



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:56 PM UTC

PDB ID : 1JZ3 / pdb_00001jz3
Title : E. COLI (lacZ) BETA-GALACTOSIDASE-TRAPPED 2-DEOXY-
GALACTOSYL ENZYME INTERMEDIATE
Authors : Juers, D.H.; Matthews, B.W.
Deposited on : 2001-09-13
Resolution : 1.75 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

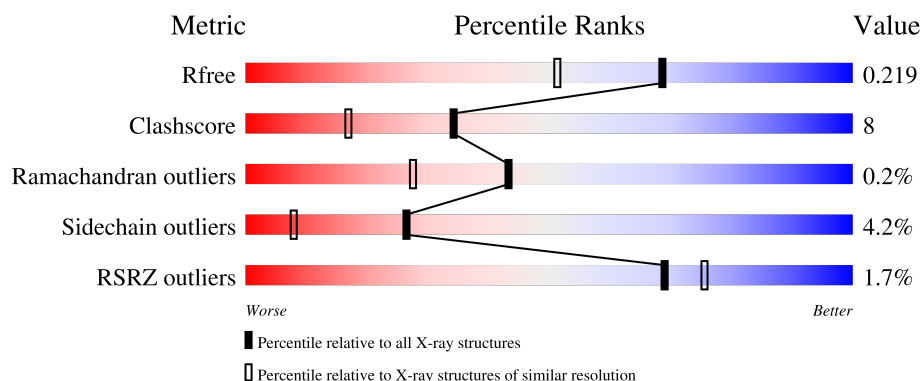
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	1023	0% 78% 17% ..
1	B	1023	2% 80% 16% ..
1	C	1023	0% 79% 17% ..
1	D	1023	2% 77% 18% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	DMS	A	8503	-	-	X	-
6	DMS	C	8425	-	-	X	-
6	DMS	D	8703	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 37369 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	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			
1	B	1011	Total	C	N	O	S	0	1	0
			8131	5144	1440	1509	38			
1	C	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			

There are 32 discrepancies between the modelled and reference sequences:

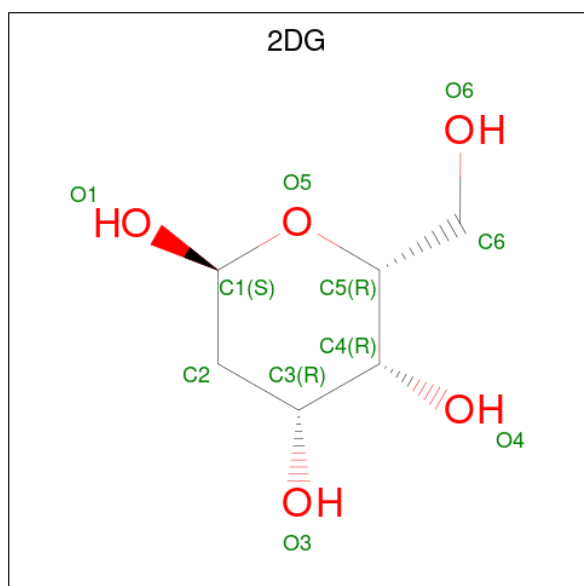
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	THR	cloning artifact	? P00722
A	2	SER	MET	cloning artifact	? P00722
A	3	HIS	ILE	cloning artifact	? P00722
A	4	MET	THR	cloning artifact	? P00722
A	5	LEU	ASP	cloning artifact	? P00722
A	6	GLU	SER	cloning artifact	? P00722
A	7	ASP	LEU	cloning artifact	? P00722
A	8	PRO	ALA	cloning artifact	? P00722
B	1	GLY	THR	cloning artifact	? P00722
B	2	SER	MET	cloning artifact	? P00722
B	3	HIS	ILE	cloning artifact	? P00722
B	4	MET	THR	cloning artifact	? P00722
B	5	LEU	ASP	cloning artifact	? P00722
B	6	GLU	SER	cloning artifact	? P00722
B	7	ASP	LEU	cloning artifact	? P00722
B	8	PRO	ALA	cloning artifact	? P00722
C	1	GLY	THR	cloning artifact	? P00722
C	2	SER	MET	cloning artifact	? P00722
C	3	HIS	ILE	cloning artifact	? P00722
C	4	MET	THR	cloning artifact	? P00722
C	5	LEU	ASP	cloning artifact	? P00722

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	6	GLU	SER	cloning artifact	? P00722
C	7	ASP	LEU	cloning artifact	? P00722
C	8	PRO	ALA	cloning artifact	? P00722
D	1	GLY	THR	cloning artifact	? P00722
D	2	SER	MET	cloning artifact	? P00722
D	3	HIS	ILE	cloning artifact	? P00722
D	4	MET	THR	cloning artifact	? P00722
D	5	LEU	ASP	cloning artifact	? P00722
D	6	GLU	SER	cloning artifact	? P00722
D	7	ASP	LEU	cloning artifact	? P00722
D	8	PRO	ALA	cloning artifact	? P00722

- Molecule 2 is 2-deoxy-alpha-D-galactopyranose (CCD ID: 2DG) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			10	6	4		
2	D	1	Total	C	O	0	0
			10	6	4		

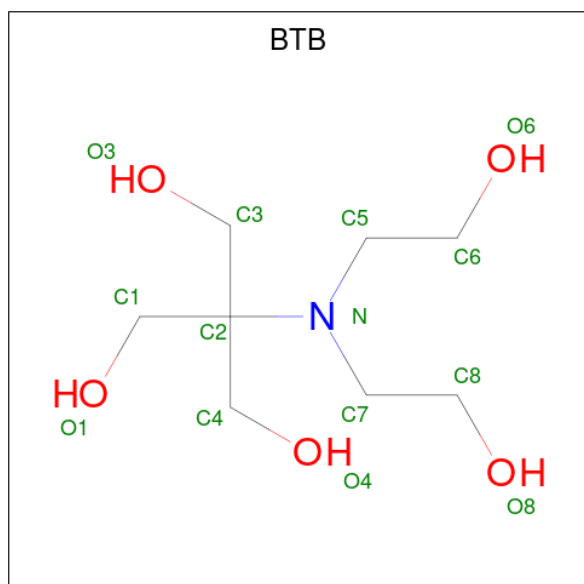
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mg	0	0
			4	4		
3	B	3	Total	Mg	0	0
			3	3		
3	C	6	Total	Mg	0	0
			6	6		
3	D	4	Total	Mg	0	0
			4	4		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Na	0	0
			4	4		
4	B	4	Total	Na	0	0
			4	4		
4	C	4	Total	Na	0	0
			4	4		
4	D	4	Total	Na	0	0
			4	4		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C₈H₁₉NO₅).



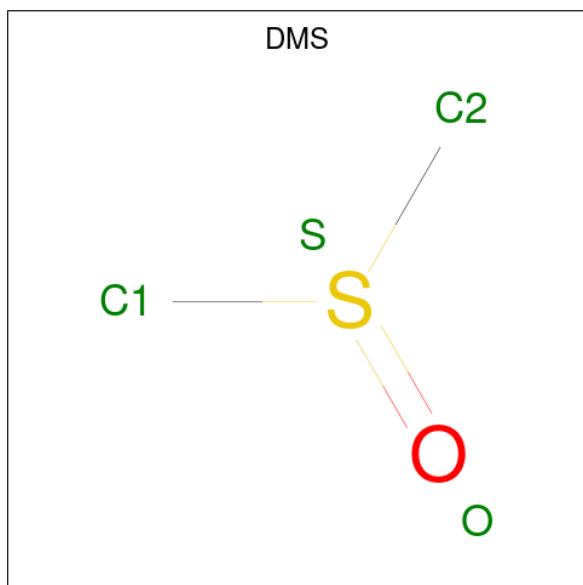
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	A	1	Total	C	O	S	0	0
			4	2	1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	B	1	Total 4	C 2	O 1	S 1	0	0
6	B	1	Total 4	C 2	O 1	S 1	0	0

Continued on next page...

Continued from previous page...

[illegible]

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total 4	C 2	O 1	S 1	0	0
6	B	1	Total 4	C 2	O 1	S 1	0	0
6	B	1	Total 4	C 2	O 1	S 1	0	0
6	B	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	C	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1090	Total 1090	O 1090	0	0

Continued on next page...

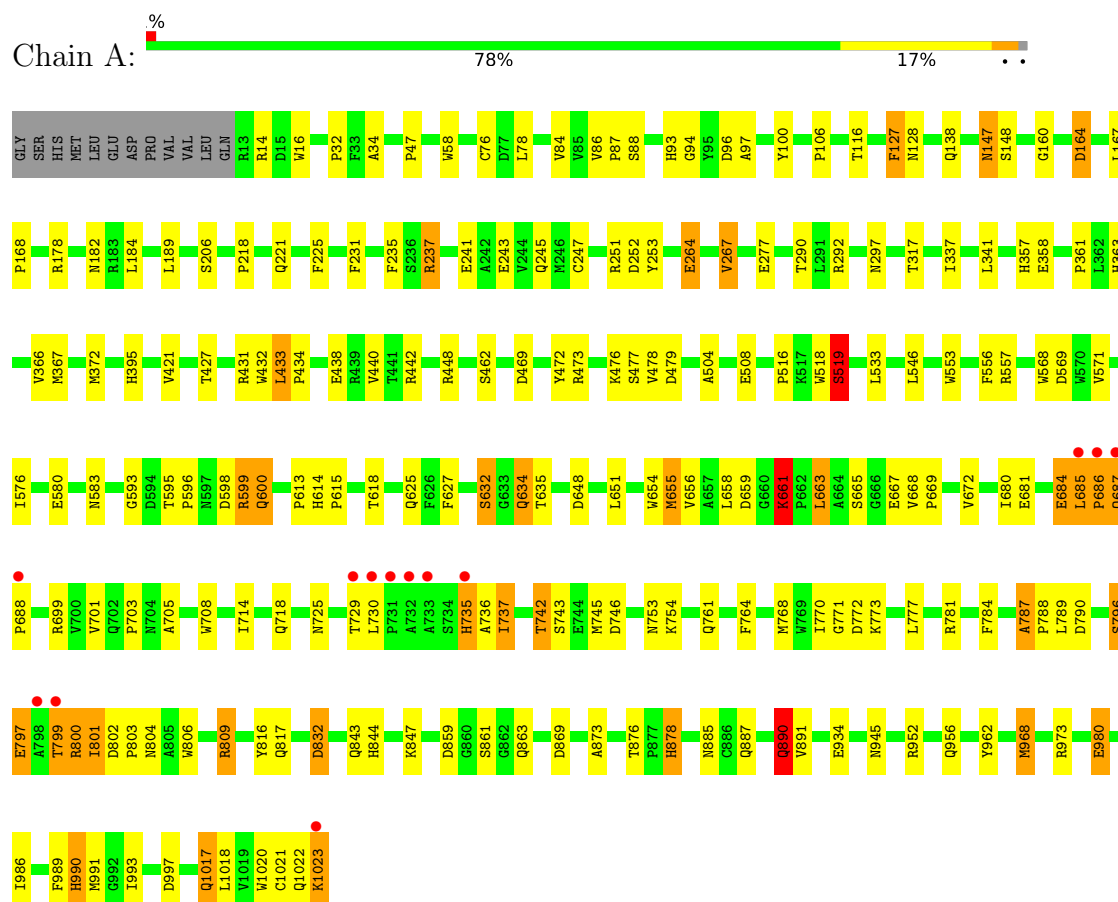
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1091	Total 1091	O 1091	0	0
7	C	1034	Total 1034	O 1034	0	0
7	D	1079	Total 1079	O 1079	0	0

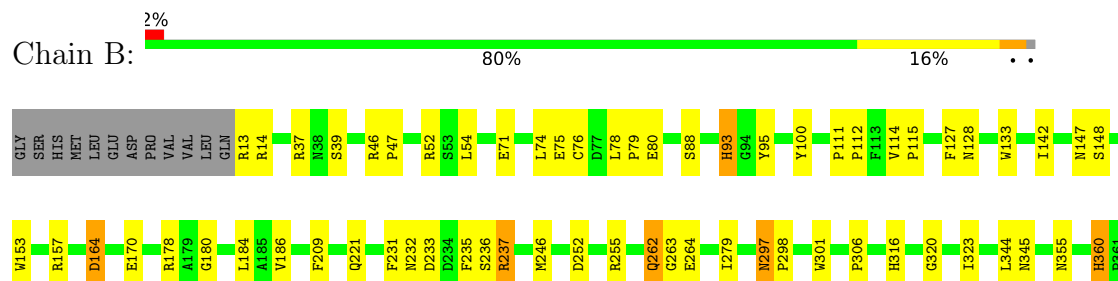
3 Residue-property plots

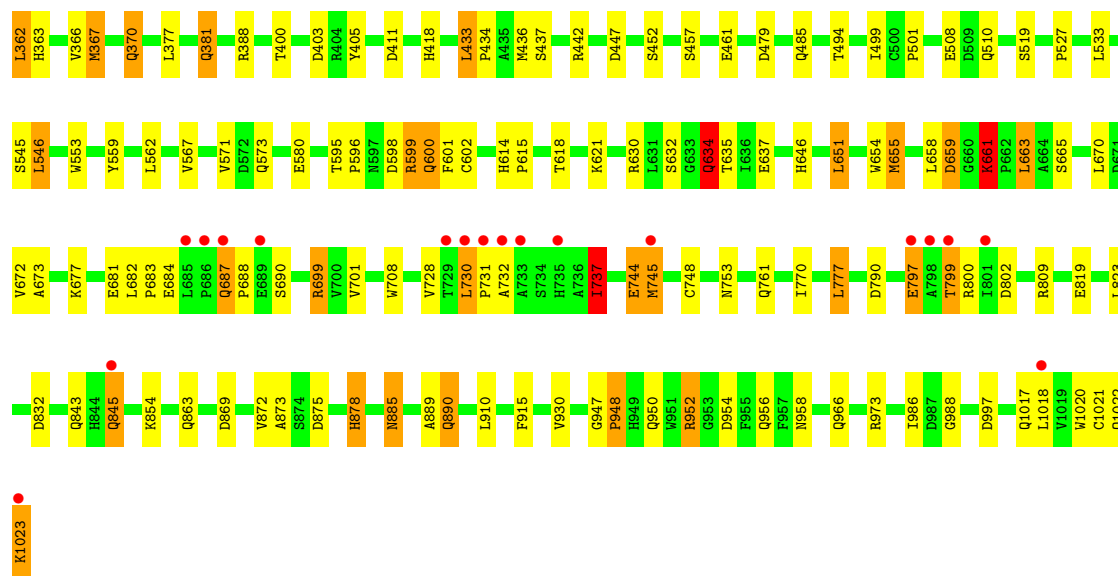
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

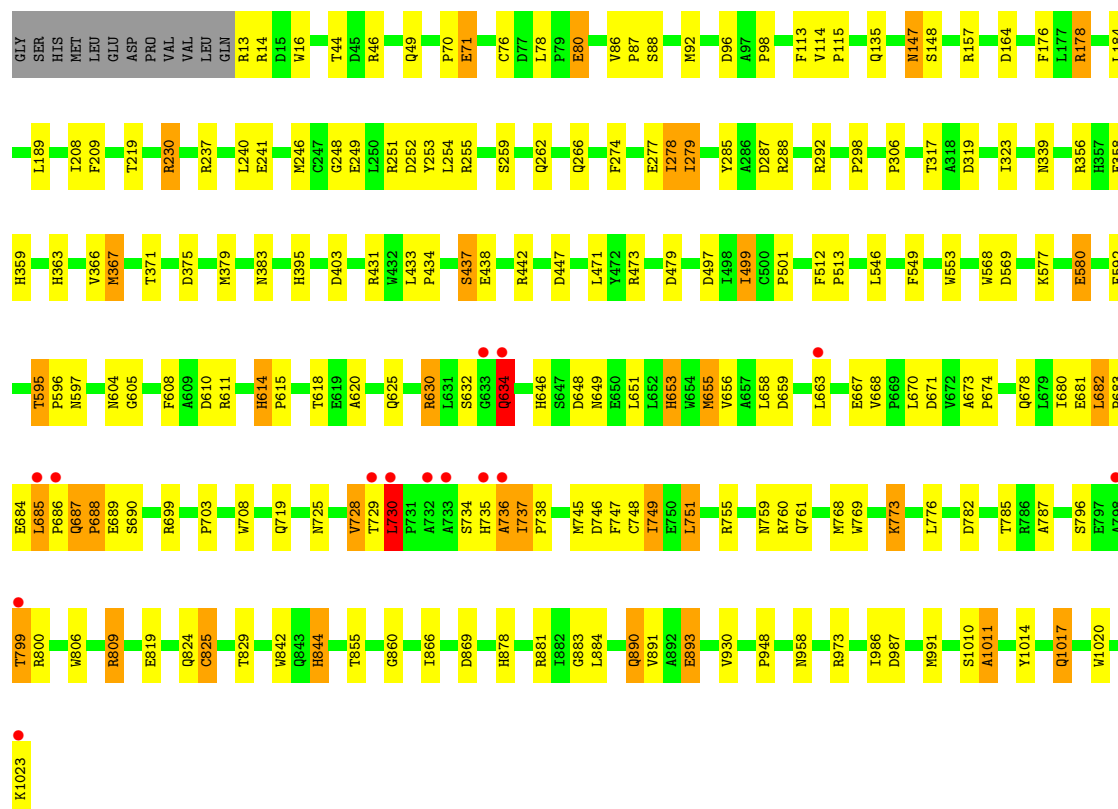
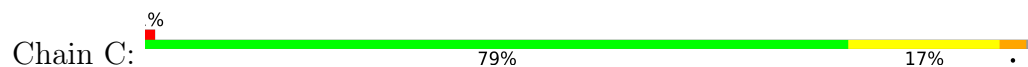


• Molecule 1: Beta-Galactosidase

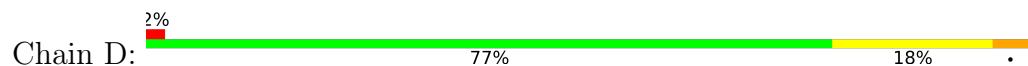


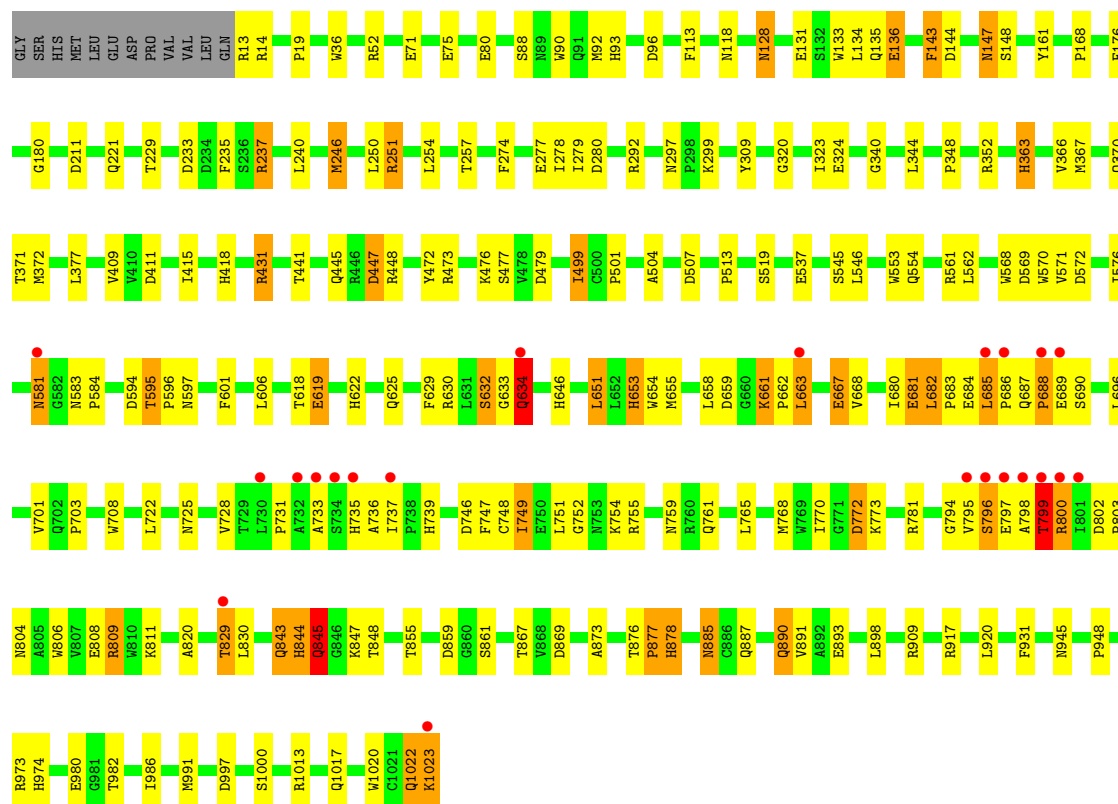


• Molecule 1: Beta-Galactosidase



• Molecule 1: Beta-Galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.56Å 168.19Å 200.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.00 – 1.75 16.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	93.8 (16.00-1.75) 93.3 (16.00-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.75Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.158 , 0.222 0.163 , 0.219	Depositor DCC
R_{free} test set	6833 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 99.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	37369	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.43 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0078e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: DMS, MG, BTB, NA, 2DG

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	1.24	4/8367 (0.0%)	1.72	101/11415 (0.9%)
1	B	1.23	3/8379 (0.0%)	1.71	88/11431 (0.8%)
1	C	1.22	3/8367 (0.0%)	1.71	94/11415 (0.8%)
1	D	1.25	5/8367 (0.1%)	1.71	109/11415 (1.0%)
All	All	1.24	15/33480 (0.0%)	1.71	392/45676 (0.9%)

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	A	1	0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	ASP	C-N	-6.70	1.27	1.34
1	D	71	GLU	CD-OE2	6.39	1.37	1.25
1	A	844	HIS	N-CA	-5.63	1.39	1.46
1	A	421	VAL	C-O	5.58	1.29	1.23
1	B	418	HIS	CE1-NE2	5.43	1.38	1.32
1	A	206	SER	N-CA	5.41	1.52	1.46
1	C	479	ASP	C-N	-5.32	1.28	1.34
1	D	537	GLU	CD-OE2	5.27	1.35	1.25
1	B	461	GLU	CD-OE2	5.22	1.35	1.25
1	D	418	HIS	CE1-NE2	5.16	1.37	1.32
1	C	80	GLU	CD-OE2	5.14	1.35	1.25
1	B	809	ARG	C-O	5.09	1.30	1.24
1	C	403	ASP	CG-OD2	5.07	1.34	1.25
1	D	75	GLU	CD-OE2	5.05	1.34	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	280	ASP	CG-OD2	5.01	1.34	1.25

All (392) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	HIS	CA-CB-CG	-13.58	100.22	113.80
1	A	634	GLN	N-CA-CB	9.62	125.65	110.73
1	B	809	ARG	NE-CZ-NH1	9.48	130.98	121.50
1	D	869	ASP	CA-CB-CG	-9.26	103.34	112.60
1	A	771	GLY	CA-C-N	-9.25	107.96	122.49
1	A	771	GLY	C-N-CA	-9.25	107.96	122.49
1	D	931	PHE	CA-CB-CG	-8.60	105.20	113.80
1	B	297	ASN	CB-CA-C	-8.33	102.88	110.71
1	B	699	ARG	NE-CZ-NH1	8.25	129.75	121.50
1	B	809	ARG	CD-NE-CZ	8.07	135.70	124.40
1	C	306	PRO	N-CA-CB	8.04	107.88	102.25
1	A	14	ARG	N-CA-CB	-8.01	100.76	110.53
1	B	699	ARG	NE-CZ-NH2	-7.98	112.02	119.20
1	D	14	ARG	N-CA-CB	-7.95	101.44	110.35
1	A	832	ASP	N-CA-CB	-7.89	100.10	111.54
1	C	680	ILE	CA-C-N	-7.78	111.98	122.72
1	C	680	ILE	C-N-CA	-7.78	111.98	122.72
1	D	770	ILE	N-CA-C	-7.76	96.42	107.75
1	B	433	LEU	CA-C-O	7.71	125.81	118.34
1	D	844	HIS	CA-CB-CG	-7.64	106.16	113.80
1	B	809	ARG	NE-CZ-NH2	-7.56	112.39	119.20
1	C	809	ARG	NE-CZ-NH1	7.47	128.97	121.50
1	A	725	ASN	CA-CB-CG	-7.42	105.18	112.60
1	A	264	GLU	CA-C-N	-7.41	112.49	122.72
1	A	264	GLU	C-N-CA	-7.41	112.49	122.72
1	A	661	LYS	CA-C-O	7.37	124.08	119.29
1	D	348	PRO	CB-CA-C	-7.27	104.78	111.40
1	B	553	TRP	CA-CB-CG	-7.27	99.79	113.60
1	D	447	ASP	N-CA-C	7.26	122.31	113.38
1	C	113	PHE	CA-CB-CG	-7.19	106.61	113.80
1	C	76	CYS	N-CA-CB	-7.17	98.19	111.53
1	C	682	LEU	CA-C-N	7.15	127.14	119.78
1	C	682	LEU	C-N-CA	7.15	127.14	119.78
1	C	363	HIS	CA-CB-CG	-7.13	106.67	113.80
1	B	571	VAL	N-CA-C	7.12	118.38	108.12
1	A	784	PHE	CA-CB-CG	-7.08	106.72	113.80
1	B	235	PHE	CA-CB-CG	-7.04	106.77	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	737	ILE	N-CA-CB	7.03	119.82	112.37
1	C	592	PHE	CA-CB-CG	-7.02	106.78	113.80
1	A	627	PHE	CA-CB-CG	-6.99	106.81	113.80
1	B	869	ASP	CA-CB-CG	-6.97	105.62	112.60
1	B	279	ILE	CA-CB-CG2	6.93	122.28	110.50
1	A	770	ILE	N-CA-C	-6.92	97.65	107.75
1	B	661	LYS	CA-C-O	6.91	124.44	119.32
1	C	274	PHE	CA-CB-CG	-6.91	106.89	113.80
1	D	633	GLY	CA-C-N	-6.87	111.71	122.49
1	D	633	GLY	C-N-CA	-6.87	111.71	122.49
1	A	614	HIS	N-CA-C	-6.86	101.17	110.36
1	C	648	ASP	CA-CB-CG	-6.84	105.76	112.60
1	C	147	ASN	N-CA-CB	-6.83	100.00	110.65
1	D	619	GLU	N-CA-C	-6.81	103.94	111.36
1	A	598	ASP	CA-CB-CG	-6.77	105.83	112.60
1	B	699	ARG	CD-NE-CZ	6.76	133.87	124.40
1	A	571	VAL	N-CA-C	6.75	117.84	108.12
1	B	823	LEU	N-CA-C	-6.73	105.60	113.88
1	A	790	ASP	CA-CB-CG	-6.73	105.87	112.60
1	C	782	ASP	CA-CB-CG	-6.72	105.88	112.60
1	D	632	SER	N-CA-CB	6.72	121.38	110.90
1	A	890	GLN	N-CA-CB	-6.71	100.09	110.29
1	D	363	HIS	CA-CB-CG	-6.70	107.10	113.80
1	A	433	LEU	CA-C-O	6.69	124.83	118.34
1	C	614	HIS	N-CA-C	-6.64	102.49	110.13
1	B	875	ASP	CA-CB-CG	-6.64	105.96	112.60
1	A	583	ASN	CA-CB-CG	-6.62	105.98	112.60
1	D	606	LEU	N-CA-C	-6.61	104.70	112.89
1	C	553	TRP	CA-CB-CG	-6.58	101.09	113.60
1	C	298	PRO	CB-CA-C	-6.56	102.99	111.39
1	B	442	ARG	NE-CZ-NH1	6.53	128.03	121.50
1	C	184	LEU	CB-CA-C	-6.52	98.48	109.50
1	D	128	ASN	CA-CB-CG	-6.52	106.08	112.60
1	B	770	ILE	CA-CB-CG1	-6.52	99.32	110.40
1	B	360	HIS	CA-CB-CG	-6.51	107.29	113.80
1	B	958	ASN	N-CA-CB	6.50	123.62	111.53
1	B	948	PRO	N-CA-C	-6.50	107.18	114.92
1	A	816	TYR	CA-C-N	-6.50	112.46	122.60
1	A	816	TYR	C-N-CA	-6.50	112.46	122.60
1	B	997	ASP	N-CA-CB	6.50	121.82	111.56
1	B	306	PRO	N-CA-CB	6.48	106.79	102.25
1	B	681	GLU	CB-CG-CD	-6.47	101.61	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	788	PRO	N-CA-CB	6.45	109.07	103.27
1	D	323	ILE	N-CA-C	-6.44	105.46	111.45
1	A	147	ASN	N-CA-CB	-6.43	100.50	110.65
1	A	235	PHE	CA-CB-CG	-6.43	107.37	113.80
1	D	877	PRO	CB-CA-C	-6.43	103.40	111.56
1	B	986	ILE	CB-CG1-CD1	-6.42	100.33	113.80
1	C	367	MET	CB-CA-C	-6.41	97.64	109.37
1	C	249	GLU	N-CA-C	6.38	119.10	108.96
1	C	632	SER	CA-C-N	-6.37	113.22	120.42
1	C	632	SER	C-N-CA	-6.37	113.22	120.42
1	D	653	HIS	N-CA-CB	6.36	121.02	110.52
1	D	820	ALA	N-CA-C	6.36	119.93	108.17
1	A	363	HIS	CA-CB-CG	-6.35	107.45	113.80
1	A	96	ASP	N-CA-CB	6.34	121.26	111.24
1	D	685	LEU	N-CA-C	6.34	118.71	110.40
1	B	885	ASN	CA-CB-CG	6.34	118.94	112.60
1	B	442	ARG	NE-CZ-NH2	-6.33	113.51	119.20
1	B	78	LEU	CA-C-O	6.32	125.39	119.76
1	B	221	GLN	N-CA-CB	-6.31	101.59	111.56
1	A	78	LEU	CA-C-O	6.30	124.31	119.46
1	D	798	ALA	CA-C-N	6.30	130.34	120.89
1	D	798	ALA	C-N-CA	6.30	130.34	120.89
1	D	513	PRO	CB-CA-C	-6.26	103.38	111.46
1	B	728	VAL	CA-C-O	6.26	125.66	119.97
1	B	545	SER	N-CA-C	6.25	116.53	108.34
1	C	442	ARG	NE-CZ-NH2	-6.25	113.57	119.20
1	D	997	ASP	N-CA-CB	6.21	121.38	111.56
1	D	948	PRO	CB-CA-C	-6.21	101.66	111.04
1	A	47	PRO	N-CA-CB	6.20	108.75	103.35
1	B	209	PHE	N-CA-C	6.20	120.98	113.17
1	D	96	ASP	N-CA-CB	6.17	121.00	111.24
1	B	878	HIS	CA-CB-CG	-6.15	107.65	113.80
1	C	890	GLN	N-CA-CB	-6.15	100.39	110.41
1	B	1020	TRP	CB-CA-C	-6.14	100.11	110.19
1	D	93	HIS	N-CA-C	-6.14	105.43	113.17
1	B	400	THR	CA-CB-OG1	-6.13	100.40	109.60
1	D	945	ASN	CA-CB-CG	-6.12	106.47	112.60
1	A	878	HIS	CA-CB-CG	-6.12	107.68	113.80
1	D	246	MET	CG-SD-CE	-6.12	87.43	100.90
1	A	472	TYR	N-CA-C	-6.10	104.54	111.07
1	A	746	ASP	CB-CA-C	-6.09	97.36	110.45
1	A	127	PHE	CA-CB-CG	-6.05	107.75	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	274	PHE	CA-CB-CG	-6.05	107.75	113.80
1	D	211	ASP	N-CA-C	6.04	118.09	110.24
1	C	359	HIS	CA-CB-CG	-6.04	107.76	113.80
1	C	893	GLU	N-CA-C	6.03	117.94	111.36
1	A	634	GLN	CB-CA-C	6.01	120.88	110.72
1	D	765	LEU	N-CA-C	-6.01	100.50	109.15
1	B	634	GLN	N-CA-C	-6.00	105.54	112.92
1	B	323	ILE	N-CA-C	-6.00	105.97	111.67
1	D	799	THR	CA-C-N	6.00	130.40	122.06
1	D	799	THR	C-N-CA	6.00	130.40	122.06
1	A	221	GLN	N-CA-CB	-5.99	102.09	111.56
1	A	477	SER	N-CA-CB	5.99	119.12	110.20
1	B	790	ASP	CA-CB-CG	-5.99	106.61	112.60
1	B	510	GLN	CA-C-O	5.98	127.76	121.00
1	C	890	GLN	N-CA-C	5.98	119.83	110.32
1	C	279	ILE	CA-CB-CG2	5.98	120.66	110.50
1	D	878	HIS	CA-CB-CG	-5.97	107.83	113.80
1	B	367	MET	CG-SD-CE	5.93	113.95	100.90
1	A	395	HIS	N-CA-C	-5.93	102.78	109.60
1	C	719	GLN	CB-CA-C	-5.93	97.03	110.07
1	C	799	THR	CA-C-O	5.91	125.89	119.15
1	A	685	LEU	N-CA-C	5.89	118.26	110.36
1	D	829	THR	N-CA-CB	5.89	120.03	110.43
1	C	259	SER	CB-CA-C	5.87	120.90	109.33
1	A	632	SER	N-CA-CB	5.87	121.10	110.95
1	C	479	ASP	CA-C-O	5.87	127.63	121.00
1	B	777	LEU	N-CA-C	-5.83	106.71	113.88
1	D	597	ASN	CA-CB-CG	-5.82	106.78	112.60
1	D	855	THR	N-CA-CB	5.81	121.53	111.13
1	C	287	ASP	CB-CA-C	-5.80	101.36	110.94
1	D	662	PRO	N-CA-CB	5.80	108.41	103.19
1	A	93	HIS	N-CA-C	-5.80	105.86	113.17
1	A	832	ASP	CA-CB-CG	-5.79	106.81	112.60
1	B	39	SER	N-CA-C	5.78	118.36	111.71
1	C	96	ASP	N-CA-CB	5.78	120.36	111.46
1	D	278	ILE	CA-C-N	-5.76	114.80	121.71
1	D	278	ILE	C-N-CA	-5.76	114.80	121.71
1	B	598	ASP	CA-CB-CG	-5.75	106.85	112.60
1	C	844	HIS	CA-CB-CG	-5.75	108.05	113.80
1	C	653	HIS	CA-CB-CG	5.74	119.54	113.80
1	B	559	TYR	CB-CA-C	-5.74	103.80	110.17
1	A	97	ALA	N-CA-C	5.73	117.29	110.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	219	THR	CA-CB-OG1	-5.73	101.01	109.60
1	C	497	ASP	CA-CB-CG	-5.72	106.88	112.60
1	A	138	GLN	N-CA-CB	-5.72	100.64	111.00
1	A	442	ARG	NE-CZ-NH2	-5.72	114.05	119.20
1	C	648	ASP	N-CA-C	5.72	119.33	112.93
1	D	221	GLN	N-CA-CB	-5.72	102.36	111.62
1	A	934	GLU	N-CA-C	-5.72	102.18	110.24
1	D	634	GLN	CB-CA-C	5.71	120.28	111.02
1	A	448	ARG	N-CA-C	5.71	119.35	112.38
1	D	772	ASP	CA-C-N	-5.71	115.17	122.77
1	D	772	ASP	C-N-CA	-5.71	115.17	122.77
1	D	809	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	D	176	PHE	CA-CB-CG	-5.71	108.09	113.80
1	A	553	TRP	CA-CB-CG	-5.70	102.77	113.60
1	C	634	GLN	CA-C-O	5.70	126.84	119.95
1	D	553	TRP	CA-CB-CG	-5.70	102.78	113.60
1	C	277	GLU	CA-CB-CG	-5.69	102.71	114.10
1	C	513	PRO	CB-CA-C	-5.69	104.12	111.46
1	C	431	ARG	NE-CZ-NH2	-5.68	114.09	119.20
1	A	997	ASP	CA-CB-CG	-5.67	106.92	112.60
1	C	252	ASP	CA-CB-CG	-5.67	106.93	112.60
1	D	297	ASN	CA-CB-CG	-5.66	106.94	112.60
1	C	383	ASN	N-CA-C	5.66	119.48	112.58
1	D	90	TRP	N-CA-C	5.65	118.21	111.71
1	B	52	ARG	CB-CA-C	-5.65	99.22	109.38
1	D	134	LEU	N-CA-C	-5.64	105.89	112.89
1	A	770	ILE	N-CA-CB	5.63	118.97	111.64
1	A	94	GLY	O-C-N	-5.63	115.28	122.43
1	A	869	ASP	CA-CB-CG	-5.62	106.98	112.60
1	B	614	HIS	N-CA-C	-5.62	102.83	110.36
1	C	728	VAL	CB-CA-C	-5.62	104.79	111.65
1	A	556	PHE	CA-CB-CG	5.62	119.42	113.80
1	D	352	ARG	CA-C-N	-5.62	116.62	122.69
1	D	352	ARG	C-N-CA	-5.62	116.62	122.69
1	A	297	ASN	CA-CB-CG	-5.62	106.98	112.60
1	B	345	ASN	CA-CB-CG	-5.62	106.98	112.60
1	C	319	ASP	CA-C-N	-5.61	113.05	122.25
1	C	319	ASP	C-N-CA	-5.61	113.05	122.25
1	D	794	GLY	CA-C-N	-5.60	111.89	121.97
1	D	794	GLY	C-N-CA	-5.60	111.89	121.97
1	C	736	ALA	CA-C-N	-5.59	118.47	123.33
1	C	736	ALA	C-N-CA	-5.59	118.47	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	431	ARG	NE-CZ-NH2	-5.58	114.17	119.20
1	B	71	GLU	CB-CG-CD	5.58	122.09	112.60
1	B	381	GLN	CA-CB-CG	-5.58	102.94	114.10
1	B	255	ARG	CA-C-N	-5.57	115.37	123.06
1	B	255	ARG	C-N-CA	-5.57	115.37	123.06
1	A	519	SER	N-CA-C	-5.57	102.39	110.24
1	D	736	ALA	N-CA-C	5.57	117.97	109.95
1	D	415	ILE	CB-CA-C	-5.56	104.07	110.41
1	C	825	CYS	O-C-N	-5.55	117.12	123.40
1	B	186	VAL	CA-C-N	-5.55	115.39	122.77
1	B	186	VAL	C-N-CA	-5.55	115.39	122.77
1	C	248	GLY	CA-C-N	-5.55	114.81	122.30
1	C	248	GLY	C-N-CA	-5.55	114.81	122.30
1	C	747	PHE	CA-CB-CG	5.55	119.35	113.80
1	A	357	HIS	CA-CB-CG	-5.54	108.26	113.80
1	B	744	GLU	CB-CG-CD	-5.54	103.18	112.60
1	D	136	GLU	N-CA-CB	-5.54	102.93	111.46
1	D	143	PHE	CA-CB-CG	-5.54	108.26	113.80
1	A	218	PRO	CB-CA-C	-5.54	102.96	110.60
1	A	599	ARG	N-CA-C	5.53	116.72	108.31
1	B	915	PHE	CA-CB-CG	-5.52	108.28	113.80
1	B	890	GLN	N-CA-C	5.52	118.69	110.52
1	A	247	CYS	CA-CB-SG	-5.51	101.72	114.40
1	D	235	PHE	CA-CB-CG	-5.50	108.30	113.80
1	D	113	PHE	CA-CB-CG	-5.50	108.30	113.80
1	B	39	SER	CA-CB-OG	-5.50	100.11	111.10
1	D	746	ASP	N-CA-C	5.50	117.43	109.07
1	D	796	SER	CA-CB-OG	-5.49	100.12	111.10
1	B	519	SER	N-CA-C	-5.49	102.51	110.24
1	C	209	PHE	N-CA-C	5.48	120.08	113.17
1	A	714	ILE	CA-CB-CG1	-5.47	101.10	110.40
1	A	116	THR	N-CA-C	-5.46	105.48	111.82
1	C	208	ILE	O-C-N	5.46	128.42	122.36
1	B	405	TYR	CA-C-O	5.45	126.22	119.79
1	D	747	PHE	N-CA-CB	5.45	119.15	110.65
1	C	246	MET	CG-SD-CE	-5.44	88.94	100.90
1	A	787	ALA	CA-C-N	5.43	125.70	119.83
1	A	787	ALA	C-N-CA	5.43	125.70	119.83
1	D	448	ARG	N-CA-C	5.43	119.01	112.38
1	D	571	VAL	N-CA-C	5.43	116.56	108.46
1	C	499	ILE	CA-C-N	-5.43	116.81	122.89
1	C	499	ILE	C-N-CA	-5.43	116.81	122.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	761	GLN	CA-CB-CG	-5.42	103.25	114.10
1	A	684	GLU	N-CA-C	-5.42	101.83	109.96
1	D	504	ALA	N-CA-C	-5.42	102.26	110.28
1	C	869	ASP	CA-CB-CG	-5.42	107.18	112.60
1	A	705	ALA	CA-C-O	-5.42	115.59	121.87
1	A	737	ILE	N-CA-CB	5.41	118.78	111.21
1	A	772	ASP	CB-CA-C	5.40	119.77	111.02
1	D	309	TYR	N-CA-C	-5.40	101.55	109.81
1	B	854	LYS	N-CA-C	5.39	117.39	109.24
1	C	842	TRP	CB-CA-C	-5.39	101.35	110.19
1	D	144	ASP	CA-CB-CG	-5.39	107.21	112.60
1	D	279	ILE	CA-CB-CG2	5.39	119.66	110.50
1	D	499	ILE	CA-C-N	-5.38	116.86	122.89
1	D	499	ILE	C-N-CA	-5.38	116.86	122.89
1	A	989	PHE	CA-CB-CG	-5.38	108.42	113.80
1	A	182	ASN	CA-CB-CG	-5.38	107.22	112.60
1	C	1011	ALA	N-CA-C	5.38	119.10	112.54
1	B	100	TYR	CA-CB-CG	-5.38	104.22	113.90
1	A	76	CYS	N-CA-C	5.37	117.23	109.07
1	A	968	MET	CA-C-N	-5.37	112.66	122.38
1	A	968	MET	C-N-CA	-5.37	112.66	122.38
1	A	440	VAL	CB-CA-C	-5.37	104.89	111.92
1	D	52	ARG	CB-CA-C	-5.35	98.78	109.33
1	B	370	GLN	CB-CG-CD	5.35	121.69	112.60
1	A	997	ASP	N-CA-CB	5.35	120.01	111.56
1	A	771	GLY	N-CA-C	-5.35	101.02	110.86
1	B	47	PRO	N-CA-CB	5.33	108.06	103.31
1	C	323	ILE	N-CA-C	-5.33	106.49	111.45
1	B	832	ASP	N-CA-CB	-5.33	103.34	111.66
1	A	990	HIS	CA-CB-CG	-5.33	108.47	113.80
1	B	95	TYR	N-CA-C	5.33	118.00	111.82
1	C	653	HIS	N-CA-CB	5.33	119.11	110.43
1	D	257	THR	CA-C-N	-5.33	116.59	123.19
1	D	257	THR	C-N-CA	-5.33	116.59	123.19
1	A	945	ASN	CA-CB-CG	-5.32	107.28	112.60
1	A	106	PRO	N-CA-CB	5.32	108.25	103.20
1	D	479	ASP	CA-CB-CG	-5.32	107.28	112.60
1	D	728	VAL	CB-CA-C	-5.32	105.17	111.65
1	A	438	GLU	CG-CD-OE2	-5.31	106.18	118.40
1	A	997	ASP	CB-CG-OD2	-5.31	106.19	118.40
1	B	546	LEU	N-CA-CB	5.30	119.45	110.49
1	D	477	SER	N-CA-CB	5.30	118.10	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	447	ASP	N-CA-C	5.30	119.84	113.17
1	D	731	PRO	N-CA-CB	5.30	107.96	103.35
1	A	504	ALA	N-CA-C	-5.29	102.44	110.28
1	C	884	LEU	CA-C-N	-5.29	112.59	121.75
1	C	884	LEU	C-N-CA	-5.29	112.59	121.75
1	B	403	ASP	CB-CA-C	-5.29	102.02	110.79
1	C	751	LEU	N-CA-CB	5.29	118.80	110.71
1	D	320	GLY	CA-C-N	-5.28	114.75	122.19
1	D	320	GLY	C-N-CA	-5.28	114.75	122.19
1	B	164	ASP	N-CA-CB	5.28	119.41	110.49
1	B	527	PRO	N-CA-CB	5.28	107.94	103.19
1	D	477	SER	CB-CA-C	-5.28	101.05	110.70
1	A	160	GLY	O-C-N	5.27	129.68	123.62
1	D	147	ASN	N-CA-CB	-5.27	102.27	110.55
1	D	147	ASN	O-C-N	-5.26	117.06	123.27
1	C	339	ASN	CA-CB-CG	-5.25	107.34	112.60
1	B	954	ASP	N-CA-C	-5.25	99.62	110.80
1	C	773	LYS	N-CA-C	5.24	117.26	108.73
1	C	776	LEU	N-CA-C	5.23	117.92	109.40
1	B	748	CYS	N-CA-CB	5.22	119.21	110.85
1	C	279	ILE	N-CA-CB	-5.22	103.09	111.82
1	C	958	ASN	N-CA-CB	5.22	121.25	111.53
1	D	733	ALA	N-CA-C	5.22	117.60	110.24
1	C	689	GLU	N-CA-C	5.22	116.97	111.28
1	B	479	ASP	CA-CB-CG	-5.22	107.38	112.60
1	A	225	PHE	N-CA-CB	5.21	120.21	110.99
1	D	409	VAL	N-CA-C	5.21	115.98	108.48
1	C	176	PHE	CA-C-N	-5.21	113.66	122.67
1	C	176	PHE	C-N-CA	-5.21	113.66	122.67
1	C	358	GLU	N-CA-CB	-5.21	102.78	110.49
1	D	562	LEU	N-CA-CB	5.21	118.11	110.35
1	C	98	PRO	O-C-N	-5.20	116.57	123.13
1	C	164	ASP	N-CA-CB	5.20	119.27	110.49
1	B	1018	LEU	CB-CA-C	-5.20	98.03	109.56
1	D	845	GLN	CB-CA-C	-5.19	104.36	111.73
1	A	686	PRO	N-CA-CB	5.18	107.92	103.31
1	B	988	GLY	N-CA-C	-5.18	106.14	112.77
1	A	34	ALA	N-CA-C	-5.18	106.77	114.64
1	C	395	HIS	ND1-CG-CD2	5.17	111.27	106.10
1	B	632	SER	N-CA-CB	5.16	119.88	110.95
1	C	499	ILE	N-CA-C	-5.16	102.03	108.84
1	C	809	ARG	NE-CZ-NH2	-5.16	114.56	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	75	GLU	CA-C-N	-5.16	112.82	121.75
1	D	75	GLU	C-N-CA	-5.16	112.82	121.75
1	D	581	ASN	CA-CB-CG	5.16	117.76	112.60
1	C	688	PRO	CB-CA-C	-5.16	104.81	111.46
1	A	116	THR	CA-CB-OG1	-5.15	101.87	109.60
1	B	93	HIS	CA-CB-CG	-5.15	108.65	113.80
1	C	512	PHE	CA-C-O	5.15	126.31	120.70
1	C	597	ASN	CA-CB-CG	-5.15	107.45	112.60
1	A	432	TRP	N-CA-C	-5.14	106.69	113.17
1	B	753	ASN	N-CA-CB	5.14	118.36	110.70
1	C	725	ASN	CA-CB-CG	-5.14	107.45	112.60
1	B	843	GLN	O-C-N	5.14	129.84	123.15
1	A	516	PRO	CB-CA-C	-5.14	104.65	111.23
1	D	229	THR	CA-C-O	-5.13	114.80	120.24
1	D	867	THR	CA-C-O	-5.13	114.78	120.38
1	A	252	ASP	CA-CB-CG	-5.13	107.47	112.60
1	D	890	GLN	N-CA-CB	-5.13	102.79	110.17
1	D	1000	SER	N-CA-C	-5.12	103.61	108.22
1	D	324	GLU	N-CA-CB	5.12	120.18	111.57
1	A	164	ASP	N-CA-CB	5.12	119.14	110.49
1	C	787	ALA	N-CA-C	-5.12	100.62	109.58
1	D	118	ASN	O-C-N	5.12	127.41	121.47
1	A	100	TYR	CA-CB-CG	-5.12	104.69	113.90
1	A	746	ASP	N-CA-C	5.12	116.85	109.07
1	D	917	ARG	CD-NE-CZ	-5.11	117.24	124.40
1	C	730	LEU	CB-CA-C	5.11	117.44	109.42
1	A	593	GLY	CA-C-O	5.11	124.69	119.02
1	C	614	HIS	CB-CA-C	-5.10	101.44	110.47
1	C	438	GLU	CG-CD-OE2	-5.10	106.68	118.40
1	D	974	HIS	CA-CB-CG	-5.10	108.70	113.80
1	B	659	ASP	CA-C-N	-5.09	114.61	122.86
1	B	659	ASP	C-N-CA	-5.09	114.61	122.86
1	B	635	THR	N-CA-C	5.09	117.54	109.24
1	A	613	PRO	N-CA-CB	5.09	108.06	103.33
1	A	1021	CYS	CA-CB-SG	-5.09	102.70	114.40
1	B	237	ARG	CA-CB-CG	-5.08	103.94	114.10
1	D	601	PHE	CA-CB-CG	-5.08	108.72	113.80
1	D	572	ASP	CB-CA-C	-5.07	101.99	109.90
1	D	982	THR	N-CA-C	5.07	117.17	108.90
1	A	980	GLU	O-C-N	-5.07	116.88	122.86
1	D	570	TRP	CA-C-N	-5.07	115.89	122.94
1	D	570	TRP	C-N-CA	-5.07	115.89	122.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	842	TRP	CA-CB-CG	-5.06	103.98	113.60
1	B	567	VAL	CB-CA-C	-5.06	103.65	111.08
1	D	507	ASP	N-CA-CB	-5.05	103.64	110.67
1	A	184	LEU	CB-CA-C	-5.05	100.88	109.51
1	A	469	ASP	CA-CB-CG	-5.04	107.56	112.60
1	D	920	LEU	CB-CA-C	-5.04	101.56	109.22
1	D	19	PRO	N-CA-CB	5.04	108.14	103.41
1	A	796	SER	N-CA-CB	5.03	117.39	109.69
1	B	76	CYS	CA-CB-SG	-5.03	102.84	114.40
1	A	742	THR	N-CA-CB	-5.03	103.06	111.20
1	A	317	THR	N-CA-C	-5.02	103.77	110.55
1	A	625	GLN	CA-CB-CG	-5.02	104.06	114.10
1	D	885	ASN	CA-CB-CG	5.02	117.62	112.60
1	B	54	LEU	N-CA-C	-5.02	107.00	112.72
1	C	604	ASN	CA-C-N	-5.01	116.45	122.16
1	C	604	ASN	C-N-CA	-5.01	116.45	122.16
1	C	855	THR	N-CA-CB	5.01	120.09	111.13
1	A	742	THR	CB-CA-C	-5.00	99.95	109.66
1	D	161	TYR	N-CA-CB	-5.00	102.22	111.53

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	634	GLN	CA

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	8125	0	7716	122	0
1	B	8131	0	7721	104	0
1	C	8125	0	7716	118	0
1	D	8125	0	7716	122	0
2	A	10	0	9	0	0
2	B	10	0	9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10	0	9	0	0
2	D	10	0	10	0	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	6	0	0	0	0
3	D	4	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	14	0	19	0	0
5	B	14	0	19	0	0
5	C	14	0	19	1	0
5	D	14	0	19	1	0
6	A	108	0	162	20	0
6	B	108	0	162	21	0
6	C	112	0	168	17	0
6	D	112	0	168	17	0
7	A	1090	0	0	18	1
7	B	1091	0	0	13	1
7	C	1034	0	0	20	0
7	D	1079	0	0	23	0
All	All	37369	0	31642	491	1

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 8.

All (491) 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)
6:B:8508:DMS:C1	6:B:8508:DMS:S	2.06	1.42
6:B:8407:DMS:C2	6:B:8407:DMS:S	2.10	1.39
1:C:634:GLN:H	1:C:634:GLN:NE2	1.37	1.21
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.41	1.16
1:D:804:ASN:ND2	1:D:809:ARG:HH21	1.41	1.16
1:B:655:MET:HE2	1:B:665:SER:HB3	1.29	1.12
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.32	1.03
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.25	1.02
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.25	0.97
1:A:473:ARG:NH1	1:A:476:LYS:HB2	1.84	0.92
1:D:809:ARG:HH11	1:D:809:ARG:HG2	1.34	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:ASN:HA	1:A:809:ARG:NH1	1.87	0.89
1:B:233:ASP:HA	6:B:8417:DMS:H13	1.53	0.88
1:A:777:LEU:CD1	1:A:980:GLU:HG2	2.04	0.88
1:B:600:GLN:H	1:B:600:GLN:HE21	1.18	0.87
1:B:655:MET:CE	1:B:665:SER:HB3	2.04	0.87
1:C:634:GLN:NE2	1:C:634:GLN:N	2.22	0.87
1:C:687:GLN:HG3	1:C:688:PRO:HD2	1.57	0.86
6:A:8420:DMS:H22	7:D:9523:HOH:O	1.77	0.84
6:D:8703:DMS:H21	7:D:9706:HOH:O	1.79	0.83
1:B:599:ARG:HG3	1:B:599:ARG:HH11	1.40	0.82
1:D:237:ARG:HH11	1:D:237:ARG:HG2	1.44	0.82
1:D:658:LEU:O	1:D:661:LYS:HG3	1.81	0.81
1:A:787:ALA:HA	1:A:968:MET:HG3	1.63	0.81
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.16	0.81
1:A:267:VAL:O	6:A:8602:DMS:H23	1.81	0.80
1:C:703:PRO:HG2	6:C:8425:DMS:H11	1.63	0.80
1:B:797:GLU:HG2	1:B:799:THR:HG23	1.62	0.80
1:D:663:LEU:CD1	1:D:686:PRO:HG2	2.11	0.80
1:A:237:ARG:HB3	1:A:237:ARG:NH1	1.97	0.80
6:C:8417:DMS:H22	7:C:9238:HOH:O	1.82	0.78
1:A:797:GLU:O	1:A:801:ILE:HD13	1.83	0.77
1:B:651:LEU:O	1:B:651:LEU:HD23	1.83	0.77
1:B:651:LEU:HD21	1:B:701:VAL:HB	1.65	0.77
1:D:663:LEU:HD13	1:D:686:PRO:HG2	1.66	0.77
1:A:237:ARG:HH11	1:A:237:ARG:CB	1.98	0.77
1:A:797:GLU:HB3	1:A:799:THR:HG23	1.66	0.76
1:A:973:ARG:O	6:A:8423:DMS:H12	1.85	0.76
1:C:634:GLN:H	1:C:634:GLN:HE21	1.27	0.76
1:D:133:TRP:HE1	6:D:8703:DMS:H23	1.52	0.75
1:D:629:PHE:O	1:D:630:ARG:HD3	1.86	0.75
1:A:777:LEU:HD13	1:A:980:GLU:HG2	1.68	0.75
1:C:737:ILE:HD12	1:C:738:PRO:HD2	1.67	0.74
1:D:887:GLN:NE2	1:D:980:GLU:O	2.20	0.74
1:D:748:CYS:C	1:D:749:ILE:HD12	2.13	0.74
1:B:737:ILE:HD11	7:B:9591:HOH:O	1.88	0.74
1:A:600:GLN:H	1:A:600:GLN:HE21	1.35	0.73
6:A:8503:DMS:H22	7:A:9021:HOH:O	1.90	0.71
1:D:133:TRP:NE1	6:D:8703:DMS:H23	2.04	0.71
1:C:230:ARG:HD2	7:C:8959:HOH:O	1.89	0.71
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.72	0.70
1:C:824:GLN:HG2	1:C:825:CYS:N	2.05	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.27	0.70
6:B:8410:DMS:H22	7:B:8882:HOH:O	1.92	0.70
1:C:703:PRO:HG2	6:C:8425:DMS:C1	2.20	0.70
1:A:768:MET:HE1	1:A:1020:TRP:CE2	2.27	0.69
1:A:277:GLU:H	1:A:277:GLU:CD	1.99	0.69
1:A:777:LEU:HD11	1:A:980:GLU:HG2	1.72	0.69
1:C:748:CYS:C	1:C:749:ILE:HD12	2.17	0.69
1:D:653:HIS:ND1	1:D:701:VAL:HG21	2.08	0.69
1:C:768:MET:HE1	1:C:1020:TRP:CZ2	2.27	0.69
1:A:800:ARG:HB3	7:A:9395:HOH:O	1.92	0.68
1:D:973:ARG:O	6:D:8423:DMS:H12	1.94	0.68
1:A:832:ASP:OD1	1:A:832:ASP:N	2.27	0.68
1:D:749:ILE:HD12	1:D:749:ILE:N	2.08	0.68
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.75	0.68
1:B:262:GLN:HE21	1:B:263:GLY:N	1.92	0.68
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.24	0.68
1:B:878:HIS:HD2	7:B:8695:HOH:O	1.76	0.68
1:C:237:ARG:NH1	1:C:237:ARG:HB3	2.08	0.68
1:C:651:LEU:HD12	1:C:651:LEU:C	2.17	0.68
1:A:1022:GLN:HG2	1:A:1023:LYS:N	1.99	0.67
1:B:262:GLN:HE21	1:B:262:GLN:C	2.01	0.67
1:D:847:LYS:NZ	7:D:9499:HOH:O	2.28	0.67
1:D:292:ARG:HH12	6:D:8412:DMS:H23	1.58	0.67
6:B:8410:DMS:H11	7:B:8964:HOH:O	1.95	0.67
1:C:749:ILE:HD12	1:C:749:ILE:N	2.10	0.67
1:C:878:HIS:HD2	7:C:8695:HOH:O	1.76	0.67
1:A:718:GLN:NE2	6:A:8503:DMS:H11	2.09	0.66
1:B:845:GLN:OE1	1:B:845:GLN:HA	1.95	0.66
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.07	0.66
1:A:878:HIS:HD2	7:A:8674:HOH:O	1.78	0.66
1:B:744:GLU:HB2	1:B:745:MET:HE3	1.77	0.66
1:D:128:ASN:HB3	1:D:180:GLY:O	1.95	0.66
1:B:494:THR:HB	1:C:473:ARG:NH2	2.11	0.66
1:C:690:SER:HB2	7:C:9380:HOH:O	1.95	0.66
1:D:804:ASN:HA	1:D:809:ARG:CZ	2.26	0.66
1:D:804:ASN:HA	1:D:809:ARG:NH2	2.11	0.66
1:D:237:ARG:NH1	7:D:9273:HOH:O	2.28	0.66
1:A:473:ARG:HH11	1:A:476:LYS:HB2	1.60	0.65
1:D:135:GLN:C	1:D:136:GLU:HG2	2.22	0.65
1:A:754:LYS:NZ	7:A:9527:HOH:O	2.30	0.65
1:D:685:LEU:HB3	1:D:686:PRO:HD2	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:8427:DMS:H13	7:B:9052:HOH:O	1.95	0.65
1:D:651:LEU:HD11	1:D:653:HIS:CE1	2.31	0.65
1:A:887:GLN:NE2	1:A:980:GLU:O	2.29	0.65
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.77	0.65
1:D:653:HIS:CE1	1:D:701:VAL:HG21	2.32	0.64
1:D:237:ARG:HG2	1:D:237:ARG:NH1	2.08	0.64
6:D:8421:DMS:H12	7:D:9361:HOH:O	1.97	0.64
1:C:651:LEU:HD12	1:C:651:LEU:O	1.98	0.64
1:D:254:LEU:HD12	7:D:9641:HOH:O	1.97	0.63
1:A:431:ARG:HG3	7:A:9378:HOH:O	1.97	0.63
1:A:648:ASP:OD2	7:A:9548:HOH:O	2.15	0.63
1:C:595:THR:HA	1:C:596:PRO:C	2.23	0.63
6:A:8503:DMS:H21	7:A:8976:HOH:O	1.99	0.62
1:C:278:ILE:HD13	1:C:278:ILE:N	2.13	0.62
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.80	0.62
1:B:797:GLU:CG	1:B:799:THR:HG23	2.28	0.62
1:B:637:GLU:OE2	1:B:677:LYS:HE3	2.00	0.62
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.80	0.62
1:D:292:ARG:HH12	6:D:8412:DMS:C2	2.11	0.62
1:D:595:THR:HA	1:D:596:PRO:C	2.25	0.62
1:D:725:ASN:HB2	7:D:9581:HOH:O	1.99	0.61
1:A:804:ASN:OD1	1:A:809:ARG:NH2	2.33	0.61
1:C:240:LEU:C	1:C:240:LEU:HD23	2.25	0.61
1:D:1022:GLN:O	1:D:1022:GLN:HG3	1.98	0.61
6:B:8508:DMS:H13	7:B:8732:HOH:O	2.00	0.61
1:A:962:TYR:OH	6:A:8423:DMS:H21	2.01	0.61
1:A:658:LEU:O	1:A:661:LYS:HG3	2.01	0.61
1:C:88:SER:HA	1:C:366:VAL:HG21	1.82	0.61
1:D:878:HIS:HD2	7:D:8814:HOH:O	1.83	0.61
1:A:651:LEU:C	1:A:651:LEU:HD12	2.26	0.61
1:C:730:LEU:N	1:C:730:LEU:HD23	2.16	0.60
1:B:863:GLN:HG2	1:B:1021:CYS:HB3	1.83	0.60
1:C:237:ARG:HH11	1:C:237:ARG:CB	2.13	0.60
1:D:233:ASP:HA	6:D:8417:DMS:H13	1.84	0.60
1:D:367:MET:HE1	1:D:371:THR:HG22	1.84	0.60
1:A:241:GLU:OE2	1:A:292:ARG:NE	2.28	0.60
1:A:809:ARG:HH11	1:A:809:ARG:CG	2.15	0.60
1:D:663:LEU:HD13	1:D:686:PRO:CG	2.32	0.59
1:B:316:HIS:CD2	6:B:8406:DMS:H23	2.37	0.59
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.85	0.59
1:B:133:TRP:CD1	6:B:8504:DMS:H12	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:618:THR:HG21	7:D:9054:HOH:O	2.02	0.59
1:D:809:ARG:HG2	1:D:809:ARG:NH1	2.09	0.59
1:C:890:GLN:HG3	1:C:891:VAL:N	2.18	0.59
1:C:703:PRO:HD2	6:C:8425:DMS:H12	1.84	0.59
1:B:599:ARG:NH1	1:B:601[A]:PHE:CD1	2.71	0.59
1:C:266:GLN:HE21	6:C:8602:DMS:H23	1.67	0.59
1:A:687:GLN:HG3	7:A:9467:HOH:O	2.02	0.59
1:A:595:THR:HA	1:A:596:PRO:C	2.27	0.59
1:B:595:THR:HA	1:B:596:PRO:C	2.28	0.59
1:B:890:GLN:OE1	1:B:947:GLY:HA3	2.03	0.58
6:C:8427:DMS:H22	7:C:9057:HOH:O	2.02	0.58
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.39	0.58
1:A:699:ARG:NH2	7:A:9471:HOH:O	2.35	0.57
1:C:646:HIS:CE1	1:C:673:ALA:HB2	2.39	0.57
1:D:703:PRO:HG2	6:D:8425:DMS:H12	1.86	0.57
1:D:809:ARG:HH11	1:D:809:ARG:CG	2.14	0.57
1:C:806:TRP:CE2	1:C:809:ARG:NH2	2.73	0.57
1:A:237:ARG:NH1	7:A:9138:HOH:O	2.29	0.57
1:B:508:GLU:OE2	6:B:8407:DMS:H11	2.04	0.57
1:C:687:GLN:HE21	1:C:687:GLN:HA	1.69	0.57
1:B:651:LEU:HD23	1:B:651:LEU:C	2.29	0.57
1:C:730:LEU:HD23	1:C:730:LEU:H	1.67	0.57
1:A:1022:GLN:C	1:A:1023:LYS:HG3	2.30	0.56
1:C:730:LEU:H	1:C:730:LEU:CD2	2.18	0.56
5:C:2002:BTB:O8	5:C:2002:BTB:H62	2.05	0.56
1:D:799:THR:OG1	1:D:800:ARG:N	2.38	0.56
6:B:8420:DMS:H13	7:C:9229:HOH:O	2.05	0.56
1:A:789:LEU:HD11	1:A:993:ILE:HG22	1.88	0.56
1:B:654:TRP:CZ3	1:B:665:SER:HA	2.39	0.56
1:C:866:ILE:O	1:C:1017:GLN:NE2	2.36	0.56
1:D:795:VAL:HG12	6:D:8506:DMS:H11	1.87	0.56
1:A:231:PHE:O	6:A:8417:DMS:H23	2.06	0.56
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.88	0.56
1:D:802:ASP:OD1	1:D:803:PRO:HD2	2.06	0.56
1:A:803:PRO:O	1:A:809:ARG:NH1	2.38	0.55
1:A:473:ARG:HH12	1:A:476:LYS:HB2	1.71	0.55
1:B:157:ARG:HD3	7:B:9476:HOH:O	2.05	0.55
1:D:708:TRP:CZ2	6:D:8403:DMS:H13	2.42	0.55
1:B:75:GLU:HA	1:B:75:GLU:OE1	2.06	0.55
1:C:70:PRO:HG2	1:C:78:LEU:HD21	1.88	0.55
1:C:649:ASN:HA	6:C:8425:DMS:C1	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:950:GLN:OE1	1:B:952:ARG:HD3	2.07	0.55
1:B:615:PRO:O	1:B:618:THR:HG22	2.08	0.54
1:B:646:HIS:CE1	1:B:673:ALA:HA	2.43	0.54
1:C:13:ARG:O	1:C:14:ARG:C	2.50	0.54
1:A:178:ARG:HD2	7:A:9497:HOH:O	2.07	0.54
1:D:133:TRP:HE1	6:D:8703:DMS:C2	2.20	0.54
1:D:653:HIS:CD2	1:D:667:GLU:HB3	2.42	0.54
1:B:79:PRO:HD2	1:B:80:GLU:OE2	2.07	0.54
1:D:878:HIS:HE1	7:D:9399:HOH:O	1.91	0.54
1:B:320:GLY:O	6:B:8406:DMS:O	2.26	0.54
1:D:473:ARG:HH11	1:D:476:LYS:HB2	1.73	0.54
1:A:88:SER:HA	1:A:366:VAL:HG21	1.90	0.54
7:B:9403:HOH:O	6:C:8420:DMS:H22	2.07	0.54
1:D:367:MET:HE1	1:D:371:THR:CG2	2.38	0.54
1:A:655:MET:HE2	1:A:656:VAL:O	2.08	0.53
1:B:178:ARG:O	1:B:178:ARG:HG3	2.08	0.53
1:C:649:ASN:HA	6:C:8425:DMS:H13	1.90	0.53
1:D:135:GLN:O	1:D:136:GLU:HG2	2.07	0.53
1:A:735:HIS:O	1:A:736:ALA:HB2	2.07	0.53
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.76	0.53
1:C:634:GLN:H	1:C:634:GLN:CD	2.08	0.53
1:B:37:ARG:NH1	6:B:8504:DMS:H21	2.24	0.53
1:B:231:PHE:O	6:B:8417:DMS:H23	2.09	0.53
1:B:316:HIS:CG	6:B:8406:DMS:H23	2.43	0.53
1:C:241:GLU:OE1	1:C:292:ARG:NE	2.41	0.53
1:D:651:LEU:C	1:D:651:LEU:HD12	2.33	0.53
1:D:685:LEU:HB3	1:D:686:PRO:CD	2.39	0.52
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.44	0.52
1:C:745:MET:CA	1:C:745:MET:HE3	2.40	0.52
1:C:178:ARG:HD2	7:C:9553:HOH:O	2.09	0.52
1:D:554:GLN:NE2	7:D:9666:HOH:O	2.24	0.52
1:B:634:GLN:HG2	1:B:682:LEU:O	2.10	0.52
1:B:596:PRO:HB3	7:B:9423:HOH:O	2.09	0.52
6:C:8407:DMS:H22	7:C:9561:HOH:O	2.08	0.52
1:B:599:ARG:HH11	1:B:599:ARG:CG	2.16	0.51
1:C:46:ARG:HG2	7:C:9538:HOH:O	2.10	0.51
1:C:745:MET:HE3	1:C:745:MET:HA	1.92	0.51
1:A:615:PRO:O	1:A:618:THR:HG22	2.11	0.51
1:B:797:GLU:HG2	1:B:799:THR:CG2	2.38	0.51
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.92	0.51
1:D:749:ILE:N	1:D:749:ILE:CD1	2.73	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:8407:DMS:C2	6:B:8407:DMS:C1	2.88	0.51
1:A:264:GLU:HG3	7:A:9518:HOH:O	2.11	0.51
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.46	0.51
1:C:768:MET:HE1	1:C:1020:TRP:CH2	2.46	0.51
1:B:599:ARG:HH12	1:B:601[A]:PHE:HE1	1.50	0.50
6:C:8409:DMS:H23	7:C:8960:HOH:O	2.11	0.50
1:D:584:PRO:HD2	7:D:9453:HOH:O	2.11	0.50
1:D:754:LYS:HE2	1:D:1022:GLN:HG2	1.92	0.50
1:C:630:ARG:HH11	1:C:630:ARG:CB	2.25	0.50
1:D:651:LEU:HD12	1:D:651:LEU:O	2.11	0.50
1:A:863:GLN:NE2	1:A:952:ARG:HH22	2.09	0.50
1:C:736:ALA:O	1:C:860:GLY:HA3	2.12	0.50
1:D:363:HIS:HD2	7:D:9324:HOH:O	1.93	0.50
1:D:92:MET:HA	1:D:92:MET:HE2	1.93	0.50
1:D:688:PRO:C	1:D:690:SER:H	2.20	0.50
1:C:375:ASP:HB3	1:C:379:MET:HE3	1.93	0.49
1:C:16:TRP:CG	1:C:189:LEU:HD13	2.47	0.49
1:C:759:ASN:OD1	1:C:761:GLN:N	2.44	0.49
1:B:13:ARG:HG3	1:C:13:ARG:CZ	2.42	0.49
1:A:508:GLU:OE2	6:A:8407:DMS:H11	2.12	0.49
1:C:608:PHE:CE1	1:C:614:HIS:HD2	2.30	0.49
1:D:367:MET:HB3	1:D:372:MET:HE3	1.95	0.49
1:D:131:GLU:O	1:D:131:GLU:OE2	2.30	0.49
1:D:859:ASP:OD1	1:D:861:SER:HB2	2.12	0.49
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.95	0.49
1:B:37:ARG:HH12	6:B:8504:DMS:H21	1.77	0.49
1:C:667:GLU:C	1:C:668:VAL:HG23	2.38	0.49
1:D:797:GLU:HB3	1:D:799:THR:HG23	1.95	0.49
1:D:844:HIS:O	1:D:845:GLN:HB2	2.13	0.49
1:A:718:GLN:CD	6:A:8503:DMS:H11	2.37	0.49
1:B:74:LEU:HD22	1:B:153:TRP:CG	2.47	0.49
1:B:232:ASN:ND2	1:B:237:ARG:HG3	2.28	0.49
1:D:237:ARG:CG	1:D:237:ARG:NH1	2.73	0.49
1:A:680:ILE:HG12	7:A:9249:HOH:O	2.13	0.48
1:C:728:VAL:O	1:C:730:LEU:HD23	2.13	0.48
1:D:809:ARG:NH1	1:D:809:ARG:CG	2.75	0.48
1:C:651:LEU:CD1	1:C:653:HIS:CE1	2.95	0.48
1:C:708:TRP:CZ2	6:C:8403:DMS:H13	2.48	0.48
1:D:1022:GLN:O	1:D:1023:LYS:HB2	2.14	0.48
1:A:708:TRP:CZ2	6:A:8403:DMS:H13	2.49	0.48
1:B:88:SER:HA	1:B:366:VAL:HG21	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:THR:O	1:D:445:GLN:HG3	2.13	0.48
1:D:843:GLN:HB3	1:D:847:LYS:O	2.13	0.48
1:C:890:GLN:OE1	1:C:948:PRO:HD3	2.13	0.48
1:D:634:GLN:NE2	1:D:682:LEU:O	2.46	0.48
1:D:795:VAL:HG12	6:D:8506:DMS:C1	2.43	0.48
1:A:745:MET:HE1	1:A:761:GLN:HB2	1.96	0.48
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.32	0.48
1:C:266:GLN:HB3	6:C:8602:DMS:H23	1.95	0.48
1:B:381:GLN:O	1:B:621:LYS:HE3	2.14	0.48
1:B:630:ARG:HH21	1:B:637:GLU:CD	2.21	0.48
1:C:671:ASP:N	1:C:678:GLN:OE1	2.28	0.48
1:A:809:ARG:HH11	1:A:809:ARG:HG3	1.79	0.48
1:A:890:GLN:HG3	1:A:891:VAL:N	2.28	0.48
1:B:93:HIS:ND1	6:B:8414:DMS:H12	2.29	0.47
1:C:44:THR:OG1	1:C:46:ARG:HD3	2.14	0.47
1:A:358:GLU:C	1:A:367:MET:HE3	2.40	0.47
1:D:651:LEU:C	1:D:651:LEU:CD1	2.87	0.47
1:D:739:HIS:HB2	7:D:9753:HOH:O	2.15	0.47
1:A:599:ARG:HD2	1:A:600:GLN:HE22	1.79	0.47
1:B:573:GLN:HB2	1:B:602:CYS:O	2.13	0.47
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.49	0.47
1:B:1022:GLN:CG	1:B:1023:LYS:N	2.77	0.47
6:C:8503:DMS:H13	7:C:9040:HOH:O	2.14	0.47
1:D:890:GLN:HG3	1:D:891:VAL:N	2.30	0.47
1:A:668:VAL:HG12	1:A:669:PRO:O	2.14	0.47
1:B:13:ARG:O	1:B:14:ARG:C	2.57	0.47
1:C:92:MET:HE2	1:C:92:MET:HA	1.94	0.47
1:A:658:LEU:O	1:A:659:ASP:C	2.55	0.47
1:A:768:MET:CE	1:A:1020:TRP:CZ2	2.92	0.47
1:B:1017:GLN:HB2	7:B:9592:HOH:O	2.14	0.47
1:C:356:ARG:HD2	1:C:379:MET:CE	2.23	0.47
1:C:615:PRO:O	1:C:618:THR:HG22	2.14	0.47
1:C:651:LEU:CD1	1:C:653:HIS:ND1	2.77	0.47
1:C:824:GLN:CG	1:C:825:CYS:N	2.75	0.47
1:D:340:GLY:O	1:D:561:ARG:HG2	2.15	0.47
6:D:8415:DMS:H11	7:D:9784:HOH:O	2.13	0.47
1:A:147:ASN:HA	1:A:148:SER:HA	1.58	0.47
1:A:685:LEU:HB3	1:A:686:PRO:CD	2.43	0.47
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.95	0.47
1:C:86:VAL:HG13	1:C:87:PRO:HA	1.97	0.47
1:C:237:ARG:NH1	1:C:237:ARG:CB	2.73	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:749:ILE:N	1:C:749:ILE:CD1	2.77	0.47
1:A:654:TRP:CZ3	1:A:665:SER:HA	2.49	0.47
1:A:806:TRP:CD2	1:A:991:MET:HE1	2.50	0.47
1:D:768:MET:HE1	1:D:1020:TRP:CE2	2.50	0.47
1:A:290:THR:O	6:A:8412:DMS:H23	2.16	0.46
1:A:599:ARG:HD2	1:A:600:GLN:NE2	2.30	0.46
6:A:8409:DMS:O	7:A:9110:HOH:O	2.20	0.46
6:A:8420:DMS:H23	7:D:9246:HOH:O	2.15	0.46
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.97	0.46
1:B:127:PHE:CD2	1:B:127:PHE:N	2.83	0.46
1:A:167:LEU:HB3	1:A:168:PRO:HD2	1.98	0.46
1:B:730:LEU:H	1:B:730:LEU:HG	1.27	0.46
1:C:367:MET:HE1	1:C:371:THR:CG2	2.45	0.46
1:A:809:ARG:NH1	1:A:809:ARG:CG	2.78	0.46
1:B:595:THR:O	1:B:595:THR:HG23	2.15	0.46
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.97	0.46
1:C:610:ASP:O	1:C:611:ARG:HB2	2.16	0.46
1:D:653:HIS:ND1	1:D:701:VAL:CG2	2.77	0.46
1:D:696:LEU:HB2	1:D:722:LEU:HD11	1.98	0.46
1:A:1022:GLN:CG	1:A:1023:LYS:N	2.75	0.46
1:B:494:THR:HB	1:C:473:ARG:HH21	1.81	0.46
1:B:670:LEU:HA	1:B:670:LEU:HD23	1.66	0.46
1:C:16:TRP:CG	1:C:189:LEU:CD1	2.98	0.46
1:C:751:LEU:HD21	1:C:860:GLY:O	2.16	0.46
1:D:250:LEU:O	1:D:251:ARG:HG2	2.17	0.45
1:D:147:ASN:HA	1:D:148:SER:HA	1.75	0.45
1:A:663:LEU:HD11	1:A:688:PRO:HG3	1.96	0.45
1:B:658:LEU:O	1:B:659:ASP:C	2.58	0.45
1:B:777:LEU:HG	1:B:889:ALA:HA	1.99	0.45
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.34	0.45
1:D:240:LEU:HD23	1:D:240:LEU:C	2.41	0.45
1:A:178:ARG:HG3	7:A:9497:HOH:O	2.16	0.45
1:B:147:ASN:HA	1:B:148:SER:HA	1.59	0.45
1:A:128:ASN:HB2	7:A:9543:HOH:O	2.17	0.45
1:C:646:HIS:HB3	7:C:9488:HOH:O	2.17	0.45
1:A:58:TRP:CD1	1:A:86:VAL:HB	2.52	0.45
1:B:377:LEU:O	1:B:381:GLN:HG3	2.16	0.45
1:D:658:LEU:O	1:D:659:ASP:C	2.59	0.45
1:C:755:ARG:HG2	1:C:769:TRP:CE3	2.52	0.45
1:A:243:GLU:OE2	1:A:245:GLN:NE2	2.43	0.45
1:B:599:ARG:NH1	1:B:601[A]:PHE:CE1	2.74	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:TYR:CD1	1:C:317:THR:HG22	2.52	0.45
1:C:658:LEU:O	1:C:659:ASP:C	2.57	0.45
1:D:545:SER:O	1:D:909:ARG:HD3	2.17	0.45
1:D:847:LYS:HG3	1:D:848:THR:N	2.17	0.45
1:A:361:PRO:HB2	1:A:576:ILE:HG12	1.99	0.44
1:A:1017:GLN:HG3	1:A:1018:LEU:N	2.16	0.44
1:B:910:LEU:C	1:B:910:LEU:HD12	2.42	0.44
1:C:114:VAL:HB	1:C:115:PRO:CD	2.47	0.44
1:C:237:ARG:HB3	1:C:237:ARG:HH11	1.72	0.44
6:D:8410:DMS:H11	7:D:9083:HOH:O	2.16	0.44
1:A:742:THR:HG22	1:A:743:SER:N	2.31	0.44
1:C:147:ASN:HA	1:C:148:SER:HA	1.60	0.44
1:C:433:LEU:O	1:C:437:SER:HB3	2.17	0.44
1:D:808:GLU:OE2	1:D:811:LYS:NZ	2.49	0.44
1:B:262:GLN:CA	1:B:262:GLN:NE2	2.80	0.44
1:C:577:LYS:HB3	1:C:577:LYS:HE3	1.88	0.44
1:D:668:VAL:HG11	1:D:680:ILE:HG12	1.99	0.44
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.52	0.44
1:A:84:VAL:HA	6:A:8414:DMS:O	2.17	0.44
1:A:685:LEU:HD23	1:A:686:PRO:HD3	1.99	0.44
1:B:872:VAL:O	1:B:873:ALA:C	2.60	0.44
6:C:8410:DMS:H11	7:C:8966:HOH:O	2.17	0.44
1:C:844:HIS:HD2	7:C:9471:HOH:O	2.01	0.44
1:B:687:GLN:HE21	1:B:687:GLN:N	2.15	0.44
1:C:651:LEU:C	1:C:651:LEU:CD1	2.88	0.44
1:D:651:LEU:CD1	1:D:653:HIS:CE1	3.00	0.44
1:D:663:LEU:HD11	1:D:686:PRO:HG2	1.96	0.44
1:B:252:ASP:OD2	6:B:8416:DMS:H12	2.17	0.44
1:B:599:ARG:NH1	1:B:601[A]:PHE:HD1	2.16	0.43
1:B:708:TRP:CZ2	6:B:8403:DMS:H13	2.53	0.43
1:D:292:ARG:NH1	6:D:8412:DMS:H23	2.28	0.43
1:D:806:TRP:CD2	1:D:991:MET:HE1	2.53	0.43
1:A:32:PRO:HB2	6:A:8404:DMS:H13	1.99	0.43
1:A:859:ASP:OD1	1:A:861:SER:OG	2.28	0.43
1:C:92:MET:HE2	1:C:92:MET:CA	2.48	0.43
1:C:569:ASP:O	1:C:605:GLY:HA2	2.19	0.43
1:C:634:GLN:CD	1:C:634:GLN:C	2.86	0.43
1:D:802:ASP:O	1:D:808:GLU:HG3	2.18	0.43
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.54	0.43
1:C:866:ILE:C	1:C:1017:GLN:NE2	2.77	0.43
6:C:8427:DMS:H11	7:C:8832:HOH:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:659:ASP:HB3	1:D:898:LEU:HD21	2.01	0.43
1:A:127:PHE:N	1:A:127:PHE:CD2	2.86	0.43
1:A:843:GLN:HA	1:A:847:LYS:O	2.18	0.43
1:B:114:VAL:HB	1:B:115:PRO:HD2	2.01	0.43
1:B:533:LEU:HD23	1:B:533:LEU:C	2.44	0.43
1:B:890:GLN:OE1	1:B:948:PRO:HD2	2.18	0.43
1:B:128:ASN:HA	1:B:180:GLY:O	2.19	0.43
1:D:246:MET:HE3	1:D:250:LEU:HD23	2.00	0.43
1:D:576:ILE:HD13	1:D:576:ILE:HA	1.86	0.43
1:D:829:THR:O	1:D:830:LEU:HD23	2.19	0.43
1:C:375:ASP:O	1:C:379:MET:HG3	2.18	0.43
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.54	0.43
1:A:433:LEU:N	1:A:434:PRO:CD	2.82	0.43
1:B:93:HIS:CE1	6:B:8414:DMS:H12	2.54	0.43
1:B:236:SER:C	1:B:237:ARG:HG2	2.30	0.43
1:A:600:GLN:HE21	1:A:600:GLN:N	2.09	0.42
1:B:661:LYS:NZ	7:B:9522:HOH:O	2.52	0.42
1:B:745:MET:N	1:B:745:MET:SD	2.75	0.42
1:D:843:GLN:HA	1:D:847:LYS:O	2.19	0.42
1:D:873:ALA:O	1:D:876:THR:HG22	2.19	0.42
1:A:802:ASP:OD1	1:A:802:ASP:C	2.62	0.42
1:C:49:GLN:HG2	7:C:9326:HOH:O	2.18	0.42
1:C:230:ARG:HB3	7:C:9557:HOH:O	2.18	0.42
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.54	0.42
1:D:88:SER:HA	1:D:366:VAL:HG21	2.01	0.42
6:A:8416:DMS:H22	7:A:9270:HOH:O	2.18	0.42
1:B:663:LEU:HD22	1:B:663:LEU:HA	1.60	0.42
1:D:646:HIS:ND1	7:D:9585:HOH:O	2.37	0.42
1:A:873:ALA:O	1:A:876:THR:HG22	2.20	0.42
1:A:685:LEU:CB	1:A:686:PRO:HD2	2.45	0.42
1:A:701:VAL:O	1:A:703:PRO:HD3	2.20	0.42
1:B:802:ASP:OD1	1:B:802:ASP:C	2.62	0.42
1:C:682:LEU:HA	1:C:683:PRO:HD3	1.84	0.42
1:C:785:THR:O	1:C:881:ARG:HD2	2.19	0.42
1:C:930:VAL:HA	1:C:973:ARG:HD3	2.02	0.42
1:A:251:ARG:HH11	6:A:8416:DMS:C1	2.33	0.42
1:D:681:GLU:HG2	7:D:9468:HOH:O	2.19	0.42
1:B:297:ASN:N	1:B:298:PRO:CD	2.83	0.42
1:D:619:GLU:HG2	1:D:909:ARG:HG3	2.02	0.42
5:D:2002:BTB:H31	5:D:2002:BTB:H51	1.73	0.42
1:A:781:ARG:NH1	7:A:9346:HOH:O	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:LEU:N	1:B:434:PRO:CD	2.83	0.42
1:D:751:LEU:O	1:D:752:GLY:C	2.63	0.42
1:A:267:VAL:C	6:A:8602:DMS:H23	2.42	0.42
1:C:254:LEU:C	1:C:255:ARG:HG2	2.44	0.42
1:C:580:GLU:H	1:C:580:GLU:HG3	1.26	0.42
1:D:622:HIS:O	1:D:625:GLN:HG3	2.20	0.42
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.84	0.41
1:A:685:LEU:HD22	1:A:686:PRO:HD2	2.01	0.41
1:B:46:ARG:HH11	1:B:46:ARG:HD2	1.57	0.41
1:C:285:TYR:HB3	1:C:288:ARG:HG3	2.01	0.41
1:D:377:LEU:HD22	1:D:708:TRP:HA	2.02	0.41
1:A:742:THR:CG2	1:A:743:SER:N	2.84	0.41
1:D:499:ILE:HG22	1:D:501:PRO:HD3	2.02	0.41
1:D:682:LEU:HD23	1:D:682:LEU:HA	1.77	0.41
1:C:653:HIS:ND1	1:C:667:GLU:HG2	2.35	0.41
1:A:990:HIS:HD2	1:A:991:MET:O	2.03	0.41
1:B:966:GLN:HG3	7:B:9663:HOH:O	2.20	0.41
1:A:685:LEU:CD2	1:A:686:PRO:HD3	2.51	0.41
1:A:753:ASN:OD1	1:A:753:ASN:N	2.53	0.41
1:C:670:LEU:HD23	1:C:670:LEU:HA	1.89	0.41
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.55	0.41
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.20	0.41
1:C:279:ILE:HD13	1:C:279:ILE:HA	1.87	0.41
1:C:625:GLN:NE2	7:C:8824:HOH:O	2.50	0.41
1:D:654:TRP:CZ2	1:D:683:PRO:HG2	2.56	0.41
1:D:781:ARG:NH1	7:D:9479:HOH:O	2.36	0.41
1:A:16:TRP:CG	1:A:189:LEU:HD13	2.55	0.41
1:A:533:LEU:C	1:A:533:LEU:HD23	2.46	0.41
1:A:753:ASN:OD1	1:A:754:LYS:HG3	2.20	0.41
1:B:436:MET:O	1:B:437:SER:C	2.63	0.41
1:B:890:GLN:HB3	7:B:9443:HOH:O	2.21	0.41
1:C:655:MET:SD	1:C:656:VAL:N	2.93	0.41
1:D:618:THR:HG23	7:D:9070:HOH:O	2.20	0.41
1:D:651:LEU:CD1	1:D:701:VAL:HB	2.50	0.41
1:A:427:THR:HG21	1:A:462:SER:HB3	2.02	0.41
1:D:802:ASP:OD1	1:D:802:ASP:C	2.64	0.41
1:A:367:MET:HB3	1:A:372:MET:HE3	2.02	0.41
1:A:685:LEU:CD2	1:A:686:PRO:CD	2.99	0.41
1:A:718:GLN:CD	6:A:8503:DMS:C1	2.94	0.41
1:A:804:ASN:HA	1:A:809:ARG:CZ	2.50	0.41
1:B:683:PRO:O	1:B:684:GLU:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:730:LEU:N	1:C:730:LEU:CD2	2.78	0.41
1:C:883:GLY:HA3	1:C:987:ASP:HA	2.03	0.41
1:D:143:PHE:O	1:D:168:PRO:HA	2.20	0.41
1:D:472:TYR:O	1:D:476:LYS:HG2	2.20	0.41
1:A:473:ARG:HA	1:A:473:ARG:HD2	1.85	0.41
1:B:1023:LYS:HE3	1:B:1023:LYS:HB3	1.66	0.41
1:A:253:TYR:CD1	1:A:253:TYR:C	2.99	0.40
1:C:71:GLU:N	7:C:9383:HOH:O	2.53	0.40
1:C:806:TRP:CD2	1:C:991:MET:HE1	2.55	0.40
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.21	0.40
1:A:768:MET:HE1	1:A:1020:TRP:CH2	2.56	0.40
6:C:8421:DMS:H23	7:C:9139:HOH:O	2.20	0.40
1:A:337:ILE:HA	1:A:341:LEU:O	2.21	0.40
1:A:518:TRP:O	1:A:519:SER:C	2.64	0.40
1:B:301:TRP:CH2	1:B:452:SER:HA	2.56	0.40
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.21	0.40
1:B:562:LEU:HD23	1:B:562:LEU:HA	1.83	0.40
1:B:930:VAL:HA	1:B:973:ARG:HD3	2.03	0.40
1:C:471:LEU:HD23	1:C:471:LEU:HA	1.95	0.40
1:B:111:PRO:HA	1:B:112:PRO:HA	1.86	0.40
1:B:142:ILE:HG12	1:B:170:GLU:HG2	2.02	0.40
1:B:457:SER:HA	1:B:485:GLN:O	2.22	0.40
1:A:557:ARG:HH11	1:A:557:ARG:HD2	1.72	0.40
1:A:685:LEU:CB	1:A:686:PRO:CD	2.99	0.40
1:A:861:SER:OG	1:A:863:GLN:HG3	2.22	0.40
1:D:36:TRP:HH2	6:D:8404:DMS:H21	1.86	0.40
1:D:431:ARG:HD2	7:D:9514:HOH:O	2.21	0.40
1:D:583:ASN:HB3	7:D:9453:HOH:O	2.20	0.40
1:D:759:ASN:OD1	1:D:761:GLN:N	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:9544:HOH:O	7:B:9658:HOH:O[2_454]	2.18	0.02

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	1009/1023 (99%)	974 (96%)	34 (3%)	1 (0%)	48	32
1	B	1010/1023 (99%)	969 (96%)	36 (4%)	5 (0%)	24	11
1	C	1009/1023 (99%)	975 (97%)	34 (3%)	0	100	100
1	D	1009/1023 (99%)	970 (96%)	38 (4%)	1 (0%)	48	32
All	All	4037/4092 (99%)	3888 (96%)	142 (4%)	7 (0%)	43	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	731	PRO
1	B	732	ALA
1	D	688	PRO
1	B	690	SER
1	A	164	ASP
1	B	164	ASP
1	B	688	PRO

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	864/875 (99%)	830 (96%)	34 (4%)	28	9
1	B	865/875 (99%)	834 (96%)	31 (4%)	31	11
1	C	864/875 (99%)	826 (96%)	38 (4%)	25	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	864/875 (99%)	821 (95%)	43 (5%)	22	5
All	All	3457/3500 (99%)	3311 (96%)	146 (4%)	26	8

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	ARG
1	A	267	VAL
1	A	478	VAL
1	A	519	SER
1	A	546	LEU
1	A	580	GLU
1	A	600	GLN
1	A	632	SER
1	A	634	GLN
1	A	655	MET
1	A	661	LYS
1	A	663	LEU
1	A	667	GLU
1	A	672	VAL
1	A	684	GLU
1	A	687	GLN
1	A	729	THR
1	A	730	LEU
1	A	735	HIS
1	A	737	ILE
1	A	773	LYS
1	A	796	SER
1	A	797	GLU
1	A	799	THR
1	A	800	ARG
1	A	801	ILE
1	A	809	ARG
1	A	817	GLN
1	A	885	ASN
1	A	890	GLN
1	A	956	GLN
1	A	986	ILE
1	A	1017	GLN
1	A	1023	LYS
1	B	246	MET
1	B	262	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	264	GLU
1	B	344	LEU
1	B	362	LEU
1	B	367	MET
1	B	370	GLN
1	B	546	LEU
1	B	580	GLU
1	B	599	ARG
1	B	600	GLN
1	B	634	GLN
1	B	651	LEU
1	B	655	MET
1	B	661	LYS
1	B	663	LEU
1	B	672	VAL
1	B	687	GLN
1	B	699	ARG
1	B	730	LEU
1	B	737	ILE
1	B	745	MET
1	B	797	GLU
1	B	799	THR
1	B	800	ARG
1	B	819	GLU
1	B	845	GLN
1	B	885	ASN
1	B	952	ARG
1	B	956	GLN
1	B	1023	LYS
1	C	71	GLU
1	C	80	GLU
1	C	135	GLN
1	C	157	ARG
1	C	178	ARG
1	C	230	ARG
1	C	251	ARG
1	C	262	GLN
1	C	278	ILE
1	C	437	SER
1	C	546	LEU
1	C	580	GLU
1	C	595	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	630	ARG
1	C	634	GLN
1	C	655	MET
1	C	663	LEU
1	C	681	GLU
1	C	684	GLU
1	C	685	LEU
1	C	687	GLN
1	C	699	ARG
1	C	729	THR
1	C	730	LEU
1	C	734	SER
1	C	735	HIS
1	C	737	ILE
1	C	749	ILE
1	C	773	LYS
1	C	796	SER
1	C	799	THR
1	C	800	ARG
1	C	819	GLU
1	C	829	THR
1	C	893	GLU
1	C	986	ILE
1	C	1017	GLN
1	C	1023	LYS
1	D	13	ARG
1	D	80	GLU
1	D	237	ARG
1	D	251	ARG
1	D	277	GLU
1	D	299	LYS
1	D	344	LEU
1	D	370	GLN
1	D	519	SER
1	D	546	LEU
1	D	581	ASN
1	D	594	ASP
1	D	595	THR
1	D	632	SER
1	D	634	GLN
1	D	651	LEU
1	D	655	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	661	LYS
1	D	663	LEU
1	D	667	GLU
1	D	681	GLU
1	D	682	LEU
1	D	684	GLU
1	D	687	GLN
1	D	689	GLU
1	D	735	HIS
1	D	737	ILE
1	D	749	ILE
1	D	755	ARG
1	D	772	ASP
1	D	773	LYS
1	D	796	SER
1	D	799	THR
1	D	800	ARG
1	D	843	GLN
1	D	845	GLN
1	D	885	ASN
1	D	893	GLU
1	D	986	ILE
1	D	1013	ARG
1	D	1017	GLN
1	D	1022	GLN
1	D	1023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	294	ASN
1	A	485	GLN
1	A	600	GLN
1	A	624	GLN
1	A	757	GLN
1	A	817	GLN
1	A	843	GLN
1	A	844	HIS
1	A	863	GLN
1	A	878	HIS
1	A	903	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	163	GLN
1	B	262	GLN
1	B	363	HIS
1	B	485	GLN
1	B	554	GLN
1	B	583	ASN
1	B	600	GLN
1	B	624	GLN
1	B	646	HIS
1	B	687	GLN
1	B	757	GLN
1	B	843	GLN
1	B	844	HIS
1	B	863	GLN
1	B	878	HIS
1	B	903	GLN
1	B	977	HIS
1	C	147	ASN
1	C	163	GLN
1	C	266	GLN
1	C	394	ASN
1	C	485	GLN
1	C	624	GLN
1	C	628	GLN
1	C	634	GLN
1	C	646	HIS
1	C	687	GLN
1	C	704	ASN
1	C	817	GLN
1	C	878	HIS
1	C	903	GLN
1	C	977	HIS
1	D	135	GLN
1	D	262	GLN
1	D	266	GLN
1	D	297	ASN
1	D	363	HIS
1	D	365	GLN
1	D	394	ASN
1	D	485	GLN
1	D	624	GLN
1	D	628	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	634	GLN
1	D	653	HIS
1	D	804	ASN
1	D	843	GLN
1	D	878	HIS
1	D	903	GLN
1	D	977	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 151 ligands modelled in this entry, 33 are monoatomic - leaving 118 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	DMS	A	8404	-	3,3,3	1.14	0	3,3,3	0.19	0
6	DMS	A	8602	-	3,3,3	0.68	0	3,3,3	0.29	0
6	DMS	D	8416	-	3,3,3	0.60	0	3,3,3	0.49	0
6	DMS	C	8427	-	3,3,3	0.42	0	3,3,3	0.22	0
6	DMS	D	8423	-	3,3,3	1.35	0	3,3,3	0.34	0
6	DMS	A	8409	-	3,3,3	2.43	1 (33%)	3,3,3	0.20	0
6	DMS	A	8410	-	3,3,3	0.76	0	3,3,3	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	DMS	B	8508	-	3,3,3	2.72	1 (33%)	3,3,3	0.61	0
2	2DG	D	2001	1,4	10,10,11	0.72	0	13,13,15	2.06	2 (15%)
6	DMS	C	8503	-	3,3,3	0.90	0	3,3,3	0.56	0
6	DMS	D	8412	-	3,3,3	0.62	0	3,3,3	0.76	0
6	DMS	C	8402	-	3,3,3	1.44	1 (33%)	3,3,3	0.13	0
6	DMS	A	8407	-	3,3,3	1.60	0	3,3,3	0.67	0
6	DMS	B	8407	-	3,3,3	3.03	2 (66%)	3,3,3	0.31	0
6	DMS	C	8407	-	3,3,3	1.41	0	3,3,3	0.05	0
6	DMS	C	8415	-	3,3,3	1.12	0	3,3,3	0.38	0
6	DMS	B	8403	-	3,3,3	1.07	0	3,3,3	0.24	0
6	DMS	D	8425	4	3,3,3	0.27	0	3,3,3	0.37	0
6	DMS	B	8420	-	3,3,3	1.72	1 (33%)	3,3,3	0.80	0
6	DMS	C	8501	-	3,3,3	0.91	0	3,3,3	0.85	0
6	DMS	C	8411	-	3,3,3	0.98	0	3,3,3	0.34	0
6	DMS	D	8508	-	3,3,3	1.74	1 (33%)	3,3,3	0.54	0
6	DMS	A	8504	-	3,3,3	0.64	0	3,3,3	0.27	0
6	DMS	C	8421	-	3,3,3	0.59	0	3,3,3	0.56	0
6	DMS	D	8403	-	3,3,3	0.60	0	3,3,3	0.20	0
5	BTB	B	2002	-	13,13,13	1.44	2 (15%)	7,16,16	0.92	0
6	DMS	B	8408	-	3,3,3	0.46	0	3,3,3	0.05	0
6	DMS	C	8419	-	3,3,3	0.72	0	3,3,3	0.25	0
6	DMS	B	8502	-	3,3,3	0.78	0	3,3,3	1.29	1 (33%)
6	DMS	C	8420	-	3,3,3	1.31	1 (33%)	3,3,3	0.34	0
6	DMS	B	8401	-	3,3,3	0.35	0	3,3,3	0.36	0
6	DMS	A	8425	4	3,3,3	1.41	1 (33%)	3,3,3	0.56	0
5	BTB	D	2002	-	13,13,13	1.42	3 (23%)	7,16,16	1.18	1 (14%)
6	DMS	C	8504	-	3,3,3	0.55	0	3,3,3	0.20	0
6	DMS	B	8409	-	3,3,3	1.49	1 (33%)	3,3,3	0.77	0
6	DMS	C	8401	-	3,3,3	0.71	0	3,3,3	0.14	0
6	DMS	C	8506	-	3,3,3	1.23	0	3,3,3	0.46	0
6	DMS	A	8503	-	3,3,3	0.49	0	3,3,3	0.31	0
6	DMS	D	8404	-	3,3,3	1.46	1 (33%)	3,3,3	0.28	0
6	DMS	C	8404	-	3,3,3	0.50	0	3,3,3	1.06	0
6	DMS	C	8412	-	3,3,3	0.90	0	3,3,3	0.58	0
6	DMS	D	8407	-	3,3,3	0.82	0	3,3,3	0.64	0
6	DMS	A	8401	-	3,3,3	0.74	0	3,3,3	0.48	0
6	DMS	A	8406	-	3,3,3	0.65	0	3,3,3	0.88	0
6	DMS	B	8406	-	3,3,3	1.23	0	3,3,3	0.44	0
6	DMS	D	8410	-	3,3,3	0.95	0	3,3,3	0.23	0
6	DMS	D	8409	-	3,3,3	1.42	1 (33%)	3,3,3	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	DMS	D	8408	-	3,3,3	1.24	0	3,3,3	0.31	0
6	DMS	A	8413	-	3,3,3	1.61	0	3,3,3	0.08	0
6	DMS	B	8410	-	3,3,3	0.61	0	3,3,3	0.48	0
6	DMS	B	8601	-	3,3,3	1.59	1 (33%)	3,3,3	0.47	0
6	DMS	C	8602	-	3,3,3	0.94	0	3,3,3	0.15	0
6	DMS	D	8419	-	3,3,3	0.99	0	3,3,3	0.10	0
6	DMS	A	8414	-	3,3,3	1.16	0	3,3,3	0.23	0
6	DMS	A	8421	-	3,3,3	0.81	0	3,3,3	0.51	0
6	DMS	B	8402	-	3,3,3	1.00	0	3,3,3	0.71	0
6	DMS	B	8405	-	3,3,3	1.38	1 (33%)	3,3,3	0.54	0
6	DMS	A	8419	-	3,3,3	0.61	0	3,3,3	0.33	0
6	DMS	D	8406	-	3,3,3	1.01	0	3,3,3	0.68	0
6	DMS	C	8601	-	3,3,3	1.46	1 (33%)	3,3,3	0.78	0
6	DMS	A	8417	-	3,3,3	1.31	0	3,3,3	0.14	0
6	DMS	B	8423	-	3,3,3	0.56	0	3,3,3	0.59	0
6	DMS	A	8405	-	3,3,3	0.51	0	3,3,3	0.49	0
6	DMS	C	8405	-	3,3,3	1.09	0	3,3,3	0.61	0
6	DMS	B	8506	-	3,3,3	1.03	0	3,3,3	0.50	0
6	DMS	A	8502	-	3,3,3	2.02	1 (33%)	3,3,3	1.09	0
6	DMS	C	8417	-	3,3,3	0.79	0	3,3,3	0.30	0
6	DMS	C	8423	-	3,3,3	0.69	0	3,3,3	0.10	0
6	DMS	D	8402	-	3,3,3	1.10	0	3,3,3	0.21	0
6	DMS	C	8408	-	3,3,3	0.62	0	3,3,3	0.74	0
6	DMS	C	8403	-	3,3,3	0.87	0	3,3,3	0.66	0
6	DMS	B	8427	-	3,3,3	0.76	0	3,3,3	0.16	0
5	BTB	C	2002	-	13,13,13	1.85	4 (30%)	7,16,16	1.11	1 (14%)
6	DMS	A	8416	-	3,3,3	0.51	0	3,3,3	0.36	0
6	DMS	C	8425	4	3,3,3	1.45	1 (33%)	3,3,3	0.23	0
6	DMS	A	8501	-	3,3,3	1.18	0	3,3,3	0.12	0
6	DMS	A	8423	-	3,3,3	1.33	1 (33%)	3,3,3	0.27	0
6	DMS	D	8506	-	3,3,3	1.05	0	3,3,3	0.17	0
6	DMS	A	8506	-	3,3,3	1.06	0	3,3,3	0.43	0
6	DMS	A	8412	-	3,3,3	0.39	0	3,3,3	0.25	0
6	DMS	D	8415	-	3,3,3	2.93	1 (33%)	3,3,3	0.34	0
6	DMS	B	8411	-	3,3,3	1.25	0	3,3,3	0.57	0
6	DMS	B	8413	-	3,3,3	1.90	1 (33%)	3,3,3	0.44	0
6	DMS	D	8703	-	3,3,3	1.64	1 (33%)	3,3,3	0.29	0
6	DMS	D	8411	-	3,3,3	0.49	0	3,3,3	0.22	0
6	DMS	B	8421	-	3,3,3	0.28	0	3,3,3	0.45	0
2	2DG	A	2001	1,4	10,10,11	0.80	0	13,13,15	1.77	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	DMS	A	8411	-	3,3,3	0.93	0	3,3,3	0.39	0
6	DMS	C	8413	-	3,3,3	2.33	1 (33%)	3,3,3	0.13	0
2	2DG	C	2001	1,4	10,10,11	1.00	1 (10%)	13,13,15	2.24	2 (15%)
6	DMS	C	8409	-	3,3,3	1.36	1 (33%)	3,3,3	1.26	1 (33%)
6	DMS	C	8410	-	3,3,3	1.10	0	3,3,3	0.20	0
6	DMS	B	8414	-	3,3,3	1.00	0	3,3,3	0.34	0
6	DMS	A	8402	-	3,3,3	1.02	0	3,3,3	0.50	0
6	DMS	D	8413	-	3,3,3	0.97	0	3,3,3	0.25	0
6	DMS	B	8417	-	3,3,3	0.47	0	3,3,3	0.49	0
6	DMS	A	8403	-	3,3,3	2.09	2 (66%)	3,3,3	0.48	0
6	DMS	A	8420	-	3,3,3	0.81	0	3,3,3	1.08	0
6	DMS	D	8501	-	3,3,3	0.57	0	3,3,3	0.42	0
6	DMS	D	8421	-	3,3,3	0.31	0	3,3,3	0.15	0
6	DMS	C	8414	-	3,3,3	0.54	0	3,3,3	0.79	0
6	DMS	D	8701	-	3,3,3	2.29	2 (66%)	3,3,3	0.46	0
6	DMS	D	8405	-	3,3,3	0.72	0	3,3,3	0.83	0
6	DMS	D	8414	-	3,3,3	0.27	0	3,3,3	0.34	0
6	DMS	D	8503	-	3,3,3	0.64	0	3,3,3	0.96	0
6	DMS	B	8504	-	3,3,3	0.69	0	3,3,3	0.68	0
6	DMS	D	8417	-	3,3,3	1.70	1 (33%)	3,3,3	0.60	0
6	DMS	D	8705	-	3,3,3	1.96	1 (33%)	3,3,3	0.62	0
5	BTB	A	2002	-	13,13,13	1.63	4 (30%)	7,16,16	1.26	1 (14%)
6	DMS	B	8416	-	3,3,3	1.49	1 (33%)	3,3,3	0.52	0
6	DMS	A	8408	-	3,3,3	0.71	0	3,3,3	0.45	0
6	DMS	D	8401	-	3,3,3	1.04	0	3,3,3	0.16	0
6	DMS	B	8415	-	3,3,3	2.05	2 (66%)	3,3,3	1.21	0
2	2DG	B	2001	1,4	10,10,11	0.93	0	13,13,15	1.07	0
6	DMS	B	8404	-	3,3,3	0.78	0	3,3,3	0.23	0
6	DMS	B	8412	-	3,3,3	0.93	0	3,3,3	0.28	0
6	DMS	C	8416	-	3,3,3	0.60	0	3,3,3	0.38	0
6	DMS	B	8425	4	3,3,3	2.35	2 (66%)	3,3,3	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BTB	B	2002	-	-	3/21/21/21	-
2	2DG	B	2001	1,4	-	1/2/16/18	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BTB	A	2002	-	-	3/21/21/21	-
5	BTB	D	2002	-	-	3/21/21/21	-
2	2DG	A	2001	1,4	-	1/2/16/18	0/1/1/1
2	2DG	D	2001	1,4	-	1/2/16/18	0/1/1/1
2	2DG	C	2001	1,4	-	1/2/16/18	0/1/1/1
5	BTB	C	2002	-	-	2/21/21/21	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	8407	DMS	C2-S	4.80	2.10	1.76
6	D	8415	DMS	O-S	4.65	1.80	1.50
5	C	2002	BTB	C1-C2	-4.35	1.48	1.53
6	B	8508	DMS	C1-S	4.18	2.06	1.76
6	A	8409	DMS	O-S	3.86	1.75	1.50
6	C	8413	DMS	O-S	3.50	1.73	1.50
6	B	8425	DMS	O-S	3.37	1.72	1.50
5	C	2002	BTB	C3-C2	3.15	1.57	1.53
5	A	2002	BTB	C1-C2	-3.15	1.49	1.53
5	D	2002	BTB	C1-C2	-2.95	1.49	1.53
6	D	8705	DMS	O-S	2.93	1.69	1.50
6	B	8420	DMS	C2-S	2.82	1.96	1.76
6	A	8403	DMS	O-S	2.82	1.68	1.50
6	A	8502	DMS	C1-S	2.82	1.96	1.76
5	A	2002	BTB	C5-N	2.81	1.51	1.48
5	B	2002	BTB	C1-C2	-2.80	1.50	1.53
6	D	8701	DMS	O-S	2.77	1.68	1.50
6	D	8508	DMS	O-S	2.74	1.68	1.50
5	B	2002	BTB	C3-C2	2.59	1.56	1.53
6	B	8416	DMS	O-S	2.50	1.66	1.50
5	C	2002	BTB	C7-N	2.49	1.51	1.48
6	C	8402	DMS	C2-S	2.49	1.93	1.76
5	A	2002	BTB	C3-C2	2.46	1.56	1.53
6	B	8409	DMS	O-S	2.45	1.66	1.50
6	C	8601	DMS	C2-S	2.38	1.93	1.76
6	D	8701	DMS	C1-S	2.34	1.92	1.76
6	C	8409	DMS	O-S	2.30	1.65	1.50
6	C	8425	DMS	O-S	2.29	1.65	1.50
6	A	8403	DMS	C2-S	2.26	1.92	1.76
6	B	8425	DMS	C2-S	2.25	1.92	1.76
6	D	8404	DMS	C2-S	2.24	1.92	1.76
6	B	8601	DMS	C2-S	2.22	1.91	1.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	8405	DMS	O-S	2.22	1.64	1.50
6	A	8423	DMS	C1-S	2.21	1.91	1.76
6	B	8415	DMS	C2-S	2.19	1.91	1.76
6	D	8409	DMS	O-S	2.18	1.64	1.50
6	C	8420	DMS	O-S	2.18	1.64	1.50
2	C	2001	2DG	C3-C4	2.17	1.55	1.52
5	D	2002	BTB	C7-N	2.15	1.51	1.48
5	A	2002	BTB	C2-N	2.15	1.52	1.48
6	D	8703	DMS	O-S	2.14	1.64	1.50
6	B	8413	DMS	O-S	2.14	1.64	1.50
6	B	8407	DMS	O-S	2.12	1.64	1.50
5	D	2002	BTB	C5-N	2.11	1.50	1.48
6	D	8417	DMS	O-S	2.10	1.64	1.50
6	A	8425	DMS	O-S	2.05	1.63	1.50
5	C	2002	BTB	O3-C3	2.04	1.48	1.42
6	B	8415	DMS	O-S	2.03	1.63	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	2DG	C3-C4-C5	-6.78	103.19	109.99
2	D	2001	2DG	C3-C4-C5	-4.69	105.28	109.99
2	D	2001	2DG	C1-O5-C5	4.48	119.89	112.01
2	A	2001	2DG	C3-C4-C5	-4.32	105.65	109.99
2	A	2001	2DG	O5-C5-C6	-3.14	101.55	107.66
2	C	2001	2DG	C1-O5-C5	2.50	116.41	112.01
5	C	2002	BTB	O1-C1-C2	-2.37	105.82	111.40
5	A	2002	BTB	O3-C3-C2	-2.35	105.88	111.40
6	B	8502	DMS	C2-S-C1	2.19	109.66	98.42
6	C	8409	DMS	C2-S-C1	2.07	109.02	98.42
5	D	2002	BTB	O1-C1-C2	-2.05	106.57	111.40

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2002	BTB	C1-C2-C3-O3
5	A	2002	BTB	C4-C2-C3-O3
5	A	2002	BTB	N-C2-C3-O3
5	B	2002	BTB	N-C2-C3-O3
5	C	2002	BTB	N-C2-C3-O3
5	D	2002	BTB	N-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	2001	2DG	O5-C5-C6-O6
2	B	2001	2DG	O5-C5-C6-O6
5	C	2002	BTB	N-C7-C8-O8
2	C	2001	2DG	O5-C5-C6-O6
5	D	2002	BTB	N-C7-C8-O8
2	D	2001	2DG	O5-C5-C6-O6
5	B	2002	BTB	N-C7-C8-O8
5	D	2002	BTB	C4-C2-C3-O3
5	B	2002	BTB	C4-C2-C3-O3

There are no ring outliers.

47 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	8404	DMS	1	0
6	A	8602	DMS	2	0
6	C	8427	DMS	2	0
6	D	8423	DMS	1	0
6	A	8409	DMS	1	0
6	B	8508	DMS	2	0
6	C	8503	DMS	1	0
6	D	8412	DMS	3	0
6	A	8407	DMS	1	0
6	B	8407	DMS	3	0
6	C	8407	DMS	1	0
6	B	8403	DMS	1	0
6	D	8425	DMS	1	0
6	B	8420	DMS	1	0
6	C	8421	DMS	1	0
6	D	8403	DMS	1	0
6	C	8420	DMS	1	0
5	D	2002	BTB	1	0
6	A	8503	DMS	5	0
6	D	8404	DMS	1	0
6	B	8406	DMS	3	0
6	D	8410	DMS	1	0
6	B	8410	DMS	2	0
6	C	8602	DMS	2	0
6	A	8414	DMS	1	0
6	A	8417	DMS	1	0
6	C	8417	DMS	1	0
6	C	8403	DMS	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	8427	DMS	1	0
5	C	2002	BTB	1	0
6	A	8416	DMS	2	0
6	C	8425	DMS	5	0
6	A	8423	DMS	2	0
6	D	8506	DMS	2	0
6	A	8412	DMS	1	0
6	D	8415	DMS	1	0
6	D	8703	DMS	4	0
6	C	8409	DMS	1	0
6	C	8410	DMS	1	0
6	B	8414	DMS	2	0
6	B	8417	DMS	2	0
6	A	8403	DMS	1	0
6	A	8420	DMS	2	0
6	D	8421	DMS	1	0
6	B	8504	DMS	3	0
6	D	8417	DMS	1	0
6	B	8416	DMS	1	0

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	1011/1023 (98%)	-0.63	13 (1%) 75 81	11, 18, 46, 98	0
1	B	1011/1023 (98%)	-0.60	18 (1%) 67 74	10, 18, 47, 97	1 (0%)
1	C	1011/1023 (98%)	-0.59	14 (1%) 73 80	11, 19, 49, 100	0
1	D	1011/1023 (98%)	-0.58	22 (2%) 62 69	10, 18, 50, 100	0
All	All	4044/4092 (98%)	-0.60	67 (1%) 69 75	10, 18, 48, 100	1 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	686	PRO	5.9
1	D	801	ILE	4.7
1	A	730	LEU	4.5
1	B	730	LEU	4.4
1	D	798	ALA	3.9
1	A	799	THR	3.8
1	B	685	LEU	3.7
1	B	733	ALA	3.6
1	A	798	ALA	3.5
1	D	732	ALA	3.4
1	D	685	LEU	3.4
1	D	686	PRO	3.4
1	C	732	ALA	3.3
1	D	735	HIS	3.3
1	A	732	ALA	3.2
1	B	798	ALA	3.2
1	D	688	PRO	3.1
1	D	797	GLU	3.1
1	D	730	LEU	3.1
1	C	736	ALA	3.1
1	B	799	THR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	732	ALA	3.1
1	C	733	ALA	3.1
1	C	799	THR	3.1
1	C	634	GLN	2.9
1	D	734	SER	2.9
1	A	1023	LYS	2.8
1	B	1023	LYS	2.7
1	D	795	VAL	2.7
1	A	735	HIS	2.7
1	C	730	LEU	2.7
1	B	797	GLU	2.6
1	D	737	ILE	2.6
1	D	799	THR	2.6
1	A	685	LEU	2.6
1	C	735	HIS	2.6
1	C	686	PRO	2.6
1	B	735	HIS	2.5
1	D	796	SER	2.5
1	D	663	LEU	2.5
1	B	731	PRO	2.5
1	C	1023	LYS	2.4
1	B	687	GLN	2.4
1	D	634	GLN	2.4
1	B	801	ILE	2.4
1	C	798	ALA	2.3
1	D	800	ARG	2.3
1	D	581	ASN	2.3
1	B	689	GLU	2.3
1	A	731	PRO	2.3
1	D	733	ALA	2.3
1	C	685	LEU	2.3
1	B	845	GLN	2.2
1	B	745	MET	2.2
1	D	1023	LYS	2.2
1	A	687	GLN	2.2
1	A	688	PRO	2.2
1	D	829	THR	2.2
1	B	1018	LEU	2.1
1	B	729	THR	2.1
1	B	686	PRO	2.1
1	A	733	ALA	2.1
1	D	689	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	663	LEU	2.1
1	A	729	THR	2.1
1	C	633	GLY	2.0
1	C	729	THR	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 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
3	MG	C	3105	1/1	0.75	0.20	47,47,47,47	1
6	DMS	D	8407	4/4	0.78	0.17	21,34,71,100	0
6	DMS	B	8413	4/4	0.82	0.16	50,55,58,70	0
6	DMS	C	8419	4/4	0.83	0.13	38,51,67,78	0
6	DMS	D	8417	4/4	0.84	0.19	27,29,72,94	0
6	DMS	D	8503	4/4	0.84	0.17	41,57,72,74	0
6	DMS	B	8406	4/4	0.86	0.16	32,40,52,59	0
6	DMS	A	8417	4/4	0.86	0.16	32,34,90,100	0
6	DMS	A	8413	4/4	0.87	0.17	36,70,79,100	0
6	DMS	C	8417	4/4	0.87	0.11	27,37,45,68	0
6	DMS	A	8423	4/4	0.88	0.19	39,68,81,100	0
3	MG	B	3003	1/1	0.88	0.08	25,25,25,25	1
6	DMS	B	8410	4/4	0.88	0.14	34,36,57,82	0
3	MG	A	3003	1/1	0.89	0.19	26,26,26,26	1
6	DMS	A	8416	4/4	0.89	0.13	23,38,47,100	0
3	MG	D	3003	1/1	0.89	0.12	30,30,30,30	1
6	DMS	D	8415	4/4	0.89	0.15	29,37,68,100	0
6	DMS	A	8421	4/4	0.89	0.18	54,67,79,94	0
6	DMS	D	8423	4/4	0.89	0.13	39,55,62,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	DMS	B	8420	4/4	0.89	0.17	52,54,69,77	0
6	DMS	B	8423	4/4	0.90	0.13	34,35,59,100	0
6	DMS	B	8427	4/4	0.90	0.10	35,38,53,66	0
6	DMS	B	8415	4/4	0.90	0.11	27,28,42,56	0
6	DMS	A	8502	4/4	0.90	0.13	23,31,54,67	0
6	DMS	C	8503	4/4	0.90	0.13	36,58,65,76	0
6	DMS	D	8703	4/4	0.90	0.15	31,48,50,51	0
3	MG	C	3004	1/1	0.91	0.09	51,51,51,51	0
6	DMS	A	8503	4/4	0.91	0.20	26,100,100,100	0
6	DMS	C	8423	4/4	0.91	0.10	39,39,54,61	0
6	DMS	B	8425	4/4	0.91	0.11	23,34,44,50	0
6	DMS	A	8420	4/4	0.91	0.14	37,43,45,66	0
6	DMS	B	8416	4/4	0.92	0.12	36,45,53,68	0
6	DMS	A	8406	4/4	0.92	0.13	23,33,65,73	0
6	DMS	B	8421	4/4	0.92	0.11	28,56,60,67	0
6	DMS	D	8416	4/4	0.92	0.13	28,30,51,100	0
5	BTB	C	2002	14/14	0.93	0.11	14,25,38,98	14
6	DMS	B	8508	4/4	0.93	0.09	30,40,45,49	0
6	DMS	D	8413	4/4	0.93	0.13	39,44,45,83	0
6	DMS	C	8416	4/4	0.93	0.12	59,65,71,72	0
6	DMS	A	8506	4/4	0.93	0.11	35,35,36,38	0
6	DMS	A	8602	4/4	0.93	0.16	41,45,100,100	0
6	DMS	C	8421	4/4	0.93	0.15	38,48,94,100	0
6	DMS	D	8425	4/4	0.93	0.20	21,31,44,76	4
6	DMS	A	8414	4/4	0.93	0.13	31,43,51,100	0
6	DMS	C	8427	4/4	0.93	0.12	42,55,62,70	0
6	DMS	D	8705	4/4	0.93	0.10	21,33,40,43	0
6	DMS	C	8506	4/4	0.94	0.09	22,30,37,38	0
6	DMS	C	8413	4/4	0.94	0.15	30,41,52,95	0
6	DMS	C	8415	4/4	0.94	0.10	26,38,38,46	0
6	DMS	A	8425	4/4	0.94	0.10	31,38,42,43	0
6	DMS	A	8407	4/4	0.94	0.10	29,40,41,45	0
6	DMS	B	8414	4/4	0.94	0.12	30,32,51,100	0
6	DMS	D	8419	4/4	0.94	0.07	23,41,52,62	0
6	DMS	D	8421	4/4	0.94	0.12	43,48,50,100	0
3	MG	C	3003	1/1	0.94	0.07	24,24,24,24	1
6	DMS	B	8407	4/4	0.94	0.11	34,34,41,47	0
6	DMS	B	8504	4/4	0.94	0.10	27,44,46,47	0
6	DMS	D	8506	4/4	0.94	0.06	19,25,31,40	0
6	DMS	B	8417	4/4	0.94	0.12	25,34,62,100	0
6	DMS	C	8504	4/4	0.94	0.10	30,39,48,58	0
6	DMS	D	8404	4/4	0.95	0.11	24,24,49,100	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BTB	B	2002	14/14	0.95	0.09	13,23,30,99	14
6	DMS	B	8409	4/4	0.95	0.08	29,31,35,39	0
3	MG	C	3006	1/1	0.95	0.06	43,43,43,43	0
4	NA	B	3104	1/1	0.95	0.07	33,33,33,33	0
6	DMS	C	8420	4/4	0.95	0.14	44,46,79,100	0
5	BTB	A	2002	14/14	0.95	0.08	11,20,31,34	14
6	DMS	B	8502	4/4	0.95	0.10	25,30,42,46	0
6	DMS	C	8425	4/4	0.95	0.14	34,43,58,100	0
6	DMS	A	8419	4/4	0.95	0.09	43,46,51,56	0
6	DMS	D	8501	4/4	0.95	0.07	23,35,42,54	0
6	DMS	A	8409	4/4	0.95	0.09	26,37,45,47	0
6	DMS	C	8410	4/4	0.95	0.10	30,37,45,45	0
6	DMS	D	8508	4/4	0.95	0.09	37,39,45,47	0
6	DMS	A	8410	4/4	0.95	0.11	25,30,46,55	0
6	DMS	C	8601	4/4	0.95	0.09	28,47,53,57	0
6	DMS	D	8409	4/4	0.96	0.09	30,32,36,36	0
6	DMS	D	8410	4/4	0.96	0.09	33,35,39,44	0
6	DMS	A	8404	4/4	0.96	0.07	23,27,36,37	0
6	DMS	D	8414	4/4	0.96	0.14	27,45,89,100	0
6	DMS	A	8412	4/4	0.96	0.11	31,33,39,100	0
4	NA	D	3104	1/1	0.96	0.06	35,35,35,35	0
6	DMS	B	8506	4/4	0.96	0.10	31,32,33,47	0
6	DMS	B	8404	4/4	0.96	0.06	22,22,32,36	0
6	DMS	B	8601	4/4	0.96	0.08	29,36,40,48	0
6	DMS	C	8501	4/4	0.96	0.08	20,30,36,46	0
6	DMS	C	8407	4/4	0.96	0.13	29,32,44,100	0
3	MG	A	3005	1/1	0.96	0.05	30,30,30,30	0
6	DMS	A	8408	4/4	0.96	0.08	19,31,40,59	0
6	DMS	B	8408	4/4	0.96	0.11	28,34,40,90	0
6	DMS	C	8602	4/4	0.96	0.09	39,45,60,72	0
6	DMS	A	8501	4/4	0.96	0.07	20,32,36,41	0
5	BTB	D	2002	14/14	0.96	0.08	15,22,29,95	14
6	DMS	B	8412	4/4	0.97	0.07	28,34,34,36	0
6	DMS	C	8409	4/4	0.97	0.07	30,32,39,39	0
6	DMS	A	8504	4/4	0.97	0.10	18,38,53,89	0
6	DMS	C	8412	4/4	0.97	0.10	32,35,36,100	0
3	MG	D	3005	1/1	0.97	0.05	25,25,25,25	0
6	DMS	C	8414	4/4	0.97	0.10	21,40,71,100	0
4	NA	C	3104	1/1	0.97	0.07	30,30,30,30	0
6	DMS	C	8402	4/4	0.97	0.07	18,28,30,32	0
6	DMS	C	8405	4/4	0.98	0.05	24,24,25,29	0
6	DMS	D	8412	4/4	0.98	0.06	27,30,31,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	DMS	A	8411	4/4	0.98	0.08	28,29,31,45	0
6	DMS	C	8408	4/4	0.98	0.06	25,34,39,40	0
6	DMS	A	8405	4/4	0.98	0.07	18,25,28,45	0
6	DMS	B	8411	4/4	0.98	0.10	27,30,30,87	0
4	NA	A	3103	1/1	0.98	0.07	28,28,28,28	0
6	DMS	B	8402	4/4	0.98	0.05	17,17,23,25	0
4	NA	D	3103	1/1	0.98	0.05	30,30,30,30	0
6	DMS	B	8405	4/4	0.98	0.07	27,29,32,32	0
4	NA	A	3104	1/1	0.98	0.05	25,25,25,25	0
6	DMS	D	8402	4/4	0.98	0.05	18,22,23,24	0
6	DMS	A	8402	4/4	0.98	0.06	16,18,23,29	0
6	DMS	D	8406	4/4	0.98	0.07	24,26,26,28	0
2	2DG	C	2001	10/11	0.98	0.05	8,15,17,18	0
6	DMS	D	8701	4/4	0.98	0.06	14,17,20,31	0
6	DMS	D	8408	4/4	0.98	0.05	24,31,32,40	0
6	DMS	C	8404	4/4	0.98	0.05	19,24,25,31	0
6	DMS	C	8401	4/4	0.99	0.03	16,16,21,22	0
4	NA	B	3103	1/1	0.99	0.03	23,23,23,23	0
6	DMS	D	8401	4/4	0.99	0.04	16,18,19,23	0
6	DMS	C	8403	4/4	0.99	0.04	20,21,24,28	0
6	DMS	D	8403	4/4	0.99	0.05	19,29,29,37	0
3	MG	A	3001	1/1	0.99	0.02	16,16,16,16	0
6	DMS	D	8405	4/4	0.99	0.07	23,26,31,52	0
4	NA	C	3102	1/1	0.99	0.03	17,17,17,17	0
4	NA	C	3103	1/1	0.99	0.05	24,24,24,24	0
3	MG	A	3002	1/1	0.99	0.03	17,17,17,17	0
4	NA	D	3101	1/1	0.99	0.02	16,16,16,16	0
4	NA	D	3102	1/1	0.99	0.02	15,15,15,15	0
6	DMS	D	8411	4/4	0.99	0.06	20,27,28,55	0
6	DMS	C	8411	4/4	0.99	0.06	24,29,35,45	0
2	2DG	B	2001	10/11	0.99	0.04	5,9,12,13	10
2	2DG	A	2001	10/11	0.99	0.04	9,13,20,23	0
3	MG	D	3001	1/1	0.99	0.02	15,15,15,15	0
3	MG	D	3002	1/1	0.99	0.05	17,17,17,17	0
3	MG	B	3002	1/1	0.99	0.03	19,19,19,19	0
2	2DG	D	2001	10/11	0.99	0.03	9,11,17,18	0
6	DMS	A	8401	4/4	0.99	0.04	14,15,17,19	0
4	NA	A	3101	1/1	0.99	0.03	16,16,16,16	0
6	DMS	A	8403	4/4	0.99	0.04	21,22,25,28	0
4	NA	A	3102	1/1	0.99	0.03	14,14,14,14	0
3	MG	C	3001	1/1	0.99	0.03	15,15,15,15	0
3	MG	C	3002	1/1	0.99	0.05	15,15,15,15	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	DMS	B	8401	4/4	0.99	0.04	15,17,21,21	0
4	NA	B	3101	1/1	0.99	0.02	15,15,15,15	0
6	DMS	B	8403	4/4	0.99	0.04	18,24,26,26	0
4	NA	B	3102	1/1	0.99	0.04	16,16,16,16	0
4	NA	C	3101	1/1	1.00	0.02	15,15,15,15	0
3	MG	B	3001	1/1	1.00	0.02	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.