Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 11:13 am BST

PDB ID	:	6SD0
Title	:	Structure of beta-galactosidase from Thermotoga maritima.
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Deposited on	:	2019-07-26
Resolution	:	3.70 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 following versions of software and data (see references (1)) were used in the production of this report:

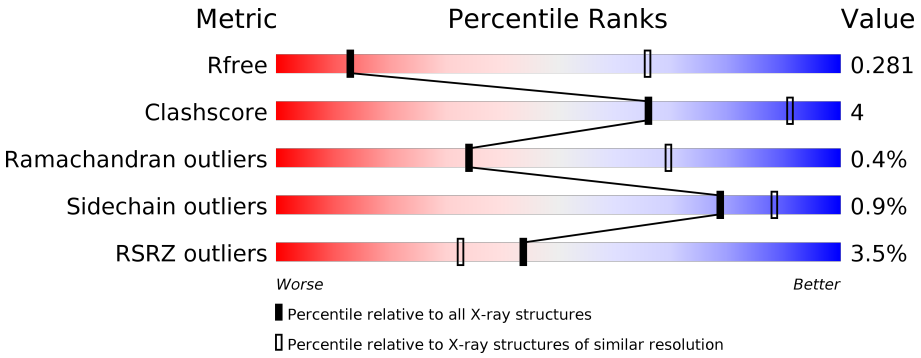
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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	1084	2% 91% 9%
1	B	1084	3% 93% 7%
1	C	1084	4% 90% 9%
1	D	1084	5% 94% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 36135 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1083	Total	C	N	O	S	0	1	0
			9032	5833	1516	1656	27			
1	B	1083	Total	C	N	O	S	0	1	0
			9032	5833	1516	1656	27			
1	C	1083	Total	C	N	O	S	0	1	0
			9032	5833	1516	1656	27			
1	D	1083	Total	C	N	O	S	0	1	0
			9032	5833	1516	1656	27			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

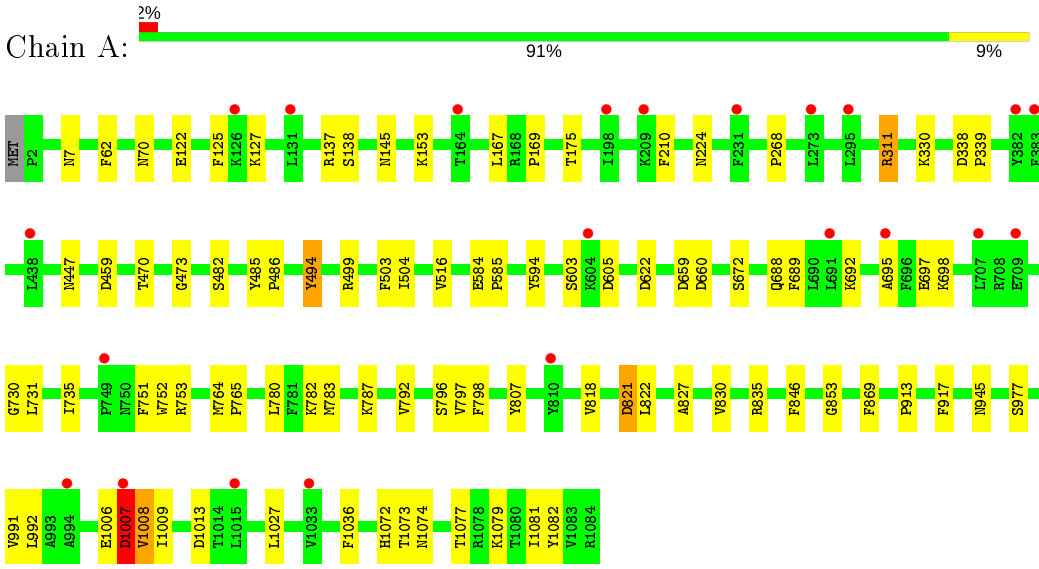
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	1	Total	O	0	0
			1	1		
3	C	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

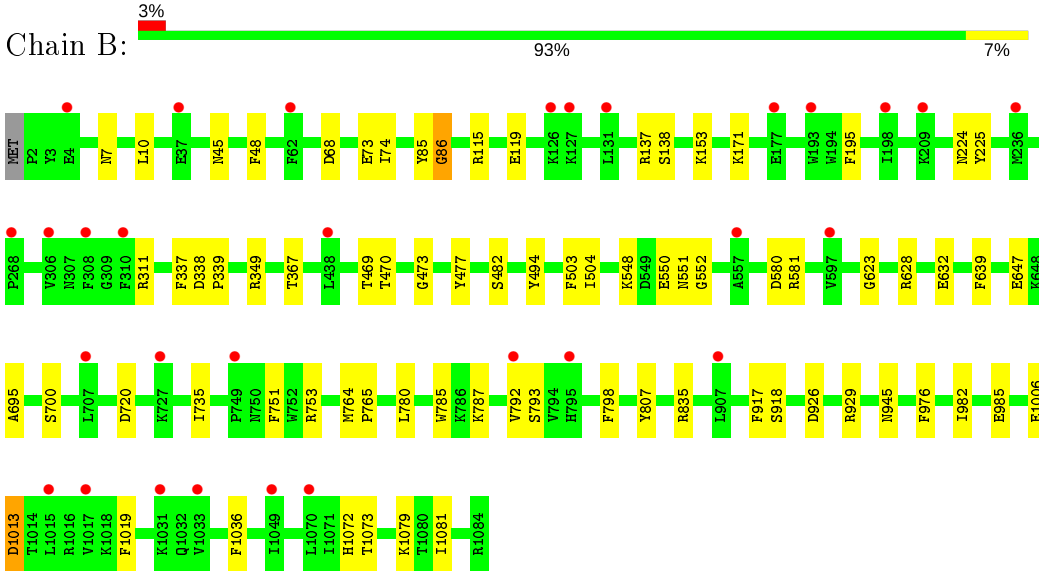
- Molecule 1: Beta-galactosidase

Chain A:



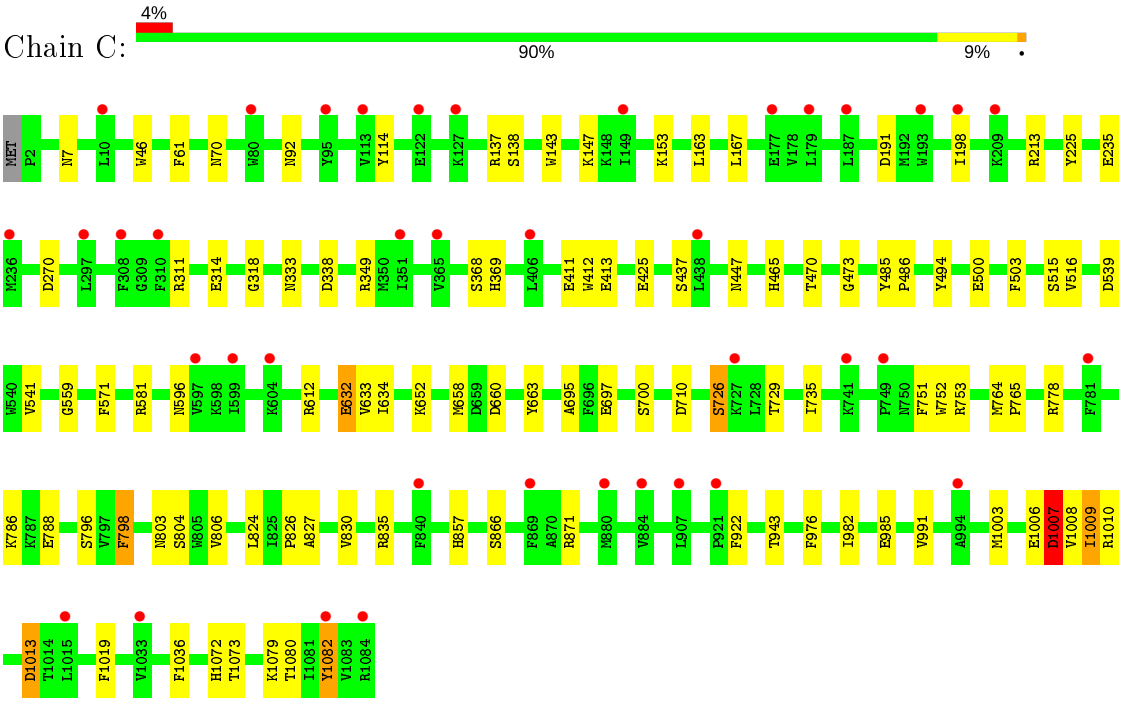
- Molecule 1: Beta-galactosidase

Chain B:



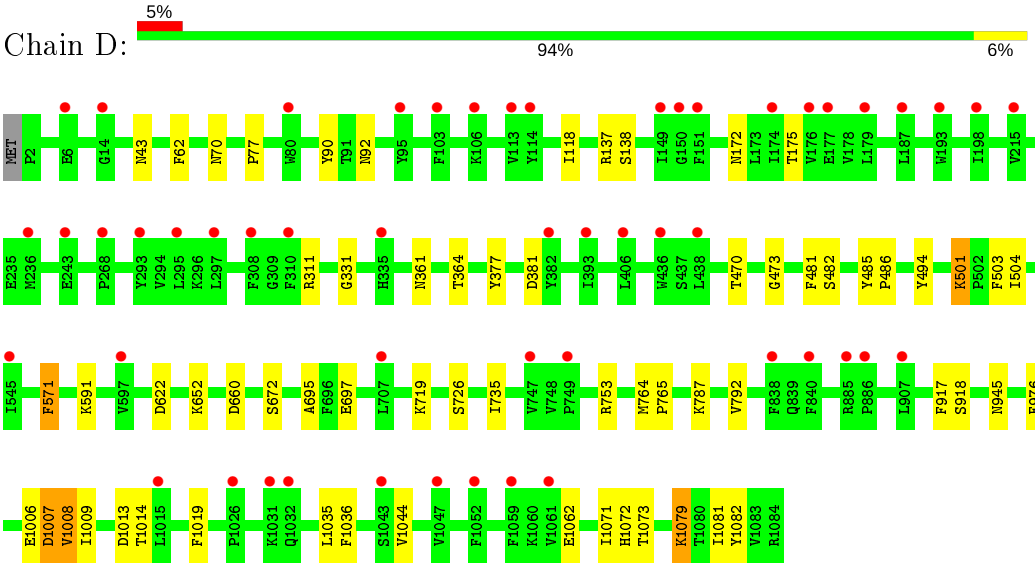
- Molecule 1: Beta-galactosidase

Chain C:



• Molecule 1: Beta-galactosidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	167.85Å 167.85Å 519.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.70 40.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-3.70) 99.9 (40.00-3.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 3.66Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.241 , 0.285 0.241 , 0.281	Depositor DCC
R_{free} test set	3721 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	126.6	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 82.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.104 for -h,k,-l	Xtriage
Reported twinning fraction	0.158 for H, K, L 0.842 for -K, -H, -L	Depositor
Outliers	0 of 76049 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	36135	wwPDB-VP
Average B, all atoms (Å^2)	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% 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	0.66	0/9303	0.82	2/12600 (0.0%)
1	B	0.67	0/9303	0.82	1/12600 (0.0%)
1	C	0.67	0/9303	0.81	3/12600 (0.0%)
1	D	0.70	0/9303	0.82	2/12600 (0.0%)
All	All	0.68	0/37212	0.82	8/50400 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1007	ASP	CB-CA-C	7.09	124.57	110.40
1	A	1007	ASP	CB-CA-C	6.64	123.68	110.40
1	C	1082	TYR	CB-CA-C	5.78	121.96	110.40
1	D	1082	TYR	CB-CA-C	5.74	121.87	110.40
1	C	798	PHE	CB-CA-C	-5.48	99.43	110.40
1	C	1007	ASP	CB-CA-C	5.38	121.16	110.40
1	D	1007	ASP	CB-CA-C	5.25	120.89	110.40
1	A	1082	TYR	CB-CA-C	5.10	120.61	110.40

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	9032	0	8777	118	0
1	B	9032	0	8777	77	0
1	C	9032	0	8777	71	0
1	D	9032	0	8777	50	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
All	All	36135	0	35108	285	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 4.

All (285) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:TRP:CZ2	1:B:119:GLU:HG3	1.47	1.47
1:A:410:TRP:CH2	1:B:119:GLU:HG3	1.75	1.22
1:C:541:VAL:HG21	1:C:581:ARG:NH2	1.62	1.13
1:A:494:TYR:HD1	1:A:503:PHE:CD2	1.66	1.13
1:A:338:ASP:OD1	1:A:339:PRO:HD2	1.50	1.07
1:A:410:TRP:CE2	1:B:119:GLU:HG3	1.90	1.06
1:A:169:PRO:HG3	1:B:551:ASN:O	1.56	1.05
1:C:1008:VAL:O	1:C:1009:ILE:HG23	1.57	1.04
1:A:494:TYR:CD1	1:A:503:PHE:CD2	2.47	1.02
1:A:410:TRP:CZ2	1:B:119:GLU:CG	2.41	1.02
1:A:494:TYR:CD1	1:A:503:PHE:HD2	1.77	1.01
1:C:1008:VAL:HG22	1:C:1009:ILE:H	1.30	0.97
1:A:410:TRP:CH2	1:B:119:GLU:CG	2.51	0.94
1:A:1008:VAL:O	1:A:1009:ILE:HG23	1.71	0.91
1:D:494:TYR:OH	1:D:501:LYS:HG2	1.73	0.89
1:A:494:TYR:CE1	1:A:503:PHE:HB2	2.10	0.86
1:A:494:TYR:HE2	1:A:499:ARG:HD2	1.41	0.85
1:B:548:LYS:HG2	1:B:552:GLY:O	1.75	0.85
1:C:1008:VAL:HG22	1:C:1009:ILE:N	1.91	0.85
1:A:494:TYR:HE2	1:A:499:ARG:CD	1.90	0.85
1:A:821:ASP:OD1	1:A:977:SER:HB3	1.77	0.84
1:C:1008:VAL:O	1:C:1009:ILE:CG2	2.25	0.84
1:A:167:LEU:O	1:B:548:LYS:CE	2.25	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:C	1:B:548:LYS:HE2	1.99	0.83
1:A:1073:THR:HG22	1:A:1074:ASN:H	1.43	0.83
1:D:92:ASN:ND2	1:D:571:PHE:CE2	2.46	0.83
1:A:1073:THR:HG22	1:A:1074:ASN:N	1.96	0.80
1:A:1008:VAL:CG2	1:A:1009:ILE:N	2.45	0.79
1:D:1036:PHE:HB2	1:D:1072:HIS:CE1	2.18	0.79
1:A:494:TYR:CE2	1:A:499:ARG:HG3	2.17	0.78
1:A:821:ASP:OD1	1:A:977:SER:CB	2.32	0.78
1:B:224:ASN:OD1	1:D:652:LYS:HE3	1.83	0.78
1:A:167:LEU:O	1:B:548:LYS:HE2	1.84	0.78
1:D:1008:VAL:O	1:D:1009:ILE:HG23	1.85	0.76
1:D:1008:VAL:CG2	1:D:1009:ILE:N	2.48	0.76
1:C:541:VAL:HG21	1:C:581:ARG:HH22	1.51	0.75
1:D:1079:LYS:HD3	1:D:1081:ILE:HD11	1.68	0.75
1:A:167:LEU:C	1:B:548:LYS:CE	2.57	0.73
1:D:1036:PHE:CB	1:D:1072:HIS:CE1	2.72	0.73
1:A:729:THR:O	1:A:731:LEU:HG	1.89	0.73
1:A:1008:VAL:HG22	1:A:1009:ILE:N	2.01	0.72
1:A:494:TYR:CE2	1:A:499:ARG:CD	2.72	0.72
1:D:92:ASN:ND2	1:D:571:PHE:HE2	1.84	0.72
1:A:1008:VAL:O	1:A:1009:ILE:CG2	2.37	0.72
1:C:1036:PHE:HB2	1:C:1072:HIS:CE1	2.25	0.72
1:A:167:LEU:N	1:B:548:LYS:HE2	2.05	0.71
1:C:1008:VAL:C	1:C:1009:ILE:HG23	2.08	0.71
1:C:1080:THR:HG22	1:C:1082:TYR:CZ	2.26	0.71
1:C:1007:ASP:N	1:C:1007:ASP:OD1	2.23	0.70
1:B:780:LEU:HB2	1:B:798:PHE:HE1	1.56	0.70
1:A:494:TYR:CD1	1:A:503:PHE:HB2	2.25	0.70
1:B:751:PHE:HA	1:B:835:ARG:O	1.91	0.70
1:A:494:TYR:CE2	1:A:499:ARG:CG	2.75	0.70
1:A:1036:PHE:HB2	1:A:1072:HIS:CE1	2.27	0.70
1:A:167:LEU:O	1:B:548:LYS:HE3	1.91	0.70
1:A:494:TYR:CE2	1:A:499:ARG:HD2	2.25	0.69
1:C:1008:VAL:CG2	1:C:1009:ILE:H	2.04	0.69
1:A:494:TYR:HE2	1:A:499:ARG:CG	2.04	0.69
1:C:1036:PHE:CB	1:C:1072:HIS:CE1	2.76	0.69
1:A:338:ASP:OD1	1:A:339:PRO:CD	2.37	0.68
1:D:1008:VAL:HG23	1:D:1009:ILE:H	1.59	0.68
1:A:821:ASP:OD1	1:A:1027:LEU:HD22	1.93	0.67
1:B:224:ASN:OD1	1:D:652:LYS:CE	2.43	0.66
1:A:796:SER:HB2	1:A:798:PHE:HE2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1008:VAL:C	1:D:1009:ILE:HG23	2.17	0.66
1:A:410:TRP:CE2	1:B:119:GLU:CG	2.74	0.65
1:A:780:LEU:HD13	1:A:798:PHE:CE1	2.31	0.65
1:D:1008:VAL:HG23	1:D:1009:ILE:N	2.11	0.65
1:D:1008:VAL:O	1:D:1009:ILE:CG2	2.45	0.64
1:A:1008:VAL:C	1:A:1009:ILE:HG23	2.17	0.64
1:D:1079:LYS:HD3	1:D:1081:ILE:CD1	2.28	0.64
1:A:796:SER:CB	1:A:798:PHE:CE2	2.82	0.63
1:A:1007:ASP:OD2	1:A:1007:ASP:N	2.32	0.63
1:A:1036:PHE:CB	1:A:1072:HIS:CE1	2.81	0.63
1:B:780:LEU:HA	1:B:798:PHE:CD1	2.33	0.63
1:A:1073:THR:CG2	1:A:1074:ASN:H	2.12	0.62
1:A:1008:VAL:CG2	1:A:1009:ILE:H	2.13	0.62
1:A:780:LEU:HD13	1:A:798:PHE:CZ	2.35	0.61
1:A:796:SER:HB3	1:A:798:PHE:CE2	2.36	0.61
1:C:633:VAL:HG12	1:C:634:ILE:N	2.16	0.61
1:C:541:VAL:CG2	1:C:581:ARG:NH2	2.54	0.61
1:A:169:PRO:HD3	1:B:552:GLY:C	2.21	0.60
1:B:68:ASP:OD2	1:B:115:ARG:NE	2.30	0.60
1:A:1008:VAL:HG23	1:A:1009:ILE:H	1.67	0.60
1:C:541:VAL:HG21	1:C:581:ARG:HH21	1.58	0.60
1:C:596:ASN:O	1:C:612:ARG:HB2	2.02	0.60
1:D:660:ASP:HB3	1:D:695:ALA:HB3	1.84	0.59
1:A:410:TRP:CZ3	1:B:119:GLU:HG3	2.37	0.59
1:D:90:TYR:OH	1:D:571:PHE:HB3	2.02	0.59
1:D:92:ASN:HD21	1:D:571:PHE:HE2	1.51	0.58
1:A:122:GLU:HG2	1:B:551:ASN:HB3	1.85	0.58
1:A:494:TYR:CE1	1:A:503:PHE:HD2	2.21	0.57
1:C:660:ASP:HB3	1:C:695:ALA:HB3	1.85	0.57
1:D:494:TYR:OH	1:D:501:LYS:HE3	2.04	0.57
1:A:169:PRO:HG3	1:B:551:ASN:C	2.23	0.57
1:C:1080:THR:CG2	1:C:1082:TYR:CZ	2.87	0.57
1:A:1006:GLU:OE1	1:A:1006:GLU:N	2.33	0.56
1:C:632:GLU:OE2	1:C:871:ARG:HD3	2.05	0.56
1:D:1081:ILE:HG22	1:D:1081:ILE:O	2.04	0.56
1:A:730:GLY:HA2	1:A:783:MET:SD	2.46	0.55
1:B:1019:PHE:CE1	1:B:1073:THR:HG21	2.42	0.55
1:B:224:ASN:O	1:B:225:TYR:HB2	2.06	0.55
1:C:857:HIS:CE1	1:C:866:SER:O	2.60	0.55
1:D:1044:VAL:HG13	1:D:1044:VAL:O	2.06	0.55
1:A:821:ASP:OD1	1:A:977:SER:HB2	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:TYR:OH	1:C:314:GLU:OE2	2.20	0.54
1:B:1007:ASP:OD1	1:B:1079:LYS:NZ	2.37	0.54
1:A:787:LYS:HG3	1:A:792:VAL:HG22	1.88	0.54
1:C:1019:PHE:CE1	1:C:1073:THR:HG21	2.43	0.54
1:A:210:PHE:CZ	1:A:268:PRO:HA	2.43	0.53
1:A:917:PHE:HA	1:A:945:ASN:O	2.08	0.53
1:B:1019:PHE:CZ	1:B:1073:THR:HG21	2.43	0.53
1:D:361:ASN:ND2	1:D:591:LYS:HG3	2.23	0.53
1:D:43:ASN:ND2	1:D:77:PRO:HD3	2.23	0.53
1:A:827:ALA:O	1:A:830:VAL:HG22	2.08	0.53
1:C:751:PHE:HA	1:C:835:ARG:O	2.08	0.53
1:B:628:ARG:HA	1:B:632:GLU:O	2.09	0.52
1:A:167:LEU:CA	1:B:548:LYS:HE2	2.39	0.52
1:A:7:ASN:O	1:A:153:LYS:NZ	2.43	0.52
1:B:720:ASP:OD1	1:B:720:ASP:N	2.42	0.52
1:C:824:LEU:O	1:C:826:PRO:HD3	2.09	0.52
1:A:796:SER:HB2	1:A:798:PHE:CE2	2.41	0.52
1:D:494:TYR:CE2	1:D:503:PHE:HB2	2.44	0.52
1:A:410:TRP:HB2	1:B:171:LYS:HD2	1.92	0.52
1:B:119:GLU:OE2	1:B:171:LYS:HG3	2.10	0.52
1:C:658:MET:HB3	1:C:663:TYR:CE1	2.45	0.51
1:C:1019:PHE:CZ	1:C:1073:THR:HG21	2.45	0.51
1:A:660:ASP:HB3	1:A:695:ALA:HB3	1.92	0.51
1:B:1036:PHE:HB2	1:B:1072:HIS:CE1	2.45	0.51
1:A:1081:ILE:HG22	1:A:1081:ILE:O	2.10	0.51
1:A:622:ASP:OD2	1:A:672:SER:HA	2.10	0.51
1:B:1006:GLU:OE1	1:B:1006:GLU:N	2.41	0.51
1:C:1006:GLU:OE1	1:C:1006:GLU:N	2.31	0.51
1:C:425:GLU:OE1	1:C:425:GLU:HA	2.10	0.51
1:C:786:LYS:HE3	1:C:788:GLU:OE1	2.10	0.51
1:D:1008:VAL:HG22	1:D:1009:ILE:N	2.26	0.50
1:D:735:ILE:HG21	1:D:982:ILE:HD12	1.93	0.50
1:A:224:ASN:OD1	1:C:652:LYS:HE3	2.12	0.50
1:A:698:LYS:HA	1:A:992:LEU:O	2.11	0.50
1:D:917:PHE:HA	1:D:945:ASN:O	2.11	0.50
1:D:481:PHE:HB2	1:D:501:LYS:HG3	1.93	0.50
1:C:1019:PHE:CZ	1:C:1073:THR:CG2	2.95	0.50
1:C:1082:TYR:N	1:C:1082:TYR:CD1	2.79	0.50
1:C:633:VAL:CG1	1:C:634:ILE:N	2.75	0.50
1:C:1080:THR:HG22	1:C:1082:TYR:CE1	2.47	0.49
1:D:1019:PHE:CE1	1:D:1073:THR:HG21	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1073:THR:CG2	1:A:1074:ASN:N	2.65	0.49
1:A:821:ASP:CG	1:A:977:SER:HB3	2.31	0.49
1:A:410:TRP:CZ3	1:B:119:GLU:CG	2.94	0.49
1:A:796:SER:HB3	1:A:798:PHE:CZ	2.48	0.49
1:C:922:PHE:O	1:C:943:THR:OG1	2.26	0.49
1:B:660:ASP:HB3	1:B:695:ALA:HB3	1.94	0.49
1:A:459:ASP:C	1:A:459:ASP:OD1	2.49	0.49
1:A:470:THR:HA	1:A:473:GLY:O	2.13	0.48
1:A:735:ILE:HG21	1:A:982:ILE:HD12	1.95	0.48
1:B:764:MET:N	1:B:765:PRO:CD	2.76	0.48
1:A:125:PHE:HE1	1:A:167:LEU:O	1.96	0.48
1:D:470:THR:HA	1:D:473:GLY:O	2.14	0.48
1:B:338:ASP:CG	1:B:339:PRO:HD2	2.33	0.48
1:D:735:ILE:HG21	1:D:982:ILE:CD1	2.43	0.48
1:B:917:PHE:HA	1:B:945:ASN:O	2.14	0.48
1:A:822:LEU:C	1:A:822:LEU:HD23	2.35	0.47
1:A:167:LEU:H	1:B:548:LYS:HE2	1.75	0.47
1:A:330:LYS:HB3	1:A:594:TYR:CD2	2.49	0.47
1:A:584:GLU:O	1:A:585:PRO:C	2.53	0.47
1:C:1003:MET:SD	1:C:1019:PHE:CZ	3.08	0.47
1:A:125:PHE:CE1	1:A:167:LEU:O	2.68	0.47
1:B:580:ASP:O	1:B:581:ARG:HB2	2.15	0.47
1:D:697:GLU:HG2	1:D:991:VAL:HG13	1.97	0.47
1:A:853:GLY:O	1:A:869:PHE:HA	2.15	0.47
1:B:470:THR:HA	1:B:473:GLY:O	2.15	0.46
1:A:735:ILE:HG21	1:A:982:ILE:CD1	2.45	0.46
1:A:122:GLU:OE1	1:B:551:ASN:HA	2.16	0.46
1:B:780:LEU:CB	1:B:798:PHE:HE1	2.25	0.46
1:D:1036:PHE:HB2	1:D:1072:HIS:ND1	2.31	0.46
1:B:7:ASN:O	1:B:153:LYS:NZ	2.48	0.46
1:B:85:TYR:O	1:B:86:GLY:O	2.33	0.46
1:B:482:SER:HA	1:B:504:ILE:O	2.16	0.46
1:A:167:LEU:C	1:B:548:LYS:HE3	2.33	0.46
1:B:137:ARG:HA	1:B:138:SER:HA	1.78	0.46
1:D:331:GLY:HA2	1:D:364:THR:O	2.16	0.46
1:B:1019:PHE:CZ	1:B:1073:THR:CG2	2.98	0.46
1:C:726:SER:HG	1:C:729:THR:H	1.60	0.45
1:D:622:ASP:OD2	1:D:672:SER:HA	2.16	0.45
1:A:751:PHE:HA	1:A:835:ARG:O	2.17	0.45
1:C:338:ASP:OD1	1:C:349:ARG:NH1	2.50	0.45
1:C:485:TYR:N	1:C:486:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1036:PHE:HB3	1:C:1072:HIS:CE1	2.50	0.45
1:A:311:ARG:O	1:A:311:ARG:HD2	2.16	0.45
1:D:137:ARG:HA	1:D:138:SER:HA	1.79	0.45
1:B:1036:PHE:CB	1:B:1072:HIS:CE1	3.00	0.45
1:A:125:PHE:HB2	1:B:550:GLU:O	2.17	0.45
1:A:494:TYR:CE1	1:A:503:PHE:CD2	3.02	0.44
1:A:821:ASP:CG	1:A:1027:LEU:HD22	2.37	0.44
1:B:780:LEU:HA	1:B:798:PHE:HD1	1.78	0.44
1:C:318:GLY:HA2	1:C:500:GLU:O	2.17	0.44
1:B:623:GLY:O	1:B:639:PHE:N	2.43	0.44
1:B:48:PHE:HB2	1:B:74:ILE:HG22	2.00	0.44
1:B:780:LEU:HA	1:B:798:PHE:CE1	2.51	0.44
1:C:752:TRP:O	1:C:835:ARG:HD2	2.17	0.44
1:B:1012:GLY:O	1:B:1013:ASP:O	2.36	0.44
1:B:735:ILE:HG21	1:B:982:ILE:HD12	2.00	0.44
1:B:119:GLU:OE2	1:B:171:LYS:CB	2.65	0.44
1:B:137:ARG:HD2	1:B:195:PHE:O	2.18	0.44
1:C:494:TYR:CE2	1:C:503:PHE:HB2	2.52	0.44
1:C:92:ASN:ND2	1:C:571:PHE:CE2	2.86	0.44
1:C:735:ILE:HG21	1:C:982:ILE:HD12	2.00	0.43
1:D:482:SER:HA	1:D:504:ILE:O	2.18	0.43
1:A:410:TRP:CZ2	1:B:119:GLU:CB	3.00	0.43
1:B:469:THR:HB	1:B:477:TYR:OH	2.18	0.43
1:B:45:ASN:HB3	1:B:73:GLU:OE1	2.18	0.43
1:B:926:ASP:OD1	1:B:929:ARG:NH1	2.50	0.43
1:A:482:SER:HA	1:A:504:ILE:O	2.18	0.43
1:A:764:MET:N	1:A:765:PRO:CD	2.81	0.43
1:B:787:LYS:HG3	1:B:792:VAL:HG22	1.99	0.43
1:C:7:ASN:O	1:C:153:LYS:NZ	2.52	0.43
1:D:1006:GLU:OE1	1:D:1006:GLU:N	2.52	0.43
1:C:137:ARG:HA	1:C:138:SER:HA	1.77	0.43
1:C:827:ALA:O	1:C:830:VAL:HG22	2.18	0.43
1:D:485:TYR:N	1:D:486:PRO:CD	2.82	0.43
1:A:494:TYR:CD2	1:A:499:ARG:HG3	2.51	0.43
1:C:710:ASP:C	1:C:710:ASP:OD1	2.57	0.43
1:D:118:ILE:HG13	1:D:172:ASN:O	2.18	0.43
1:A:797:VAL:HG13	1:A:807:TYR:CE2	2.53	0.43
1:D:1008:VAL:C	1:D:1009:ILE:CG2	2.84	0.43
1:A:485:TYR:N	1:A:486:PRO:CD	2.82	0.43
1:C:778:ARG:CD	1:C:798:PHE:CE1	3.02	0.43
1:D:377:TYR:O	1:D:381:ASP:OD2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:697:GLU:HG2	1:C:991:VAL:HG13	2.01	0.42
1:B:785:TRP:HA	1:B:793:SER:O	2.19	0.42
1:A:1008:VAL:C	1:A:1009:ILE:CG2	2.85	0.42
1:C:213:ARG:NH1	1:C:235:GLU:OE2	2.46	0.42
1:A:697:GLU:HG2	1:A:991:VAL:HG13	2.02	0.42
1:A:125:PHE:CD2	1:B:551:ASN:O	2.72	0.42
1:B:494:TYR:CE2	1:B:503:PHE:HB2	2.54	0.42
1:C:143:TRP:HA	1:C:147:LYS:O	2.20	0.42
1:C:368:SER:HA	1:C:369:HIS:HA	1.86	0.42
1:D:787:LYS:HG3	1:D:792:VAL:HG22	2.01	0.42
1:A:516:VAL:HG12	1:A:516:VAL:O	2.20	0.42
1:B:7:ASN:HD22	1:B:10:LEU:HD22	1.85	0.42
1:B:807:TYR:CD1	1:B:807:TYR:N	2.88	0.42
1:C:163:LEU:O	1:C:167:LEU:HB2	2.20	0.42
1:C:470:THR:HA	1:C:473:GLY:O	2.20	0.42
1:A:603:SER:OG	1:A:605:ASP:OD1	2.38	0.42
1:D:1014:THR:OG1	1:D:1062:GLU:OE1	2.24	0.42
1:A:752:TRP:O	1:A:835:ARG:HD2	2.19	0.42
1:B:647:GLU:OE1	1:B:649:ARG:NH1	2.53	0.42
1:D:660:ASP:CB	1:D:695:ALA:HB3	2.49	0.42
1:A:137:ARG:HA	1:A:138:SER:HA	1.77	0.42
1:C:726:SER:HG	1:C:729:THR:N	2.17	0.42
1:A:410:TRP:CD2	1:B:119:GLU:HG3	2.50	0.41
1:D:62:PHE:HA	1:D:175:THR:HG21	2.01	0.41
1:A:1072:HIS:HA	1:A:1077:THR:O	2.20	0.41
1:A:494:TYR:CD2	1:A:499:ARG:NE	2.88	0.41
1:A:659:ASP:O	1:A:692:LYS:HE2	2.20	0.41
1:A:807:TYR:N	1:A:807:TYR:CD1	2.88	0.41
1:D:1036:PHE:HB3	1:D:1072:HIS:CE1	2.53	0.41
1:C:764:MET:N	1:C:765:PRO:CD	2.83	0.41
1:D:1019:PHE:CZ	1:D:1073:THR:HG21	2.55	0.41
1:C:413:GLU:HA	1:C:447:ASN:OD1	2.21	0.41
1:A:407:ALA:O	1:A:447:ASN:HB2	2.20	0.41
1:C:515:SER:OG	1:C:516:VAL:N	2.48	0.41
1:C:1007:ASP:HA	1:C:1079:LYS:NZ	2.35	0.41
1:C:1080:THR:HG21	1:C:1082:TYR:OH	2.20	0.41
1:D:764:MET:N	1:D:765:PRO:CD	2.84	0.41
1:A:688:GLN:C	1:A:689:PHE:CD1	2.94	0.41
1:C:411:GLU:HG2	1:C:412:TRP:CD1	2.55	0.41
1:C:61:PHE:CD1	1:C:61:PHE:C	2.94	0.41
1:A:62:PHE:HA	1:A:175:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:PHE:CD1	1:B:338:ASP:N	2.89	0.41
1:A:125:PHE:C	1:A:127:LYS:H	2.23	0.41
1:B:338:ASP:OD2	1:B:349:ARG:NH1	2.53	0.41
1:A:122:GLU:CD	1:B:551:ASN:OD1	2.59	0.41
1:C:857:HIS:HE1	1:C:866:SER:O	2.04	0.41
1:A:1007:ASP:HA	1:A:1079:LYS:HZ1	1.86	0.40
1:A:818:VAL:HG13	1:A:818:VAL:O	2.21	0.40
1:B:1081:ILE:HG22	1:B:1081:ILE:O	2.20	0.40
1:C:46:TRP:CE3	1:C:114:TYR:HB3	2.56	0.40
1:D:1035:LEU:HD11	1:D:1071:ILE:CG2	2.51	0.40
1:C:437:SER:HA	1:C:465:HIS:O	2.21	0.40
1:C:333:ASN:O	1:C:539:ASP:HB2	2.22	0.40
1:A:780:LEU:HD11	1:A:782:LYS:O	2.22	0.40
1:C:1008:VAL:CG2	1:C:1009:ILE:N	2.63	0.40
1:C:1010:ARG:O	1:C:1013:ASP:HB2	2.21	0.40
1:C:798:PHE:HB2	1:C:806:VAL:HG13	2.02	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	1082/1084 (100%)	1001 (92%)	78 (7%)	3 (0%)	41	74
1	B	1082/1084 (100%)	1021 (94%)	57 (5%)	4 (0%)	34	69
1	C	1082/1084 (100%)	1017 (94%)	59 (6%)	6 (1%)	25	62
1	D	1082/1084 (100%)	1020 (94%)	58 (5%)	4 (0%)	34	69
All	All	4328/4336 (100%)	4059 (94%)	252 (6%)	17 (0%)	34	69

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1013	ASP
1	A	846	PHE
1	A	1013	ASP
1	B	86	GLY
1	B	367	THR
1	C	191	ASP
1	C	803	ASN
1	D	976	PHE
1	C	976	PHE
1	D	1013	ASP
1	A	145	ASN
1	B	976	PHE
1	D	719	LYS
1	C	198	ILE
1	C	1009	ILE
1	C	559	GLY
1	D	516	VAL

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	983/983 (100%)	973 (99%)	10 (1%)	76	86
1	B	983/983 (100%)	978 (100%)	5 (0%)	88	94
1	C	983/983 (100%)	971 (99%)	12 (1%)	71	84
1	D	983/983 (100%)	973 (99%)	10 (1%)	76	86
All	All	3932/3932 (100%)	3895 (99%)	37 (1%)	78	88

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	311	ARG
1	A	494	TYR
1	A	726	SER
1	A	753	ARG

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Mol	Chain	Res	Type
1	A	821	ASP
1	A	913	PRO
1	A	985	GLU
1	A	1007	ASP
1	A	1008	VAL
1	B	311	ARG
1	B	700	SER
1	B	753	ARG
1	B	918	SER
1	B	985	GLU
1	C	70	ASN
1	C	270	ASP
1	C	311	ARG
1	C	632	GLU
1	C	700	SER
1	C	726	SER
1	C	753	ARG
1	C	796	SER
1	C	804	SER
1	C	985	GLU
1	C	1007	ASP
1	C	1013	ASP
1	D	70	ASN
1	D	311	ARG
1	D	501	LYS
1	D	571	PHE
1	D	726	SER
1	D	753	ARG
1	D	918	SER
1	D	1007	ASP
1	D	1008	VAL
1	D	1079	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	518	ASN
1	A	1072	HIS
1	B	7	ASN
1	B	79	ASN
1	B	518	ASN

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Mol	Chain	Res	Type
1	B	750	ASN
1	B	931	GLN
1	B	1072	HIS
1	C	79	ASN
1	C	518	ASN
1	C	574	ASN
1	C	931	GLN
1	C	1072	HIS
1	D	7	ASN
1	D	79	ASN
1	D	92	ASN
1	D	361	ASN
1	D	518	ASN
1	D	1072	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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	1083/1084 (99%)	0.39	23 (2%)	63	52	108, 147, 188, 220	0
1	B	1083/1084 (99%)	0.36	33 (3%)	50	37	111, 152, 192, 233	0
1	C	1083/1084 (99%)	0.35	39 (3%)	42	32	113, 154, 196, 236	0
1	D	1083/1084 (99%)	0.37	56 (5%)	27	20	126, 162, 202, 233	0
All	All	4332/4336 (99%)	0.37	151 (3%)	44	33	108, 154, 196, 236	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	150	GLY	5.1
1	D	149	ILE	4.9
1	D	293	TYR	4.2
1	D	198	ILE	3.7
1	D	193	TRP	3.7
1	D	436	TRP	3.7
1	C	177	GLU	3.7
1	B	209	LYS	3.5
1	D	1015	LEU	3.4
1	D	406	LEU	3.4
1	D	236	MET	3.3
1	B	1015	LEU	3.3
1	D	382	TYR	3.2
1	B	1008	VAL	3.2
1	B	126	LYS	3.2
1	A	709	GLU	3.2
1	D	335	HIS	3.2
1	D	114	TYR	3.1
1	A	1015	LEU	3.0
1	D	80	TRP	3.0
1	D	234	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	438	LEU	3.0
1	D	14	GLY	3.0
1	A	198	ILE	2.9
1	C	209	LYS	2.9
1	D	179	LEU	2.9
1	D	1052	PHE	2.9
1	D	393	ILE	2.9
1	D	438	LEU	2.9
1	B	707	LEU	2.9
1	A	438	LEU	2.9
1	D	113	VAL	2.9
1	A	164	THR	2.8
1	D	543	GLN	2.8
1	A	707	LEU	2.7
1	D	840	PHE	2.7
1	C	198	ILE	2.7
1	D	295	LEU	2.7
1	C	727	LYS	2.7
1	D	106	LYS	2.7
1	C	113	VAL	2.7
1	D	886	PRO	2.7
1	B	438	LEU	2.7
1	D	597	VAL	2.7
1	C	365[A]	VAL	2.7
1	D	177	GLU	2.7
1	C	406	LEU	2.6
1	A	1007	ASP	2.6
1	A	810	TYR	2.6
1	B	1033	VAL	2.6
1	B	727	LYS	2.6
1	D	838	PHE	2.6
1	A	994	ALA	2.6
1	B	240	GLY	2.5
1	A	131	LEU	2.5
1	D	176	VAL	2.5
1	C	95	TYR	2.5
1	D	103	PHE	2.5
1	D	707	LEU	2.5
1	A	749	PRO	2.5
1	D	230	ILE	2.5
1	B	127	LYS	2.5
1	C	179	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	994	ALA	2.5
1	A	695	ALA	2.5
1	A	382	TYR	2.4
1	B	1031	LYS	2.4
1	D	174	ILE	2.4
1	D	6	GLU	2.4
1	D	268	PRO	2.4
1	C	10	LEU	2.4
1	C	1033	VAL	2.4
1	A	209	LYS	2.4
1	D	1047	VAL	2.4
1	B	236	MET	2.4
1	C	781	PHE	2.4
1	C	297	LEU	2.4
1	D	187	LEU	2.4
1	A	725	PHE	2.4
1	C	351	ILE	2.4
1	C	193	TRP	2.4
1	C	749	PRO	2.4
1	C	921	PRO	2.4
1	B	1070	LEU	2.3
1	D	215	VAL	2.3
1	D	749	PRO	2.3
1	C	869	PHE	2.3
1	C	149	ILE	2.3
1	C	127	LYS	2.3
1	D	310	PHE	2.3
1	B	749	PRO	2.3
1	C	840	PHE	2.3
1	C	604	LYS	2.3
1	B	193	TRP	2.3
1	A	604	LYS	2.3
1	C	1082	TYR	2.3
1	B	242	GLU	2.3
1	A	295	LEU	2.3
1	C	1015	LEU	2.3
1	D	545	ILE	2.2
1	B	1017	VAL	2.2
1	C	597	VAL	2.2
1	C	599	ILE	2.2
1	D	95	TYR	2.2
1	C	187	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	122	GLU	2.2
1	C	1084	ARG	2.2
1	D	308	PHE	2.2
1	C	236	MET	2.2
1	B	308	PHE	2.2
1	B	557	ALA	2.2
1	D	1032	GLN	2.2
1	D	1059	PHE	2.2
1	B	310	PHE	2.2
1	B	907	LEU	2.2
1	B	198	ILE	2.2
1	C	80	TRP	2.2
1	B	268	PRO	2.2
1	D	151	PHE	2.2
1	C	884	VAL	2.2
1	D	243	GLU	2.2
1	D	747	VAL	2.1
1	A	231	PHE	2.1
1	B	1049	ILE	2.1
1	A	383	PHE	2.1
1	B	37	GLU	2.1
1	A	1033	VAL	2.1
1	D	231	PHE	2.1
1	C	741	LYS	2.1
1	C	310	PHE	2.1
1	D	907	LEU	2.1
1	D	1026	PRO	2.1
1	D	1061	VAL	2.1
1	B	62	PHE	2.1
1	D	297	LEU	2.1
1	A	126	LYS	2.1
1	D	1031	LYS	2.1
1	B	177	GLU	2.1
1	D	1043	SER	2.0
1	B	131	LEU	2.0
1	B	792	VAL	2.0
1	C	880	MET	2.0
1	B	597	VAL	2.0
1	A	691	LEU	2.0
1	B	795	HIS	2.0
1	C	907	LEU	2.0
1	B	306	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	308	PHE	2.0
1	D	885	ARG	2.0
1	A	273	LEU	2.0
1	B	4	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 carbohydrates in this entry.

6.4 Ligands (i)

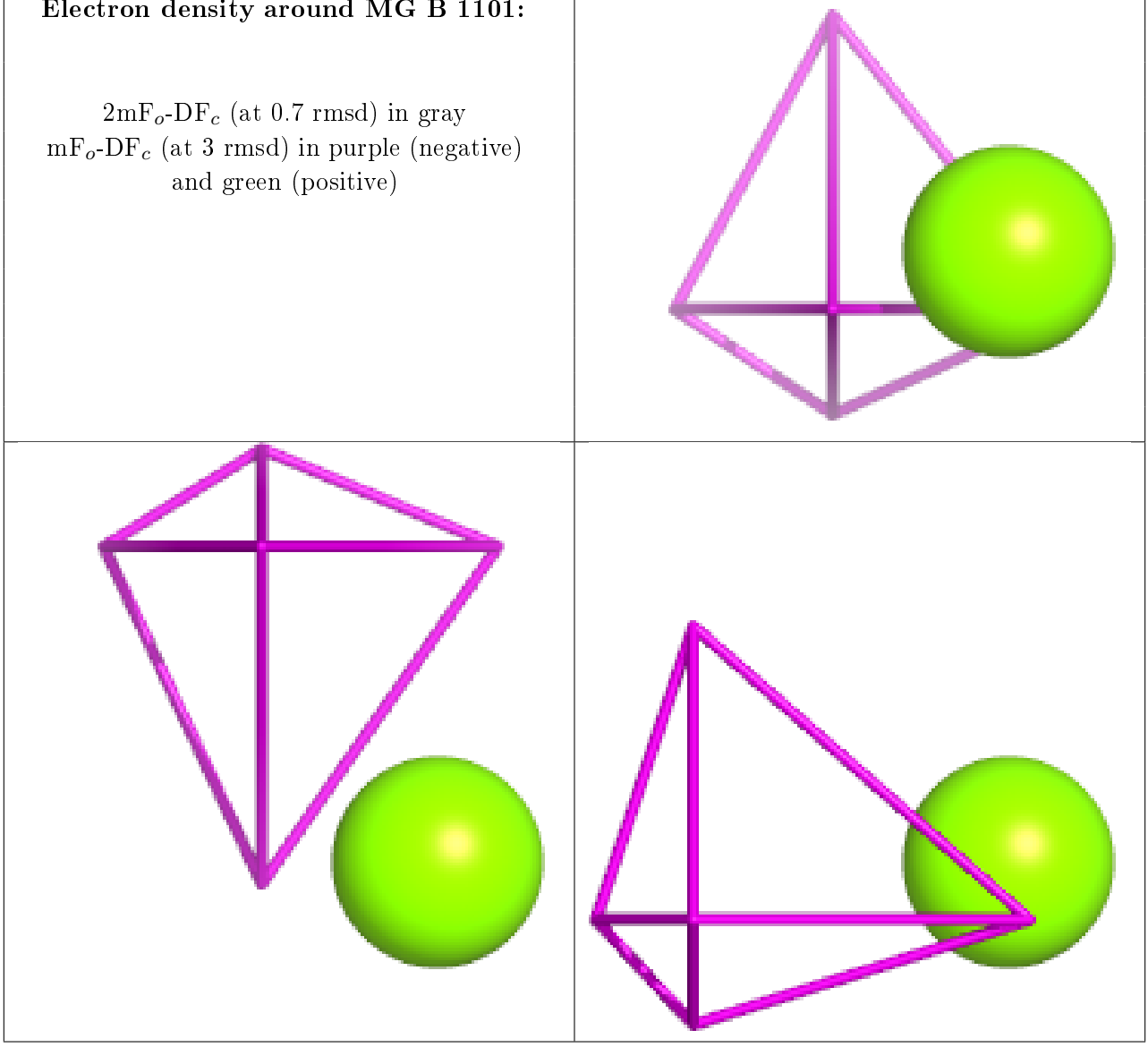
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	1101	1/1	0.88	0.17	41,41,41,41	0
2	MG	C	1101	1/1	0.93	0.15	40,40,40,40	0
2	MG	D	1101	1/1	0.96	0.14	41,41,41,41	0
2	MG	A	1101	1/1	0.98	0.13	39,39,39,39	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.

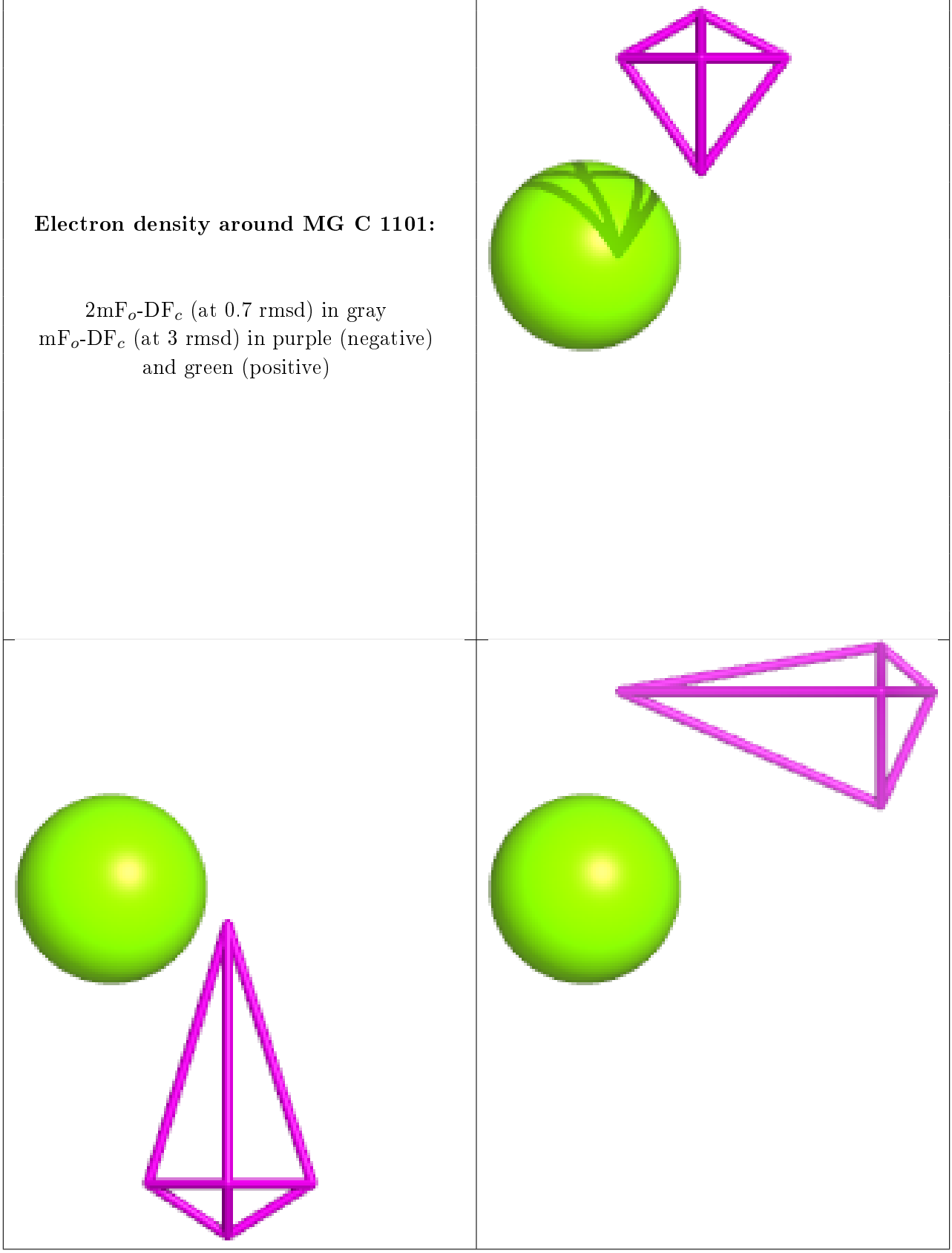
Electron density around MG B 1101:

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



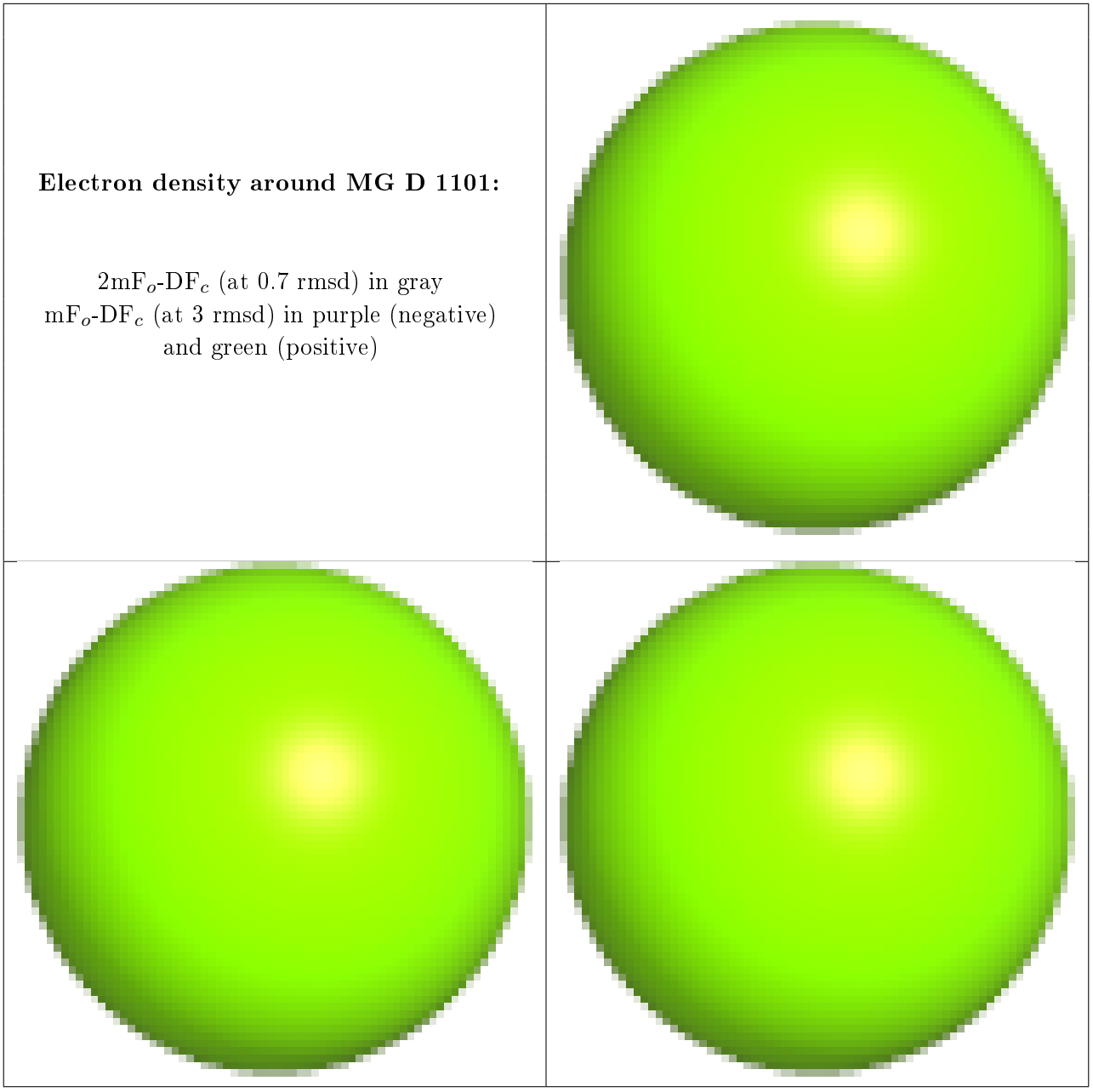
Electron density around MG C 1101:

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



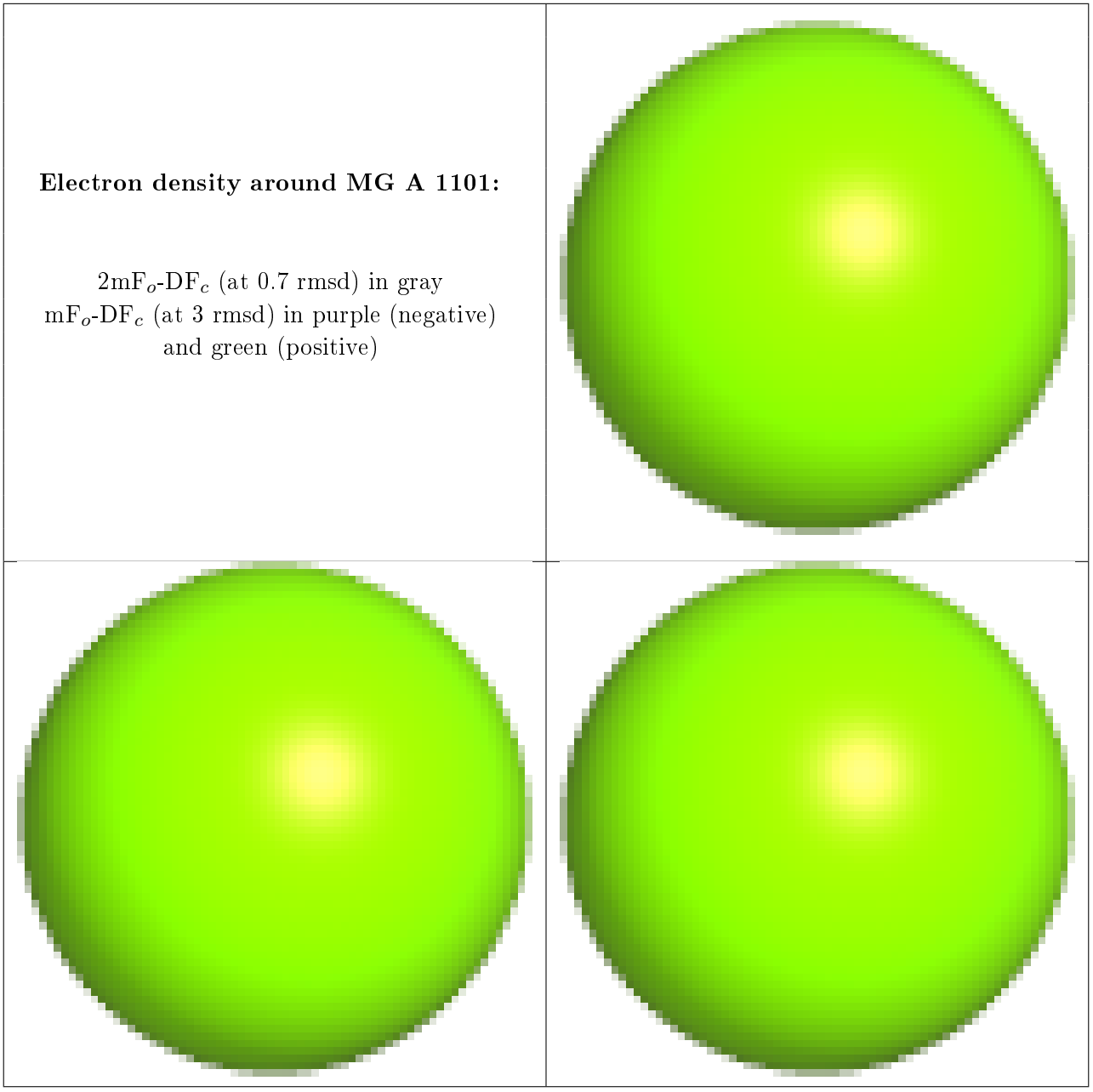
Electron density around MG D 1101:

$2mF_o$-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 1101:

$2mF_o$-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.