



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 28, 2024 – 12:43 AM EST

PDB ID : 1DQ9
Title : COMPLEX OF CATALYTIC PORTION OF HUMAN HMG-COA REDUC-TASE WITH HMG-COA
Authors : Istvan, E.S.; Palnitkar, M.; Buchanan, S.K.; Deisenhofer, J.
Deposited on : 1999-12-30
Resolution : 2.80 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

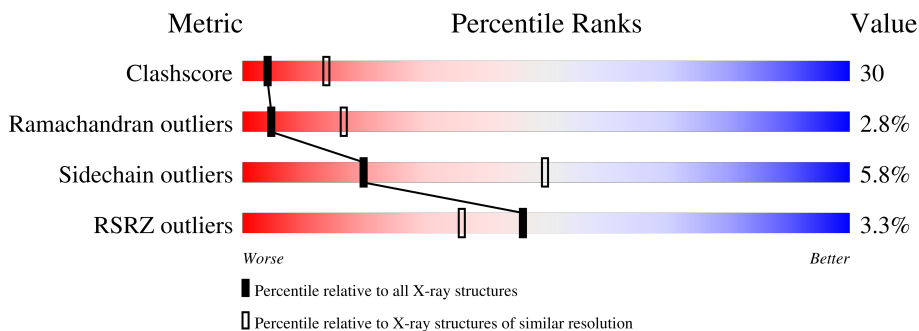
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	467	 2% 49% 33% 5% 13%
1	B	467	 2% 45% 38% • 13%
1	C	467	 3% 48% 33% 6% 13%
1	D	467	 3% 48% 34% 6% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12351 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.

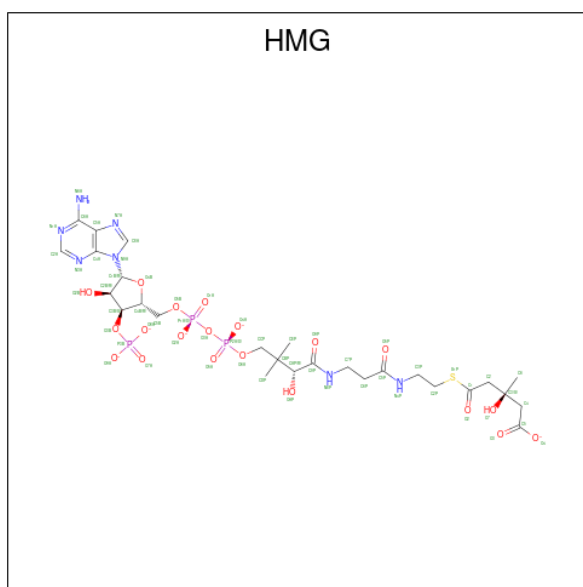
- Molecule 1 is a protein called PROTEIN (HMG-COA REDUCTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	405	3011	1879	528	575	29	0	0	0
1	B	405	3014	1882	529	574	29	0	0	0
1	C	407	3030	1891	533	577	29	0	0	0
1	D	413	3064	1910	539	586	29	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	485	ILE	MET	engineered mutation	UNP P04035
B	485	ILE	MET	engineered mutation	UNP P04035
C	485	ILE	MET	engineered mutation	UNP P04035
D	485	ILE	MET	engineered mutation	UNP P04035

- Molecule 2 is 3-HYDROXY-3-METHYLGLUTARYL-COENZYME A (three-letter code: HMG) (formula: $C_{27}H_{39}N_7O_{20}P_3S$).

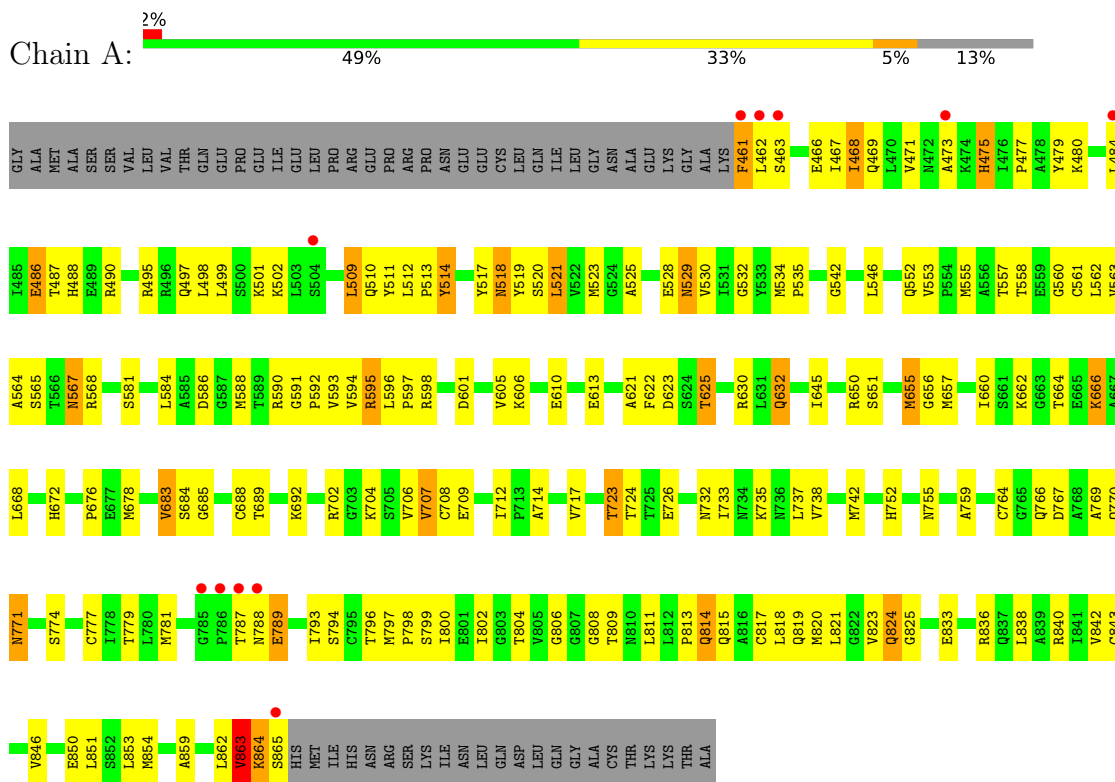


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf		
			Total	C	N	O	P			S	
2	A	1	Total	58	27	7	20	3	1	0	0
2	B	1	Total	58	27	7	20	3	1	0	0
2	C	1	Total	58	27	7	20	3	1	0	0
2	D	1	Total	58	27	7	20	3	1	0	0

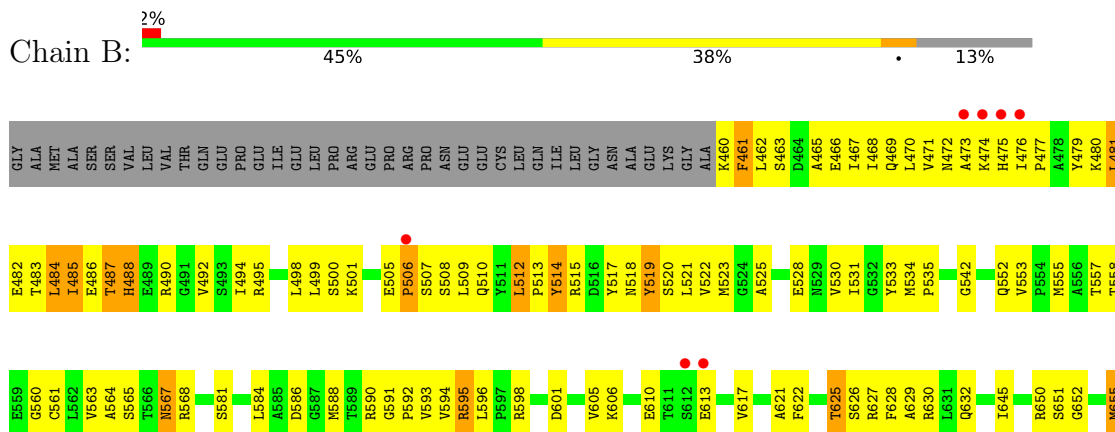
3 Residue-property plots i

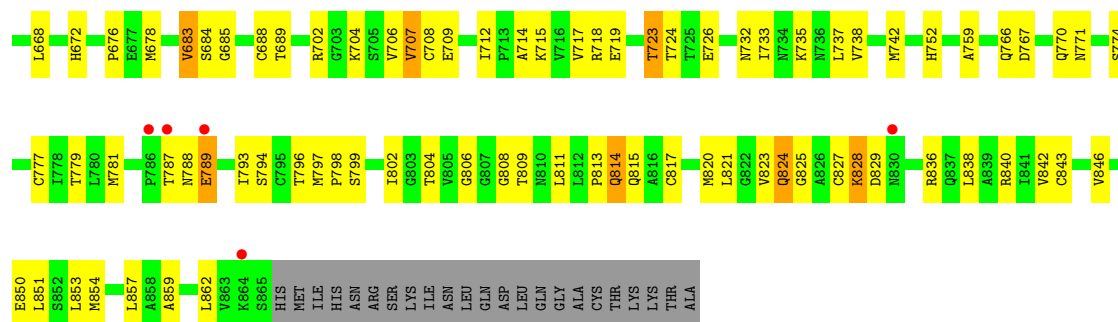
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PROTEIN (HMG-COA REDUCTASE)



• Molecule 1: PROTEIN (HMG-COA REDUCTASE)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.58Å 171.20Å 80.37Å 90.00° 116.59° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80 24.79 – 2.81	Depositor EDS
% Data completeness (in resolution range)	85.1 (25.00-2.80) 42.6 (24.79-2.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.80Å)	Xtrriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.207 , 0.247 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtrriage
Anisotropy	0.262	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 65.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.057 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12351	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.56	1/3055 (0.0%)	0.75	1/4131 (0.0%)
1	B	0.55	0/3058	0.74	0/4134
1	C	0.54	1/3075 (0.0%)	0.72	0/4157
1	D	0.53	0/3108	0.72	1/4200 (0.0%)
All	All	0.54	2/12296 (0.0%)	0.73	2/16622 (0.0%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	527	CYS	CB-SG	-5.35	1.73	1.81
1	A	771	ASN	CG-OD1	5.03	1.35	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	863	VAL	CB-CA-C	6.13	123.04	111.40
1	D	568	ARG	NE-CZ-NH2	5.27	122.93	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	479	TYR	Sidechain

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	3011	0	3054	184	0
1	B	3014	0	3062	206	0
1	C	3030	0	3074	206	0
1	D	3064	0	3108	190	0
2	A	58	0	39	3	0
2	B	58	0	39	5	0
2	C	58	0	39	5	0
2	D	58	0	39	5	0
All	All	12351	0	12454	739	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (739) 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:518:ASN:HD21	1:A:521:LEU:HD22	1.05	1.17
1:A:732:ASN:HB2	1:A:781:MET:HE2	1.33	1.11
1:C:584:LEU:HD11	1:C:707:VAL:HG22	1.33	1.10
1:B:584:LEU:HD11	1:B:707:VAL:HG22	1.37	1.06
1:A:584:LEU:HD11	1:A:707:VAL:HG22	1.36	1.06
1:B:732:ASN:HB2	1:B:781:MET:HE2	1.38	1.05
1:D:584:LEU:HD11	1:D:707:VAL:HG22	1.38	1.03
1:A:499:LEU:HD11	1:B:552:GLN:HG3	1.40	1.02
1:D:732:ASN:HB2	1:D:781:MET:HE2	1.45	0.98
1:B:467:ILE:HD11	1:B:490:ARG:NH2	1.80	0.96
1:A:518:ASN:ND2	1:A:521:LEU:HD22	1.84	0.93
1:B:461:PHE:N	1:B:461:PHE:HD1	1.67	0.91
1:C:732:ASN:HB2	1:C:781:MET:HE2	1.52	0.89
1:D:806:GLY:O	1:D:809:THR:HB	1.70	0.89
1:C:806:GLY:O	1:C:809:THR:HB	1.72	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:LYS:NZ	1:C:474:LYS:HA	1.88	0.88
1:A:484:LEU:HD23	1:A:484:LEU:O	1.74	0.88
1:A:463:SER:OG	1:A:466:GLU:HG3	1.74	0.88
1:A:564:ALA:HB2	1:B:528:GLU:HG2	1.55	0.87
1:A:806:GLY:O	1:A:809:THR:HB	1.74	0.87
1:C:465:ALA:HA	1:C:468:ILE:HG12	1.56	0.87
1:A:862:LEU:O	1:A:863:VAL:C	2.07	0.86
1:B:806:GLY:O	1:B:809:THR:HB	1.74	0.86
1:D:596:LEU:HD23	1:D:601:ASP:HB3	1.57	0.86
1:C:477:PRO:HD2	1:C:480:LYS:HG3	1.58	0.85
1:B:461:PHE:N	1:B:461:PHE:CD1	2.41	0.84
1:A:509:LEU:HD12	1:A:509:LEU:H	1.41	0.84
1:B:724:THR:HG22	1:B:726:GLU:H	1.43	0.83
1:B:596:LEU:HD23	1:B:601:ASP:HB3	1.59	0.83
1:C:724:THR:HG22	1:C:726:GLU:H	1.42	0.83
1:B:660:ILE:O	1:B:664:THR:HG23	1.78	0.83
1:A:596:LEU:HD23	1:A:601:ASP:HB3	1.61	0.83
1:C:482:GLU:HG2	1:C:523:MET:HG2	1.61	0.83
1:D:470:LEU:HD12	1:D:470:LEU:H	1.44	0.83
1:C:534:MET:CE	1:D:813:PRO:HB2	2.09	0.82
1:B:485:ILE:HD13	1:B:494:ILE:HD12	1.60	0.82
1:D:660:ILE:O	1:D:664:THR:HG23	1.79	0.82
1:D:787:THR:HB	1:D:789:GLU:HG2	1.61	0.82
1:A:666:LYS:NZ	1:A:666:LYS:HB3	1.95	0.82
1:C:474:LYS:HA	1:C:474:LYS:HZ2	1.43	0.81
1:C:596:LEU:HD23	1:C:601:ASP:HB3	1.59	0.81
1:A:813:PRO:HB2	1:B:534:MET:HE1	1.63	0.81
1:B:461:PHE:HD1	1:B:461:PHE:H	1.24	0.81
1:A:813:PRO:HB2	1:B:534:MET:CE	2.11	0.81
1:C:486:GLU:O	1:C:487:THR:HB	1.81	0.81
1:C:593:VAL:CG2	1:C:685:GLY:HA3	2.10	0.81
1:D:492:VAL:O	1:D:496:ARG:HG3	1.80	0.80
1:A:660:ILE:O	1:A:664:THR:HG23	1.81	0.80
1:C:660:ILE:O	1:C:664:THR:HG23	1.80	0.80
1:D:724:THR:HG22	1:D:726:GLU:H	1.44	0.80
1:A:724:THR:HG22	1:A:726:GLU:H	1.45	0.80
1:B:593:VAL:CG2	1:B:685:GLY:HA3	2.12	0.80
1:A:593:VAL:CG2	1:A:685:GLY:HA3	2.12	0.79
1:D:593:VAL:CG2	1:D:685:GLY:HA3	2.13	0.79
1:A:666:LYS:HB3	1:A:666:LYS:HZ3	1.48	0.79
1:A:819:GLN:HB3	1:B:508:SER:HB2	1.63	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:518:ASN:HD21	1:D:521:LEU:HD22	1.48	0.78
1:A:534:MET:CE	1:B:813:PRO:HB2	2.14	0.78
1:C:813:PRO:HB2	1:D:534:MET:CE	2.14	0.78
1:B:519:TYR:O	1:B:523:MET:HG2	1.83	0.78
1:C:474:LYS:HB2	1:C:476:ILE:HG13	1.66	0.77
1:C:704:LYS:HE3	1:C:836:ARG:HG3	1.66	0.77
1:C:478:ALA:O	1:C:481:LEU:HG	1.85	0.77
1:D:655:MET:HE2	1:D:657:MET:H	1.50	0.77
1:D:655:MET:HE2	1:D:657:MET:N	2.00	0.77
1:A:473:ALA:C	1:A:475:HIS:H	1.88	0.76
1:A:655:MET:HE2	1:A:657:MET:N	2.00	0.76
1:C:655:MET:HE2	1:C:657:MET:N	1.99	0.76
1:A:862:LEU:O	1:A:863:VAL:O	2.02	0.76
1:C:534:MET:HE1	1:D:813:PRO:HB2	1.66	0.76
1:C:787:THR:HB	1:C:789:GLU:HG3	1.68	0.75
1:B:804:THR:HG21	1:B:823:VAL:O	1.85	0.75
1:A:565:SER:HB2	2:A:101:HMG:H6P1	1.67	0.75
1:D:565:SER:HB2	2:D:104:HMG:H6P1	1.68	0.75
1:A:779:THR:HG21	1:A:850:GLU:OE1	1.87	0.74
1:B:621:ALA:HB2	1:B:670:LYS:HD2	1.67	0.74
1:B:655:MET:HE2	1:B:657:MET:N	2.01	0.74
1:A:461:PHE:HD1	1:A:462:LEU:N	1.85	0.74
1:C:828:LYS:HG3	1:C:829:ASP:H	1.52	0.74
1:C:655:MET:HE2	1:C:657:MET:H	1.52	0.74
1:C:593:VAL:HG23	1:C:685:GLY:HA3	1.70	0.74
1:A:517:TYR:O	1:A:518:ASN:HB3	1.87	0.73
1:C:565:SER:HB2	2:C:103:HMG:H6P1	1.70	0.73
1:A:655:MET:HE2	1:A:657:MET:H	1.53	0.72
1:B:534:MET:HE3	1:B:535:PRO:HD2	1.70	0.72
1:C:804:THR:HG21	1:C:823:VAL:O	1.89	0.72
1:A:477:PRO:HD2	1:A:480:LYS:HD2	1.69	0.72
1:B:655:MET:HE2	1:B:657:MET:H	1.54	0.72
1:C:528:GLU:HG2	1:D:564:ALA:HB2	1.72	0.72
1:C:494:ILE:HA	1:C:497:GLN:HE21	1.55	0.71
1:D:811:LEU:HB2	1:D:814:GLN:HG2	1.71	0.71
1:C:463:SER:OG	1:C:466:GLU:HB2	1.90	0.71
1:C:461:PHE:H	1:C:462:LEU:HD12	1.56	0.71
1:D:493:SER:O	1:D:497:GLN:HG3	1.90	0.71
1:A:804:THR:HG21	1:A:823:VAL:O	1.90	0.71
1:D:787:THR:HB	1:D:789:GLU:CG	2.20	0.70
1:B:565:SER:HB2	2:B:102:HMG:H6P1	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:ALA:HB2	1:A:789:GLU:HB3	1.73	0.70
1:B:811:LEU:HB2	1:B:814:GLN:HG2	1.72	0.70
1:C:499:LEU:HD23	1:C:509:LEU:HD11	1.73	0.70
1:B:477:PRO:HG2	1:B:480:LYS:HG3	1.74	0.70
1:C:584:LEU:HD11	1:C:707:VAL:CG2	2.16	0.70
1:C:811:LEU:HB2	1:C:814:GLN:HG2	1.72	0.70
1:D:555:MET:CE	1:D:563:VAL:HA	2.21	0.70
1:D:559:GLU:OE2	2:D:104:HMG:H2P1	1.91	0.70
1:A:468:ILE:O	1:A:471:VAL:N	2.25	0.70
1:B:555:MET:CE	1:B:563:VAL:HA	2.22	0.70
1:B:476:ILE:HD13	1:B:484:LEU:HD21	1.74	0.69
1:C:779:THR:HG21	1:C:850:GLU:OE1	1.92	0.69
1:C:467:ILE:HG21	1:C:485:ILE:HD11	1.72	0.69
1:D:804:THR:HG21	1:D:823:VAL:O	1.92	0.69
1:B:487:THR:HG22	1:B:487:THR:O	1.93	0.69
1:D:485:ILE:HG22	1:D:486:GLU:N	2.07	0.69
1:A:534:MET:HE3	1:A:535:PRO:HD2	1.74	0.69
1:D:496:ARG:O	1:D:500:SER:HB2	1.91	0.69
1:C:534:MET:HE3	1:C:535:PRO:HD2	1.74	0.69
1:C:555:MET:CE	1:C:563:VAL:HA	2.22	0.68
1:C:523:MET:CE	1:C:530:VAL:HG21	2.23	0.68
1:D:804:THR:HG22	1:D:804:THR:O	1.92	0.68
1:C:813:PRO:HB2	1:D:534:MET:HE1	1.76	0.68
1:A:528:GLU:HG2	1:B:564:ALA:HB2	1.75	0.68
1:B:593:VAL:HG23	1:B:685:GLY:HA3	1.76	0.68
1:A:555:MET:CE	1:A:563:VAL:HA	2.24	0.68
1:B:482:GLU:OE2	1:B:495:ARG:NH2	2.25	0.68
1:D:724:THR:HG22	1:D:726:GLU:N	2.09	0.68
1:B:460:LYS:HA	1:B:460:LYS:HE2	1.76	0.68
1:A:534:MET:HE1	1:B:813:PRO:HB2	1.75	0.67
1:D:534:MET:HE3	1:D:535:PRO:HD2	1.75	0.67
1:A:724:THR:HG22	1:A:726:GLU:N	2.10	0.67
1:C:724:THR:HG22	1:C:726:GLU:N	2.09	0.67
1:A:479:TYR:HB3	1:A:529:ASN:ND2	2.09	0.67
1:D:779:THR:HG21	1:D:850:GLU:OE1	1.94	0.67
1:B:724:THR:HG22	1:B:726:GLU:N	2.09	0.67
1:C:465:ALA:HA	1:C:468:ILE:CG1	2.25	0.67
1:B:779:THR:HG21	1:B:850:GLU:OE1	1.94	0.67
1:A:593:VAL:HG23	1:A:685:GLY:HA3	1.75	0.66
1:A:811:LEU:HB2	1:A:814:GLN:HG2	1.75	0.66
1:A:804:THR:HG22	1:A:804:THR:O	1.94	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:ILE:HD13	1:B:484:LEU:CD2	2.25	0.66
1:C:804:THR:O	1:C:804:THR:HG22	1.94	0.66
1:B:787:THR:HB	1:B:789:GLU:HG3	1.76	0.66
1:D:593:VAL:HG23	1:D:685:GLY:HA3	1.75	0.66
1:B:477:PRO:HG3	1:B:480:LYS:HE3	1.78	0.66
1:A:584:LEU:HD11	1:A:707:VAL:CG2	2.20	0.65
1:C:518:ASN:ND2	1:C:521:LEU:HD22	2.10	0.65
1:B:467:ILE:CD1	1:B:490:ARG:NH2	2.59	0.65
1:A:755:ASN:HD21	1:B:691:LYS:NZ	1.94	0.65
1:D:485:ILE:HG22	1:D:486:GLU:H	1.62	0.65
1:A:509:LEU:HD12	1:A:509:LEU:N	2.12	0.65
1:B:804:THR:HG22	1:B:804:THR:O	1.94	0.65
1:C:518:ASN:HD22	1:C:521:LEU:HD22	1.60	0.65
1:C:712:ILE:HG22	1:C:717:VAL:HG23	1.79	0.64
1:A:723:THR:HG23	1:A:859:ALA:HB2	1.78	0.64
1:D:584:LEU:HD11	1:D:707:VAL:CG2	2.22	0.64
1:A:461:PHE:CD1	1:A:462:LEU:N	2.64	0.64
1:D:478:ALA:O	1:D:481:LEU:HG	1.98	0.64
1:A:595:ARG:O	1:A:596:LEU:HD12	1.98	0.64
1:A:712:ILE:HG22	1:A:717:VAL:HG23	1.80	0.64
1:C:466:GLU:O	1:C:470:LEU:HB2	1.98	0.64
1:D:463:SER:OG	1:D:465:ALA:HB3	1.97	0.64
1:C:523:MET:HE1	1:C:530:VAL:HG21	1.80	0.63
1:C:655:MET:CE	1:C:657:MET:HB2	2.28	0.63
1:C:489:GLU:OE2	1:C:515:ARG:HG3	1.98	0.63
1:C:793:ILE:HD12	1:C:851:LEU:HD13	1.81	0.63
1:D:712:ILE:HG22	1:D:717:VAL:HG23	1.80	0.63
1:A:586:ASP:CG	1:A:704:LYS:HE3	2.19	0.63
1:D:463:SER:O	1:D:467:ILE:HG13	1.99	0.62
1:D:586:ASP:CG	1:D:704:LYS:HE3	2.20	0.62
1:D:723:THR:HG23	1:D:859:ALA:HB2	1.80	0.62
1:A:473:ALA:C	1:A:475:HIS:N	2.52	0.62
1:C:485:ILE:HG21	1:C:490:ARG:HG2	1.81	0.62
1:C:813:PRO:HB2	1:D:534:MET:HE3	1.79	0.62
1:A:595:ARG:C	1:A:596:LEU:HD12	2.19	0.62
1:B:584:LEU:HD11	1:B:707:VAL:CG2	2.22	0.62
1:B:586:ASP:CG	1:B:704:LYS:HE3	2.19	0.62
1:B:593:VAL:HG22	1:B:685:GLY:HA3	1.81	0.62
1:D:472:ASN:O	1:D:474:LYS:HG3	2.00	0.62
1:A:519:TYR:O	1:A:523:MET:HG2	2.00	0.62
1:B:817:CYS:HA	1:B:820:MET:HE3	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:738:VAL:O	1:B:742:MET:HG2	1.99	0.62
1:A:534:MET:HE3	1:B:813:PRO:HB2	1.81	0.62
1:A:542:GLY:H	1:A:567:ASN:ND2	1.98	0.62
1:B:655:MET:CE	1:B:657:MET:HB2	2.30	0.62
1:B:777:CYS:HB2	1:B:797:MET:HG2	1.82	0.62
1:B:828:LYS:HE2	1:B:828:LYS:N	2.14	0.62
1:C:462:LEU:HD12	1:C:462:LEU:N	2.14	0.62
1:A:499:LEU:O	1:A:499:LEU:HG	1.99	0.62
1:B:542:GLY:H	1:B:567:ASN:ND2	1.98	0.61
1:A:793:ILE:HD12	1:A:851:LEU:HD13	1.81	0.61
1:D:593:VAL:HG22	1:D:685:GLY:HA3	1.81	0.61
1:D:594:VAL:HG13	1:D:678:MET:HG3	1.83	0.61
1:D:655:MET:CE	1:D:657:MET:HB2	2.30	0.61
1:D:777:CYS:HB2	1:D:797:MET:HG2	1.82	0.61
1:B:712:ILE:HG22	1:B:717:VAL:HG23	1.82	0.61
1:C:542:GLY:H	1:C:567:ASN:ND2	1.98	0.61
1:D:793:ILE:HD12	1:D:851:LEU:HD13	1.83	0.61
1:C:464:ASP:HA	1:C:490:ARG:HH21	1.66	0.60
1:A:672:HIS:CD2	1:A:676:PRO:HA	2.35	0.60
1:B:591:GLY:HA2	1:B:645:ILE:O	1.99	0.60
1:C:462:LEU:HD12	1:C:462:LEU:H	1.66	0.60
1:D:715:LYS:HA	1:D:718:ARG:NH2	2.16	0.60
1:C:817:CYS:HA	1:C:820:MET:HE3	1.83	0.60
1:B:617:VAL:HG23	1:B:670:LYS:HD3	1.84	0.60
1:A:593:VAL:HG22	1:A:685:GLY:HA3	1.81	0.60
1:C:534:MET:HE3	1:D:813:PRO:HB2	1.81	0.60
1:D:672:HIS:CD2	1:D:676:PRO:HA	2.37	0.60
1:B:470:LEU:HD12	1:B:470:LEU:H	1.66	0.60
1:D:811:LEU:HB2	1:D:814:GLN:CG	2.32	0.60
1:B:672:HIS:CD2	1:B:676:PRO:HA	2.36	0.59
1:C:590:ARG:HB3	1:C:664:THR:HG21	1.84	0.59
1:D:542:GLY:H	1:D:567:ASN:ND2	1.99	0.59
1:D:622:PHE:O	1:D:625:THR:HB	2.02	0.59
1:A:501:LYS:H	1:A:501:LYS:HD2	1.67	0.59
1:C:591:GLY:HA2	1:C:645:ILE:O	2.02	0.59
1:C:732:ASN:HB2	1:C:781:MET:CE	2.27	0.59
1:C:777:CYS:HB2	1:C:797:MET:HG2	1.84	0.59
1:A:622:PHE:O	1:A:625:THR:HB	2.02	0.59
1:A:655:MET:CE	1:A:657:MET:HB2	2.33	0.59
1:B:595:ARG:O	1:B:596:LEU:HD12	2.02	0.59
1:D:732:ASN:HB2	1:D:781:MET:CE	2.25	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:GLY:HA2	1:A:645:ILE:O	2.02	0.59
1:C:471:VAL:O	1:C:475:HIS:N	2.34	0.59
1:D:479:TYR:HB3	1:D:529:ASN:OD1	2.02	0.59
1:C:495:ARG:HA	1:C:498:LEU:HD23	1.85	0.59
1:A:512:LEU:HD12	1:A:513:PRO:HD2	1.83	0.59
1:B:480:LYS:O	1:B:481:LEU:C	2.40	0.59
1:C:672:HIS:CD2	1:C:676:PRO:HA	2.38	0.59
1:D:591:GLY:HA2	1:D:645:ILE:O	2.03	0.59
1:B:628:PHE:O	1:B:630:ARG:HG2	2.03	0.59
1:C:723:THR:HG23	1:C:859:ALA:HB2	1.84	0.59
1:C:595:ARG:C	1:C:596:LEU:HD12	2.23	0.58
1:B:595:ARG:C	1:B:596:LEU:HD12	2.23	0.58
1:D:853:LEU:HD13	2:D:104:HMG:O5P	2.03	0.58
1:B:811:LEU:HB2	1:B:814:GLN:CG	2.34	0.58
1:D:595:ARG:C	1:D:596:LEU:HD12	2.24	0.58
1:D:857:LEU:HD21	1:D:862:LEU:HD22	1.84	0.58
1:C:622:PHE:O	1:C:625:THR:HB	2.04	0.58
1:B:467:ILE:O	1:B:471:VAL:HG23	2.03	0.58
1:A:823:VAL:HG11	1:A:838:LEU:HB2	1.85	0.58
1:A:804:THR:C	1:A:809:THR:HG21	2.25	0.57
1:C:470:LEU:O	1:C:474:LYS:HG2	2.04	0.57
1:C:866:HIS:CE1	2:C:103:HMG:H4	2.22	0.57
1:C:593:VAL:HG22	1:C:685:GLY:HA3	1.83	0.57
1:C:804:THR:C	1:C:809:THR:HG21	2.24	0.57
1:A:815:GLN:HG2	1:A:824:GLN:HE21	1.69	0.57
1:A:819:GLN:CB	1:B:508:SER:HB2	2.34	0.57
1:C:522:VAL:HB	1:C:523:MET:HE3	1.86	0.57
1:B:476:ILE:HG21	1:B:484:LEU:CD2	2.35	0.57
1:B:460:LYS:HE2	1:B:460:LYS:CA	2.34	0.57
1:C:704:LYS:HE3	1:C:836:ARG:CG	2.35	0.57
1:B:804:THR:C	1:B:809:THR:HG21	2.25	0.57
1:A:590:ARG:HB3	1:A:664:THR:HG21	1.87	0.57
1:B:480:LYS:O	1:B:482:GLU:N	2.38	0.57
1:C:595:ARG:O	1:C:596:LEU:HD12	2.05	0.57
1:C:619:LYS:HZ1	1:C:630:ARG:HG3	1.68	0.57
1:D:590:ARG:HB3	1:D:664:THR:HG21	1.86	0.56
1:B:500:SER:HB3	1:B:506:PRO:O	2.05	0.56
1:B:517:TYR:HE2	1:B:522:VAL:HG21	1.70	0.56
1:B:590:ARG:HB3	1:B:664:THR:HG21	1.86	0.56
1:D:823:VAL:HG11	1:D:838:LEU:HB2	1.87	0.56
1:B:630:ARG:HH21	1:B:652:GLY:H	1.52	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:ILE:O	1:C:498:LEU:HD22	2.05	0.56
1:C:593:VAL:HG23	1:C:685:GLY:CA	2.36	0.56
1:D:455:ALA:O	1:D:456:GLU:HG3	2.05	0.56
1:D:523:MET:SD	1:D:530:VAL:HG21	2.45	0.56
1:D:655:MET:HE3	1:D:655:MET:O	2.06	0.56
1:A:471:VAL:O	1:A:475:HIS:N	2.39	0.56
1:B:863:VAL:O	1:B:864:LYS:HB3	2.05	0.56
1:A:787:THR:CG2	1:A:789:GLU:OE1	2.54	0.56
1:B:793:ILE:HD12	1:B:851:LEU:HD13	1.87	0.56
1:C:513:PRO:O	1:C:514:TYR:HB3	2.05	0.56
1:D:738:VAL:O	1:D:742:MET:HG2	2.05	0.56
1:D:828:LYS:HE2	1:D:828:LYS:N	2.20	0.56
1:A:471:VAL:O	1:A:475:HIS:HA	2.05	0.56
1:B:853:LEU:HD21	2:B:102:HMG:H63	1.87	0.56
1:D:815:GLN:HG2	1:D:824:GLN:HE21	1.71	0.56
1:B:672:HIS:HD2	1:B:676:PRO:HA	1.70	0.56
1:B:823:VAL:HG11	1:B:838:LEU:HB2	1.87	0.56
1:C:811:LEU:HB2	1:C:814:GLN:CG	2.35	0.56
1:A:672:HIS:HD2	1:A:676:PRO:HA	1.69	0.56
1:B:842:VAL:O	1:B:846:VAL:HG23	2.06	0.56
1:B:622:PHE:O	1:B:625:THR:HB	2.05	0.55
1:B:723:THR:HG23	1:B:859:ALA:HB2	1.86	0.55
1:B:534:MET:CE	1:B:535:PRO:HD2	2.36	0.55
1:B:732:ASN:HB2	1:B:781:MET:CE	2.24	0.55
1:C:485:ILE:HG22	1:C:486:GLU:N	2.22	0.55
1:D:528:GLU:O	1:D:529:ASN:HB2	2.06	0.55
1:A:461:PHE:CD1	1:A:461:PHE:C	2.80	0.55
1:D:518:ASN:HD21	1:D:521:LEU:HB2	1.72	0.55
1:D:804:THR:C	1:D:809:THR:HG21	2.27	0.55
1:B:594:VAL:HG13	1:B:678:MET:HG3	1.89	0.55
1:B:469:GLN:O	1:B:469:GLN:OE1	2.25	0.55
1:C:467:ILE:HG21	1:C:485:ILE:CD1	2.36	0.55
1:C:766:GLN:OE1	1:C:802:ILE:HG13	2.07	0.55
1:D:595:ARG:O	1:D:596:LEU:HD12	2.06	0.55
1:C:594:VAL:HG13	1:C:678:MET:HG3	1.89	0.55
1:C:505:GLU:C	1:C:505:GLU:OE1	2.45	0.55
1:C:815:GLN:HG2	1:C:824:GLN:HE21	1.71	0.55
1:D:623:ASP:OD1	1:D:630:ARG:HA	2.07	0.55
1:B:507:SER:O	1:B:510:GLN:HB2	2.08	0.54
1:B:586:ASP:O	1:B:650:ARG:HD3	2.07	0.54
1:C:581:SER:OG	1:C:840:ARG:HD2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:823:VAL:HG11	1:C:838:LEU:HB2	1.89	0.54
1:A:811:LEU:HB2	1:A:814:GLN:CG	2.37	0.54
1:D:672:HIS:HD2	1:D:676:PRO:HA	1.71	0.54
1:A:606:LYS:O	1:A:610:GLU:HG3	2.07	0.54
1:C:517:TYR:CD1	1:C:518:ASN:N	2.75	0.54
1:C:560:GLY:O	1:C:561:CYS:HB2	2.08	0.54
1:C:864:LYS:HE2	1:C:864:LYS:HA	1.90	0.54
1:A:462:LEU:O	1:A:463:SER:HB3	2.07	0.54
2:A:101:HMG:H3B	1:B:479:TYR:OH	2.08	0.54
1:C:672:HIS:HD2	1:C:676:PRO:HA	1.71	0.54
1:D:518:ASN:ND2	1:D:521:LEU:HD22	2.20	0.54
1:D:732:ASN:CB	1:D:781:MET:HE2	2.30	0.54
1:A:656:GLY:O	1:A:660:ILE:HG12	2.08	0.54
1:A:815:GLN:HG2	1:A:824:GLN:NE2	2.23	0.54
1:B:477:PRO:HG2	1:B:480:LYS:CG	2.38	0.54
1:B:606:LYS:O	1:B:610:GLU:HG3	2.07	0.54
1:B:518:ASN:O	1:B:520:SER:N	2.41	0.54
1:B:815:GLN:HG2	1:B:824:GLN:HE21	1.72	0.54
1:C:500:SER:HB3	1:C:506:PRO:O	2.08	0.53
1:D:456:GLU:O	1:D:457:LYS:HB2	2.08	0.53
1:A:842:VAL:O	1:A:846:VAL:HG23	2.07	0.53
1:D:497:GLN:O	1:D:500:SER:HB3	2.08	0.53
1:C:474:LYS:HA	1:C:474:LYS:HZ3	1.70	0.53
1:D:470:LEU:HD12	1:D:470:LEU:N	2.19	0.53
1:A:534:MET:CE	1:A:535:PRO:HD2	2.38	0.53
1:C:485:ILE:HG21	1:C:490:ARG:CG	2.37	0.53
1:A:513:PRO:O	1:A:514:TYR:HB3	2.08	0.53
1:B:463:SER:O	1:B:467:ILE:HG13	2.09	0.53
1:D:733:ILE:O	1:D:737:LEU:HB2	2.09	0.53
1:A:499:LEU:HD11	1:B:552:GLN:CG	2.28	0.53
1:C:462:LEU:HB2	1:C:467:ILE:HD11	1.90	0.53
1:C:606:LYS:O	1:C:610:GLU:HG3	2.09	0.53
1:B:470:LEU:O	1:B:473:ALA:HB3	2.08	0.53
1:B:613:GLU:H	1:B:613:GLU:CD	2.12	0.53
1:C:733:ILE:O	1:C:737:LEU:HB2	2.09	0.53
1:A:613:GLU:CD	1:A:613:GLU:H	2.12	0.53
1:A:509:LEU:O	1:A:510:GLN:C	2.47	0.52
1:D:842:VAL:O	1:D:846:VAL:HG23	2.09	0.52
1:B:704:LYS:HE2	1:B:836:ARG:HG3	1.91	0.52
1:C:771:ASN:HD22	1:D:771:ASN:HB3	1.74	0.52
1:D:485:ILE:HD11	1:D:494:ILE:HD12	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:529:ASN:ND2	2:D:104:HMG:H2A1	2.25	0.52
1:C:534:MET:CE	1:C:535:PRO:HD2	2.40	0.52
1:D:606:LYS:O	1:D:610:GLU:HG3	2.10	0.52
1:D:706:VAL:HG22	1:D:843:CYS:SG	2.50	0.52
1:D:467:ILE:CD1	1:D:490:ARG:NH2	2.73	0.52
1:B:498:LEU:O	1:B:501:LYS:CG	2.57	0.52
1:A:704:LYS:HE2	1:A:836:ARG:HG3	1.92	0.52
1:A:732:ASN:CB	1:A:781:MET:HE2	2.22	0.52
1:A:813:PRO:HB2	1:B:534:MET:HE3	1.88	0.52
1:B:560:GLY:O	1:B:561:CYS:HB2	2.10	0.52
1:B:480:LYS:O	1:B:483:THR:N	2.42	0.52
1:C:623:ASP:OD1	1:C:630:ARG:HA	2.09	0.52
1:D:534:MET:CE	1:D:535:PRO:HD2	2.38	0.52
1:C:461:PHE:O	1:C:462:LEU:O	2.27	0.52
1:C:488:HIS:O	1:C:492:VAL:HG13	2.09	0.52
1:C:656:GLY:O	1:C:660:ILE:HG12	2.10	0.52
1:C:863:VAL:O	1:C:863:VAL:HG12	2.11	0.52
1:D:485:ILE:CD1	1:D:494:ILE:HD12	2.40	0.52
1:D:632:GLN:HE21	1:D:650:ARG:HG2	1.73	0.52
1:A:552:GLN:HG3	1:B:499:LEU:HD11	1.92	0.51
1:B:815:GLN:HG2	1:B:824:GLN:NE2	2.25	0.51
1:D:656:GLY:O	1:D:660:ILE:HG12	2.09	0.51
1:C:808:GLY:O	1:C:814:GLN:HG3	2.10	0.51
1:A:738:VAL:O	1:A:742:MET:HG2	2.10	0.51
1:A:509:LEU:H	1:A:509:LEU:CD1	2.18	0.51
1:B:596:LEU:HD21	1:B:605:VAL:HG21	1.93	0.51
1:D:467:ILE:HD11	1:D:490:ARG:NH2	2.26	0.51
1:D:815:GLN:HG2	1:D:824:GLN:NE2	2.26	0.51
1:A:684:SER:O	1:B:735:LYS:NZ	2.43	0.51
1:C:738:VAL:O	1:C:742:MET:HG2	2.11	0.51
1:D:593:VAL:HG23	1:D:685:GLY:CA	2.40	0.51
1:B:514:TYR:CE1	1:B:515:ARG:HG2	2.46	0.51
1:D:586:ASP:O	1:D:650:ARG:HD3	2.11	0.51
1:D:613:GLU:CD	1:D:613:GLU:H	2.13	0.51
1:D:463:SER:O	1:D:464:ASP:C	2.48	0.51
1:A:777:CYS:HB2	1:A:797:MET:HG2	1.93	0.51
1:D:704:LYS:HE2	1:D:836:ARG:HG3	1.92	0.51
1:A:817:CYS:HA	1:A:820:MET:HE3	1.94	0.50
1:B:518:ASN:CG	1:B:520:SER:HG	2.15	0.50
1:D:555:MET:HE1	1:D:563:VAL:HA	1.93	0.50
1:A:487:THR:OG1	1:A:490:ARG:HG2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:VAL:HG13	1:A:678:MET:HG3	1.94	0.50
1:A:767:ASP:HB3	1:A:770:GLN:HG3	1.93	0.50
1:C:815:GLN:HG2	1:C:824:GLN:NE2	2.26	0.50
1:D:592:PRO:HG3	1:D:668:LEU:HD11	1.92	0.50
1:B:466:GLU:C	1:B:468:ILE:N	2.65	0.50
1:A:561:CYS:H	1:B:528:GLU:CD	2.13	0.50
1:C:461:PHE:O	1:C:462:LEU:C	2.49	0.50
1:C:715:LYS:HE2	1:C:719:GLU:OE1	2.11	0.50
1:B:766:GLN:OE1	1:B:802:ILE:HG13	2.12	0.50
1:B:774:SER:HA	1:B:799:SER:O	2.12	0.50
1:B:828:LYS:N	1:B:828:LYS:CE	2.75	0.50
1:C:842:VAL:O	1:C:846:VAL:HG23	2.12	0.50
1:D:455:ALA:O	1:D:456:GLU:CG	2.60	0.50
1:D:714:ALA:HB2	1:D:789:GLU:HB2	1.92	0.50
1:A:467:ILE:O	1:A:471:VAL:HG23	2.11	0.50
1:A:530:VAL:HG12	1:A:532:GLY:H	1.77	0.50
1:B:863:VAL:O	1:B:864:LYS:CB	2.59	0.50
1:A:597:PRO:O	1:A:598:ARG:HD3	2.11	0.50
1:A:766:GLN:OE1	1:A:802:ILE:HG13	2.12	0.50
1:B:596:LEU:HD21	1:B:605:VAL:CG2	2.42	0.50
1:B:732:ASN:CB	1:B:781:MET:HE2	2.25	0.50
1:C:479:TYR:HA	1:C:495:ARG:HH12	1.76	0.50
1:D:804:THR:HG22	1:D:825:GLY:O	2.12	0.50
1:C:684:SER:O	1:D:735:LYS:NZ	2.42	0.50
1:D:655:MET:HE2	1:D:657:MET:HB2	1.93	0.50
1:B:498:LEU:O	1:B:501:LYS:HG3	2.12	0.49
1:B:827:CYS:HA	1:B:828:LYS:NZ	2.26	0.49
1:C:485:ILE:CG2	1:C:490:ARG:HG2	2.42	0.49
1:D:461:PHE:C	1:D:462:LEU:HG	2.32	0.49
1:D:804:THR:O	1:D:804:THR:CG2	2.59	0.49
2:B:102:HMG:S1P	2:B:102:HMG:H62	2.52	0.49
1:C:588:MET:CE	1:C:655:MET:HE3	2.43	0.49
1:C:804:THR:O	1:C:809:THR:HG21	2.12	0.49
1:B:656:GLY:O	1:B:660:ILE:HG12	2.12	0.49
1:C:462:LEU:HB3	1:C:466:GLU:CD	2.33	0.49
1:C:495:ARG:HD2	1:C:531:ILE:HG22	1.95	0.49
1:C:619:LYS:NZ	1:C:630:ARG:HG3	2.27	0.49
1:A:497:GLN:O	1:A:501:LYS:HD2	2.13	0.49
1:A:593:VAL:HG23	1:A:685:GLY:CA	2.42	0.49
1:B:706:VAL:HG22	1:B:843:CYS:SG	2.52	0.49
1:A:596:LEU:HD21	1:A:605:VAL:HG21	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:HIS:CE1	1:B:520:SER:HA	2.48	0.49
1:B:655:MET:HE2	1:B:657:MET:HB2	1.94	0.49
1:C:477:PRO:HD2	1:C:480:LYS:CG	2.36	0.49
1:C:735:LYS:NZ	1:D:684:SER:O	2.44	0.49
1:D:485:ILE:CG2	1:D:486:GLU:H	2.26	0.49
1:D:485:ILE:CG2	1:D:486:GLU:N	2.75	0.49
1:A:581:SER:OG	1:A:840:ARG:HD2	2.12	0.49
1:B:733:ILE:O	1:B:737:LEU:HB2	2.11	0.49
1:B:808:GLY:O	1:B:814:GLN:HG3	2.12	0.49
1:C:804:THR:O	1:C:804:THR:CG2	2.61	0.49
1:D:469:GLN:HA	1:D:472:ASN:HD22	1.77	0.49
1:A:473:ALA:O	1:A:475:HIS:N	2.46	0.49
1:A:733:ILE:O	1:A:737:LEU:HB2	2.12	0.49
1:A:808:GLY:O	1:A:814:GLN:HG3	2.12	0.49
1:B:632:GLN:HE21	1:B:650:ARG:HG2	1.78	0.49
1:D:560:GLY:O	1:D:561:CYS:HB2	2.13	0.49
1:A:560:GLY:O	1:A:561:CYS:HB2	2.13	0.49
1:A:804:THR:O	1:A:804:THR:CG2	2.61	0.49
1:C:771:ASN:HB3	1:D:771:ASN:HD22	1.78	0.49
1:A:471:VAL:O	1:A:475:HIS:CA	2.60	0.48
1:B:534:MET:HE3	1:B:535:PRO:CD	2.42	0.48
1:C:474:LYS:O	1:C:475:HIS:HB3	2.13	0.48
1:C:535:PRO:HB2	1:D:517:TYR:HE2	1.78	0.48
1:B:555:MET:HE1	1:B:563:VAL:HA	1.93	0.48
1:B:565:SER:CB	2:B:102:HMG:H6P1	2.41	0.48
1:A:461:PHE:HD1	1:A:462:LEU:CA	2.26	0.48
1:A:804:THR:O	1:A:809:THR:HG21	2.13	0.48
1:D:476:ILE:HG23	1:D:484:LEU:HD23	1.96	0.48
1:D:456:GLU:O	1:D:457:LYS:CB	2.61	0.48
1:B:469:GLN:O	1:B:470:LEU:C	2.52	0.48
1:D:555:MET:HB3	1:D:759:ALA:HB1	1.95	0.48
1:A:555:MET:HB3	1:A:759:ALA:HB1	1.96	0.48
1:A:732:ASN:HA	1:A:854:MET:HE1	1.95	0.48
1:B:520:SER:OG	1:B:521:LEU:N	2.47	0.48
1:D:808:GLY:O	1:D:814:GLN:HG3	2.13	0.48
1:B:513:PRO:HB2	1:B:533:TYR:CZ	2.49	0.48
1:C:553:VAL:HA	1:C:821:LEU:HD21	1.96	0.48
1:D:688:CYS:HB2	1:D:689:THR:CA	2.42	0.48
1:A:771:ASN:HB3	1:B:771:ASN:HD22	1.78	0.48
1:B:476:ILE:HG21	1:B:484:LEU:HD21	1.95	0.48
1:B:555:MET:HB3	1:B:759:ALA:HB1	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:752:HIS:HD2	1:C:755:ASN:HD22	1.62	0.48
1:C:471:VAL:HG13	1:C:476:ILE:O	2.13	0.48
1:C:787:THR:CB	1:C:789:GLU:HG3	2.42	0.48
1:D:518:ASN:HD21	1:D:521:LEU:CD2	2.22	0.48
1:A:510:GLN:NE2	1:A:511:TYR:CE1	2.82	0.48
1:A:864:LYS:O	1:A:865:SER:CB	2.61	0.48
1:A:477:PRO:CD	1:A:480:LYS:HD2	2.40	0.47
1:A:706:VAL:HG22	1:A:843:CYS:SG	2.54	0.47
1:B:519:TYR:HB3	1:B:523:MET:SD	2.54	0.47
1:C:715:LYS:HE2	1:C:719:GLU:CD	2.34	0.47
1:C:728:MET:HB3	1:C:781:MET:HE3	1.95	0.47
1:D:596:LEU:HD21	1:D:605:VAL:CG2	2.44	0.47
1:A:709:GLU:HA	1:A:793:ILE:O	2.14	0.47
1:D:774:SER:HA	1:D:799:SER:O	2.14	0.47
1:B:655:MET:HE3	1:B:655:MET:O	2.14	0.47
1:C:592:PRO:HG3	1:C:668:LEU:HD11	1.95	0.47
1:A:479:TYR:HA	1:A:495:ARG:HH12	1.79	0.47
1:A:774:SER:HA	1:A:799:SER:O	2.15	0.47
1:C:485:ILE:HG22	1:C:486:GLU:H	1.80	0.47
1:D:817:CYS:HA	1:D:820:MET:HE3	1.95	0.47
1:A:714:ALA:CB	1:A:789:GLU:HB3	2.42	0.47
1:B:804:THR:O	1:B:809:THR:HG21	2.14	0.47
1:C:477:PRO:HB2	1:C:480:LYS:HG2	1.96	0.47
1:A:632:GLN:HE21	1:A:650:ARG:HG2	1.80	0.47
1:C:517:TYR:HE2	1:D:535:PRO:HB2	1.80	0.47
1:D:565:SER:CB	2:D:104:HMG:H6P1	2.41	0.47
1:B:828:LYS:HE2	1:B:829:ASP:H	1.80	0.47
1:C:523:MET:CE	1:C:523:MET:H	2.28	0.47
1:C:793:ILE:CD1	1:C:851:LEU:HD13	2.44	0.47
1:D:827:CYS:HA	1:D:828:LYS:NZ	2.30	0.47
1:A:519:TYR:HB3	1:A:523:MET:SD	2.55	0.47
1:B:494:ILE:HG22	1:B:498:LEU:HD12	1.97	0.47
1:B:586:ASP:OD1	1:B:704:LYS:HE3	2.14	0.47
1:B:492:VAL:HG13	1:B:531:ILE:HA	1.97	0.46
1:D:804:THR:O	1:D:809:THR:HG21	2.15	0.46
1:A:662:LYS:HG2	1:B:863:VAL:HG11	1.97	0.46
1:B:593:VAL:HG23	1:B:685:GLY:CA	2.43	0.46
1:D:470:LEU:H	1:D:470:LEU:CD1	2.22	0.46
1:D:709:GLU:HA	1:D:793:ILE:O	2.15	0.46
1:A:755:ASN:HD21	1:B:691:LYS:HZ3	1.61	0.46
1:C:688:CYS:HB2	1:C:689:THR:CA	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:814:GLN:CD	1:D:534:MET:HE1	2.36	0.46
1:D:508:SER:O	1:D:510:GLN:N	2.48	0.46
1:A:520:SER:OG	1:A:521:LEU:N	2.48	0.46
1:A:596:LEU:HD21	1:A:605:VAL:CG2	2.44	0.46
1:A:708:CYS:O	1:A:794:SER:HA	2.15	0.46
1:B:581:SER:OG	1:B:840:ARG:HD2	2.15	0.46
1:D:466:GLU:O	1:D:470:LEU:HD12	2.14	0.46
1:A:732:ASN:HA	1:A:854:MET:CE	2.46	0.46
1:C:464:ASP:HA	1:C:490:ARG:NH2	2.30	0.46
1:C:514:TYR:O	1:C:519:TYR:OH	2.29	0.46
1:B:553:VAL:HA	1:B:821:LEU:HD21	1.97	0.46
1:C:752:HIS:CD2	1:C:755:ASN:HD22	2.34	0.46
1:D:581:SER:OG	1:D:840:ARG:HD2	2.15	0.46
1:A:586:ASP:O	1:A:650:ARG:HD3	2.16	0.46
1:A:592:PRO:HG3	1:A:668:LEU:HD11	1.97	0.46
1:A:820:MET:CE	1:B:509:LEU:HD21	2.45	0.46
1:D:488:HIS:HD2	1:D:523:MET:HG3	1.81	0.46
1:A:555:MET:HE1	1:A:563:VAL:HA	1.98	0.46
1:A:688:CYS:HB2	1:A:689:THR:CA	2.46	0.46
1:C:804:THR:HG22	1:C:825:GLY:O	2.16	0.46
1:A:623:ASP:OD1	1:A:630:ARG:HA	2.16	0.46
1:B:480:LYS:C	1:B:482:GLU:N	2.69	0.46
1:C:593:VAL:CG2	1:C:685:GLY:CA	2.90	0.46
1:C:732:ASN:CB	1:C:781:MET:HE2	2.36	0.46
1:C:814:GLN:NE2	1:D:534:MET:HE1	2.31	0.46
1:D:464:ASP:O	1:D:465:ALA:C	2.54	0.46
1:B:804:THR:HG22	1:B:825:GLY:O	2.17	0.45
1:C:586:ASP:OD1	1:C:704:LYS:NZ	2.49	0.45
1:C:702:ARG:O	1:C:799:SER:HA	2.16	0.45
1:D:495:ARG:HG2	1:D:531:ILE:HG22	1.97	0.45
1:A:468:ILE:HG23	1:A:498:LEU:CD1	2.45	0.45
1:A:553:VAL:HA	1:A:821:LEU:HD21	1.99	0.45
1:B:475:HIS:C	1:B:476:ILE:HG13	2.36	0.45
1:C:518:ASN:HD21	1:C:521:LEU:HD13	1.80	0.45
1:C:732:ASN:HA	1:C:854:MET:CE	2.47	0.45
1:D:553:VAL:HA	1:D:821:LEU:HD21	1.98	0.45
1:D:592:PRO:HB3	1:D:683:VAL:HA	1.99	0.45
1:C:522:VAL:HB	1:C:523:MET:CE	2.46	0.45
1:D:484:LEU:HD22	1:D:484:LEU:H	1.82	0.45
1:D:505:GLU:OE1	1:D:505:GLU:HA	2.17	0.45
1:D:632:GLN:NE2	1:D:650:ARG:HG2	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:MET:O	1:A:655:MET:HE3	2.16	0.45
1:B:513:PRO:O	1:B:514:TYR:HB3	2.17	0.45
1:B:712:ILE:HG22	1:B:717:VAL:CG2	2.46	0.45
1:C:494:ILE:O	1:C:497:GLN:HB2	2.17	0.45
1:C:555:MET:HE1	1:C:563:VAL:HA	1.95	0.45
1:D:596:LEU:HD21	1:D:605:VAL:HG21	1.97	0.45
1:D:787:THR:O	1:D:788:ASN:HB2	2.15	0.45
1:B:476:ILE:HG21	1:B:484:LEU:HD22	1.99	0.45
1:B:804:THR:CG2	1:B:823:VAL:O	2.62	0.45
1:C:514:TYR:HB2	1:C:532:GLY:HA2	1.99	0.45
1:C:555:MET:HB3	1:C:759:ALA:HB1	1.97	0.45
1:A:804:THR:HG22	1:A:825:GLY:O	2.16	0.45
1:B:793:ILE:CD1	1:B:851:LEU:HD13	2.47	0.45
1:A:586:ASP:OD1	1:A:704:LYS:HE3	2.17	0.45
1:B:463:SER:OG	1:B:466:GLU:HG2	2.17	0.45
1:B:804:THR:O	1:B:804:THR:CG2	2.61	0.45
1:D:466:GLU:C	1:D:468:ILE:N	2.69	0.45
1:D:767:ASP:HB3	1:D:770:GLN:HG3	1.99	0.45
1:B:463:SER:C	1:B:465:ALA:N	2.70	0.45
1:D:857:LEU:CD2	1:D:862:LEU:HD22	2.46	0.45
1:B:473:ALA:C	1:B:475:HIS:H	2.20	0.45
1:C:499:LEU:CD1	1:D:552:GLN:HG3	2.47	0.45
1:D:588:MET:CE	1:D:655:MET:HE3	2.46	0.45
1:D:828:LYS:N	1:D:828:LYS:CE	2.80	0.45
1:A:461:PHE:CE1	1:A:462:LEU:HD23	2.52	0.44
1:D:518:ASN:ND2	1:D:521:LEU:HB2	2.31	0.44
1:A:787:THR:HB	1:A:789:GLU:OE1	2.17	0.44
1:B:688:CYS:HB2	1:B:689:THR:CA	2.47	0.44
1:B:709:GLU:HA	1:B:793:ILE:O	2.17	0.44
1:C:688:CYS:N	1:C:689:THR:HA	2.32	0.44
1:C:862:LEU:HD22	1:C:866:HIS:CE1	2.53	0.44
1:C:462:LEU:O	1:C:463:SER:C	2.55	0.44
1:C:596:LEU:HD21	1:C:605:VAL:HG21	1.98	0.44
1:C:706:VAL:HG22	1:C:843:CYS:SG	2.57	0.44
1:C:815:GLN:O	1:C:819:GLN:HG3	2.16	0.44
1:D:828:LYS:HE2	1:D:829:ASP:H	1.81	0.44
1:A:468:ILE:O	1:A:471:VAL:HB	2.18	0.44
1:B:462:LEU:HB2	1:B:467:ILE:HG12	2.00	0.44
1:D:482:GLU:CD	1:D:482:GLU:H	2.21	0.44
1:D:766:GLN:OE1	1:D:802:ILE:HG13	2.18	0.44
1:C:709:GLU:HA	1:C:793:ILE:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:513:PRO:O	1:D:514:TYR:HB3	2.17	0.44
1:D:586:ASP:OD1	1:D:704:LYS:HE3	2.17	0.44
1:C:462:LEU:HB3	1:C:466:GLU:OE2	2.17	0.44
1:C:668:LEU:HB3	1:C:680:ILE:HD13	2.00	0.44
1:D:499:LEU:O	1:D:503:LEU:HG	2.18	0.44
1:D:779:THR:HG21	1:D:850:GLU:HG3	2.00	0.44
1:A:655:MET:HE2	1:A:657:MET:HB2	2.00	0.44
1:A:735:LYS:NZ	2:A:101:HMG:O3	2.46	0.44
1:B:787:THR:O	1:B:788:ASN:HB2	2.18	0.44
1:D:557:THR:OG1	1:D:558:THR:N	2.51	0.44
1:C:712:ILE:HA	1:C:713:PRO:HD3	1.90	0.44
1:D:708:CYS:O	1:D:794:SER:HA	2.18	0.44
1:A:621:ALA:O	1:A:666:LYS:NZ	2.51	0.44
1:C:496:ARG:NH1	1:C:531:ILE:O	2.49	0.44
1:C:787:THR:O	1:C:788:ASN:HB2	2.18	0.44
1:B:708:CYS:O	1:B:794:SER:HA	2.17	0.43
1:D:519:TYR:O	1:D:523:MET:HG2	2.18	0.43
1:D:853:LEU:HD12	1:D:853:LEU:O	2.18	0.43
1:A:692:LYS:HE2	1:A:692:LYS:HB2	1.88	0.43
1:A:787:THR:O	1:A:788:ASN:HB2	2.17	0.43
1:C:529:ASN:HB3	1:D:540:VAL:HG12	1.99	0.43
1:C:596:LEU:HD21	1:C:605:VAL:CG2	2.48	0.43
1:D:453:GLY:O	1:D:454:ASN:CG	2.56	0.43
1:A:688:CYS:N	1:A:689:THR:HA	2.33	0.43
1:A:820:MET:HE1	1:B:509:LEU:HD21	2.00	0.43
1:B:519:TYR:CE2	1:B:530:VAL:HG11	2.53	0.43
1:C:596:LEU:HD23	1:C:601:ASP:CB	2.41	0.43
1:D:593:VAL:HG13	1:D:644:TYR:CE2	2.54	0.43
1:A:468:ILE:O	1:A:469:GLN:C	2.56	0.43
1:A:562:LEU:HD11	1:A:755:ASN:HB3	2.00	0.43
1:A:769:ALA:C	1:A:771:ASN:H	2.21	0.43
1:B:592:PRO:HG3	1:B:668:LEU:HD11	1.99	0.43
1:C:476:ILE:HD13	1:C:484:LEU:HD11	2.00	0.43
1:C:511:TYR:O	1:C:513:PRO:HD3	2.19	0.43
1:D:529:ASN:O	1:D:531:ILE:HG23	2.19	0.43
1:A:567:ASN:HD22	1:A:567:ASN:HA	1.55	0.43
1:C:715:LYS:HE2	1:C:719:GLU:OE2	2.18	0.43
1:A:864:LYS:O	1:A:865:SER:HB2	2.18	0.43
1:B:588:MET:CE	1:B:655:MET:HE3	2.48	0.43
1:C:523:MET:HE2	1:C:523:MET:N	2.32	0.43
1:D:797:MET:HA	1:D:798:PRO:HD3	1.77	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:ARG:O	1:A:799:SER:HA	2.19	0.43
1:B:469:GLN:O	1:B:472:ASN:N	2.52	0.43
1:B:557:THR:OG1	1:B:558:THR:N	2.52	0.43
1:B:592:PRO:HB3	1:B:683:VAL:HA	2.00	0.43
1:B:797:MET:HA	1:B:798:PRO:HD3	1.75	0.43
1:C:592:PRO:HB3	1:C:683:VAL:HA	1.99	0.43
1:C:767:ASP:HB3	1:C:770:GLN:HG3	2.00	0.43
1:C:774:SER:HA	1:C:799:SER:O	2.18	0.43
1:D:480:LYS:O	1:D:483:THR:N	2.49	0.43
1:A:588:MET:CE	1:A:655:MET:HE3	2.48	0.43
1:A:793:ILE:CD1	1:A:851:LEU:HD13	2.46	0.43
1:B:688:CYS:N	1:B:689:THR:HA	2.34	0.43
1:B:732:ASN:HA	1:B:854:MET:CE	2.49	0.43
1:C:771:ASN:HD22	1:D:771:ASN:HD22	1.65	0.43
1:D:487:THR:HG22	1:D:490:ARG:H	1.84	0.43
1:D:850:GLU:O	1:D:854:MET:HG2	2.19	0.43
1:A:712:ILE:HG22	1:A:717:VAL:CG2	2.47	0.43
1:C:787:THR:HG21	1:C:789:GLU:OE2	2.19	0.43
1:C:862:LEU:CD2	1:C:866:HIS:CE1	3.02	0.43
1:B:629:ALA:HB2	1:B:659:MET:SD	2.59	0.42
1:D:732:ASN:HA	1:D:854:MET:CE	2.49	0.42
1:A:461:PHE:CD2	1:A:486:GLU:HG2	2.54	0.42
1:C:557:THR:OG1	1:C:558:THR:N	2.52	0.42
1:D:472:ASN:C	1:D:474:LYS:N	2.73	0.42
1:D:567:ASN:HD22	1:D:567:ASN:HA	1.56	0.42
1:C:564:ALA:HB2	1:D:528:GLU:HG2	2.01	0.42
1:A:592:PRO:HB3	1:A:683:VAL:HA	2.00	0.42
1:B:460:LYS:HE2	1:B:460:LYS:N	2.35	0.42
1:B:468:ILE:HG23	1:B:472:ASN:ND2	2.34	0.42
1:B:486:GLU:OE1	1:B:486:GLU:HA	2.19	0.42
1:B:626:SER:OG	1:B:627:ARG:N	2.51	0.42
1:D:459:ALA:HB3	1:D:462:LEU:HD21	2.01	0.42
1:D:712:ILE:HG22	1:D:717:VAL:CG2	2.49	0.42
1:A:546:LEU:HD11	1:A:581:SER:HB3	2.02	0.42
1:B:473:ALA:C	1:B:475:HIS:N	2.71	0.42
1:C:586:ASP:CG	1:C:704:LYS:HZ2	2.22	0.42
1:D:626:SER:OG	1:D:627:ARG:N	2.53	0.42
1:A:833:GLU:OE1	1:A:836:ARG:NH1	2.50	0.42
1:B:767:ASP:HB3	1:B:770:GLN:HG3	2.00	0.42
1:D:496:ARG:NH1	1:D:531:ILE:O	2.53	0.42
1:D:715:LYS:O	1:D:719:GLU:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:ASN:O	1:B:518:ASN:CG	2.57	0.42
1:B:725:THR:O	1:B:729:ILE:HG13	2.20	0.42
1:C:828:LYS:HG3	1:C:829:ASP:N	2.27	0.42
1:D:470:LEU:HA	1:D:473:ALA:HB3	2.02	0.42
1:A:562:LEU:CD1	1:A:755:ASN:HB3	2.49	0.42
1:A:685:GLY:HA2	1:B:735:LYS:HG3	2.02	0.42
1:A:764:CYS:HB3	1:A:818:LEU:HD21	2.02	0.42
1:B:796:THR:HG21	1:C:638:ILE:O	2.20	0.42
1:A:495:ARG:HD2	1:A:530:VAL:O	2.20	0.41
1:C:862:LEU:HD11	2:C:103:HMG:C6	2.50	0.41
1:D:688:CYS:N	1:D:689:THR:HA	2.35	0.41
1:A:853:LEU:O	1:A:853:LEU:HD12	2.21	0.41
1:B:485:ILE:O	1:B:485:ILE:HG22	2.20	0.41
1:B:460:LYS:HB3	1:B:461:PHE:CD1	2.56	0.41
1:B:466:GLU:C	1:B:468:ILE:H	2.23	0.41
1:B:715:LYS:HE2	1:B:719:GLU:OE1	2.20	0.41
1:C:560:GLY:O	1:C:561:CYS:CB	2.68	0.41
1:A:534:MET:HE1	1:B:814:GLN:CD	2.41	0.41
1:B:565:SER:HB2	2:B:102:HMG:C6P	2.46	0.41
1:B:630:ARG:HE	1:B:650:ARG:HB2	1.84	0.41
1:C:470:LEU:HD23	1:C:474:LYS:HG3	2.02	0.41
1:C:494:ILE:HG23	1:C:498:LEU:HD21	2.03	0.41
1:C:833:GLU:OE1	1:C:836:ARG:NH1	2.46	0.41
1:D:649:SER:HB3	1:D:660:ILE:CD1	2.51	0.41
1:A:517:TYR:CE1	1:B:535:PRO:HB2	2.56	0.41
1:B:509:LEU:HD22	1:B:512:LEU:CD1	2.50	0.41
1:C:590:ARG:HA	1:C:590:ARG:HD3	1.75	0.41
1:A:706:VAL:HG13	1:A:800:ILE:HD12	2.02	0.41
1:B:702:ARG:O	1:B:799:SER:HA	2.21	0.41
1:C:714:ALA:HB2	1:C:789:GLU:O	2.21	0.41
1:C:723:THR:HB	1:C:724:THR:H	1.47	0.41
1:C:764:CYS:HB3	1:C:818:LEU:HD21	2.02	0.41
1:A:534:MET:HE1	1:B:814:GLN:NE2	2.36	0.41
1:A:797:MET:HA	1:A:798:PRO:HD3	1.77	0.41
1:B:460:LYS:HB3	1:B:461:PHE:HD1	1.85	0.41
1:B:560:GLY:O	1:B:561:CYS:CB	2.69	0.41
1:C:517:TYR:HE2	1:D:535:PRO:CB	2.34	0.41
1:A:563:VAL:HB	1:B:528:GLU:HB2	2.03	0.41
1:B:833:GLU:OE1	1:B:836:ARG:NH1	2.50	0.41
1:C:562:LEU:HD11	1:C:755:ASN:HB3	2.02	0.41
1:A:512:LEU:HA	1:A:513:PRO:HD3	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:ARG:HD2	1:C:531:ILE:CG2	2.50	0.41
1:C:562:LEU:CD1	1:C:755:ASN:HB3	2.51	0.41
1:C:655:MET:HE3	1:C:655:MET:O	2.21	0.41
1:C:866:HIS:CE1	2:C:103:HMG:N4P	2.89	0.41
1:A:557:THR:OG1	1:A:558:THR:N	2.54	0.41
1:A:707:VAL:HG13	1:A:796:THR:HG23	2.03	0.41
1:B:473:ALA:O	1:B:475:HIS:N	2.53	0.41
1:B:815:GLN:O	1:B:819:GLN:HG3	2.20	0.41
1:C:514:TYR:CB	1:C:532:GLY:HA2	2.51	0.41
1:D:461:PHE:CZ	1:D:486:GLU:OE2	2.73	0.41
1:D:593:VAL:CG2	1:D:685:GLY:CA	2.92	0.41
1:D:828:LYS:CE	1:D:829:ASP:H	2.33	0.41
1:B:728:MET:HE3	1:B:791:LEU:HD21	2.03	0.40
1:C:523:MET:CE	1:C:523:MET:N	2.84	0.40
1:D:485:ILE:CG2	1:D:490:ARG:HD3	2.51	0.40
1:A:819:GLN:HB3	1:B:508:SER:CB	2.40	0.40
1:B:764:CYS:HB3	1:B:818:LEU:HD21	2.04	0.40
1:D:487:THR:O	1:D:488:HIS:C	2.59	0.40
1:D:723:THR:HB	1:D:724:THR:H	1.48	0.40
1:A:488:HIS:CE1	1:A:523:MET:HG3	2.56	0.40
1:B:617:VAL:HG23	1:B:670:LYS:CD	2.51	0.40
1:C:708:CYS:O	1:C:794:SER:HA	2.21	0.40
1:C:862:LEU:HD11	2:C:103:HMG:H62	2.04	0.40
1:D:476:ILE:HG23	1:D:484:LEU:CD2	2.50	0.40
1:A:862:LEU:HA	1:A:862:LEU:HD23	1.76	0.40
1:B:632:GLN:NE2	1:B:650:ARG:HG2	2.36	0.40
1:D:702:ARG:O	1:D:799:SER:HA	2.22	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	403/467 (86%)	361 (90%)	31 (8%)	11 (3%)	5	17
1	B	403/467 (86%)	358 (89%)	33 (8%)	12 (3%)	4	15
1	C	405/467 (87%)	356 (88%)	39 (10%)	10 (2%)	5	19
1	D	411/467 (88%)	366 (89%)	33 (8%)	12 (3%)	4	15
All	All	1622/1868 (87%)	1441 (89%)	136 (8%)	45 (3%)	5	17

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	863	VAL
1	B	485	ILE
1	B	487	THR
1	B	514	TYR
1	C	462	LEU
1	C	468	ILE
1	C	514	TYR
1	D	485	ILE
1	D	514	TYR
1	A	468	ILE
1	A	514	TYR
1	A	518	ASN
1	A	864	LYS
1	B	519	TYR
1	B	525	ALA
1	D	457	LYS
1	D	465	ALA
1	D	509	LEU
1	A	475	HIS
1	A	502	LYS
1	A	525	ALA
1	A	824	GLN
1	B	474	LYS
1	B	481	LEU
1	B	484	LEU
1	B	488	HIS
1	B	651	SER
1	C	824	GLN
1	D	479	TYR
1	D	516	ASP
1	D	824	GLN
1	A	651	SER
1	C	481	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	487	THR
1	C	651	SER
1	D	459	ALA
1	D	651	SER
1	A	632	GLN
1	B	824	GLN
1	C	632	GLN
1	D	518	ASN
1	B	506	PRO
1	D	632	GLN
1	C	506	PRO
1	C	863	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	323/375 (86%)	306 (95%)	17 (5%)	22	54
1	B	323/375 (86%)	307 (95%)	16 (5%)	24	56
1	C	325/375 (87%)	302 (93%)	23 (7%)	14	39
1	D	327/375 (87%)	308 (94%)	19 (6%)	20	50
All	All	1298/1500 (86%)	1223 (94%)	75 (6%)	20	50

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	PHE
1	A	486	GLU
1	A	509	LEU
1	A	521	LEU
1	A	529	ASN
1	A	567	ASN
1	A	568	ARG
1	A	595	ARG
1	A	625	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	655	MET
1	A	666	LYS
1	A	683	VAL
1	A	707	VAL
1	A	723	THR
1	A	752	HIS
1	A	789	GLU
1	A	814	GLN
1	B	461	PHE
1	B	505	GLU
1	B	512	LEU
1	B	567	ASN
1	B	568	ARG
1	B	595	ARG
1	B	598	ARG
1	B	625	THR
1	B	655	MET
1	B	683	VAL
1	B	707	VAL
1	B	718	ARG
1	B	723	THR
1	B	752	HIS
1	B	814	GLN
1	B	828	LYS
1	C	462	LEU
1	C	464	ASP
1	C	474	LYS
1	C	483	THR
1	C	492	VAL
1	C	494	ILE
1	C	505	GLU
1	C	515	ARG
1	C	523	MET
1	C	567	ASN
1	C	568	ARG
1	C	595	ARG
1	C	625	THR
1	C	650	ARG
1	C	655	MET
1	C	683	VAL
1	C	707	VAL
1	C	723	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	752	HIS
1	C	779	THR
1	C	814	GLN
1	C	819	GLN
1	C	851	LEU
1	D	484	LEU
1	D	487	THR
1	D	509	LEU
1	D	510	GLN
1	D	521	LEU
1	D	567	ASN
1	D	568	ARG
1	D	594	VAL
1	D	595	ARG
1	D	625	THR
1	D	655	MET
1	D	683	VAL
1	D	707	VAL
1	D	723	THR
1	D	752	HIS
1	D	789	GLU
1	D	796	THR
1	D	814	GLN
1	D	828	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	GLN
1	A	510	GLN
1	A	518	ASN
1	A	552	GLN
1	A	567	ASN
1	A	632	GLN
1	A	672	HIS
1	A	755	ASN
1	A	788	ASN
1	A	810	ASN
1	A	824	GLN
1	B	472	ASN
1	B	552	GLN
1	B	567	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	632	GLN
1	B	648	GLN
1	B	771	ASN
1	B	788	ASN
1	B	810	ASN
1	B	819	GLN
1	B	824	GLN
1	B	830	ASN
1	B	861	HIS
1	C	469	GLN
1	C	475	HIS
1	C	497	GLN
1	C	510	GLN
1	C	518	ASN
1	C	552	GLN
1	C	567	ASN
1	C	648	GLN
1	C	672	HIS
1	C	752	HIS
1	C	771	ASN
1	C	788	ASN
1	C	810	ASN
1	C	824	GLN
1	C	830	ASN
1	D	472	ASN
1	D	475	HIS
1	D	488	HIS
1	D	518	ASN
1	D	552	GLN
1	D	567	ASN
1	D	632	GLN
1	D	648	GLN
1	D	672	HIS
1	D	771	ASN
1	D	788	ASN
1	D	810	ASN
1	D	819	GLN
1	D	824	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HMG	C	103	-	52,60,60	1.91	10 (19%)	62,90,90	1.10	4 (6%)
2	HMG	B	102	-	52,60,60	2.07	14 (26%)	62,90,90	1.16	5 (8%)
2	HMG	A	101	-	52,60,60	1.88	10 (19%)	62,90,90	1.07	4 (6%)
2	HMG	D	104	-	52,60,60	1.98	12 (23%)	62,90,90	1.20	4 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HMG	C	103	-	-	11/56/77/77	0/3/3/3
2	HMG	B	102	-	-	9/56/77/77	0/3/3/3
2	HMG	A	101	-	-	10/56/77/77	0/3/3/3
2	HMG	D	104	-	-	14/56/77/77	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	103	HMG	C4A-N3A	8.67	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	102	HMG	C4A-N3A	8.60	1.47	1.35
2	D	104	HMG	C4A-N3A	8.45	1.47	1.35
2	A	101	HMG	C4A-N3A	8.19	1.47	1.35
2	B	102	HMG	C6-C3	4.21	1.57	1.52
2	B	102	HMG	C1-S1P	4.16	1.86	1.76
2	D	104	HMG	P3B-O7A	3.97	1.63	1.50
2	B	102	HMG	O2-C1	3.84	1.27	1.21
2	D	104	HMG	C1-S1P	3.63	1.84	1.76
2	A	101	HMG	P3B-O7A	3.60	1.62	1.50
2	A	101	HMG	P1A-O1A	3.54	1.63	1.50
2	C	103	HMG	P3B-O7A	3.54	1.61	1.50
2	A	101	HMG	O2-C1	3.44	1.26	1.21
2	B	102	HMG	P3B-O7A	3.34	1.61	1.50
2	A	101	HMG	C1-S1P	3.22	1.83	1.76
2	C	103	HMG	P1A-O1A	3.19	1.62	1.50
2	B	102	HMG	C2-C1	3.17	1.57	1.51
2	C	103	HMG	P2A-O5A	3.12	1.62	1.50
2	C	103	HMG	C6-C3	3.04	1.56	1.52
2	B	102	HMG	C4-C3	3.02	1.58	1.54
2	B	102	HMG	P2A-O5A	3.01	1.61	1.50
2	D	104	HMG	P1A-O1A	2.92	1.61	1.50
2	A	101	HMG	P2A-O5A	2.90	1.61	1.50
2	D	104	HMG	C6-C3	2.84	1.55	1.52
2	C	103	HMG	C1-S1P	2.78	1.82	1.76
2	D	104	HMG	P2A-O5A	2.77	1.60	1.50
2	A	101	HMG	C6-C3	2.75	1.55	1.52
2	B	102	HMG	P1A-O1A	2.73	1.60	1.50
2	C	103	HMG	O2-C1	2.49	1.25	1.21
2	D	104	HMG	O4B-C1B	2.46	1.44	1.41
2	D	104	HMG	P3B-O9A	2.35	1.63	1.54
2	C	103	HMG	O4B-C1B	2.32	1.44	1.41
2	B	102	HMG	O4-C5	2.31	1.38	1.30
2	B	102	HMG	O4B-C1B	2.24	1.44	1.41
2	D	104	HMG	C2-C3	2.23	1.57	1.54
2	C	103	HMG	C5A-C4A	2.22	1.46	1.40
2	D	104	HMG	O2-C1	2.14	1.24	1.21
2	B	102	HMG	OAP-CAP	2.12	1.46	1.42
2	A	101	HMG	O4-C5	2.10	1.37	1.30
2	A	101	HMG	C5A-C4A	2.10	1.46	1.40
2	C	103	HMG	P3B-O9A	2.09	1.62	1.54
2	D	104	HMG	C2-C1	2.06	1.55	1.51
2	B	102	HMG	C5A-C4A	2.06	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	102	HMG	C2-C3	2.05	1.57	1.54
2	A	101	HMG	P3B-O8A	2.04	1.62	1.54
2	D	104	HMG	C5A-C4A	2.03	1.46	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	104	HMG	C2-C1-S1P	4.77	119.53	113.63
2	A	101	HMG	C4A-C5A-N7A	3.82	113.38	109.40
2	B	102	HMG	C2-C1-S1P	3.82	118.35	113.63
2	D	104	HMG	C4A-C5A-N7A	3.67	113.22	109.40
2	B	102	HMG	C4A-C5A-N7A	3.60	113.15	109.40
2	C	103	HMG	P1A-O3A-P2A	-3.50	120.82	132.83
2	C	103	HMG	C2-C1-S1P	3.45	117.89	113.63
2	C	103	HMG	C4A-C5A-N7A	3.43	112.97	109.40
2	D	104	HMG	O2-C1-C2	-3.15	118.60	123.64
2	A	101	HMG	C2-C1-S1P	3.05	117.40	113.63
2	B	102	HMG	P1A-O3A-P2A	-3.00	122.53	132.83
2	C	103	HMG	O2-C1-C2	-2.90	119.00	123.64
2	B	102	HMG	O2-C1-C2	-2.81	119.14	123.64
2	A	101	HMG	P1A-O3A-P2A	-2.70	123.57	132.83
2	A	101	HMG	O2-C1-C2	-2.53	119.59	123.64
2	D	104	HMG	P1A-O3A-P2A	-2.33	124.83	132.83
2	B	102	HMG	CEP-CBP-CAP	2.16	112.57	108.82

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	101	HMG	C5B-O5B-P1A-O3A
2	A	101	HMG	C5B-O5B-P1A-O1A
2	A	101	HMG	C3P-C2P-S1P-C1
2	A	101	HMG	O2-C1-S1P-C2P
2	A	101	HMG	C2-C1-S1P-C2P
2	A	101	HMG	C1-C2-C3-O7
2	A	101	HMG	C1-C2-C3-C6
2	B	102	HMG	C5B-O5B-P1A-O3A
2	B	102	HMG	C3P-C2P-S1P-C1
2	B	102	HMG	O2-C1-S1P-C2P
2	B	102	HMG	C2-C1-S1P-C2P
2	C	103	HMG	C5B-O5B-P1A-O3A
2	C	103	HMG	C3P-C2P-S1P-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	103	HMG	O2-C1-S1P-C2P
2	C	103	HMG	C2-C1-S1P-C2P
2	C	103	HMG	O7-C3-C4-C5
2	C	103	HMG	C6-C3-C4-C5
2	D	104	HMG	C5B-O5B-P1A-O1A
2	D	104	HMG	C5B-O5B-P1A-O2A
2	D	104	HMG	C3B-O3B-P3B-O7A
2	D	104	HMG	O2-C1-S1P-C2P
2	D	104	HMG	C2-C1-S1P-C2P
2	B	102	HMG	O5P-C5P-N4P-C3P
2	B	102	HMG	C6P-C5P-N4P-C3P
2	A	101	HMG	C6P-C5P-N4P-C3P
2	A	101	HMG	O5P-C5P-N4P-C3P
2	C	103	HMG	O5P-C5P-N4P-C3P
2	A	101	HMG	P2A-O3A-P1A-O5B
2	B	102	HMG	P2A-O3A-P1A-O5B
2	C	103	HMG	P2A-O3A-P1A-O5B
2	C	103	HMG	C6P-C5P-N4P-C3P
2	B	102	HMG	C5B-O5B-P1A-O1A
2	C	103	HMG	C5B-O5B-P1A-O1A
2	D	104	HMG	S1P-C2P-C3P-N4P
2	D	104	HMG	CEP-CBP-CCP-O6A
2	D	104	HMG	P1A-O3A-P2A-O4A
2	D	104	HMG	C3P-C2P-S1P-C1
2	D	104	HMG	C6P-C7P-N8P-C9P
2	C	103	HMG	C3B-O3B-P3B-O9A
2	D	104	HMG	C5B-O5B-P1A-O3A
2	B	102	HMG	C6P-C7P-N8P-C9P
2	D	104	HMG	P1A-O3A-P2A-O5A
2	D	104	HMG	CCP-O6A-P2A-O5A
2	D	104	HMG	C1-C2-C3-O7

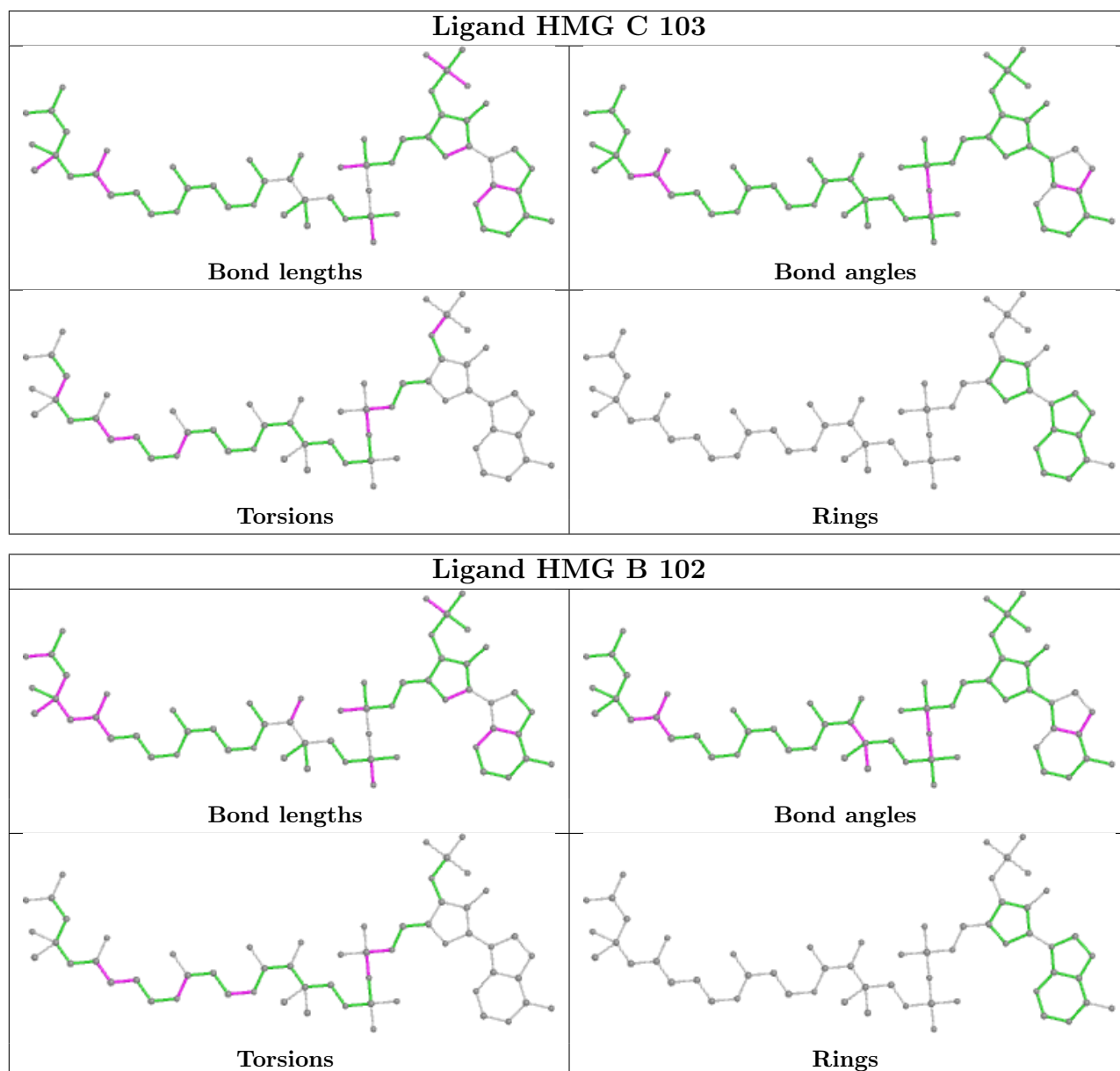
There are no ring outliers.

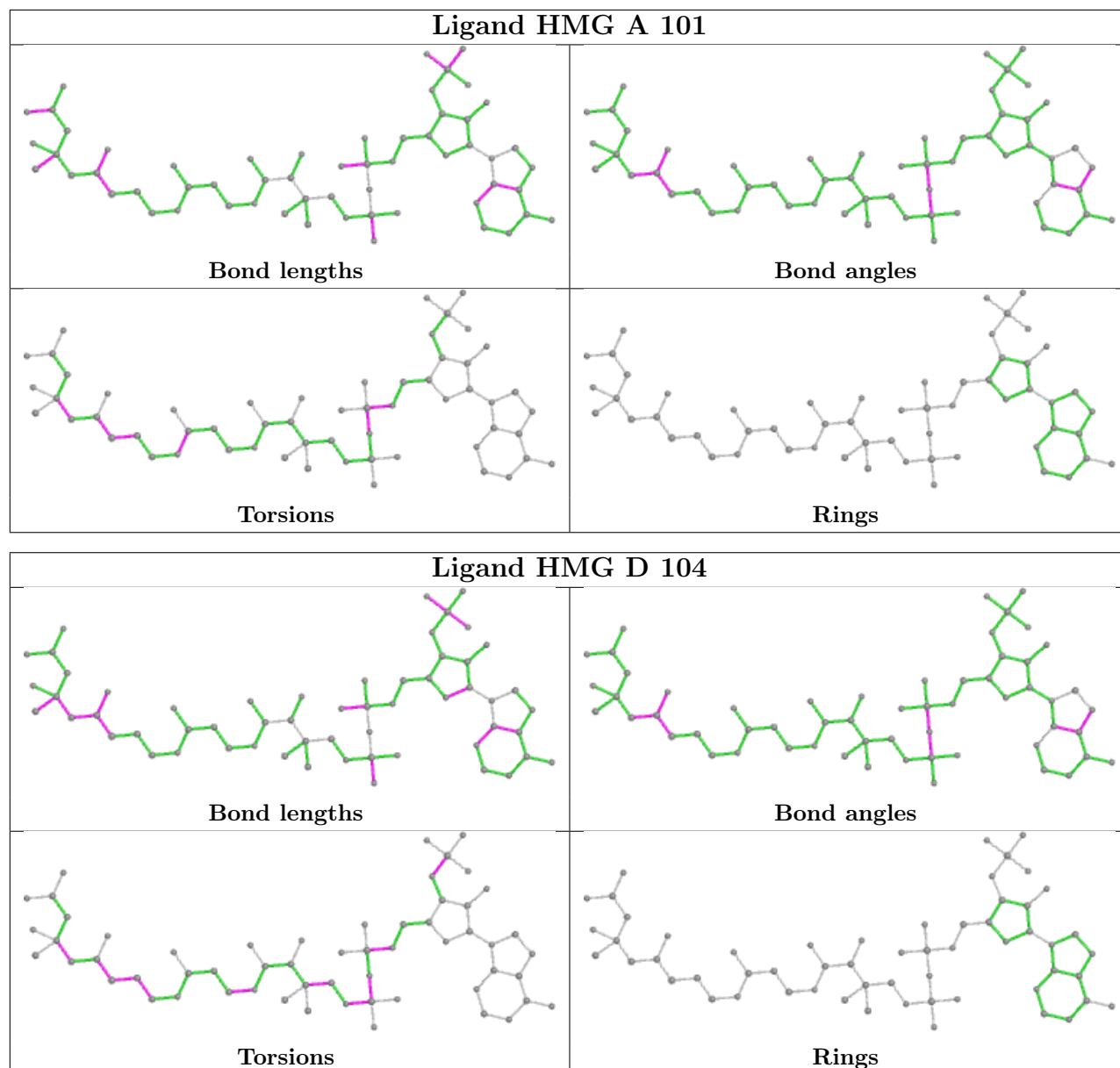
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	103	HMG	5	0
2	B	102	HMG	5	0
2	A	101	HMG	3	0
2	D	104	HMG	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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





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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	405/467 (86%)	-0.28	11 (2%) 54 44	10, 44, 79, 118	0
1	B	405/467 (86%)	-0.38	11 (2%) 54 44	11, 43, 77, 111	0
1	C	407/467 (87%)	-0.24	15 (3%) 41 31	23, 48, 84, 118	0
1	D	413/467 (88%)	-0.29	16 (3%) 39 29	13, 44, 93, 118	0
All	All	1630/1868 (87%)	-0.30	53 (3%) 46 36	10, 45, 83, 118	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	475	HIS	5.8
1	C	475	HIS	5.4
1	A	787	THR	5.1
1	D	475	HIS	4.1
1	D	786	PRO	3.9
1	A	786	PRO	3.7
1	D	474	LYS	3.7
1	D	787	THR	3.7
1	D	465	ALA	3.5
1	C	829	ASP	3.5
1	C	461	PHE	3.4
1	D	454	ASN	3.4
1	B	864	LYS	3.3
1	C	486	GLU	3.3
1	C	506	PRO	3.2
1	B	829	ASP	3.2
1	A	785	GLY	3.2
1	A	788	ASN	3.1
1	B	473	ALA	3.1
1	C	866	HIS	3.1
1	D	473	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	461	PHE	2.9
1	C	612	SER	2.8
1	D	864	LYS	2.8
1	A	473	ALA	2.7
1	B	830	ASN	2.7
1	C	473	ALA	2.7
1	D	471	VAL	2.7
1	D	453	GLY	2.7
1	D	466	GLU	2.5
1	C	786	PRO	2.5
1	C	830	ASN	2.5
1	A	461	PHE	2.5
1	B	476	ILE	2.5
1	A	865	SER	2.4
1	B	828	LYS	2.4
1	B	612	SER	2.4
1	B	613	GLU	2.4
1	C	463	SER	2.4
1	C	828	LYS	2.3
1	C	785	GLY	2.3
1	A	504	SER	2.3
1	A	462	LEU	2.3
1	D	830	ASN	2.2
1	B	506	PRO	2.2
1	D	476	ILE	2.2
1	A	484	LEU	2.1
1	A	463	SER	2.1
1	C	787	THR	2.1
1	D	789	GLU	2.1
1	D	456	GLU	2.1
1	B	474	LYS	2.1
1	C	548	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](#)

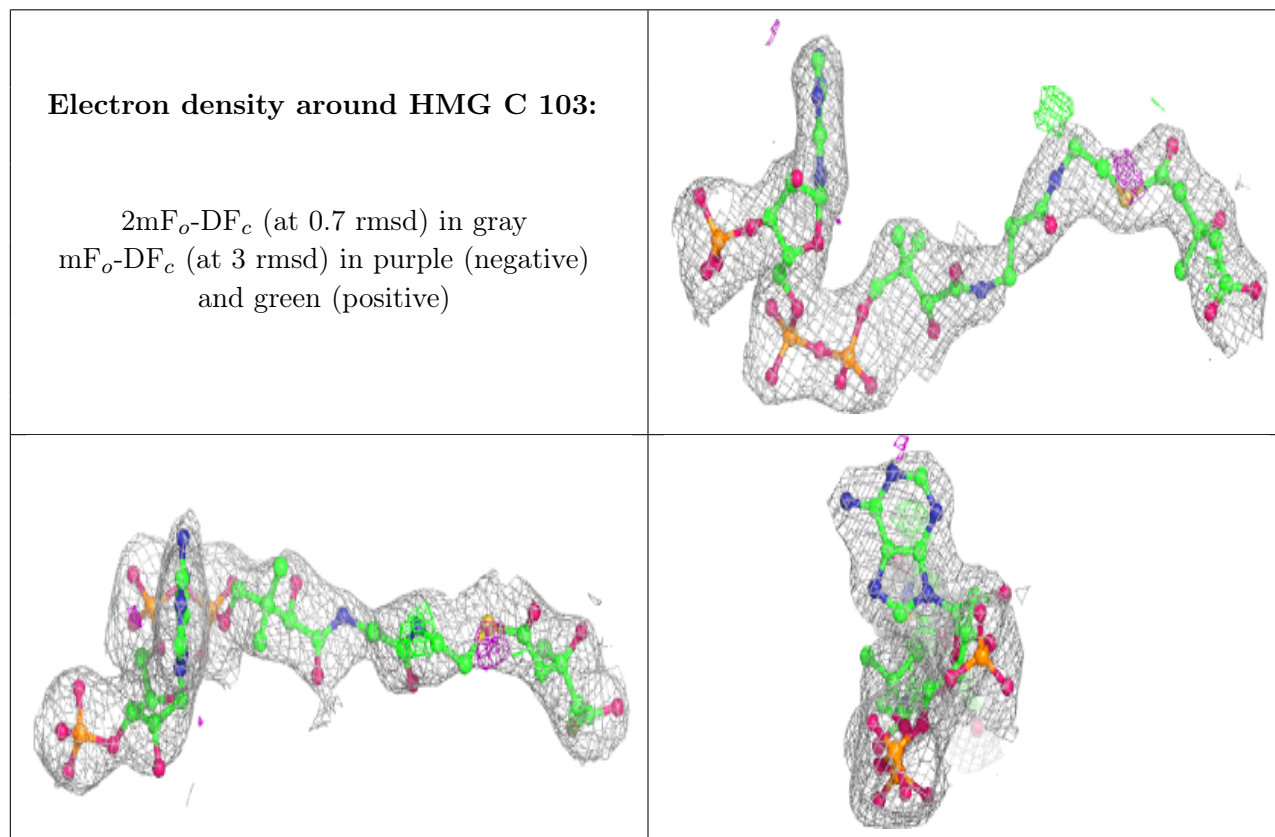
There are no monosaccharides in this entry.

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, 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.

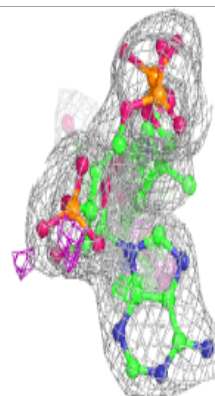
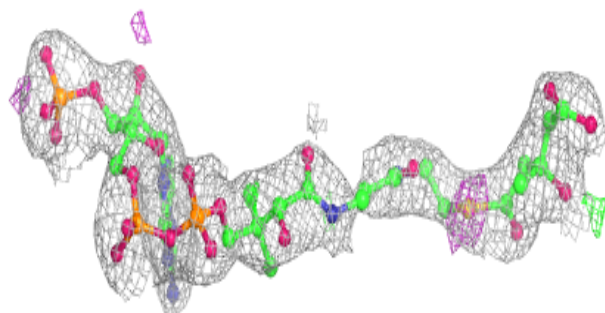
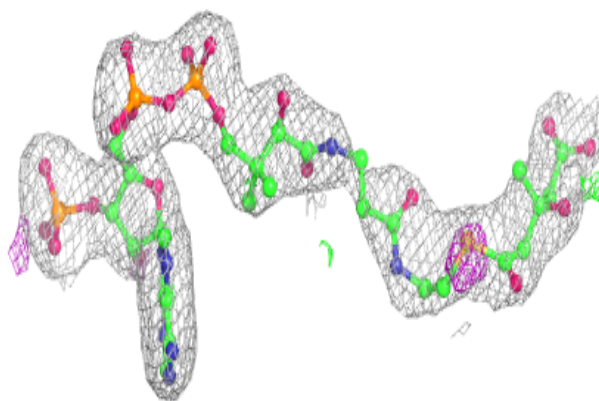
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HMG	C	103	58/58	0.94	0.15	62,62,62,62	0
2	HMG	D	104	58/58	0.94	0.16	53,53,53,53	0
2	HMG	A	101	58/58	0.95	0.14	54,54,54,54	0
2	HMG	B	102	58/58	0.95	0.15	53,53,53,53	0

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.

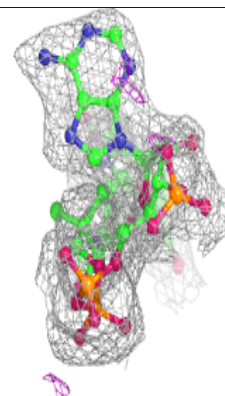
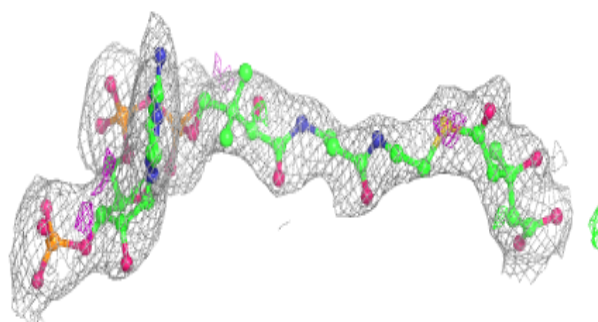
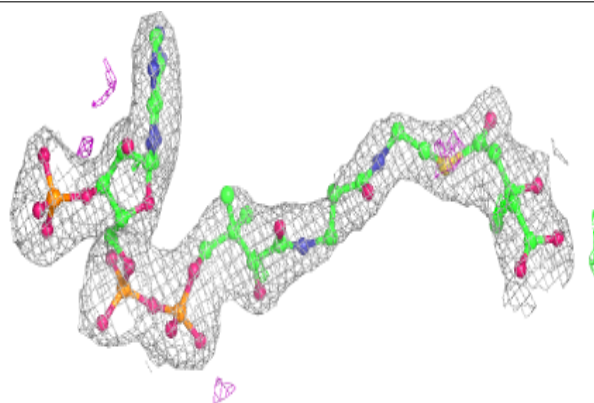


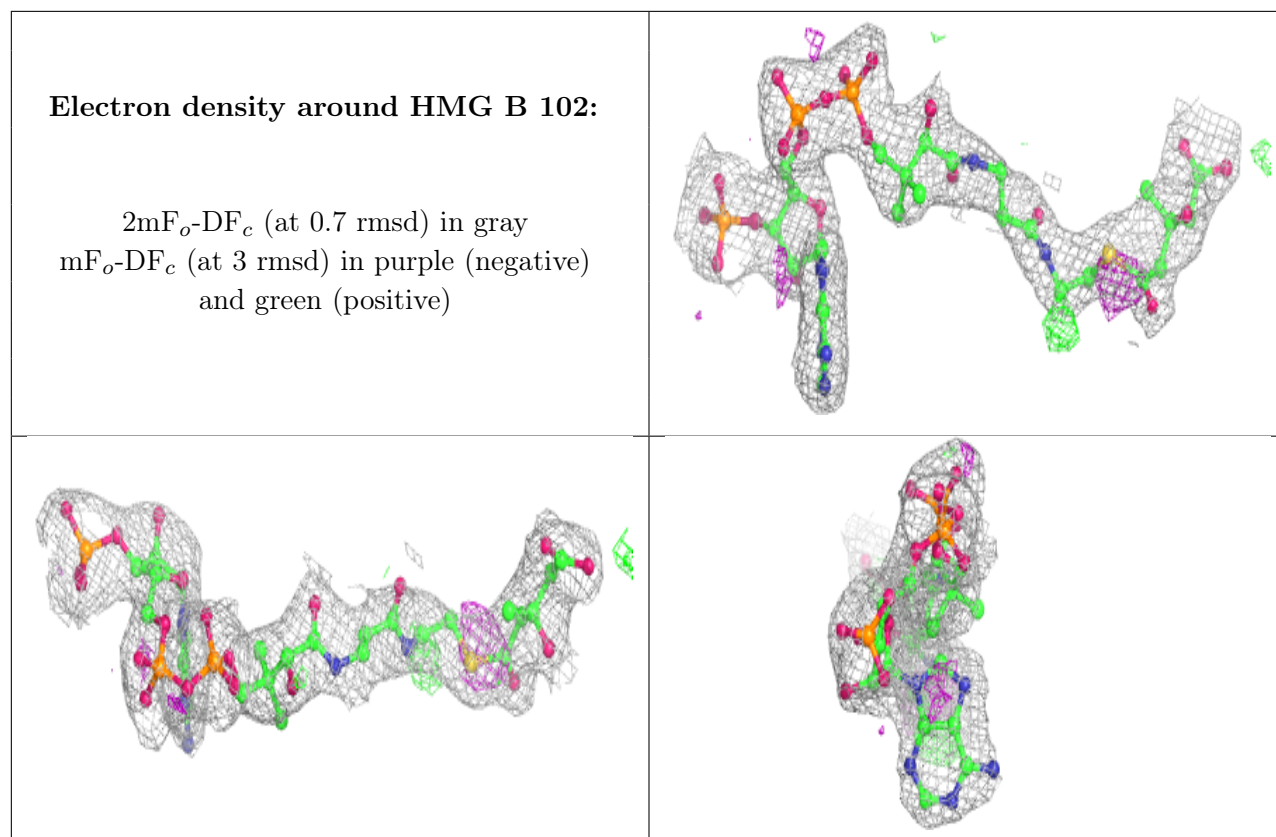
Electron density around HMG D 104:

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

**Electron density around HMG A 101:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.