TRP
1	B	555	SER
1	B	562	THR
1	C	55	HIS
1	C	69	LEU
1	C	75	GLU
1	C	81	GLU
1	C	88	ARG
1	C	112	ASP
1	C	116	VAL
1	C	119	LEU
1	C	124	LEU
1	C	151	LYS
1	C	157	CYS
1	C	178	ASP
1	C	179	ILE
1	C	230	ILE
1	C	275	LEU
1	C	277	PHE
1	C	282	LEU
1	C	283	ILE
1	C	293	LEU
1	C	317	ASP
1	C	339	ASP
1	C	341	ASN
1	C	363	ASP
1	C	377	ILE
1	C	431	VAL
1	C	439	LEU
1	C	442	VAL

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Mol	Chain	Res	Type
1	C	445	LEU
1	C	447	LEU
1	C	450	ARG
1	C	457	ARG
1	C	458	ILE
1	C	459	ILE
1	C	460	ASN
1	C	464	THR
1	C	474	ASN
1	C	475	LEU
1	C	479	GLN
1	C	485	THR
1	C	493	ARG
1	C	494	GLU
1	C	507	LEU
1	C	548	TRP
1	C	551	ASN
1	C	563	LEU
1	D	37	TRP
1	D	54	GLU
1	D	60	GLU
1	D	62	LEU
1	D	143	ARG
1	D	149	THR
1	D	152	PHE
1	D	154	ASN
1	D	185	THR
1	D	202	ASN
1	D	203	LEU
1	D	205	LYS
1	D	240	THR
1	D	277	PHE
1	D	293	LEU
1	D	295	GLU
1	D	316	ASP
1	D	317	ASP
1	D	320	ASP
1	D	337	ARG
1	D	338	TRP
1	D	339	ASP
1	D	340	ILE
1	D	341	ASN

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Mol	Chain	Res	Type
1	D	363	ASP
1	D	405	THR
1	D	411	GLU
1	D	432	ASP
1	D	445	LEU
1	D	458	ILE
1	D	474	ASN
1	D	476	LYS
1	D	507	LEU
1	D	529	VAL
1	D	532	SER
1	D	548	TRP
1	D	555	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	297	HIS
1	B	154	ASN
1	C	55	HIS
1	C	460	ASN
1	C	533	HIS
1	D	257	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, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	509/555 (91%)	-0.21	1 (0%)	95	95	23, 32, 54, 76	0
1	B	506/555 (91%)	-0.06	5 (0%)	82	81	21, 36, 57, 78	0
1	C	506/555 (91%)	0.02	8 (1%)	72	71	24, 43, 78, 102	0
1	D	504/555 (90%)	-0.12	5 (0%)	82	81	19, 38, 72, 89	0
All	All	2025/2220 (91%)	-0.09	19 (0%)	84	83	19, 37, 67, 102	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	145	GLN	3.2
1	C	50	SER	2.9
1	C	74	MET	2.7
1	D	146	ASN	2.6
1	C	485	THR	2.6
1	C	58	LEU	2.5
1	B	150	GLY	2.5
1	D	54	GLU	2.5
1	C	277	PHE	2.3
1	B	247	LEU	2.3
1	D	51	VAL	2.3
1	B	278	ALA	2.3
1	B	55	HIS	2.2
1	D	111	TYR	2.2
1	C	53	GLU	2.1
1	C	57	GLY	2.1
1	A	278	ALA	2.1
1	B	145	GLN	2.0
1	C	54	GLU	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)

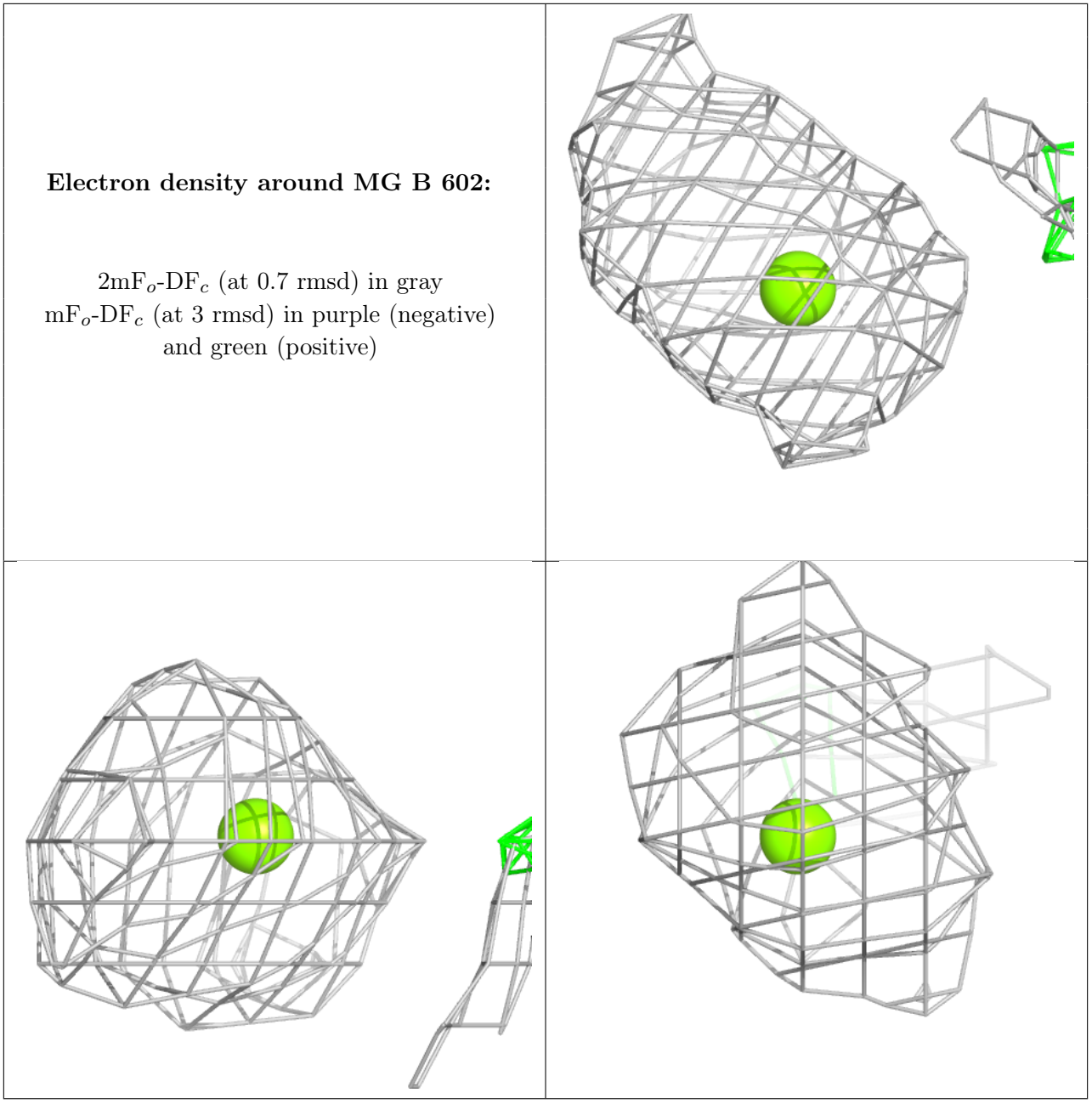
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	MG	B	602	1/1	0.88	0.15	19,19,19,19	0
2	MG	B	601	1/1	0.91	0.19	25,25,25,25	0
2	MG	A	601	1/1	0.93	0.23	19,19,19,19	0
2	MG	C	601	1/1	0.95	0.15	28,28,28,28	0
2	MG	C	602	1/1	0.95	0.23	20,20,20,20	0
2	MG	A	602	1/1	0.96	0.24	18,18,18,18	0
2	MG	D	602	1/1	0.96	0.12	9,9,9,9	0
2	MG	D	601	1/1	0.98	0.20	16,16,16,16	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.

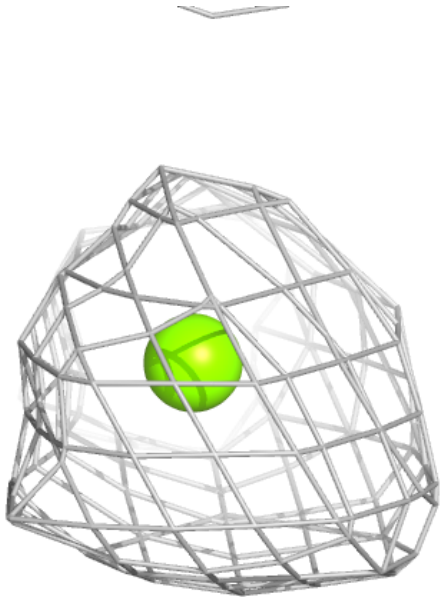
Electron density around MG B 602:

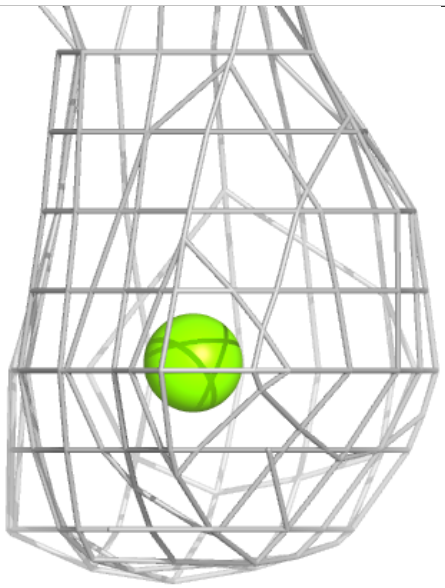
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

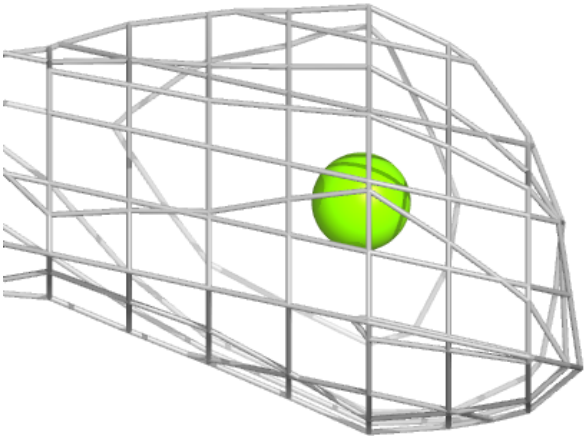


Electron density around MG B 601:

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

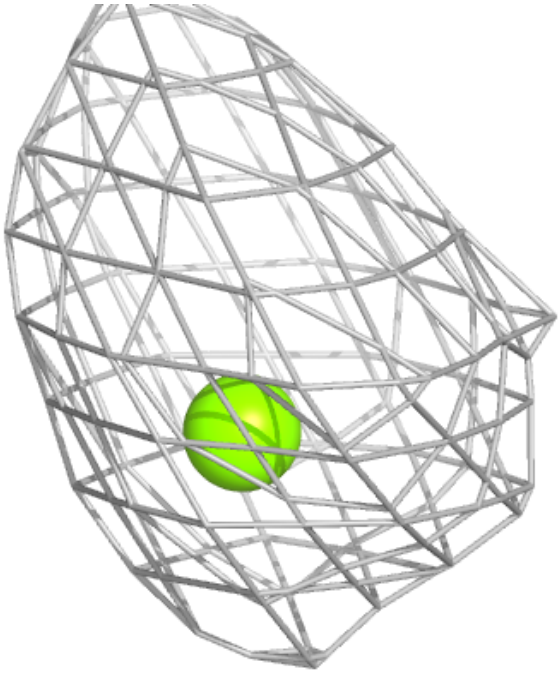


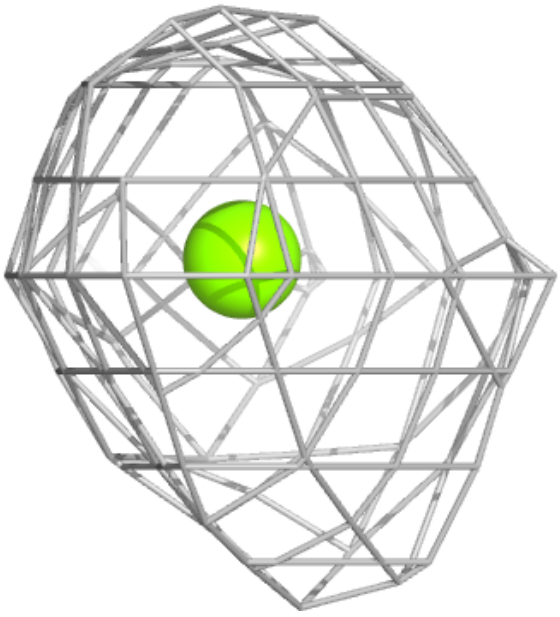


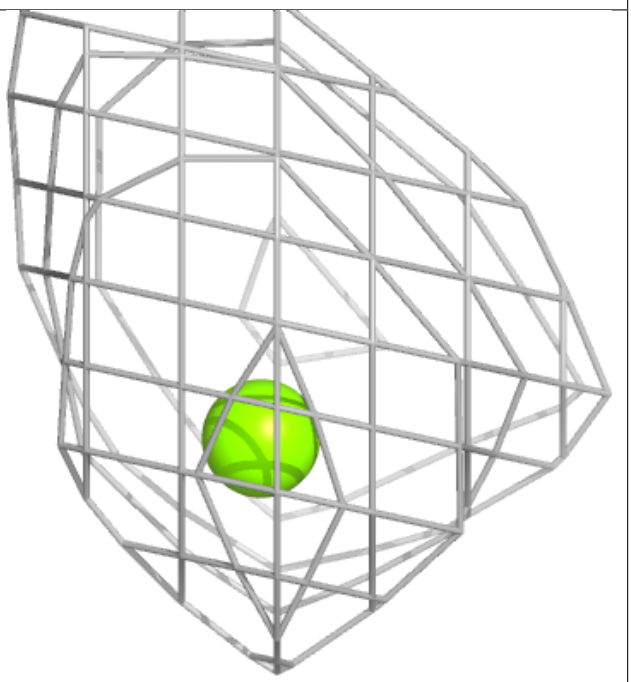


Electron density around MG A 601:

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

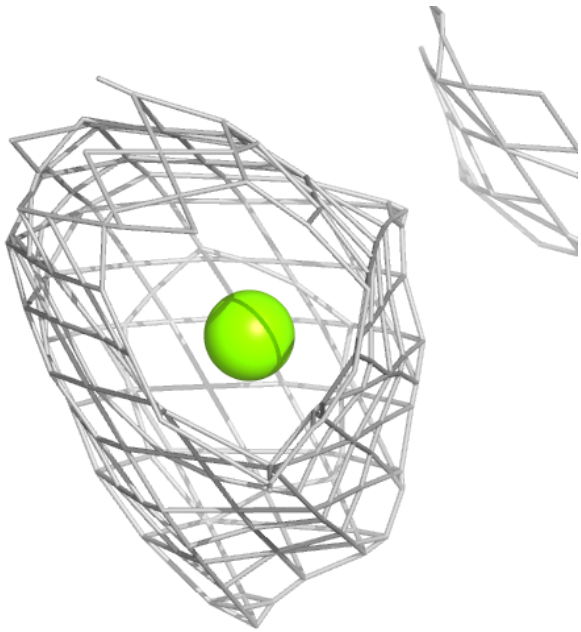


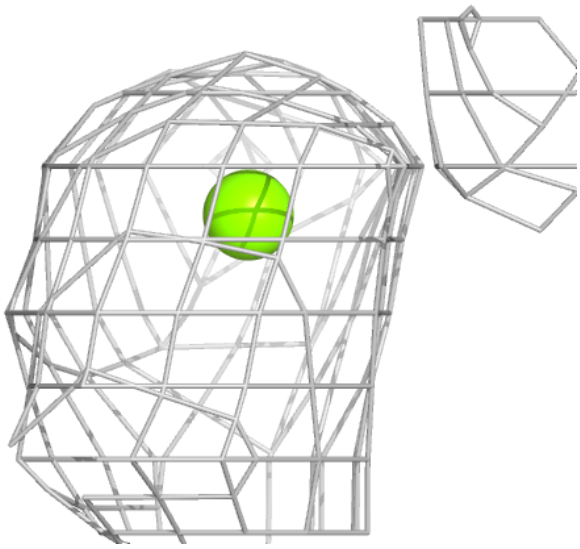


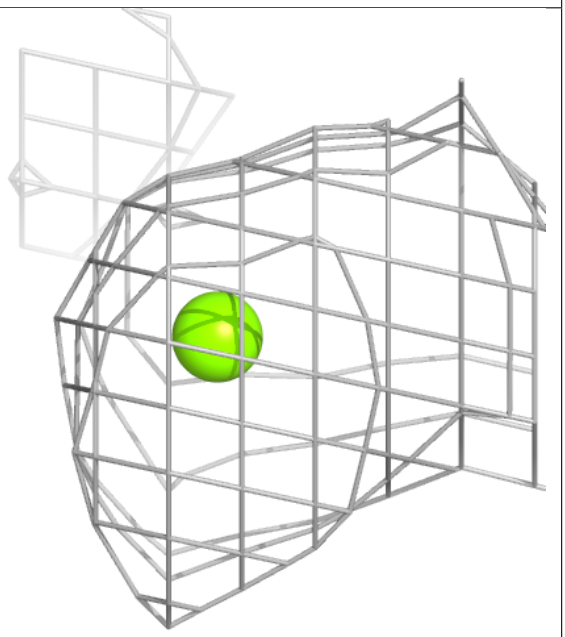


Electron density around MG C 601:

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

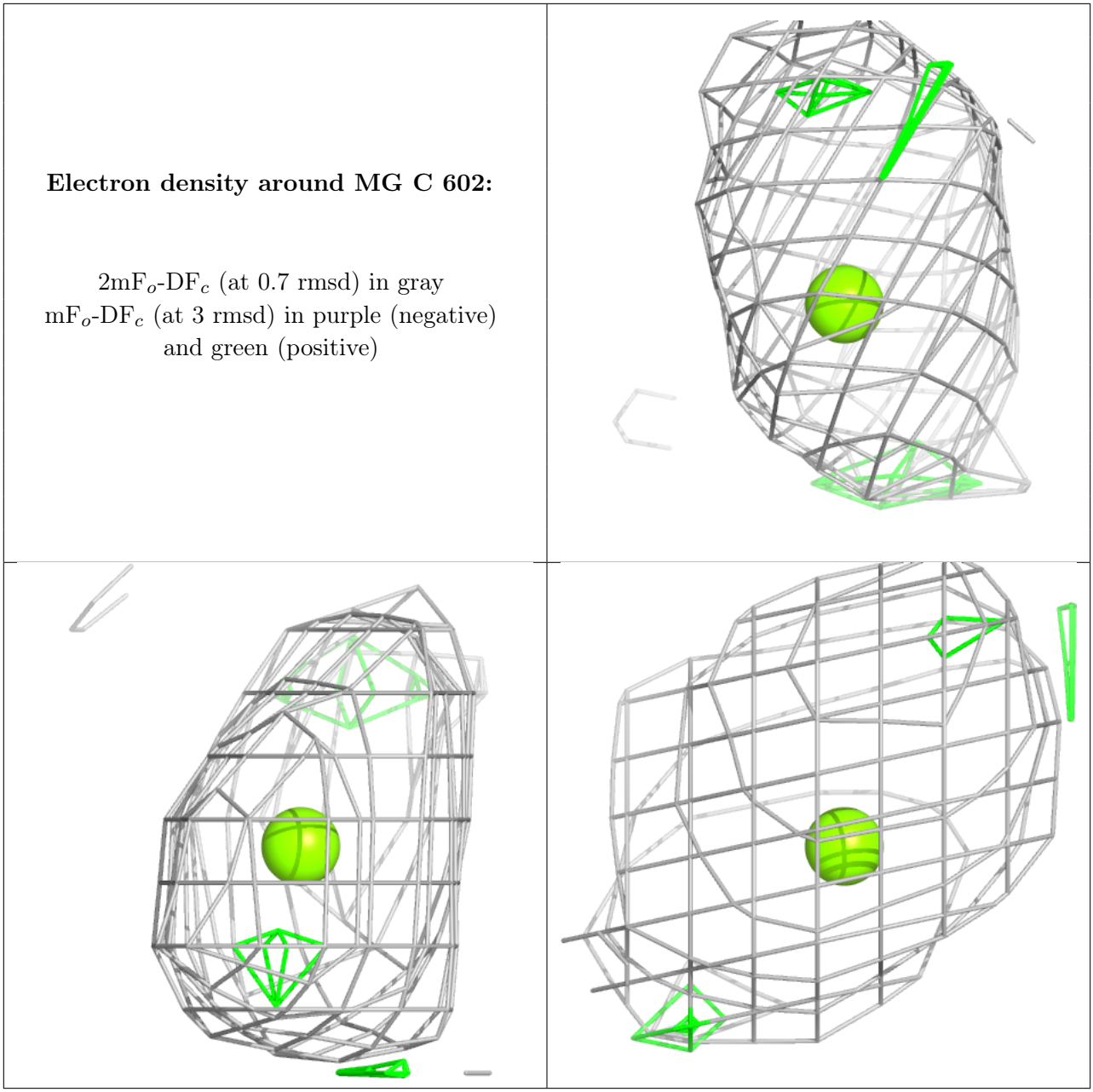






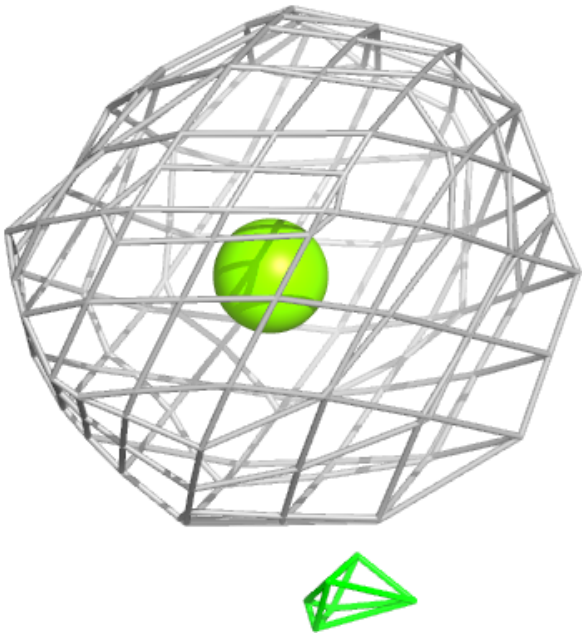
Electron density around MG C 602:

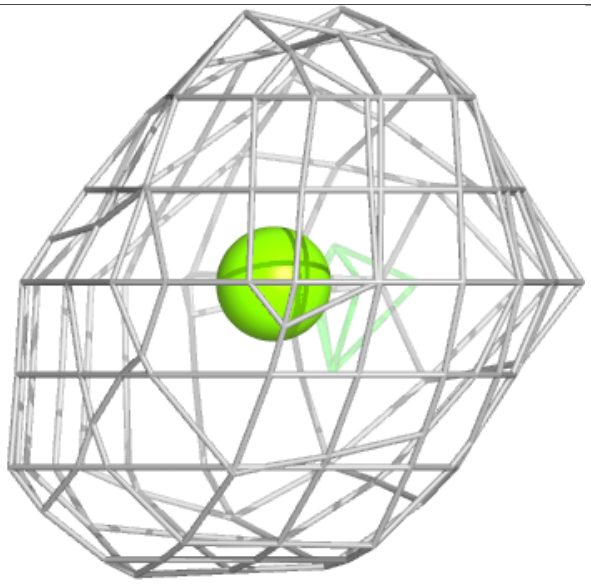
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

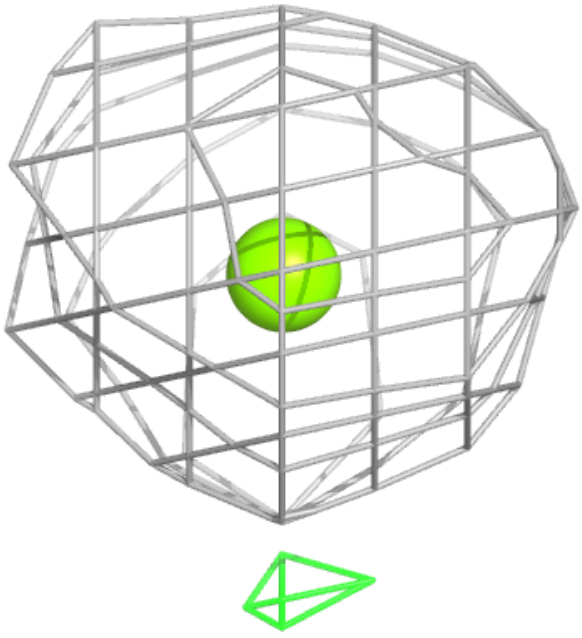


Electron density around MG A 602:

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

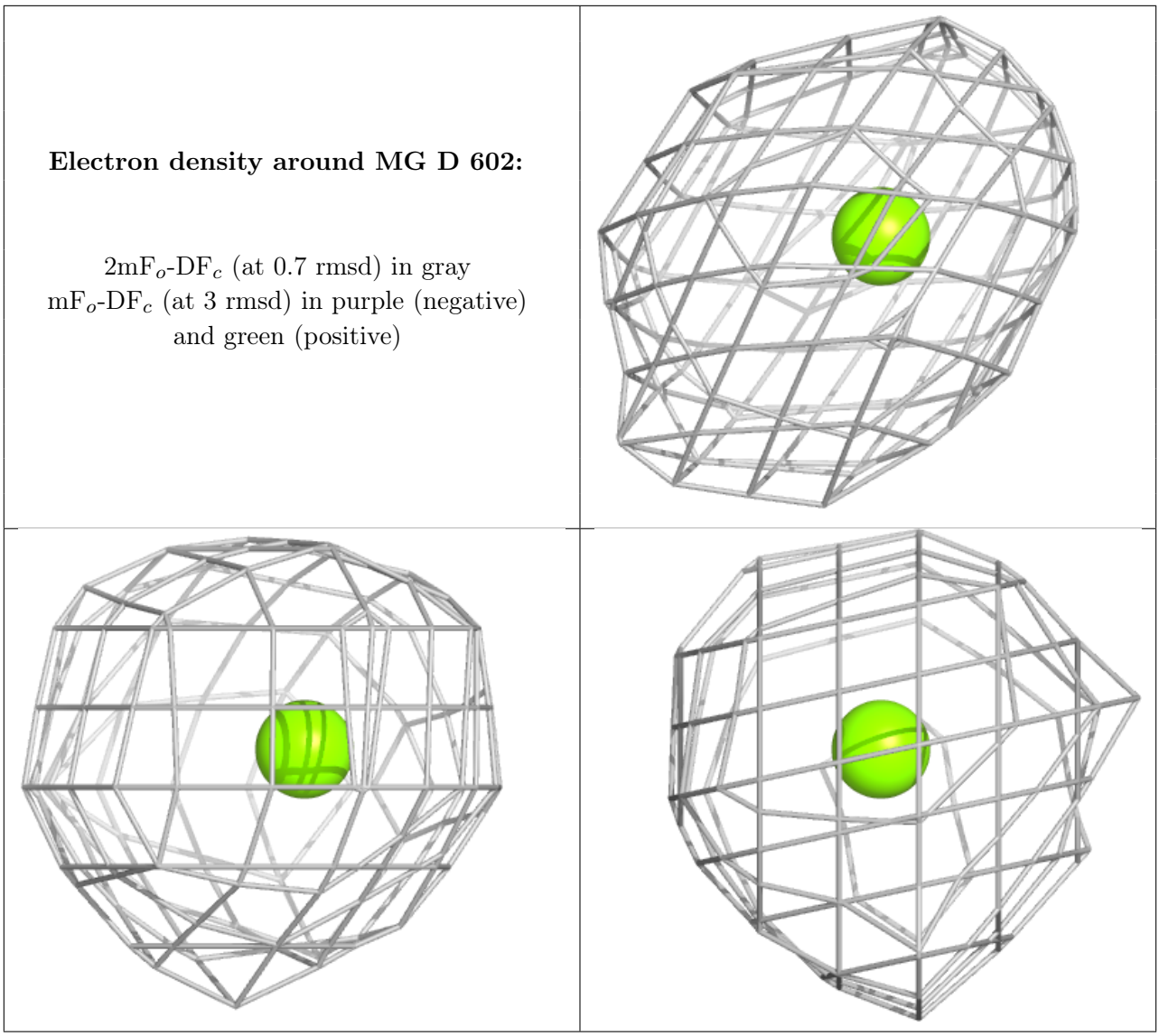






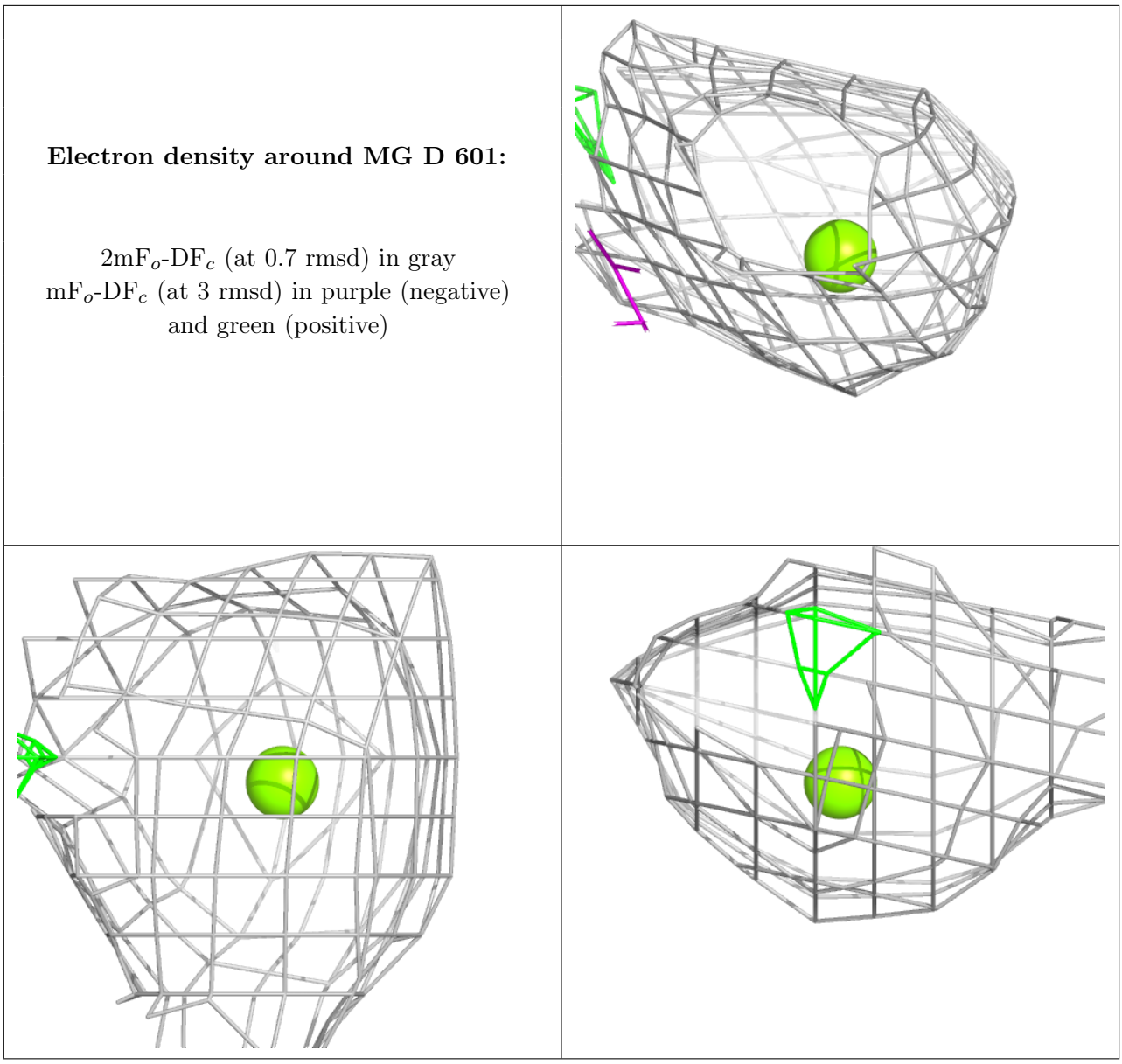
Electron density around MG D 602:

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



Electron density around MG D 601:

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



6.5 Other polymers

There are no such residues in this entry.