



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 6, 2026 – 11:26 AM UTC

PDB ID : 6SD0 / pdb_00006sd0
Title : Structure of beta-galactosidase from *Thermotoga maritima*.
Authors : Jimenez-Ortega, E.; Ramirez-Escudero, M.; Sanz-Aparicio, J.
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

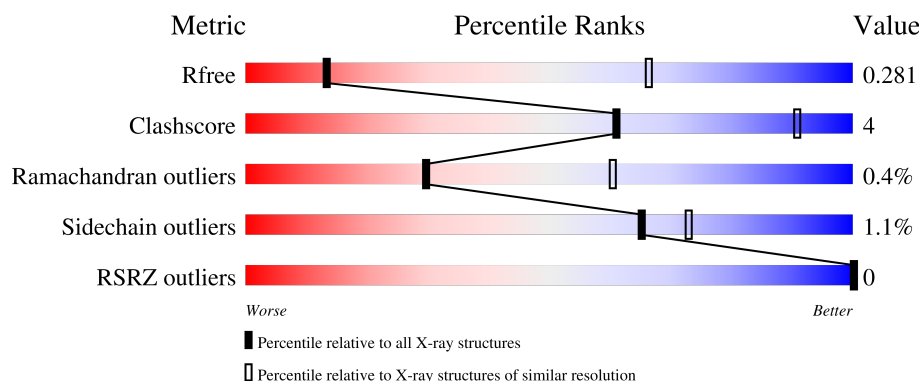
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	1084	
1	B	1084	
1	C	1084	
1	D	1084	

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 (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

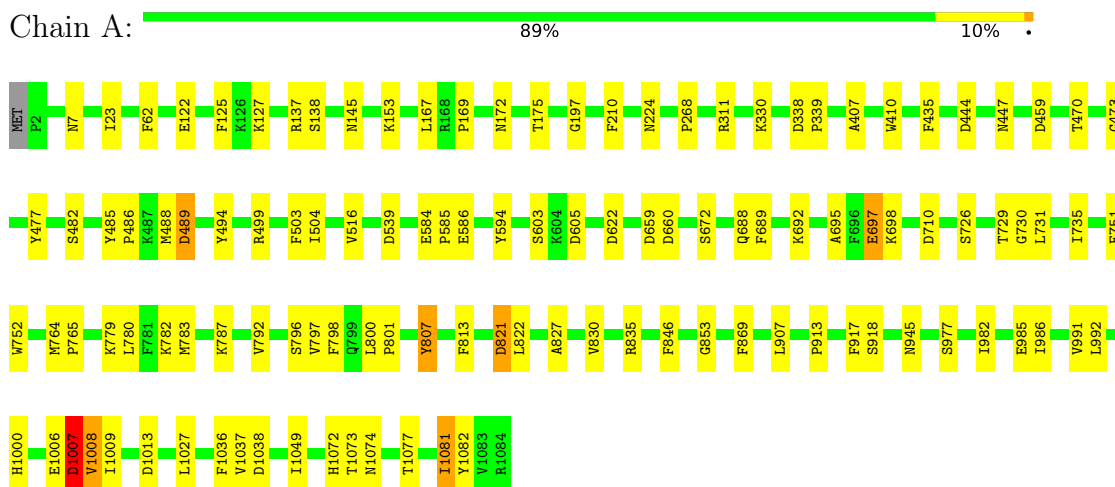
- Molecule 3 is water.

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		

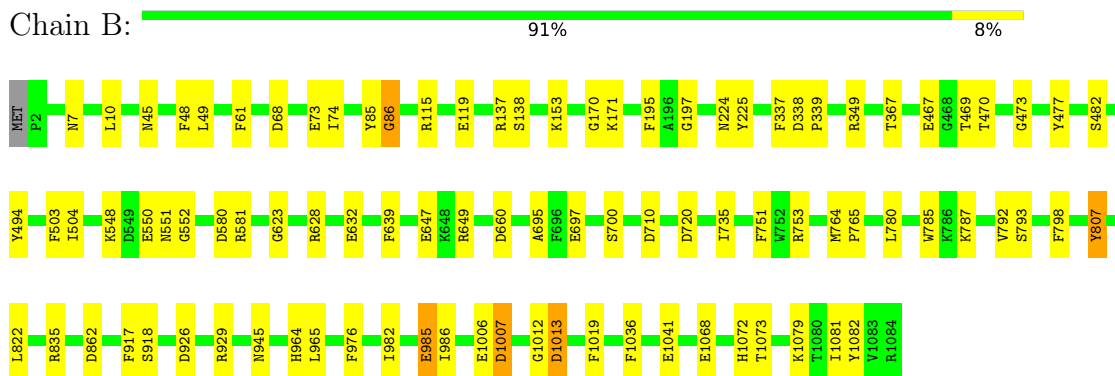
3 Residue-property plots

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.

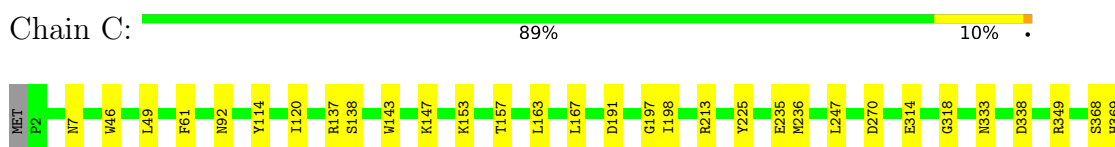
• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase

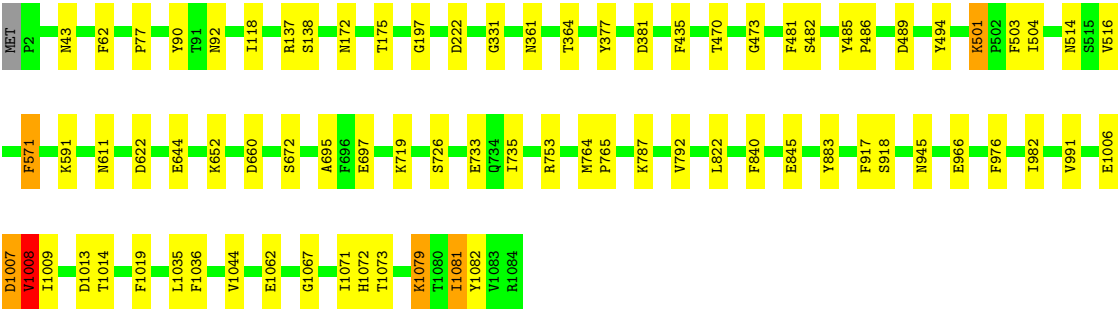


• Molecule 1: Beta-galactosidase





● Molecule 1: Beta-galactosidase



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.66Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.241 , 0.285 0.240 , 0.281	Depositor DCC
R_{free} test set	3722 reflections (4.88%)	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)	0.33 , 100.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	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	nan	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.04	2/9303 (0.0%)	1.33	15/12600 (0.1%)
1	B	1.06	1/9303 (0.0%)	1.33	10/12600 (0.1%)
1	C	1.05	2/9303 (0.0%)	1.33	10/12600 (0.1%)
1	D	1.10	1/9303 (0.0%)	1.36	8/12600 (0.1%)
All	All	1.06	6/37212 (0.0%)	1.34	43/50400 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1008	VAL	C-N	6.07	1.37	1.33
1	A	23	ILE	N-CA	5.76	1.50	1.45
1	C	986	ILE	N-CA	5.31	1.50	1.46
1	A	986	ILE	N-CA	5.24	1.50	1.46
1	C	120	ILE	N-CA	5.08	1.50	1.46
1	B	986	ILE	N-CA	5.05	1.50	1.46

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1007	ASP	CB-CA-C	7.65	124.57	110.11
1	C	798	PHE	CB-CA-C	-7.40	99.43	110.24
1	C	1082	TYR	CB-CA-C	7.37	121.96	109.80
1	D	1082	TYR	CB-CA-C	6.88	121.87	109.83
1	A	1007	ASP	CB-CA-C	6.62	123.68	110.17
1	A	1082	TYR	CB-CA-C	6.49	120.61	109.51
1	C	435	PHE	CA-CB-CG	6.04	119.84	113.80
1	A	807	TYR	CB-CA-C	5.77	119.17	109.48
1	B	1082	TYR	CB-CA-C	5.76	119.24	109.50
1	B	1041	GLU	CB-CA-C	-5.72	101.97	110.67
1	C	197	GLY	CA-C-O	-5.65	118.55	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	435	PHE	CA-CB-CG	5.62	119.42	113.80
1	B	197	GLY	CA-C-O	-5.61	118.41	122.45
1	A	435	PHE	CA-CB-CG	5.58	119.39	113.80
1	A	1007	ASP	N-CA-C	-5.57	106.33	113.01
1	D	1067	GLY	CA-C-O	-5.49	118.50	122.45
1	A	539	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	862	ASP	CA-CB-CG	5.43	118.03	112.60
1	C	985	GLU	CA-C-N	5.40	126.27	122.60
1	C	985	GLU	C-N-CA	5.40	126.27	122.60
1	B	807	TYR	CB-CA-C	5.40	119.10	109.38
1	D	1007	ASP	CB-CA-C	5.38	120.89	110.46
1	A	489	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	197	GLY	CA-C-O	-5.36	118.59	122.45
1	D	222	ASP	CA-CB-CG	5.33	117.93	112.60
1	D	840	PHE	CA-CB-CG	5.33	119.12	113.80
1	D	197	GLY	CA-C-O	-5.31	118.77	122.22
1	C	781	PHE	CA-CB-CG	5.30	119.10	113.80
1	B	985	GLU	CA-C-N	5.19	126.13	122.60
1	B	985	GLU	C-N-CA	5.19	126.13	122.60
1	A	697	GLU	CB-CA-C	5.17	118.34	109.51
1	A	1000	HIS	CB-CA-C	5.15	118.23	109.53
1	A	813	PHE	CA-C-N	5.11	125.75	120.03
1	A	813	PHE	C-N-CA	5.11	125.75	120.03
1	B	697	GLU	CB-CA-C	5.09	118.21	109.51
1	C	157	THR	CB-CA-C	5.05	116.81	109.08
1	A	710	ASP	CA-C-N	5.04	125.68	120.03
1	A	710	ASP	C-N-CA	5.04	125.68	120.03
1	B	1068	GLU	CB-CA-C	5.03	118.71	109.46
1	D	489	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	1049	ILE	CB-CA-C	5.01	116.07	110.71
1	C	697	GLU	CB-CA-C	5.01	118.08	109.51
1	C	1007	ASP	CB-CA-C	5.00	121.16	110.21

There are no chirality outliers.

There are no planarity outliers.

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	9032	0	8777	122	0
1	B	9032	0	8777	84	0
1	C	9032	0	8777	75	0
1	D	9032	0	8777	53	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	302	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 (302) 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:410:TRP:CZ2	1:B:119:GLU:CG	2.41	1.02
1:A:494:TYR:CD1	1:A:503:PHE:CD2	2.47	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:167:LEU:C	1:B:548:LYS:HE2	1.99	0.88
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:O	1:B:548:LYS:CE	2.25	0.84
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:167:LEU:C	1:B:548:LYS:CE	2.57	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:C:1008:VAL:C	1:C:1009:ILE:HG23	2.08	0.76
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: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:1080:THR:HG22	1:C:1082:TYR:CZ	2.26	0.71
1:C:1007:ASP:OD1	1:C:1007:ASP:N	2.23	0.70
1:B:780:LEU:HB2	1:B:798:PHE:HE1	1.56	0.70
1:D:1008:VAL:C	1:D:1009:ILE:HG23	2.17	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:167:LEU:O	1:B:548:LYS:HE3	1.91	0.70
1:A:1036:PHE:HB2	1:A:1072:HIS:CE1	2.27	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:A:1008:VAL:C	1:A:1009:ILE:HG23	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ASN:OD1	1:D:652:LYS:CE	2.43	0.66
1:A:169:PRO:HD3	1:B:552:GLY:C	2.21	0.66
1:A:796:SER:HB2	1:A:798:PHE:HE2	1.60	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: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:N	1:A:1007:ASP:OD2	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:169:PRO:HG3	1:B:551:ASN:C	2.23	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: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: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:224:ASN:O	1:B:225:TYR:HB2	2.06	0.55
1:B:1019:PHE:CE1	1:B:1073:THR:HG21	2.42	0.55
1:C:857:HIS:CE1	1:C:866:SER:O	2.60	0.55
1:D:1044:VAL:O	1:D:1044:VAL:HG13	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:A:821:ASP:CG	1:A:977:SER:HB3	2.31	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:A:459:ASP:C	1:A:459:ASP:OD1	2.49	0.53
1:B:1019:PHE:CZ	1:B:1073:THR:HG21	2.43	0.53
1:B:338:ASP:CG	1:B:339:PRO:HD2	2.33	0.53
1:D:43:ASN:ND2	1:D:77:PRO:HD3	2.23	0.53
1:D:361:ASN:ND2	1:D:591:LYS:HG3	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:822:LEU:C	1:A:822:LEU:HD23	2.35	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:167:LEU:C	1:B:548:LYS:HE3	2.33	0.52
1:A:410:TRP:HB2	1:B:171:LYS:HD2	1.92	0.52
1:A:584:GLU:O	1:A:585:PRO:C	2.53	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:622:ASP:OD2	1:A:672:SER:HA	2.10	0.51
1:A:1081:ILE:HG22	1:A:1081:ILE:O	2.10	0.51
1:B:1006:GLU:OE1	1:B:1006:GLU:N	2.41	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:C:1006:GLU:OE1	1:C:1006:GLU:N	2.31	0.51
1:D:735:ILE:HG21	1:D:982:ILE:HD12	1.93	0.50
1:D:1008:VAL:HG22	1:D:1009:ILE:N	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:1008:VAL:C	1:D:1009:ILE:CG2	2.84	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
1:A:410:TRP:CZ3	1:B:119:GLU:CG	2.94	0.49
1:A:1073:THR:CG2	1:A:1074:ASN:N	2.65	0.49
1:A:796:SER:HB3	1:A:798:PHE:CZ	2.48	0.49
1:A:821:ASP:CG	1:A:1027:LEU:HD22	2.37	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:C:441:GLU:OE2	1:C:484:MET:HE1	2.13	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: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:C:710:ASP:C	1:C:710:ASP:OD1	2.57	0.48
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: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: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:A:688:GLN:C	1:A:689:PHE:CD1	2.94	0.46
1:B:1019:PHE:CZ	1:B:1073:THR:CG2	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:PHE:CD1	1:C:61:PHE:C	2.94	0.46
1:D:622:ASP:OD2	1:D:672:SER:HA	2.16	0.45
1:A:122:GLU:CD	1:B:551:ASN:OD1	2.59	0.45
1:A:751:PHE:HA	1:A:835:ARG:O	2.17	0.45
1:A:125:PHE:C	1:A:127:LYS:H	2.23	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
1:C:1036:PHE:HB3	1:C:1072:HIS:CE1	2.50	0.45
1:A:311:ARG:HD2	1:A:311:ARG:O	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:B:467:GLU:CD	1:B:467:GLU:C	2.84	0.45
1:A:494:TYR:CE1	1:A:503:PHE:CD2	3.02	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:A:488:MET:O	1:A:489:ASP:C	2.60	0.44
1:B:48:PHE:HB2	1:B:74:ILE:HG22	2.00	0.44
1:B:623:GLY:O	1:B:639:PHE:N	2.43	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:735:ILE:HG21	1:B:982:ILE:HD12	2.00	0.44
1:B:1012:GLY:O	1:B:1013:ASP:O	2.36	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:B:119:GLU:OE1	1:B:170:GLY:C	2.61	0.44
1:C:92:ASN:ND2	1:C:571:PHE:CE2	2.86	0.44
1:C:494:TYR:CE2	1:C:503:PHE:HB2	2.52	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:45:ASN:HB3	1:B:73:GLU:OE1	2.18	0.43
1:B:469:THR:HB	1:B:477:TYR:OH	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:N	1:D:1006:GLU:OE1	2.52	0.43
1:A:1008:VAL:C	1:A:1009:ILE:CG2	2.85	0.43
1:C:137:ARG:HA	1:C:138:SER:HA	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:517:GLY:O	1:C:518:ASN:CG	2.62	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:A:485:TYR:N	1:A:486:PRO:CD	2.82	0.43
1:A:800:LEU:O	1:A:801:PRO:C	2.61	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
1:A:1037:VAL:O	1:A:1038:ASP:C	2.61	0.42
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:C:213:ARG:NH1	1:C:235:GLU:OE2	2.46	0.42
1:D:611:ASN:HD22	1:D:644:GLU:C	2.27	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:B:710:ASP:OD1	1:B:710:ASP:C	2.62	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:494:TYR:CD2	1:A:499:ARG:NE	2.88	0.41
1:A:1072:HIS:HA	1:A:1077:THR:O	2.20	0.41
1:A:659:ASP:O	1:A:692:LYS:HE2	2.20	0.41
1:A:807:TYR:CD1	1:A:807:TYR:N	2.88	0.41
1:B:61:PHE:CD1	1:B:61:PHE:C	2.98	0.41
1:D:1036:PHE:HB3	1:D:1072:HIS:CE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:964:HIS:O	1:B:965:LEU:C	2.64	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:A:907:LEU:HD23	1:A:907:LEU:C	2.46	0.41
1:C:515:SER:OG	1:C:516:VAL:N	2.48	0.41
1:D:514:ASN:CG	1:D:883:TYR:HH	2.28	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:B:85:TYR:C	1:B:86:GLY:O	2.64	0.41
1:B:822:LEU:HD23	1:B:822:LEU:C	2.45	0.41
1:C:411:GLU:HG2	1:C:412:TRP:CD1	2.55	0.41
1:A:62:PHE:HA	1:A:175:THR:HG21	2.02	0.41
1:B:337:PHE:CD1	1:B:338:ASP:N	2.89	0.41
1:C:236:MET:HE1	1:C:247:LEU:HD22	2.03	0.41
1:C:907:LEU:HD23	1:C:907:LEU:C	2.46	0.41
1:A:410:TRP:CE2	1:B:119:GLU:CD	2.99	0.41
1:B:338:ASP:OD2	1:B:349:ARG:NH1	2.53	0.41
1:C:857:HIS:HE1	1:C:866:SER:O	2.04	0.41
1:C:46:TRP:CE3	1:C:114:TYR:HB3	2.56	0.40
1:C:726:SER:HG	1:C:729:THR:H	1.63	0.40
1:D:1035:LEU:HD11	1:D:1071:ILE:CG2	2.51	0.40
1:C:333:ASN:O	1:C:539:ASP:HB2	2.22	0.40
1:C:437:SER:HA	1:C:465:HIS:O	2.21	0.40
1:C:726:SER:HG	1:C:729:THR:N	2.19	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:D:822:LEU:HD23	1:D:822:LEU:C	2.47	0.40
1:A:444:ASP:OD1	1:A:477:TYR:OH	2.40	0.40
1:C:798:PHE:HB2	1:C:806:VAL:HG13	2.02	0.40
1:C:1010:ARG:O	1:C:1013:ASP:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	36	65
1	B	1082/1084 (100%)	1021 (94%)	57 (5%)	4 (0%)	30	60
1	C	1082/1084 (100%)	1017 (94%)	59 (6%)	6 (1%)	21	52
1	D	1082/1084 (100%)	1020 (94%)	58 (5%)	4 (0%)	30	60
All	All	4328/4336 (100%)	4059 (94%)	252 (6%)	17 (0%)	30	60

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

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%)	972 (99%)	11 (1%)	65	73
1	B	983/983 (100%)	977 (99%)	6 (1%)	78	79
1	C	983/983 (100%)	970 (99%)	13 (1%)	61	71
1	D	983/983 (100%)	971 (99%)	12 (1%)	63	72
All	All	3932/3932 (100%)	3890 (99%)	42 (1%)	65	73

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	586	GLU
1	A	726	SER
1	A	779	LYS
1	A	821	ASP
1	A	913	PRO
1	A	918	SER
1	A	985	GLU
1	A	1007	ASP
1	A	1008	VAL
1	A	1081	ILE
1	B	49	LEU
1	B	700	SER
1	B	753	ARG
1	B	918	SER
1	B	985	GLU
1	B	1081	ILE
1	C	49	LEU
1	C	270	ASP
1	C	632	GLU
1	C	700	SER
1	C	726	SER
1	C	796	SER
1	C	804	SER
1	C	845	GLU
1	C	966	GLU
1	C	985	GLU
1	C	1007	ASP

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Mol	Chain	Res	Type
1	C	1013	ASP
1	C	1081	ILE
1	D	501	LYS
1	D	571	PHE
1	D	726	SER
1	D	733	GLU
1	D	753	ARG
1	D	845	GLU
1	D	918	SER
1	D	966	GLU
1	D	1007	ASP
1	D	1008	VAL
1	D	1079	LYS
1	D	1081	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	713	HIS
1	A	766	GLN
1	A	1072	HIS
1	B	7	ASN
1	B	79	ASN
1	B	92	ASN
1	B	307	ASN
1	B	440	ASN
1	B	518	ASN
1	B	1072	HIS
1	C	79	ASN
1	C	92	ASN
1	C	440	ASN
1	C	839	GLN
1	C	932	HIS
1	C	945	ASN
1	C	1072	HIS
1	D	7	ASN
1	D	79	ASN
1	D	92	ASN
1	D	307	ASN
1	D	361	ASN
1	D	440	ASN

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Mol	Chain	Res	Type
1	D	518	ASN
1	D	611	ASN
1	D	766	GLN
1	D	795	HIS
1	D	857	HIS
1	D	1072	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1083/1084 (99%)	-0.89	0 100 100	79, 147, 188, 220	1 (0%)
1	B	1083/1084 (99%)	-0.89	0 100 100	86, 152, 192, 233	1 (0%)
1	C	1083/1084 (99%)	-0.88	0 100 100	84, 154, 196, 236	1 (0%)
1	D	1083/1084 (99%)	-0.81	0 100 100	85, 162, 202, 233	1 (0%)
All	All	4332/4336 (99%)	-0.87	0 100 100	79, 154, 196, 236	4 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

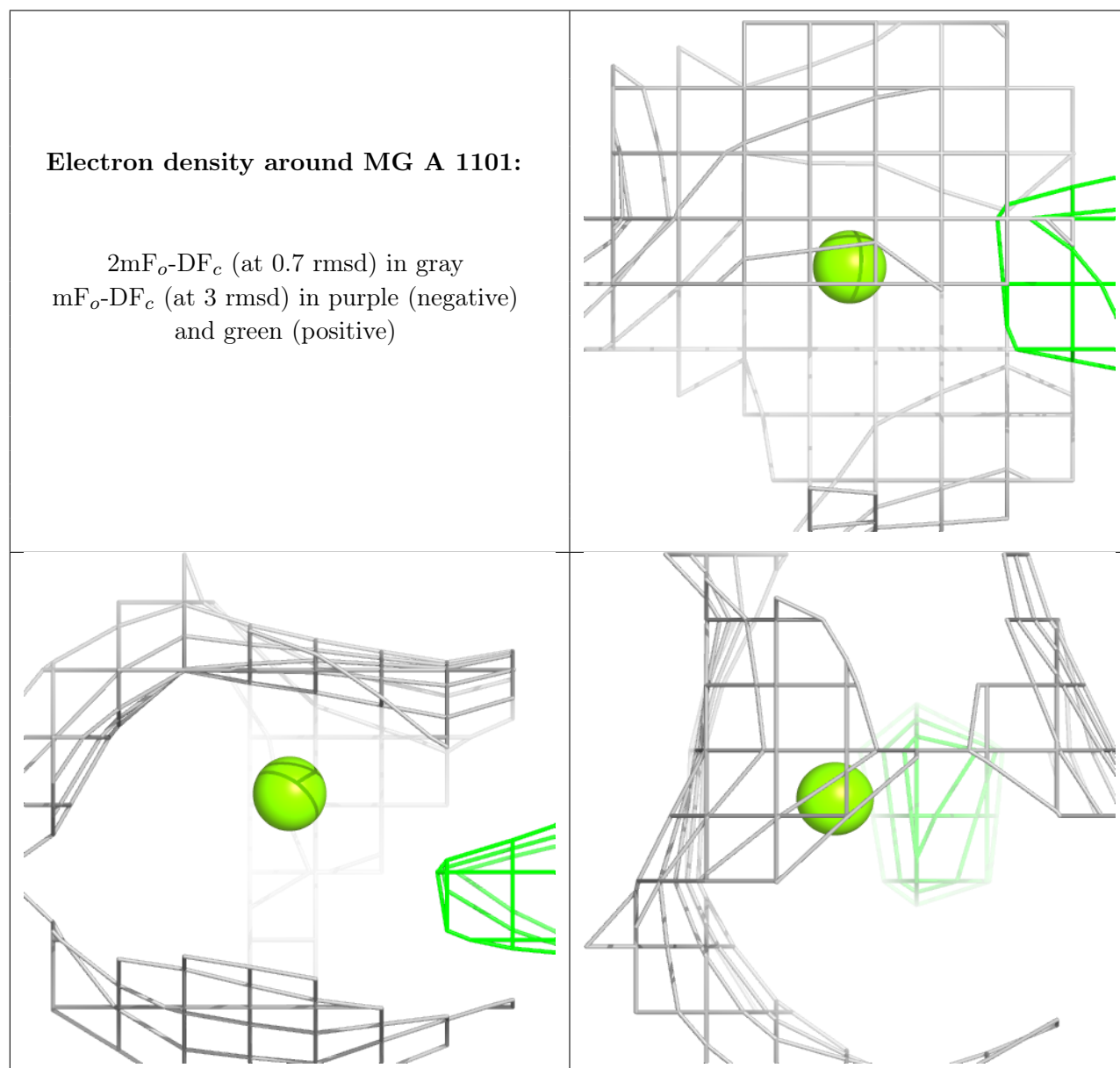
There are no oligosaccharides in this entry.

6.4 Ligands [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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

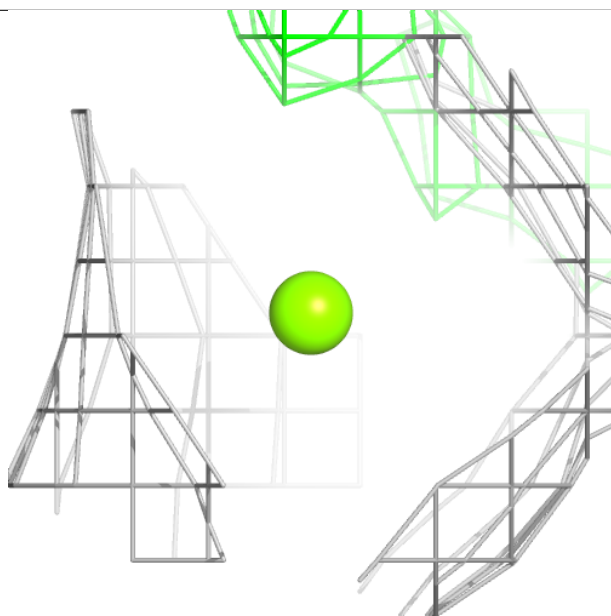
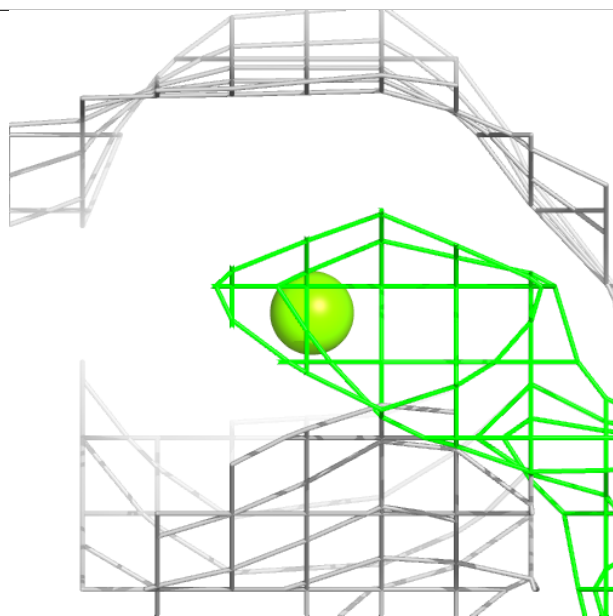
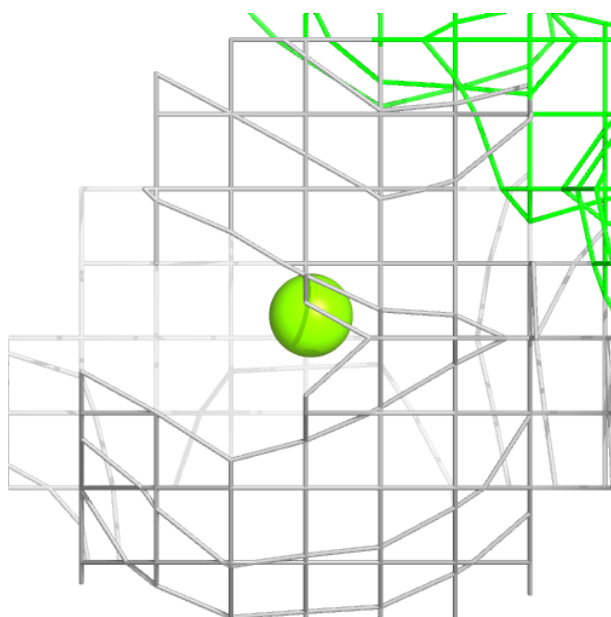
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	1101	1/1	0.99	0.03	39,39,39,39	0
2	MG	B	1101	1/1	0.99	0.03	41,41,41,41	0
2	MG	D	1101	1/1	0.99	0.02	41,41,41,41	0
2	MG	C	1101	1/1	1.00	0.02	40,40,40,40	0

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.



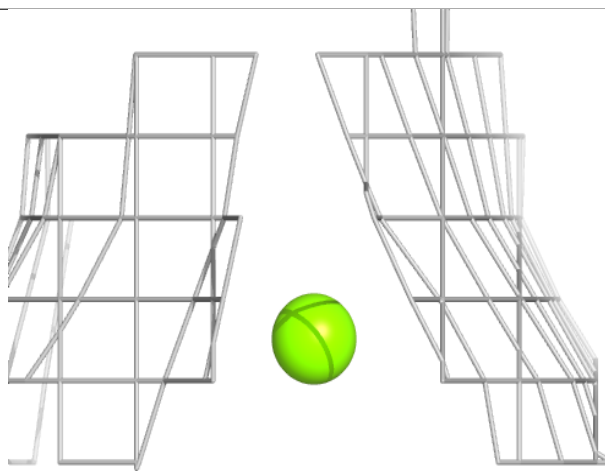
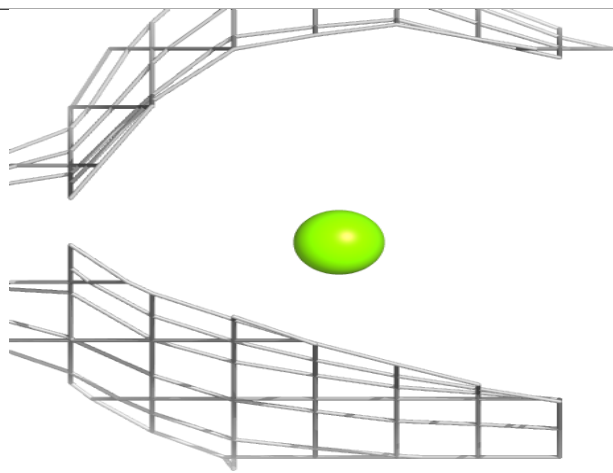
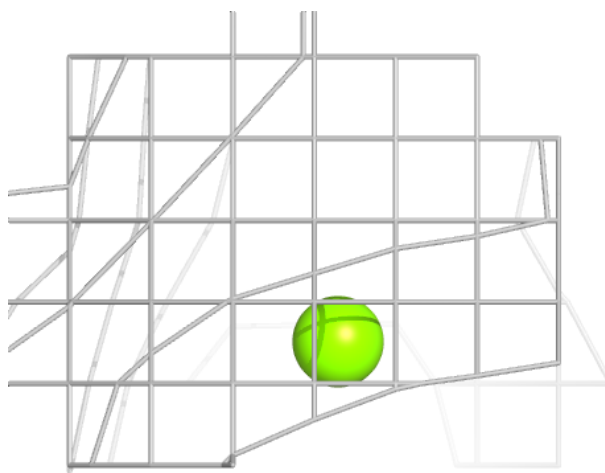
Electron density around MG B 1101:

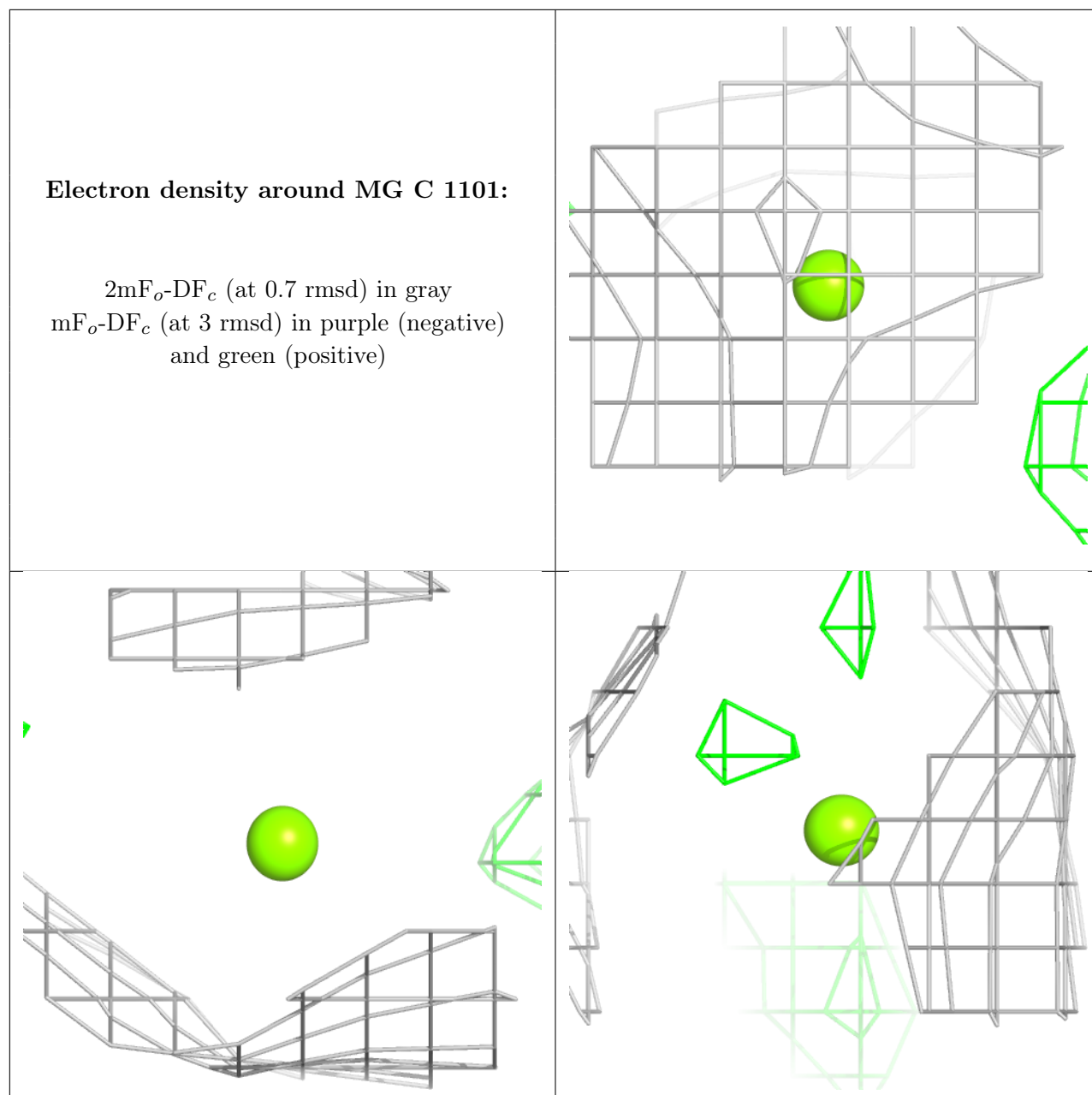
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.