



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:21 AM GMT

PDB ID : 3I3E
Title : E. COLI (lacZ) BETA-GALACTOSIDASE (M542A)
Authors : Dugdale, M.L.; Dymianiw, D.; Minhas, B.; Huber, R.E.
Deposited on : 2009-06-30
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

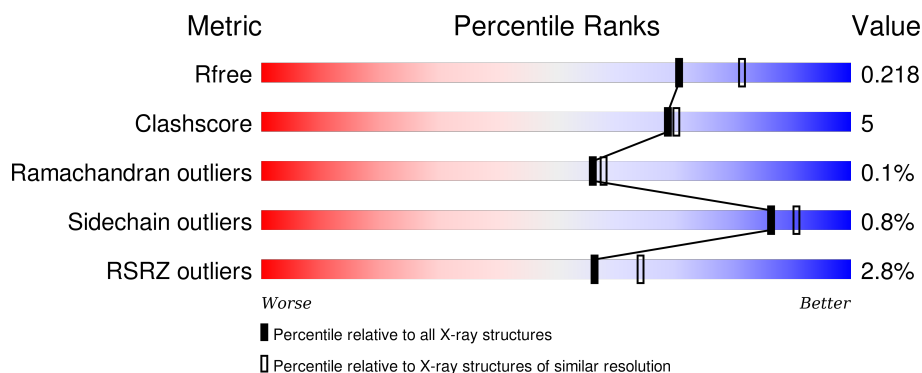
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	B	1023	<div> <div>2%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	C	1023	<div> <div>3%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	D	1023	<div> <div>3%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>

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
4	DMS	A	8404	-	-	-	X
4	DMS	A	8406	-	-	-	X
4	DMS	A	8407	-	-	-	X
4	DMS	A	8408	-	-	-	X
4	DMS	A	8419	-	-	-	X
4	DMS	A	8420	-	-	-	X
4	DMS	A	8502	-	-	-	X
4	DMS	A	8603	-	-	-	X
4	DMS	A	8604	-	-	-	X
4	DMS	A	8608	-	-	-	X
4	DMS	B	8404	-	-	-	X
4	DMS	B	8405	-	-	-	X
4	DMS	B	8406	-	-	-	X
4	DMS	B	8407	-	-	-	X
4	DMS	B	8408	-	-	-	X
4	DMS	B	8411	-	-	-	X
4	DMS	B	8413	-	-	-	X
4	DMS	B	8417	-	-	-	X
4	DMS	B	8423	-	-	-	X
4	DMS	B	8425	-	-	-	X
4	DMS	B	8502	-	-	-	X
4	DMS	B	8508	-	-	-	X
4	DMS	B	8604	-	-	-	X
4	DMS	B	8605	-	-	-	X
4	DMS	B	8610	-	-	-	X
4	DMS	C	1024	-	-	-	X
4	DMS	C	8403	-	-	-	X
4	DMS	C	8404	-	-	-	X
4	DMS	C	8405	-	-	-	X
4	DMS	C	8407	-	-	-	X
4	DMS	C	8411	-	-	-	X
4	DMS	C	8420	-	-	-	X
4	DMS	C	8423	-	-	-	X
4	DMS	C	8425	-	-	-	X
4	DMS	C	8501	-	-	-	X
4	DMS	C	8602	-	-	-	X
4	DMS	C	8604	-	-	-	X
4	DMS	C	8606	-	-	-	X
4	DMS	D	8404	-	-	-	X
4	DMS	D	8406	-	-	-	X
4	DMS	D	8407	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DMS	D	8423	-	-	-	X
4	DMS	D	8703	-	-	-	X
4	DMS	D	8705	-	-	-	X
4	DMS	D	8708	-	-	-	X
4	DMS	D	8712	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36653 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
			8122	5136	1440	1509	37			
1	B	1010	Total	C	N	O	S	0	0	0
			8113	5130	1438	1508	37			
1	C	1011	Total	C	N	O	S	0	0	0
			8122	5136	1440	1509	37			
1	D	1011	Total	C	N	O	S	0	0	0
			8122	5136	1440	1509	37			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP B8LFD6
A	2	SER	-	EXPRESSION TAG	UNP B8LFD6
A	3	HIS	-	EXPRESSION TAG	UNP B8LFD6
A	4	MET	-	EXPRESSION TAG	UNP B8LFD6
A	5	LEU	-	EXPRESSION TAG	UNP B8LFD6
A	6	GLU	-	EXPRESSION TAG	UNP B8LFD6
A	7	ASP	-	EXPRESSION TAG	UNP B8LFD6
A	8	PRO	-	EXPRESSION TAG	UNP B8LFD6
A	542	ALA	MET	ENGINEERED	UNP B8LFD6
B	1	GLY	-	EXPRESSION TAG	UNP B8LFD6
B	2	SER	-	EXPRESSION TAG	UNP B8LFD6
B	3	HIS	-	EXPRESSION TAG	UNP B8LFD6
B	4	MET	-	EXPRESSION TAG	UNP B8LFD6
B	5	LEU	-	EXPRESSION TAG	UNP B8LFD6
B	6	GLU	-	EXPRESSION TAG	UNP B8LFD6
B	7	ASP	-	EXPRESSION TAG	UNP B8LFD6
B	8	PRO	-	EXPRESSION TAG	UNP B8LFD6
B	542	ALA	MET	ENGINEERED	UNP B8LFD6
C	1	GLY	-	EXPRESSION TAG	UNP B8LFD6
C	2	SER	-	EXPRESSION TAG	UNP B8LFD6
C	3	HIS	-	EXPRESSION TAG	UNP B8LFD6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	-	EXPRESSION TAG	UNP B8LFD6
C	5	LEU	-	EXPRESSION TAG	UNP B8LFD6
C	6	GLU	-	EXPRESSION TAG	UNP B8LFD6
C	7	ASP	-	EXPRESSION TAG	UNP B8LFD6
C	8	PRO	-	EXPRESSION TAG	UNP B8LFD6
C	542	ALA	MET	ENGINEERED	UNP B8LFD6
D	1	GLY	-	EXPRESSION TAG	UNP B8LFD6
D	2	SER	-	EXPRESSION TAG	UNP B8LFD6
D	3	HIS	-	EXPRESSION TAG	UNP B8LFD6
D	4	MET	-	EXPRESSION TAG	UNP B8LFD6
D	5	LEU	-	EXPRESSION TAG	UNP B8LFD6
D	6	GLU	-	EXPRESSION TAG	UNP B8LFD6
D	7	ASP	-	EXPRESSION TAG	UNP B8LFD6
D	8	PRO	-	EXPRESSION TAG	UNP B8LFD6
D	542	ALA	MET	ENGINEERED	UNP B8LFD6

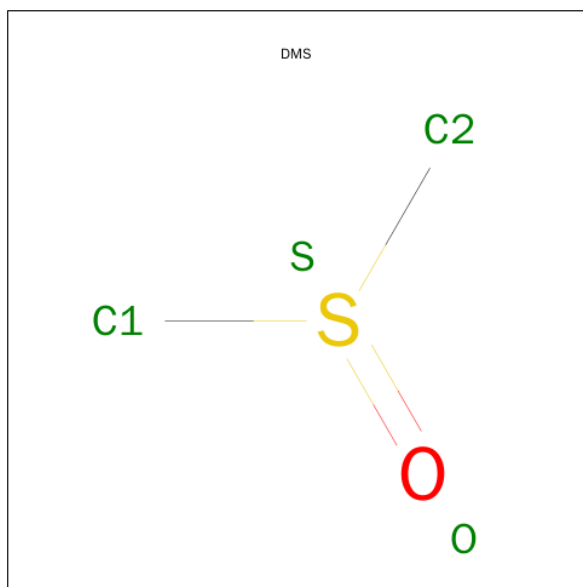
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mg 3 3	0	0
2	A	5	Total Mg 5 5	0	0
2	D	3	Total Mg 3 3	0	0
2	C	4	Total Mg 4 4	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

[illegible]

Continued on next page...

Continued from previous page...

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

- Molecule 5 is water.

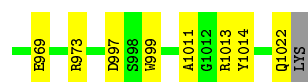
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	941	Total O 941 941	0	0
5	B	944	Total O 944 944	0	0
5	C	870	Total O 870 870	0	0
5	D	856	Total O 856 856	0	0

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

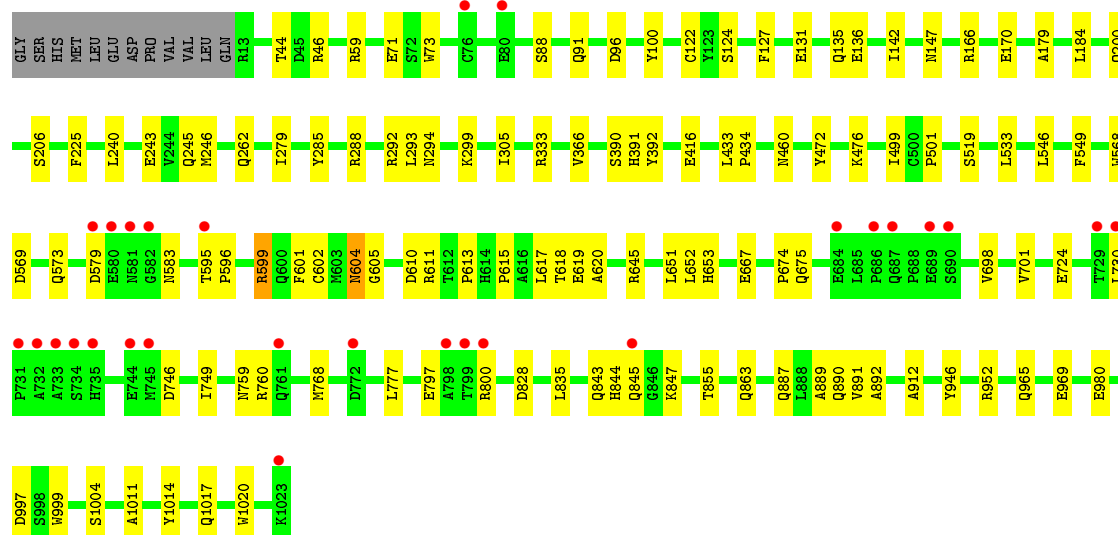
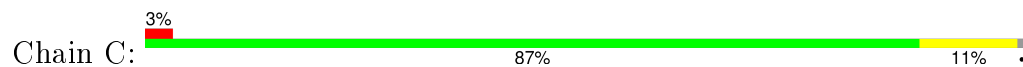
Chain A: 3% 86% 13%

GLY	SER	HIS	MET	LEU	GLU	ASP	PRO	VAL	LEU	GLN	ALA	ARG	THR	ILE	PHE	TYR																									
LYS	LEU	GLU	ASP	PRO	VAL	LEU	GLN	ALA	ARG	THR	ILE	PHE	TYR	LYS	LEU	GLU	ASP	PRO	VAL	LEU	GLN	ALA	ARG	THR	ILE	PHE	TYR	LYS	LEU	GLU	ASP	PRO	VAL	LEU	GLN	ALA	ARG	THR	ILE	PHE	TYR
LYS	LEU	GLU	ASP	PRO	VAL	LEU	GLN	ALA	ARG	THR	ILE	PHE	TYR	LYS	LEU	GLU	ASP	PRO	VAL	LEU	GLN	ALA	ARG	THR	ILE	PHE	TYR	LYS	LEU	GLU	ASP	PRO	VAL	LEU	GLN	ALA	ARG	THR	ILE	PHE	TYR
LYS	LEU	GLU	ASP	PRO	VAL	LEU	GLN	ALA	ARG	THR	ILE	PHE	TYR	LYS	LEU	GLU	ASP	PRO	VAL	LEU	GLN	ALA	ARG	THR	ILE	PHE	TYR	LYS	LEU	GLU	ASP	PRO	VAL	LEU	GLN	ALA	ARG	THR	ILE	PHE	TYR
LYS	LEU	GLU	ASP	PRO	VAL	LEU	GLN	ALA	ARG	THR	ILE	PHE	TYR	LYS	LEU	GLU	ASP	PRO	VAL	LEU	GLN	ALA	ARG	THR	ILE	PHE	TYR	LYS	LEU	GLU	ASP	PRO	VAL	LEU	GLN	ALA	ARG	THR	ILE	PHE	TYR
LYS	LEU	GLU	ASP	PRO	VAL	LEU	GLN	ALA	ARG	THR	ILE	PHE	TYR	LYS	LEU	GLU	ASP	PRO	VAL	LEU	GLN	ALA	ARG	THR	ILE	PHE	TYR	LYS	LEU	GLU	ASP	PRO	VAL	LEU	GLN	ALA	ARG	THR	ILE	PHE	TYR

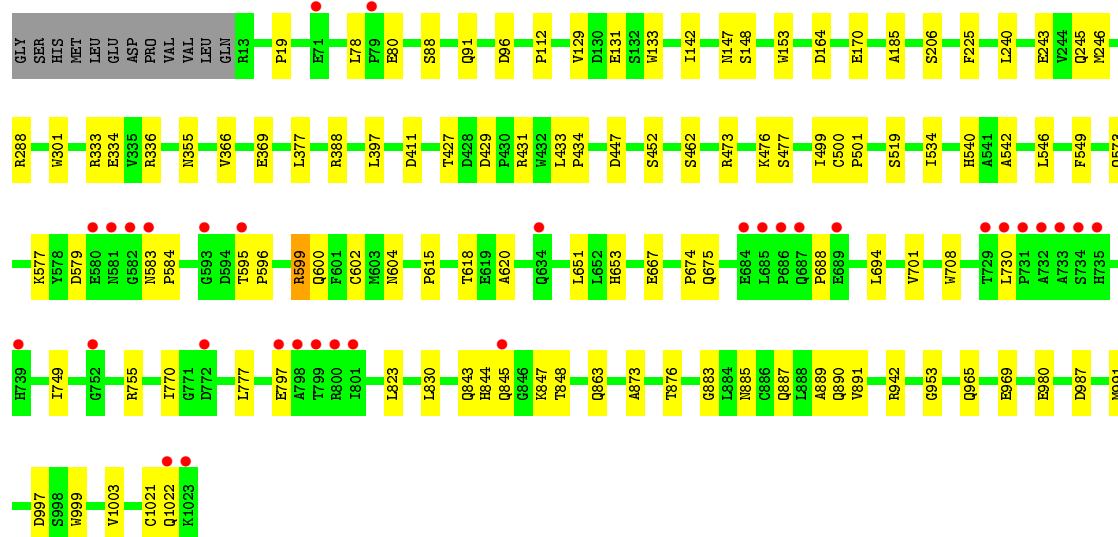
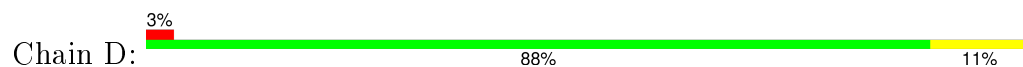
Chain B:



• 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	149.70Å 168.42Å 200.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.70 – 2.10 17.71 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (17.70-2.10) 99.9 (17.71-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.11Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.182 , 0.221 0.180 , 0.218	Depositor DCC
R_{free} test set	4227 reflections (1.44%)	DCC
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	4 of 293082 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36653	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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 36.21 % 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 5.1731e-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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, DMS

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	0.31	0/8364	0.62	0/11412
1	B	0.32	0/8355	0.62	0/11401
1	C	0.32	0/8364	0.62	0/11412
1	D	0.31	0/8364	0.62	0/11412
All	All	0.32	0/33447	0.62	0/45637

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	8122	0	7712	85	0
1	B	8113	0	7699	78	0
1	C	8122	0	7712	78	0
1	D	8122	0	7712	66	0
2	A	5	0	0	0	0
2	B	3	0	0	0	0
2	C	4	0	0	0	0
2	D	3	0	0	0	0
3	A	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	128	0	192	6	0
4	B	136	0	204	2	0
4	C	132	0	198	1	0
4	D	136	0	204	0	0
5	A	941	0	0	3	0
5	B	944	0	0	4	0
5	C	870	0	0	2	0
5	D	856	0	0	2	0
All	All	36653	0	31633	300	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 5.

All (300) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:GLN:HE21	1:C:299:LYS:HD3	1.35	0.91
1:B:245:GLN:HG2	1:B:288:ARG:HG2	1.63	0.81
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.63	0.81
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.62	0.81
1:C:262:GLN:NE2	1:C:299:LYS:HD3	1.95	0.81
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.66	0.77
1:C:142:ILE:HG12	1:C:170:GLU:HG2	1.72	0.72
1:D:153:TRP:HB2	1:D:185:ALA:HB3	1.73	0.71
1:D:599:ARG:HH21	1:D:797:GLU:HG3	1.58	0.69
1:C:579:ASP:OD2	1:C:583:ASN:HB2	1.95	0.66
1:D:651:LEU:HD12	1:D:651:LEU:O	1.96	0.66
1:C:88:SER:HA	1:C:366:VAL:HG21	1.77	0.66
1:D:615:PRO:O	1:D:618:THR:HG22	1.97	0.65
1:A:245:GLN:HG2	1:A:288:ARG:HG2	1.79	0.65
1:C:965:GLN:O	1:C:969:GLU:HG3	1.97	0.65
1:D:770:ILE:HD13	1:D:1022:GLN:NE2	2.13	0.64
1:C:245:GLN:HG2	1:C:288:ARG:HG2	1.80	0.63
1:A:844:HIS:ND1	1:A:845:GLN:HG2	2.13	0.63
1:D:599:ARG:NH2	1:D:797:GLU:HG3	2.14	0.62
1:A:751:LEU:HD23	1:A:862:GLY:HA2	1.81	0.62
1:B:88:SER:HA	1:B:366:VAL:HG21	1.81	0.62
1:C:127:PHE:CE1	1:C:184:LEU:HG	2.35	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:890:GLN:HG2	1:B:891:VAL:N	2.14	0.62
1:D:965:GLN:O	1:D:969:GLU:HG3	1.99	0.62
1:A:749:ILE:N	1:A:749:ILE:HD12	2.15	0.62
1:D:88:SER:HA	1:D:366:VAL:HG21	1.82	0.62
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.15	0.61
1:B:473:ARG:NH1	1:B:477:SER:HB2	2.16	0.61
1:A:579:ASP:OD2	1:A:583:ASN:HB2	2.00	0.61
1:C:777:LEU:HG	1:C:889:ALA:HA	1.83	0.60
1:A:304:GLU:HA	5:A:7340:HOH:O	2.02	0.60
1:B:730:LEU:HD12	1:B:730:LEU:N	2.18	0.59
1:A:277:GLU:H	1:A:277:GLU:CD	2.06	0.59
1:D:579:ASP:OD2	1:D:583:ASN:HB2	2.03	0.59
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.01	0.59
1:D:883:GLY:HA3	1:D:987:ASP:HA	1.85	0.58
1:B:131:GLU:OE1	1:B:179:ALA:HB2	2.03	0.58
1:D:245:GLN:HG2	1:D:288:ARG:HG2	1.86	0.58
1:A:615:PRO:O	1:A:618:THR:HG22	2.03	0.58
1:C:599:ARG:HH21	1:C:797:GLU:CG	2.16	0.58
1:B:165:SER:HB2	5:B:7231:HOH:O	2.04	0.58
1:D:129:VAL:HG12	1:D:133:TRP:HB2	1.86	0.57
1:B:651:LEU:HD12	1:B:651:LEU:C	2.24	0.57
1:C:730:LEU:HD21	1:D:823:LEU:O	2.05	0.57
1:B:651:LEU:HD11	1:B:653:HIS:NE2	2.20	0.57
1:A:131:GLU:O	1:A:135:GLN:HG2	2.05	0.57
1:D:749:ILE:N	1:D:749:ILE:HD12	2.21	0.56
1:B:473:ARG:HH12	1:B:477:SER:HB2	1.71	0.56
1:A:127:PHE:CE1	1:A:184:LEU:HG	2.40	0.56
1:A:91:GLN:HG3	1:A:96:ASP:OD1	2.06	0.56
1:B:890:GLN:HG2	1:B:891:VAL:H	1.72	0.55
1:A:730:LEU:HD21	1:B:823:LEU:O	2.05	0.55
1:A:830:LEU:HD22	1:B:828:ASP:HB3	1.87	0.55
1:A:887:GLN:NE2	1:A:980:GLU:O	2.36	0.55
1:B:653:HIS:ND1	1:B:667:GLU:HB3	2.22	0.55
1:A:578:TYR:CE1	1:A:584:PRO:HB3	2.41	0.55
1:C:615:PRO:O	1:C:618:THR:HG22	2.05	0.55
1:B:749:ILE:N	1:B:749:ILE:HD12	2.22	0.55
1:B:59:ARG:HB2	1:B:124:SER:OG	2.07	0.55
1:B:777:LEU:HG	1:B:889:ALA:HA	1.87	0.54
1:A:88:SER:HA	1:A:366:VAL:HG21	1.89	0.54
1:A:965:GLN:O	1:A:969:GLU:HG3	2.06	0.54
1:C:294:ASN:H	4:C:8604:DMS:H21	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:ARG:HH21	1:B:797:GLU:CG	2.21	0.54
1:C:749:ILE:HD12	1:C:749:ILE:N	2.23	0.53
1:A:13:ARG:HG2	1:A:13:ARG:O	2.08	0.53
1:D:997:ASP:HB2	1:D:999:TRP:CZ2	2.43	0.53
1:B:595:THR:HA	1:B:596:PRO:C	2.29	0.53
1:A:581:ASN:HB2	1:A:583:ASN:ND2	2.24	0.53
1:C:613:PRO:HB3	1:C:617:LEU:HD23	1.91	0.53
1:A:833:ALA:HB1	1:A:858:ILE:O	2.08	0.53
1:D:129:VAL:CG1	1:D:133:TRP:HB2	2.39	0.53
1:B:844:HIS:O	1:B:847:LYS:HB3	2.09	0.52
1:A:873:ALA:O	1:A:876:THR:HG22	2.08	0.52
1:B:973:ARG:HH22	4:B:8609:DMS:H21	1.75	0.52
1:A:595:THR:HA	1:A:596:PRO:C	2.30	0.52
1:C:136:GLU:HG3	5:C:4754:HOH:O	2.10	0.52
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.08	0.52
1:C:131:GLU:HG3	1:C:135:GLN:HG3	1.90	0.52
1:C:293:LEU:N	1:C:293:LEU:HD12	2.25	0.52
1:B:599:ARG:NH2	1:B:797:GLU:HG2	2.24	0.52
1:B:127:PHE:HE1	1:B:184:LEU:HG	1.74	0.52
1:C:651:LEU:C	1:C:651:LEU:HD12	2.30	0.52
1:C:651:LEU:HD11	1:C:653:HIS:NE2	2.25	0.52
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.92	0.52
1:B:610:ASP:O	1:B:611:ARG:HB2	2.08	0.51
1:A:844:HIS:CE1	1:A:845:GLN:HG2	2.45	0.51
1:C:416:GLU:HG3	1:C:460:ASN:O	2.10	0.51
1:B:651:LEU:HD11	1:B:653:HIS:CE1	2.46	0.51
1:C:127:PHE:HE1	1:C:184:LEU:HG	1.75	0.51
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.92	0.51
1:B:1011:ALA:HB3	1:B:1014:TYR:CZ	2.46	0.51
1:B:127:PHE:CE1	1:B:184:LEU:HG	2.45	0.51
1:C:147:ASN:HB3	1:C:206:SER:HA	1.92	0.51
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.91	0.51
1:D:653:HIS:HD2	1:D:667:GLU:HB3	1.76	0.51
1:C:653:HIS:HD2	1:C:701:VAL:HG21	1.76	0.51
1:A:599:ARG:HH21	1:A:797:GLU:CG	2.23	0.50
1:C:844:HIS:ND1	1:C:845:GLN:HG2	2.25	0.50
1:C:843:GLN:HA	1:C:847:LYS:O	2.12	0.50
1:D:991:MET:HE2	1:D:1003:VAL:HG21	1.92	0.50
1:A:755:ARG:HB2	1:A:769:TRP:HB2	1.93	0.50
1:D:91:GLN:HG3	1:D:96:ASP:OD1	2.11	0.50
1:C:240:LEU:HD23	1:C:240:LEU:C	2.32	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:800:ARG:HG2	1:C:800:ARG:HH11	1.77	0.50
1:B:674:PRO:O	1:B:675:GLN:HB2	2.12	0.50
1:D:653:HIS:CD2	1:D:667:GLU:HB3	2.47	0.50
1:A:322:LEU:HB2	4:A:8406:DMS:C1	2.41	0.50
1:D:863:GLN:HG2	1:D:1021:CYS:HB3	1.93	0.49
1:A:653:HIS:ND1	1:A:667:GLU:HB3	2.27	0.49
1:C:73:TRP:CE2	1:C:122:CYS:HB3	2.47	0.49
1:D:147:ASN:HB3	1:D:206:SER:HA	1.93	0.49
1:D:577:LYS:O	1:D:584:PRO:HA	2.12	0.49
1:B:542:ALA:HA	1:B:604:ASN:HA	1.94	0.49
1:B:245:GLN:HG2	1:B:288:ARG:CG	2.40	0.49
1:B:369:GLU:HA	1:B:372:MET:HE3	1.95	0.49
1:B:372:MET:HE3	1:B:397:LEU:HD23	1.94	0.49
1:A:651:LEU:O	1:A:651:LEU:HD12	2.13	0.49
1:C:730:LEU:N	1:C:730:LEU:HD12	2.28	0.48
1:A:863:GLN:HG2	1:A:1021:CYS:HB3	1.94	0.48
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.47	0.48
1:C:610:ASP:O	1:C:611:ARG:HB2	2.14	0.48
1:C:292:ARG:C	1:C:293:LEU:HD12	2.33	0.48
1:D:890:GLN:HG2	1:D:891:VAL:N	2.29	0.48
1:D:240:LEU:HD23	1:D:240:LEU:C	2.35	0.47
1:A:883:GLY:HA3	1:A:987:ASP:HA	1.96	0.47
1:D:540:HIS:CE1	1:D:542:ALA:HB2	2.50	0.47
1:D:369:GLU:HG3	1:D:397:LEU:HD21	1.95	0.47
1:A:59:ARG:HB2	1:A:124:SER:OG	2.13	0.47
1:C:279:ILE:HD12	1:C:285:TYR:CD2	2.49	0.47
1:A:730:LEU:HD12	1:A:730:LEU:N	2.30	0.47
1:B:651:LEU:HD11	1:B:653:HIS:CD2	2.49	0.47
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.96	0.47
1:D:730:LEU:N	1:D:730:LEU:HD12	2.29	0.47
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.50	0.47
1:A:499:ILE:HG22	1:A:501:PRO:HD3	1.96	0.47
1:B:873:ALA:O	1:B:876:THR:HG22	2.15	0.47
1:B:892:ALA:HB3	1:B:946:TYR:CE1	2.50	0.47
1:B:751:LEU:HD23	1:B:862:GLY:HA2	1.97	0.47
1:C:599:ARG:HH21	1:C:797:GLU:CD	2.18	0.47
1:D:595:THR:HA	1:D:596:PRO:C	2.35	0.47
1:D:433:LEU:HB3	1:D:434:PRO:HD3	1.96	0.47
1:A:105:TYR:CE1	1:A:199:ASP:HB2	2.50	0.47
1:C:200:GLN:HG2	1:C:391:HIS:HB2	1.97	0.47
1:B:599:ARG:NH2	1:B:797:GLU:CG	2.78	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:TRP:HB2	1:A:185:ALA:HB3	1.96	0.46
1:A:292:ARG:HH12	4:A:8412:DMS:H13	1.80	0.46
1:C:599:ARG:NH2	1:C:797:GLU:CG	2.78	0.46
1:A:240:LEU:C	1:A:240:LEU:HD23	2.35	0.46
1:A:427:THR:HG21	1:A:462:SER:HB3	1.96	0.46
1:C:568:TRP:HE1	1:C:604:ASN:ND2	2.14	0.46
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.96	0.46
1:C:569:ASP:O	1:C:605:GLY:HA2	2.15	0.46
1:B:390:SER:HA	1:B:391:HIS:HA	1.78	0.46
1:A:688:PRO:HD2	5:A:6031:HOH:O	2.16	0.46
1:D:301:TRP:CH2	1:D:452:SER:HA	2.50	0.46
1:C:828:ASP:HB3	1:D:830:LEU:HD22	1.98	0.46
1:A:610:ASP:O	1:A:611:ARG:HB2	2.16	0.46
1:A:619:GLU:HA	1:A:912:ALA:HB2	1.98	0.46
1:A:390:SER:HA	1:A:391:HIS:HA	1.78	0.46
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.98	0.46
1:A:651:LEU:C	1:A:651:LEU:HD12	2.35	0.46
1:A:223:SER:O	1:A:224:ASP:HB2	2.16	0.46
1:C:59:ARG:HB2	1:C:124:SER:OG	2.16	0.46
1:A:599:ARG:NH2	1:A:797:GLU:HG2	2.31	0.46
1:C:44:THR:OG1	1:C:46:ARG:HD3	2.16	0.46
1:D:688:PRO:HD3	1:D:694:LEU:HD11	1.98	0.46
1:C:768:MET:HE1	1:C:1020:TRP:CH2	2.51	0.46
1:D:887:GLN:NE2	1:D:980:GLU:O	2.46	0.46
1:B:476:LYS:HA	5:B:4204:HOH:O	2.16	0.46
1:C:651:LEU:HD11	1:C:653:HIS:CD2	2.51	0.45
1:D:844:HIS:CE1	1:D:845:GLN:HG2	2.51	0.45
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.98	0.45
1:B:965:GLN:O	1:B:969:GLU:HG3	2.15	0.45
1:C:844:HIS:CE1	1:C:845:GLN:HG2	2.51	0.45
1:C:746:ASP:OD1	1:C:759:ASN:HA	2.16	0.45
1:B:599:ARG:HH21	1:B:797:GLU:CD	2.20	0.45
1:C:653:HIS:ND1	1:C:667:GLU:HB3	2.31	0.45
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.52	0.45
1:C:91:GLN:HG3	1:C:96:ASP:OD1	2.16	0.45
1:A:773:LYS:HE2	1:A:774:LYS:O	2.16	0.45
1:B:100:TYR:CZ	1:B:602:CYS:HB3	2.52	0.45
1:D:473:ARG:NH1	1:D:477:SER:HB2	2.32	0.45
1:C:1017:GLN:HB2	5:C:6159:HOH:O	2.16	0.45
1:A:714:ILE:HD13	4:A:8603:DMS:H13	1.99	0.45
1:A:54:LEU:HD11	1:A:214:LEU:HG	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:991:MET:CE	1:D:1003:VAL:HG21	2.45	0.45
1:B:52:ARG:O	1:B:213:SER:HB2	2.17	0.45
1:C:835:LEU:HD11	1:C:855:THR:HB	1.98	0.45
1:D:225:PHE:HA	1:D:243:GLU:O	2.17	0.44
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.17	0.44
1:A:292:ARG:HH12	4:A:8412:DMS:C1	2.30	0.44
1:C:863:GLN:OE1	1:C:952:ARG:NH2	2.51	0.44
1:C:131:GLU:OE1	1:C:179:ALA:HB2	2.17	0.44
1:B:653:HIS:HD2	1:B:701:VAL:HG21	1.82	0.44
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.53	0.44
1:C:279:ILE:HD12	1:C:285:TYR:CE2	2.53	0.44
1:D:873:ALA:O	1:D:876:THR:HG22	2.18	0.44
1:C:652:LEU:HD11	1:C:698:VAL:HB	2.00	0.44
1:C:433:LEU:HB3	1:C:434:PRO:HD3	2.00	0.44
1:B:40:GLU:OE2	1:B:43:ARG:NH2	2.46	0.44
1:A:764:PHE:CE2	1:A:781:ARG:NH2	2.86	0.44
1:D:19:PRO:HD3	1:D:112:PRO:CB	2.48	0.44
1:C:892:ALA:HB3	1:C:946:TYR:CE1	2.52	0.44
1:C:595:THR:HA	1:C:596:PRO:C	2.38	0.43
1:A:433:LEU:HB3	1:A:434:PRO:HD3	2.00	0.43
1:B:128:ASN:HA	1:B:180:GLY:O	2.18	0.43
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.47	0.43
1:C:499:ILE:HG22	1:C:501:PRO:HD3	2.00	0.43
1:A:19:PRO:HD3	1:A:112:PRO:CB	2.49	0.43
1:D:942:ARG:HA	1:D:953:GLY:O	2.18	0.43
1:A:561:ARG:HD3	1:B:525:SER:O	2.19	0.43
1:D:429:ASP:OD1	1:D:431:ARG:HG3	2.19	0.43
1:B:896:ASN:HB3	1:B:945:ASN:HB2	2.00	0.43
1:B:499:ILE:HG22	1:B:501:PRO:HD3	2.00	0.43
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.99	0.43
1:B:764:PHE:CE2	1:B:781:ARG:NH2	2.87	0.43
1:D:843:GLN:HA	1:D:847:LYS:O	2.18	0.43
1:A:100:TYR:CZ	1:A:602:CYS:HB3	2.53	0.43
1:C:599:ARG:NH1	1:C:601:PHE:CZ	2.87	0.43
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.36	0.43
1:C:166:ARG:HG3	1:C:392:TYR:HB2	2.01	0.43
1:B:753:ASN:OD1	1:B:771:GLY:HA2	2.18	0.43
1:A:701:VAL:O	1:A:703:PRO:HD3	2.18	0.43
1:C:568:TRP:NE1	1:C:604:ASN:ND2	2.67	0.43
1:B:147:ASN:HA	1:B:148:SER:HA	1.60	0.43
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:ALA:HB2	1:A:859:ASP:HA	2.01	0.42
1:D:147:ASN:HA	1:D:148:SER:HA	1.58	0.42
1:D:843:GLN:HG2	1:D:848:THR:HA	2.01	0.42
1:B:997:ASP:HB2	1:B:999:TRP:CZ2	2.54	0.42
1:C:887:GLN:NE2	1:C:980:GLU:O	2.52	0.42
1:B:619:GLU:HA	1:B:912:ALA:HB2	2.01	0.42
1:A:599:ARG:HH21	1:A:797:GLU:HG2	1.84	0.42
1:C:724:GLU:O	1:D:847:LYS:NZ	2.52	0.42
1:A:688:PRO:HD3	1:A:694:LEU:HD11	2.01	0.42
1:D:599:ARG:HB2	1:D:600:GLN:H	1.64	0.42
1:C:573:GLN:HB2	1:C:602:CYS:O	2.19	0.42
1:B:352:ARG:HG2	1:B:553:TRP:CH2	2.54	0.42
1:B:105:TYR:CE1	1:B:199:ASP:HB2	2.55	0.42
1:B:549:PHE:CE2	1:B:620:ALA:HA	2.54	0.42
1:A:823:LEU:HD11	1:A:841:ALA:HB2	2.02	0.42
1:A:687:GLN:H	1:A:687:GLN:CD	2.22	0.42
1:C:225:PHE:HA	1:C:243:GLU:O	2.19	0.42
1:C:890:GLN:HG2	1:C:891:VAL:N	2.34	0.42
1:C:533:LEU:C	1:C:533:LEU:HD23	2.40	0.42
1:D:476:LYS:HD2	5:D:4204:HOH:O	2.19	0.42
1:D:651:LEU:HD12	1:D:651:LEU:C	2.40	0.42
1:A:892:ALA:HB3	1:A:946:TYR:CE1	2.55	0.42
1:B:615:PRO:O	1:B:618:THR:HG22	2.20	0.42
1:C:246:MET:C	1:C:246:MET:SD	2.98	0.42
1:B:973:ARG:HH22	4:B:8609:DMS:C2	2.32	0.42
1:A:991:MET:CE	1:A:1003:VAL:HG21	2.50	0.42
1:D:246:MET:SD	1:D:246:MET:C	2.99	0.42
1:B:756:TRP:CD2	1:B:858:ILE:HD13	2.55	0.42
1:D:755:ARG:HH11	1:D:755:ARG:HG3	1.85	0.42
1:B:240:LEU:HD23	1:B:240:LEU:C	2.39	0.42
1:B:755:ARG:HD3	5:B:7161:HOH:O	2.19	0.42
1:B:606:LEU:O	1:B:614:HIS:HB2	2.20	0.41
1:B:78:LEU:HD23	5:B:4504:HOH:O	2.20	0.41
1:B:651:LEU:HD23	1:B:703:PRO:HG3	2.02	0.41
1:C:100:TYR:CZ	1:C:602:CYS:HB3	2.56	0.41
1:B:755:ARG:HB2	1:B:769:TRP:HB2	2.01	0.41
1:B:570:TRP:O	1:B:607:VAL:HG22	2.20	0.41
1:B:1013:ARG:HG3	1:B:1013:ARG:HH11	1.85	0.41
1:C:619:GLU:HA	1:C:912:ALA:HB2	2.01	0.41
1:D:777:LEU:HG	1:D:889:ALA:HA	2.01	0.41
1:A:660:GLY:O	1:A:662:PRO:HD3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:LEU:HD21	1:A:986:ILE:HD11	2.02	0.41
1:A:168:PRO:O	1:A:442:ARG:NH2	2.53	0.41
1:A:352:ARG:HG2	1:A:553:TRP:CH2	2.56	0.41
1:A:746:ASP:OD1	1:A:759:ASN:HA	2.20	0.41
1:D:651:LEU:CD1	1:D:701:VAL:HB	2.51	0.41
1:A:369:GLU:HG3	1:A:397:LEU:HD21	2.02	0.41
1:D:427:THR:HG21	1:D:462:SER:HB3	2.01	0.41
1:B:656:VAL:HG21	1:B:685:LEU:HD13	2.03	0.41
1:A:127:PHE:CE2	1:A:214:LEU:HD11	2.55	0.41
1:C:390:SER:HA	1:C:391:HIS:HA	1.80	0.41
1:A:279:ILE:HD12	1:A:285:TYR:CD2	2.56	0.41
1:A:843:GLN:HA	1:A:847:LYS:O	2.20	0.41
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.56	0.41
1:A:724:GLU:O	1:B:847:LYS:NZ	2.53	0.41
1:C:844:HIS:O	1:C:847:LYS:HB3	2.21	0.41
1:A:100:TYR:CE1	1:A:602:CYS:HB3	2.56	0.41
1:B:754:LYS:HE3	1:B:1022:GLN:HG3	2.03	0.41
1:A:322:LEU:HB2	4:A:8406:DMS:H12	2.02	0.41
1:D:674:PRO:O	1:D:675:GLN:HB2	2.21	0.41
1:A:754:LYS:HE2	5:A:4766:HOH:O	2.21	0.41
1:A:533:LEU:C	1:A:533:LEU:HD23	2.41	0.41
1:A:143:PHE:O	1:A:168:PRO:HA	2.21	0.40
1:D:500:CYS:HA	1:D:534:ILE:O	2.21	0.40
1:C:674:PRO:O	1:C:675:GLN:HB2	2.21	0.40
1:A:277:GLU:N	1:A:277:GLU:CD	2.74	0.40
1:C:997:ASP:HB2	1:C:999:TRP:CZ2	2.56	0.40
1:C:472:TYR:O	1:C:476:LYS:HG2	2.21	0.40
1:A:322:LEU:HB2	4:A:8406:DMS:H13	2.02	0.40
1:A:333:ARG:HA	1:A:345:ASN:OD1	2.21	0.40
1:D:78:LEU:HD23	5:D:4504:HOH:O	2.20	0.40
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.39	0.40
1:D:573:GLN:HB2	1:D:602:CYS:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1009/1023 (99%)	970 (96%)	38 (4%)	1 (0%)	56	58
1	B	1008/1023 (98%)	969 (96%)	38 (4%)	1 (0%)	56	58
1	C	1009/1023 (99%)	968 (96%)	40 (4%)	1 (0%)	56	58
1	D	1009/1023 (99%)	961 (95%)	46 (5%)	2 (0%)	52	53
All	All	4035/4092 (99%)	3868 (96%)	162 (4%)	5 (0%)	56	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	599	ARG
1	A	599	ARG
1	B	599	ARG
1	C	599	ARG
1	D	164	ASP

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	863/874 (99%)	857 (99%)	6 (1%)	88	92
1	B	862/874 (99%)	855 (99%)	7 (1%)	86	91
1	C	863/874 (99%)	857 (99%)	6 (1%)	88	92
1	D	863/874 (99%)	856 (99%)	7 (1%)	86	91
All	All	3451/3496 (99%)	3425 (99%)	26 (1%)	86	91

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	333	ARG
1	A	519	SER
1	A	546	LEU
1	A	604	ASN
1	A	885	ASN
1	B	136	GLU
1	B	333	ARG
1	B	519	SER
1	B	546	LEU
1	B	604	ASN
1	B	768	MET
1	B	885	ASN
1	C	71	GLU
1	C	333	ARG
1	C	519	SER
1	C	546	LEU
1	C	604	ASN
1	C	1004	SER
1	D	80	GLU
1	D	131	GLU
1	D	333	ARG
1	D	519	SER
1	D	546	LEU
1	D	604	ASN
1	D	885	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	GLN
1	A	583	ASN
1	A	757	GLN
1	A	1022	GLN
1	B	554	GLN
1	B	583	ASN
1	B	804	ASN
1	B	863	GLN
1	C	163	GLN
1	D	163	GLN
1	D	583	ASN
1	D	653	HIS
1	D	757	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	804	ASN
1	D	1022	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 164 ligands modelled in this entry, 31 are monoatomic - leaving 133 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	$\# Z > 2$
4	DMS	A	8401	-	3,3,3	0.21	0	3,3,3	0.57	0
4	DMS	A	8402	-	3,3,3	0.22	0	3,3,3	0.53	0
4	DMS	A	8403	-	3,3,3	0.21	0	3,3,3	0.58	0
4	DMS	A	8404	-	3,3,3	0.20	0	3,3,3	0.58	0
4	DMS	A	8405	-	3,3,3	0.23	0	3,3,3	0.56	0
4	DMS	A	8406	-	3,3,3	0.20	0	3,3,3	0.48	0
4	DMS	A	8407	-	3,3,3	0.21	0	3,3,3	0.57	0
4	DMS	A	8408	-	3,3,3	0.23	0	3,3,3	0.61	0
4	DMS	A	8409	-	3,3,3	0.22	0	3,3,3	0.57	0
4	DMS	A	8410	-	3,3,3	0.25	0	3,3,3	0.58	0
4	DMS	A	8411	-	3,3,3	0.24	0	3,3,3	0.58	0
4	DMS	A	8412	-	3,3,3	0.22	0	3,3,3	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	A	8413	-	3,3,3	0.22	0	3,3,3	0.58	0
4	DMS	A	8414	-	3,3,3	0.23	0	3,3,3	0.57	0
4	DMS	A	8419	-	3,3,3	0.24	0	3,3,3	0.58	0
4	DMS	A	8420	-	3,3,3	0.22	0	3,3,3	0.59	0
4	DMS	A	8421	-	3,3,3	0.23	0	3,3,3	0.58	0
4	DMS	A	8425	3	3,3,3	0.21	0	3,3,3	0.57	0
4	DMS	A	8427	-	3,3,3	0.23	0	3,3,3	0.61	0
4	DMS	A	8501	-	3,3,3	0.19	0	3,3,3	0.58	0
4	DMS	A	8502	-	3,3,3	0.24	0	3,3,3	0.55	0
4	DMS	A	8503	-	3,3,3	0.25	0	3,3,3	0.57	0
4	DMS	A	8504	-	3,3,3	0.23	0	3,3,3	0.56	0
4	DMS	A	8602	-	3,3,3	0.22	0	3,3,3	0.59	0
4	DMS	A	8603	-	3,3,3	0.24	0	3,3,3	0.58	0
4	DMS	A	8604	-	3,3,3	0.24	0	3,3,3	0.58	0
4	DMS	A	8605	-	3,3,3	0.23	0	3,3,3	0.54	0
4	DMS	A	8607	-	3,3,3	0.23	0	3,3,3	0.59	0
4	DMS	A	8608	-	3,3,3	0.21	0	3,3,3	0.60	0
4	DMS	A	8609	-	3,3,3	0.24	0	3,3,3	0.60	0
4	DMS	A	8610	-	3,3,3	0.24	0	3,3,3	0.58	0
4	DMS	A	8612	-	3,3,3	0.21	0	3,3,3	0.60	0
4	DMS	B	8401	-	3,3,3	0.23	0	3,3,3	0.60	0
4	DMS	B	8402	-	3,3,3	0.18	0	3,3,3	0.52	0
4	DMS	B	8403	-	3,3,3	0.22	0	3,3,3	0.60	0
4	DMS	B	8404	-	3,3,3	0.19	0	3,3,3	0.57	0
4	DMS	B	8405	-	3,3,3	0.23	0	3,3,3	0.55	0
4	DMS	B	8406	-	3,3,3	0.26	0	3,3,3	0.58	0
4	DMS	B	8407	-	3,3,3	0.23	0	3,3,3	0.59	0
4	DMS	B	8408	-	3,3,3	0.24	0	3,3,3	0.60	0
4	DMS	B	8409	-	3,3,3	0.22	0	3,3,3	0.58	0
4	DMS	B	8410	-	3,3,3	0.20	0	3,3,3	0.57	0
4	DMS	B	8411	-	3,3,3	0.27	0	3,3,3	0.59	0
4	DMS	B	8412	-	3,3,3	0.22	0	3,3,3	0.57	0
4	DMS	B	8413	-	3,3,3	0.21	0	3,3,3	0.57	0
4	DMS	B	8414	-	3,3,3	0.23	0	3,3,3	0.57	0
4	DMS	B	8415	-	3,3,3	0.22	0	3,3,3	0.58	0
4	DMS	B	8416	-	3,3,3	0.22	0	3,3,3	0.58	0
4	DMS	B	8417	-	3,3,3	0.23	0	3,3,3	0.60	0
4	DMS	B	8421	-	3,3,3	0.24	0	3,3,3	0.58	0
4	DMS	B	8423	-	3,3,3	0.23	0	3,3,3	0.56	0
4	DMS	B	8425	3	3,3,3	0.25	0	3,3,3	0.59	0
4	DMS	B	8427	-	3,3,3	0.22	0	3,3,3	0.59	0
4	DMS	B	8502	-	3,3,3	0.26	0	3,3,3	0.62	0
4	DMS	B	8504	-	3,3,3	0.22	0	3,3,3	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	B	8508	-	3,3,3	0.24	0	3,3,3	0.61	0
4	DMS	B	8601	-	3,3,3	0.24	0	3,3,3	0.58	0
4	DMS	B	8602	-	3,3,3	0.22	0	3,3,3	0.59	0
4	DMS	B	8603	-	3,3,3	0.15	0	3,3,3	0.61	0
4	DMS	B	8604	-	3,3,3	0.24	0	3,3,3	0.61	0
4	DMS	B	8605	-	3,3,3	0.21	0	3,3,3	0.60	0
4	DMS	B	8606	-	3,3,3	0.24	0	3,3,3	0.57	0
4	DMS	B	8607	-	3,3,3	0.22	0	3,3,3	0.58	0
4	DMS	B	8608	-	3,3,3	0.21	0	3,3,3	0.57	0
4	DMS	B	8609	-	3,3,3	0.20	0	3,3,3	0.59	0
4	DMS	B	8610	-	3,3,3	0.19	0	3,3,3	0.60	0
4	DMS	C	1024	-	3,3,3	0.20	0	3,3,3	0.56	0
4	DMS	C	8401	-	3,3,3	0.20	0	3,3,3	0.62	0
4	DMS	C	8402	-	3,3,3	0.20	0	3,3,3	0.54	0
4	DMS	C	8403	-	3,3,3	0.23	0	3,3,3	0.58	0
4	DMS	C	8404	-	3,3,3	0.21	0	3,3,3	0.58	0
4	DMS	C	8405	-	3,3,3	0.20	0	3,3,3	0.57	0
4	DMS	C	8407	-	3,3,3	0.23	0	3,3,3	0.57	0
4	DMS	C	8408	-	3,3,3	0.23	0	3,3,3	0.58	0
4	DMS	C	8409	-	3,3,3	0.21	0	3,3,3	0.58	0
4	DMS	C	8410	-	3,3,3	0.25	0	3,3,3	0.57	0
4	DMS	C	8411	-	3,3,3	0.24	0	3,3,3	0.58	0
4	DMS	C	8412	-	3,3,3	0.23	0	3,3,3	0.58	0
4	DMS	C	8413	-	3,3,3	0.22	0	3,3,3	0.58	0
4	DMS	C	8414	-	3,3,3	0.20	0	3,3,3	0.57	0
4	DMS	C	8415	-	3,3,3	0.22	0	3,3,3	0.59	0
4	DMS	C	8416	-	3,3,3	0.22	0	3,3,3	0.59	0
4	DMS	C	8417	-	3,3,3	0.23	0	3,3,3	0.59	0
4	DMS	C	8419	-	3,3,3	0.24	0	3,3,3	0.59	0
4	DMS	C	8420	-	3,3,3	0.21	0	3,3,3	0.56	0
4	DMS	C	8421	-	3,3,3	0.23	0	3,3,3	0.58	0
4	DMS	C	8423	-	3,3,3	0.22	0	3,3,3	0.56	0
4	DMS	C	8425	3	3,3,3	0.24	0	3,3,3	0.57	0
4	DMS	C	8427	-	3,3,3	0.20	0	3,3,3	0.58	0
4	DMS	C	8501	-	3,3,3	0.18	0	3,3,3	0.57	0
4	DMS	C	8503	-	3,3,3	0.23	0	3,3,3	0.57	0
4	DMS	C	8504	-	3,3,3	0.21	0	3,3,3	0.58	0
4	DMS	C	8601	-	3,3,3	0.24	0	3,3,3	0.56	0
4	DMS	C	8602	-	3,3,3	0.22	0	3,3,3	0.58	0
4	DMS	C	8603	-	3,3,3	0.25	0	3,3,3	0.57	0
4	DMS	C	8604	-	3,3,3	0.20	0	3,3,3	0.57	0
4	DMS	C	8605	-	3,3,3	0.21	0	3,3,3	0.55	0
4	DMS	C	8606	-	3,3,3	0.18	0	3,3,3	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	C	8607	-	3,3,3	0.20	0	3,3,3	0.59	0
4	DMS	D	8401	-	3,3,3	0.22	0	3,3,3	0.59	0
4	DMS	D	8402	-	3,3,3	0.17	0	3,3,3	0.54	0
4	DMS	D	8403	-	3,3,3	0.20	0	3,3,3	0.58	0
4	DMS	D	8404	-	3,3,3	0.21	0	3,3,3	0.59	0
4	DMS	D	8405	-	3,3,3	0.23	0	3,3,3	0.57	0
4	DMS	D	8406	-	3,3,3	0.26	0	3,3,3	0.58	0
4	DMS	D	8407	-	3,3,3	0.24	0	3,3,3	0.58	0
4	DMS	D	8408	-	3,3,3	0.27	0	3,3,3	0.60	0
4	DMS	D	8409	-	3,3,3	0.20	0	3,3,3	0.56	0
4	DMS	D	8410	-	3,3,3	0.23	0	3,3,3	0.57	0
4	DMS	D	8411	-	3,3,3	0.24	0	3,3,3	0.59	0
4	DMS	D	8412	-	3,3,3	0.23	0	3,3,3	0.57	0
4	DMS	D	8413	-	3,3,3	0.23	0	3,3,3	0.58	0
4	DMS	D	8414	-	3,3,3	0.22	0	3,3,3	0.57	0
4	DMS	D	8415	-	3,3,3	0.21	0	3,3,3	0.59	0
4	DMS	D	8416	-	3,3,3	0.21	0	3,3,3	0.58	0
4	DMS	D	8419	-	3,3,3	0.23	0	3,3,3	0.58	0
4	DMS	D	8421	-	3,3,3	0.24	0	3,3,3	0.58	0
4	DMS	D	8423	-	3,3,3	0.23	0	3,3,3	0.57	0
4	DMS	D	8425	3	3,3,3	0.26	0	3,3,3	0.59	0
4	DMS	D	8427	-	3,3,3	0.21	0	3,3,3	0.58	0
4	DMS	D	8501	-	3,3,3	0.23	0	3,3,3	0.59	0
4	DMS	D	8503	-	3,3,3	0.20	0	3,3,3	0.58	0
4	DMS	D	8508	-	3,3,3	0.22	0	3,3,3	0.60	0
4	DMS	D	8701	-	3,3,3	0.26	0	3,3,3	0.56	0
4	DMS	D	8703	-	3,3,3	0.22	0	3,3,3	0.56	0
4	DMS	D	8705	-	3,3,3	0.24	0	3,3,3	0.58	0
4	DMS	D	8706	-	3,3,3	0.25	0	3,3,3	0.60	0
4	DMS	D	8707	-	3,3,3	0.22	0	3,3,3	0.57	0
4	DMS	D	8708	-	3,3,3	0.22	0	3,3,3	0.59	0
4	DMS	D	8709	-	3,3,3	0.23	0	3,3,3	0.59	0
4	DMS	D	8710	-	3,3,3	0.23	0	3,3,3	0.58	0
4	DMS	D	8711	-	3,3,3	0.23	0	3,3,3	0.59	0
4	DMS	D	8712	-	3,3,3	0.20	0	3,3,3	0.58	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
4	DMS	A	8401	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DMS	A	8402	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8403	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8404	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8405	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8406	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8407	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8408	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8409	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8410	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8411	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8412	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8413	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8414	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8419	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8420	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8421	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8425	3	-	0/0/0/0	0/0/0/0
4	DMS	A	8427	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8501	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8502	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8503	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8504	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8602	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8603	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8604	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8605	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8607	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8608	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8609	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8610	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8612	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8401	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8402	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8403	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8404	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8405	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8406	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8407	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8408	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8409	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8410	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8411	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DMS	B	8412	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8413	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8414	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8415	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8416	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8417	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8421	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8423	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8425	3	-	0/0/0/0	0/0/0/0
4	DMS	B	8427	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8502	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8504	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8508	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8601	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8602	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8603	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8604	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8605	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8606	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8607	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8608	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8609	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8610	-	-	0/0/0/0	0/0/0/0
4	DMS	C	1024	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8401	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8402	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8403	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8404	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8405	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8407	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8408	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8409	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8410	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8411	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8412	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8413	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8414	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8415	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8416	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8417	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8419	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8420	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DMS	C	8421	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8423	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8425	3	-	0/0/0/0	0/0/0/0
4	DMS	C	8427	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8501	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8503	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8504	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8601	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8602	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8603	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8604	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8605	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8606	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8607	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8401	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8402	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8403	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8404	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8405	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8406	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8407	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8408	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8409	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8410	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8411	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8412	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8413	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8414	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8415	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8416	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8419	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8421	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8423	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8425	3	-	0/0/0/0	0/0/0/0
4	DMS	D	8427	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8501	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8503	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8508	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8701	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8703	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8705	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8706	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DMS	D	8707	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8708	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8709	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8710	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8711	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8712	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	8406	DMS	3	0
4	A	8412	DMS	2	0
4	A	8603	DMS	1	0
4	B	8609	DMS	2	0
4	C	8604	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%)	-0.27	31 (3%)	52	61	5, 15, 33, 68	0
1	B	1010/1023 (98%)	-0.32	23 (2%)	64	70	4, 15, 31, 65	0
1	C	1011/1023 (98%)	-0.32	28 (2%)	56	64	5, 14, 33, 61	0
1	D	1011/1023 (98%)	-0.27	32 (3%)	51	60	5, 16, 34, 69	0
All	All	4043/4092 (98%)	-0.30	114 (2%)	56	64	4, 15, 33, 69	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	732	ALA	9.7
1	C	731	PRO	9.0
1	A	735	HIS	9.0
1	B	731	PRO	8.6
1	D	732	ALA	8.3
1	A	686	PRO	8.3
1	C	732	ALA	7.6
1	D	735	HIS	7.5
1	A	730	LEU	7.2
1	D	689	GLU	6.7
1	D	730	LEU	6.6
1	D	731	PRO	6.3
1	B	689	GLU	6.3
1	C	730	LEU	6.2
1	C	689	GLU	6.2
1	D	581	ASN	6.1
1	C	735	HIS	5.8
1	A	731	PRO	5.7
1	D	798	ALA	5.7
1	A	732	ALA	5.5
1	D	684	GLU	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	798	ALA	5.5
1	B	730	LEU	5.4
1	A	1023	LYS	5.3
1	D	580	GLU	5.3
1	B	684	GLU	5.3
1	B	687	GLN	5.3
1	D	687	GLN	5.2
1	D	799	THR	5.2
1	A	689	GLU	5.2
1	A	800	ARG	5.1
1	D	800	ARG	5.1
1	C	580	GLU	4.8
1	A	733	ALA	4.7
1	C	772	ASP	4.6
1	D	734	SER	4.5
1	D	685	LEU	4.4
1	D	686	PRO	4.4
1	A	687	GLN	4.4
1	B	686	PRO	4.4
1	D	733	ALA	4.3
1	B	797	GLU	4.3
1	C	800	ARG	4.3
1	B	733	ALA	4.3
1	A	798	ALA	4.2
1	B	580	GLU	4.2
1	A	734	SER	4.2
1	B	798	ALA	4.2
1	A	580	GLU	4.0
1	A	729	THR	4.0
1	A	799	THR	3.9
1	C	733	ALA	3.9
1	D	595	THR	3.8
1	A	684	GLU	3.7
1	B	800	ARG	3.7
1	D	772	ASP	3.6
1	C	684	GLU	3.6
1	C	687	GLN	3.5
1	A	581	ASN	3.4
1	B	735	HIS	3.3
1	D	71	GLU	3.3
1	A	736	ALA	3.3
1	B	729	THR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	845	GLN	3.1
1	C	595	THR	3.1
1	C	799	THR	3.1
1	B	581	ASN	3.0
1	A	846	GLY	3.0
1	B	799	THR	2.9
1	C	729	THR	2.8
1	C	745	MET	2.8
1	C	686	PRO	2.8
1	A	685	LEU	2.8
1	B	685	LEU	2.7
1	A	634	GLN	2.6
1	C	690	SER	2.5
1	B	819	GLU	2.5
1	D	583	ASN	2.5
1	B	745	MET	2.5
1	D	845	GLN	2.5
1	C	582	GLY	2.5
1	C	744	GLU	2.5
1	D	1022	GLN	2.5
1	D	801	ILE	2.5
1	A	80	GLU	2.4
1	C	1023	LYS	2.4
1	D	582	GLY	2.4
1	A	582	GLY	2.4
1	D	593	GLY	2.4
1	B	80	GLU	2.4
1	B	690	SER	2.4
1	C	734	SER	2.4
1	D	1023	LYS	2.3
1	C	76	CYS	2.3
1	A	653	HIS	2.3
1	A	595	THR	2.2
1	B	801	ILE	2.2
1	C	581	ASN	2.2
1	C	579	ASP	2.2
1	A	75	GLU	2.2
1	D	634	GLN	2.2
1	A	79	PRO	2.2
1	A	845	GLN	2.2
1	B	845	GLN	2.2
1	D	752	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	80	GLU	2.2
1	D	729	THR	2.1
1	C	761	GLN	2.1
1	D	79	PRO	2.1
1	A	753	ASN	2.0
1	A	771	GLY	2.0
1	D	797	GLU	2.0
1	D	739	HIS	2.0
1	A	797	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	DMS	A	8608	4/4	0.93	0.16	29.04	51,52,52,52	0
4	DMS	D	8407	4/4	0.72	0.32	12.30	49,50,51,51	0
4	DMS	C	8602	4/4	0.85	0.19	12.20	64,64,64,65	0
4	DMS	A	8604	4/4	0.88	0.28	11.00	74,75,75,75	0
4	DMS	B	8406	4/4	0.86	0.27	10.05	74,74,74,74	0
4	DMS	B	8508	4/4	0.87	0.23	9.90	53,54,54,55	0
4	DMS	C	8425	4/4	0.94	0.29	9.47	46,47,47,47	0
4	DMS	B	8423	4/4	0.88	0.20	8.88	70,70,71,71	0
4	DMS	A	8406	4/4	0.89	0.22	8.68	42,45,46,47	0
4	DMS	B	8407	4/4	0.91	0.21	8.14	56,56,56,57	0
4	DMS	B	8604	4/4	0.89	0.20	7.92	55,55,56,56	0
4	DMS	D	8404	4/4	0.88	0.17	7.81	46,47,47,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	DMS	C	8407	4/4	0.90	0.22	7.78	63,64,64,64	0
4	DMS	A	8407	4/4	0.88	0.26	6.57	48,48,48,49	0
4	DMS	C	8404	4/4	0.94	0.13	6.27	37,37,37,38	0
4	DMS	C	1024	4/4	0.92	0.14	5.98	60,60,60,61	0
4	DMS	A	8420	4/4	0.94	0.13	5.37	53,53,53,54	0
4	DMS	D	8712	4/4	0.88	0.22	5.32	67,67,67,68	0
4	DMS	B	8425	4/4	0.95	0.22	4.82	48,49,49,49	0
4	DMS	C	8420	4/4	0.91	0.16	4.44	56,57,57,57	0
4	DMS	D	8705	4/4	0.78	0.22	4.40	60,61,62,63	0
4	DMS	C	8501	4/4	0.93	0.13	4.37	38,39,40,40	0
4	DMS	A	8419	4/4	0.95	0.23	4.16	70,70,70,70	0
4	DMS	A	8603	4/4	0.94	0.31	3.54	80,80,80,80	0
4	DMS	B	8605	4/4	0.90	0.22	3.53	55,55,56,56	0
4	DMS	B	8610	4/4	0.77	0.21	3.26	67,67,67,68	0
4	DMS	D	8423	4/4	0.91	0.18	3.21	55,55,55,55	0
4	DMS	B	8413	4/4	0.76	0.28	3.13	64,65,65,66	0
4	DMS	C	8604	4/4	0.93	0.19	3.08	57,57,58,58	0
4	DMS	B	8404	4/4	0.92	0.12	3.04	30,31,34,34	0
4	DMS	B	8502	4/4	0.94	0.20	2.91	33,33,34,35	0
4	DMS	C	8411	4/4	0.95	0.13	2.73	36,38,39,39	0
4	DMS	A	8408	4/4	0.95	0.17	2.72	39,39,40,41	0
4	DMS	D	8406	4/4	0.93	0.14	2.72	34,34,35,36	0
4	DMS	D	8703	4/4	0.91	0.22	2.61	63,63,63,64	0
4	DMS	B	8408	4/4	0.97	0.18	2.55	30,31,31,31	0
4	DMS	C	8606	4/4	0.95	0.12	2.54	47,48,48,49	0
4	DMS	C	8403	4/4	0.97	0.12	2.49	27,28,28,30	0
4	DMS	D	8708	4/4	0.81	0.23	2.46	72,72,73,73	0
4	DMS	B	8411	4/4	0.95	0.15	2.33	36,37,38,39	0
4	DMS	C	8423	4/4	0.90	0.14	2.21	63,63,63,63	0
4	DMS	A	8404	4/4	0.93	0.11	2.21	40,41,42,43	0
4	DMS	B	8417	4/4	0.89	0.18	2.19	54,54,55,56	0
4	DMS	C	8405	4/4	0.96	0.12	2.17	30,31,32,32	0
4	DMS	B	8405	4/4	0.96	0.16	2.15	35,35,36,36	0
4	DMS	A	8502	4/4	0.78	0.30	2.10	51,53,53,54	0
4	DMS	D	8425	4/4	0.93	0.22	1.88	36,36,36,36	4
4	DMS	D	8711	4/4	0.86	0.22	1.86	49,50,51,51	0
4	DMS	D	8508	4/4	0.94	0.16	1.83	56,56,57,57	0
4	DMS	D	8501	4/4	0.93	0.14	1.81	52,52,53,54	0
4	DMS	C	8417	4/4	0.94	0.14	1.71	55,55,55,55	0
4	DMS	B	8607	4/4	0.93	0.18	1.65	69,69,69,70	0
4	DMS	D	8408	4/4	0.97	0.15	1.57	34,34,35,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	DMS	D	8419	4/4	0.95	0.14	1.55	62,62,63,63	0
4	DMS	D	8701	4/4	0.96	0.12	1.52	29,29,29,30	0
4	DMS	B	8602	4/4	0.89	0.13	1.16	46,47,48,49	0
4	DMS	B	8410	4/4	0.88	0.14	1.12	73,73,74,74	0
4	DMS	A	8401	4/4	0.98	0.10	1.08	18,18,20,21	0
4	DMS	A	8501	4/4	0.95	0.12	0.93	37,37,38,39	0
4	DMS	C	8603	4/4	0.95	0.17	0.92	47,47,47,47	0
4	DMS	B	8603	4/4	0.87	0.18	0.91	41,42,44,44	0
4	DMS	D	8707	4/4	0.92	0.14	0.91	53,54,54,54	0
4	DMS	A	8412	4/4	0.97	0.16	0.76	43,43,43,43	0
4	DMS	A	8403	4/4	0.97	0.10	0.76	31,32,33,34	0
4	DMS	A	8504	4/4	0.97	0.10	0.75	47,47,47,47	0
4	DMS	A	8402	4/4	0.97	0.11	0.67	21,21,22,24	0
4	DMS	D	8411	4/4	0.96	0.12	0.65	36,37,39,39	0
4	DMS	C	8402	4/4	0.96	0.09	0.65	19,20,23,24	0
4	DMS	B	8504	4/4	0.95	0.13	0.63	46,47,47,48	0
4	DMS	A	8610	4/4	0.89	0.15	0.52	44,45,45,46	0
4	DMS	A	8425	4/4	0.95	0.17	0.49	45,45,46,46	0
4	DMS	D	8405	4/4	0.97	0.11	0.42	29,29,29,29	0
4	DMS	D	8412	4/4	0.98	0.14	0.38	34,35,36,36	0
4	DMS	C	8401	4/4	0.97	0.09	0.35	14,17,20,21	0
4	DMS	B	8403	4/4	0.97	0.09	0.31	28,29,29,30	0
4	DMS	D	8401	4/4	0.97	0.08	0.31	16,17,21,22	0
3	NA	C	3104	1/1	0.96	0.12	0.26	26,26,26,26	0
4	DMS	D	8403	4/4	0.97	0.08	0.19	31,31,32,33	0
4	DMS	C	8419	4/4	0.94	0.11	0.15	75,75,76,76	0
4	DMS	A	8405	4/4	0.97	0.09	0.07	23,24,25,26	0
4	DMS	A	8612	4/4	0.94	0.14	0.03	63,63,63,63	0
4	DMS	C	8607	4/4	0.90	0.13	-0.03	37,37,38,41	0
4	DMS	A	8609	4/4	0.90	0.13	-0.09	58,58,58,60	0
4	DMS	B	8412	4/4	0.97	0.11	-0.10	31,32,32,34	0
4	DMS	C	8412	4/4	0.98	0.10	-0.13	38,38,39,39	0
4	DMS	C	8408	4/4	0.98	0.09	-0.13	33,34,34,35	0
4	DMS	B	8402	4/4	0.97	0.09	-0.22	15,18,18,20	0
4	DMS	A	8411	4/4	0.98	0.09	-0.23	44,44,44,45	0
4	DMS	D	8709	4/4	0.96	0.17	-0.29	69,70,70,70	0
3	NA	C	3101	1/1	0.85	0.09	-0.53	35,35,35,35	0
3	NA	C	3103	1/1	0.98	0.09	-0.78	28,28,28,28	0
4	DMS	D	8402	4/4	0.97	0.08	-0.82	16,17,17,19	0
3	NA	D	3104	1/1	0.95	0.06	-0.91	30,30,30,30	0
3	NA	B	3104	1/1	0.94	0.09	-0.92	28,28,28,28	0
3	NA	D	3101	1/1	0.94	0.07	-0.97	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NA	B	3103	1/1	0.96	0.08	-1.07	30,30,30,30	0
3	NA	A	3104	1/1	0.98	0.07	-1.11	28,28,28,28	0
3	NA	D	3103	1/1	0.98	0.07	-1.13	31,31,31,31	0
3	NA	A	3102	1/1	0.98	0.06	-1.32	9,9,9,9	0
4	DMS	B	8401	4/4	0.99	0.06	-1.32	12,16,19,21	0
3	NA	A	3103	1/1	0.98	0.07	-1.50	29,29,29,29	0
3	NA	A	3101	1/1	0.90	0.06	-1.59	36,36,36,36	0
3	NA	C	3102	1/1	0.97	0.05	-1.85	9,9,9,9	0
3	NA	D	3102	1/1	0.98	0.06	-1.89	9,9,9,9	0
2	MG	A	3001	1/1	0.96	0.04	-2.17	17,17,17,17	0
2	MG	A	3002	1/1	0.99	0.06	-2.59	15,15,15,15	0
3	NA	B	3101	1/1	0.92	0.04	-3.01	26,26,26,26	0
2	MG	D	3002	1/1	0.99	0.05	-3.20	14,14,14,14	0
2	MG	B	3002	1/1	0.98	0.03	-3.70	11,11,11,11	0
2	MG	D	3001	1/1	0.97	0.05	-3.72	16,16,16,16	0
2	MG	C	3002	1/1	0.98	0.05	-3.73	13,13,13,13	0
2	MG	B	3001	1/1	0.97	0.04	-3.87	14,14,14,14	0
2	MG	C	3001	1/1	0.98	0.05	-4.40	14,14,14,14	0
3	NA	B	3102	1/1	0.99	0.03	-8.16	12,12,12,12	0
4	DMS	B	8421	4/4	0.96	0.10	-	57,57,57,58	0
4	DMS	B	8415	4/4	0.88	0.22	-	63,63,64,64	0
4	DMS	D	8427	4/4	0.91	0.24	-	69,69,69,70	0
4	DMS	A	8421	4/4	0.94	0.26	-	56,56,56,57	0
4	DMS	A	8602	4/4	0.91	0.23	-	65,65,65,65	0
4	DMS	C	8427	4/4	0.95	0.17	-	52,52,52,52	0
2	MG	C	3006	1/1	0.93	0.05	-	37,37,37,37	0
4	DMS	C	8421	4/4	0.96	0.17	-	51,51,51,51	0
4	DMS	C	8416	4/4	0.92	0.26	-	53,53,54,54	0
4	DMS	D	8706	4/4	0.88	0.19	-	54,54,54,55	0
4	DMS	A	8605	4/4	0.86	0.36	-	49,50,51,51	0
4	DMS	D	8415	4/4	0.80	0.27	-	59,59,59,61	0
4	DMS	D	8416	4/4	0.91	0.20	-	47,48,49,50	0
4	DMS	A	8409	4/4	0.96	0.18	-	43,43,43,44	0
4	DMS	A	8413	4/4	0.64	0.36	-	99,99,99,99	0
4	DMS	B	8608	4/4	0.81	0.29	-	75,75,75,75	0
4	DMS	C	8605	4/4	0.93	0.23	-	54,54,55,55	0
4	DMS	A	8410	4/4	0.85	0.20	-	54,54,55,55	0
4	DMS	C	8413	4/4	0.85	0.25	-	79,79,79,79	0
2	MG	D	3003	1/1	0.88	0.23	-	48,48,48,48	0
4	DMS	A	8414	4/4	0.85	0.22	-	60,61,61,61	0
4	DMS	C	8414	4/4	0.96	0.19	-	42,43,43,43	0
4	DMS	D	8414	4/4	0.88	0.23	-	49,50,50,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	DMS	A	8427	4/4	0.83	0.25	-	84,84,84,84	0
4	DMS	D	8409	4/4	0.95	0.18	-	40,40,41,41	0
4	DMS	B	8601	4/4	0.95	0.17	-	50,50,50,50	0
2	MG	A	3003	1/1	0.83	0.24	-	56,56,56,56	0
4	DMS	C	8409	4/4	0.95	0.15	-	39,40,40,41	0
4	DMS	A	8607	4/4	0.89	0.16	-	71,71,71,71	0
4	DMS	D	8503	4/4	0.95	0.17	-	53,53,54,54	0
4	DMS	D	8410	4/4	0.96	0.19	-	42,43,43,44	0
4	DMS	D	8413	4/4	0.76	0.41	-	83,84,84,84	0
2	MG	A	3009	1/1	0.93	0.07	-	43,43,43,43	0
4	DMS	B	8414	4/4	0.97	0.14	-	46,46,47,47	0
4	DMS	B	8609	4/4	0.26	0.40	-	74,75,75,76	0
4	DMS	B	8606	4/4	0.93	0.21	-	59,60,60,60	0
4	DMS	B	8416	4/4	0.93	0.19	-	57,57,58,58	0
2	MG	A	3005	1/1	0.92	0.06	-	40,40,40,40	0
4	DMS	C	8504	4/4	0.93	0.17	-	48,48,49,50	0
4	DMS	C	8410	4/4	0.94	0.21	-	48,48,49,49	0
2	MG	B	3003	1/1	0.88	0.16	-	38,38,38,38	0
4	DMS	B	8427	4/4	0.92	0.20	-	52,53,53,54	0
4	DMS	C	8503	4/4	0.92	0.24	-	64,64,64,65	0
4	DMS	D	8710	4/4	0.85	0.20	-	60,60,60,60	0
2	MG	C	3003	1/1	0.83	0.14	-	24,24,24,24	1
4	DMS	C	8601	4/4	0.89	0.23	-	45,45,46,47	0
4	DMS	C	8415	4/4	0.79	0.27	-	53,55,55,56	0
4	DMS	D	8421	4/4	0.89	0.21	-	67,67,67,67	0
4	DMS	A	8503	4/4	0.94	0.34	-	58,58,58,59	0
4	DMS	B	8409	4/4	0.94	0.16	-	35,35,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.