W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 6, 2023 – 08:41 AM EDT

|		
PDB ID	:	3VD5
Title	:	E. coli (lacZ) beta-galactosidase (N460S)
Authors	:	Wheatley, R.W.; Kappelhoff, J.C.; Hahn, J.N.; Dugdale, M.L.; Dutkoski, M.J.; Tamman, S.D.; Fraser, M.E.; Huber, R.E.
Deposited on	:	2012-01-04
Resolution	:	2.70 Å(reported)

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 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
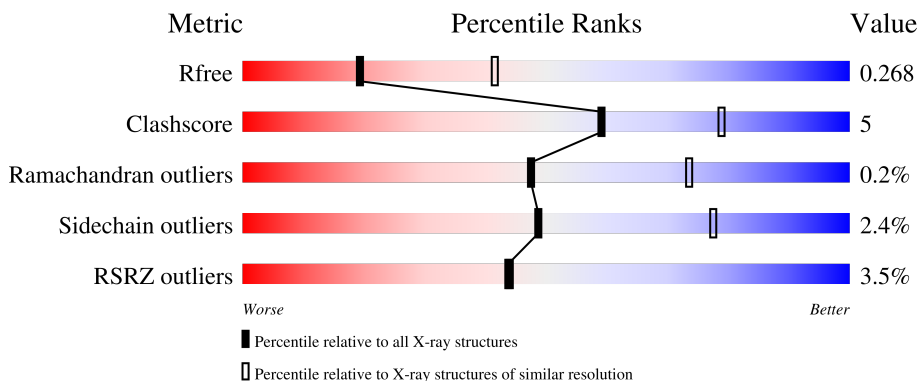
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	1052	2% / 86% / 10% / •
1	B	1052	2% / 82% / 14% / •
1	C	1052	4% / 81% / 15% / •
1	D	1052	5% / 81% / 14% / • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 33647 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
			8124	5137	1439	1510	38			
1	C	1011	Total	C	N	O	S	0	0	0
			8124	5137	1439	1510	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8124	5137	1439	1510	38			
1	B	1011	Total	C	N	O	S	0	0	0
			8124	5137	1439	1510	38			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	expression tag	UNP P00722
A	-27	GLY	-	expression tag	UNP P00722
A	-26	GLY	-	expression tag	UNP P00722
A	-25	SER	-	expression tag	UNP P00722
A	-24	HIS	-	expression tag	UNP P00722
A	-23	HIS	-	expression tag	UNP P00722
A	-22	HIS	-	expression tag	UNP P00722
A	-21	HIS	-	expression tag	UNP P00722
A	-20	HIS	-	expression tag	UNP P00722
A	-19	HIS	-	expression tag	UNP P00722
A	-18	GLY	-	expression tag	UNP P00722
A	-17	MET	-	expression tag	UNP P00722
A	-16	ALA	-	expression tag	UNP P00722
A	-15	SER	-	expression tag	UNP P00722
A	-14	MET	-	expression tag	UNP P00722
A	-13	THR	-	expression tag	UNP P00722
A	-12	GLY	-	expression tag	UNP P00722
A	-11	GLY	-	expression tag	UNP P00722
A	-10	GLN	-	expression tag	UNP P00722
A	-9	GLN	-	expression tag	UNP P00722
A	-8	MET	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP P00722
A	-6	ARG	-	expression tag	UNP P00722
A	-5	ASP	-	expression tag	UNP P00722
A	-4	LEU	-	expression tag	UNP P00722
A	-3	TYR	-	expression tag	UNP P00722
A	-2	ASP	-	expression tag	UNP P00722
A	-1	ASP	-	expression tag	UNP P00722
A	0	ASP	-	expression tag	UNP P00722
A	1	ASP	-	expression tag	UNP P00722
A	2	LYS	-	expression tag	UNP P00722
A	3	ASP	-	expression tag	UNP P00722
A	4	PRO	-	expression tag	UNP P00722
A	5	MET	-	expression tag	UNP P00722
A	6	ILE	-	expression tag	UNP P00722
A	7	ASP	-	expression tag	UNP P00722
A	8	PRO	-	expression tag	UNP P00722
A	460	SER	ASN	engineered mutation	UNP P00722
C	-28	MET	-	expression tag	UNP P00722
C	-27	GLY	-	expression tag	UNP P00722
C	-26	GLY	-	expression tag	UNP P00722
C	-25	SER	-	expression tag	UNP P00722
C	-24	HIS	-	expression tag	UNP P00722
C	-23	HIS	-	expression tag	UNP P00722
C	-22	HIS	-	expression tag	UNP P00722
C	-21	HIS	-	expression tag	UNP P00722
C	-20	HIS	-	expression tag	UNP P00722
C	-19	HIS	-	expression tag	UNP P00722
C	-18	GLY	-	expression tag	UNP P00722
C	-17	MET	-	expression tag	UNP P00722
C	-16	ALA	-	expression tag	UNP P00722
C	-15	SER	-	expression tag	UNP P00722
C	-14	MET	-	expression tag	UNP P00722
C	-13	THR	-	expression tag	UNP P00722
C	-12	GLY	-	expression tag	UNP P00722
C	-11	GLY	-	expression tag	UNP P00722
C	-10	GLN	-	expression tag	UNP P00722
C	-9	GLN	-	expression tag	UNP P00722
C	-8	MET	-	expression tag	UNP P00722
C	-7	GLY	-	expression tag	UNP P00722
C	-6	ARG	-	expression tag	UNP P00722
C	-5	ASP	-	expression tag	UNP P00722
C	-4	LEU	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	TYR	-	expression tag	UNP P00722
C	-2	ASP	-	expression tag	UNP P00722
C	-1	ASP	-	expression tag	UNP P00722
C	0	ASP	-	expression tag	UNP P00722
C	1	ASP	-	expression tag	UNP P00722
C	2	LYS	-	expression tag	UNP P00722
C	3	ASP	-	expression tag	UNP P00722
C	4	PRO	-	expression tag	UNP P00722
C	5	MET	-	expression tag	UNP P00722
C	6	ILE	-	expression tag	UNP P00722
C	7	ASP	-	expression tag	UNP P00722
C	8	PRO	-	expression tag	UNP P00722
C	460	SER	ASN	engineered mutation	UNP P00722
D	-28	MET	-	expression tag	UNP P00722
D	-27	GLY	-	expression tag	UNP P00722
D	-26	GLY	-	expression tag	UNP P00722
D	-25	SER	-	expression tag	UNP P00722
D	-24	HIS	-	expression tag	UNP P00722
D	-23	HIS	-	expression tag	UNP P00722
D	-22	HIS	-	expression tag	UNP P00722
D	-21	HIS	-	expression tag	UNP P00722
D	-20	HIS	-	expression tag	UNP P00722
D	-19	HIS	-	expression tag	UNP P00722
D	-18	GLY	-	expression tag	UNP P00722
D	-17	MET	-	expression tag	UNP P00722
D	-16	ALA	-	expression tag	UNP P00722
D	-15	SER	-	expression tag	UNP P00722
D	-14	MET	-	expression tag	UNP P00722
D	-13	THR	-	expression tag	UNP P00722
D	-12	GLY	-	expression tag	UNP P00722
D	-11	GLY	-	expression tag	UNP P00722
D	-10	GLN	-	expression tag	UNP P00722
D	-9	GLN	-	expression tag	UNP P00722
D	-8	MET	-	expression tag	UNP P00722
D	-7	GLY	-	expression tag	UNP P00722
D	-6	ARG	-	expression tag	UNP P00722
D	-5	ASP	-	expression tag	UNP P00722
D	-4	LEU	-	expression tag	UNP P00722
D	-3	TYR	-	expression tag	UNP P00722
D	-2	ASP	-	expression tag	UNP P00722
D	-1	ASP	-	expression tag	UNP P00722
D	0	ASP	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	ASP	-	expression tag	UNP P00722
D	2	LYS	-	expression tag	UNP P00722
D	3	ASP	-	expression tag	UNP P00722
D	4	PRO	-	expression tag	UNP P00722
D	5	MET	-	expression tag	UNP P00722
D	6	ILE	-	expression tag	UNP P00722
D	7	ASP	-	expression tag	UNP P00722
D	8	PRO	-	expression tag	UNP P00722
D	460	SER	ASN	engineered mutation	UNP P00722
B	-28	MET	-	expression tag	UNP P00722
B	-27	GLY	-	expression tag	UNP P00722
B	-26	GLY	-	expression tag	UNP P00722
B	-25	SER	-	expression tag	UNP P00722
B	-24	HIS	-	expression tag	UNP P00722
B	-23	HIS	-	expression tag	UNP P00722
B	-22	HIS	-	expression tag	UNP P00722
B	-21	HIS	-	expression tag	UNP P00722
B	-20	HIS	-	expression tag	UNP P00722
B	-19	HIS	-	expression tag	UNP P00722
B	-18	GLY	-	expression tag	UNP P00722
B	-17	MET	-	expression tag	UNP P00722
B	-16	ALA	-	expression tag	UNP P00722
B	-15	SER	-	expression tag	UNP P00722
B	-14	MET	-	expression tag	UNP P00722
B	-13	THR	-	expression tag	UNP P00722
B	-12	GLY	-	expression tag	UNP P00722
B	-11	GLY	-	expression tag	UNP P00722
B	-10	GLN	-	expression tag	UNP P00722
B	-9	GLN	-	expression tag	UNP P00722
B	-8	MET	-	expression tag	UNP P00722
B	-7	GLY	-	expression tag	UNP P00722
B	-6	ARG	-	expression tag	UNP P00722
B	-5	ASP	-	expression tag	UNP P00722
B	-4	LEU	-	expression tag	UNP P00722
B	-3	TYR	-	expression tag	UNP P00722
B	-2	ASP	-	expression tag	UNP P00722
B	-1	ASP	-	expression tag	UNP P00722
B	0	ASP	-	expression tag	UNP P00722
B	1	ASP	-	expression tag	UNP P00722
B	2	LYS	-	expression tag	UNP P00722
B	3	ASP	-	expression tag	UNP P00722
B	4	PRO	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	MET	-	expression tag	UNP P00722
B	6	ILE	-	expression tag	UNP P00722
B	7	ASP	-	expression tag	UNP P00722
B	8	PRO	-	expression tag	UNP P00722
B	460	SER	ASN	engineered mutation	UNP P00722

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Na 3	0	0
3	C	3	Total 3	Na 3	0	0
3	D	2	Total 2	Na 2	0	0
3	B	3	Total 3	Na 3	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).

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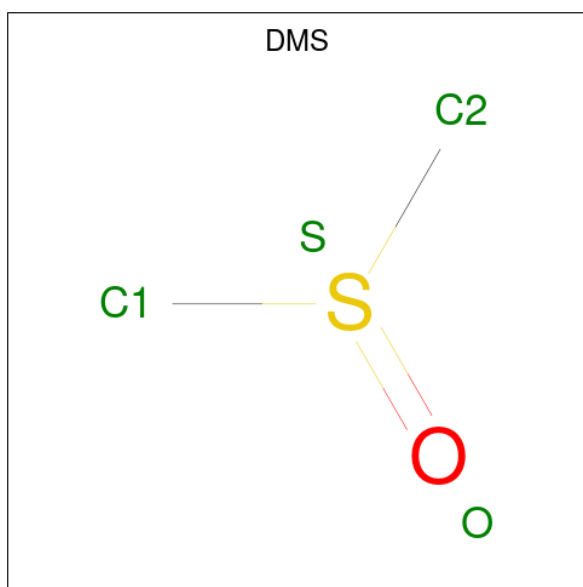
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	314	Total	O	0	0
			314	314		
5	C	204	Total	O	0	0
			204	204		
5	D	272	Total	O	0	0
			272	272		
5	B	246	Total	O	0	0
			246	246		

# 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.

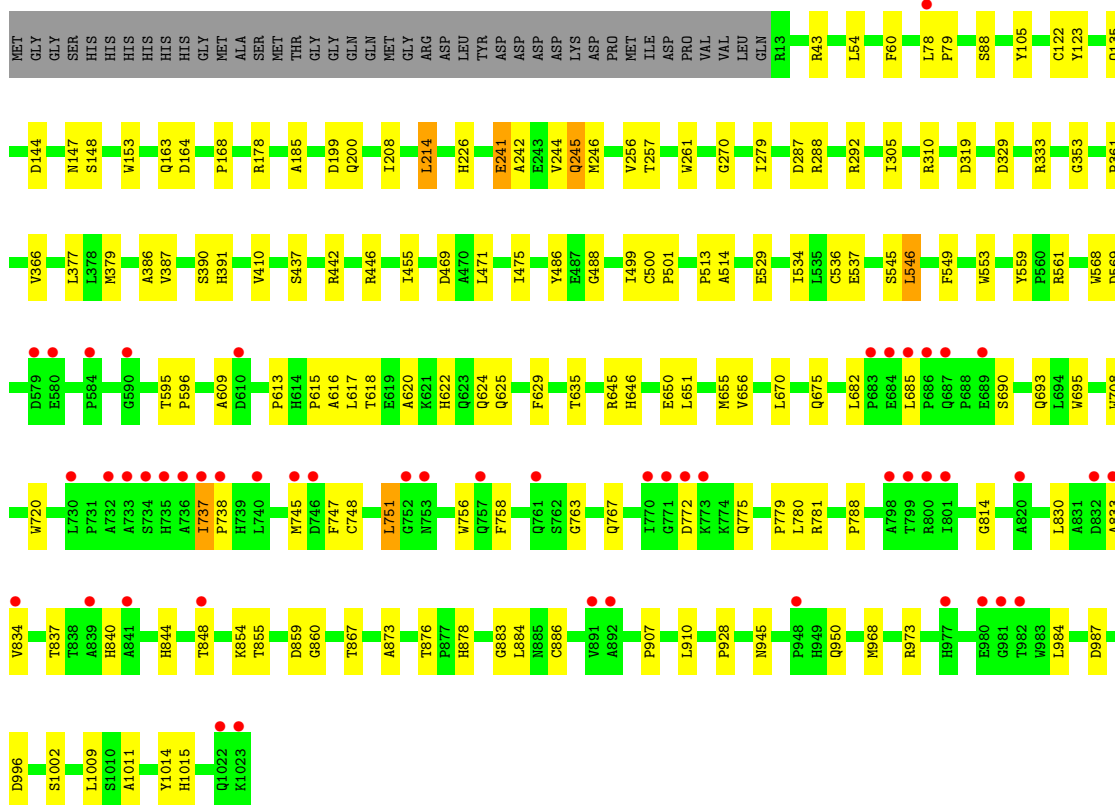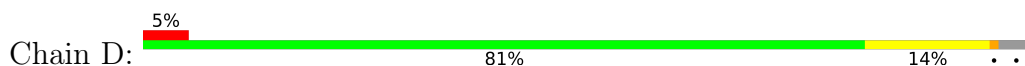- Molecule 1: Beta-galactosidase
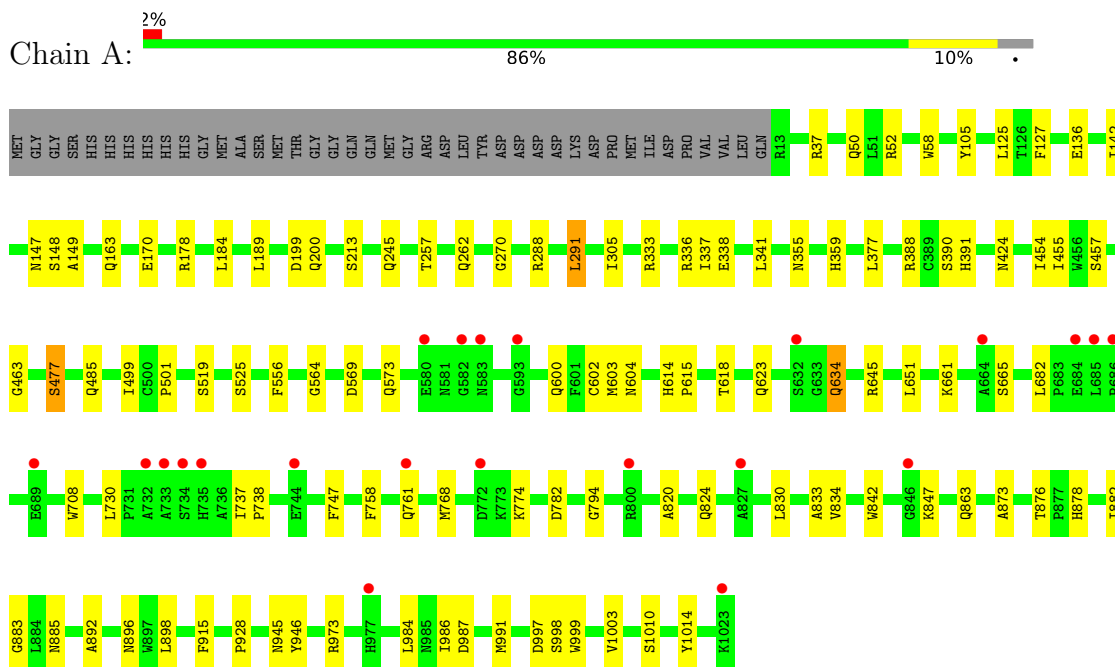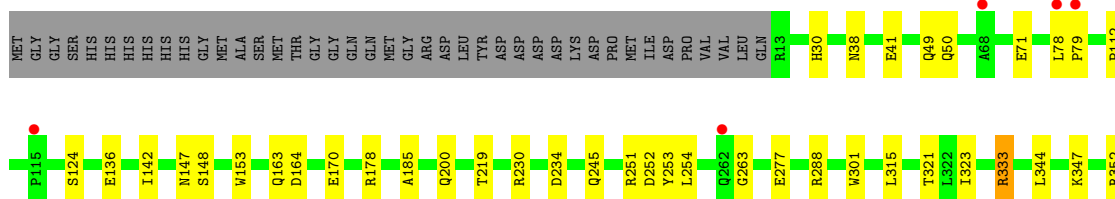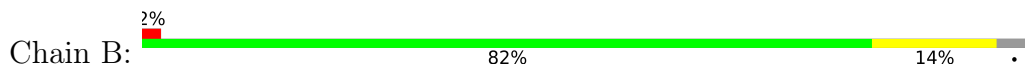

- Molecule 1: Beta-galactosidase

• Molecule 1: Beta-galactosidase

Chain D:

• Molecule 1: Beta-galactosidase

Chain B:
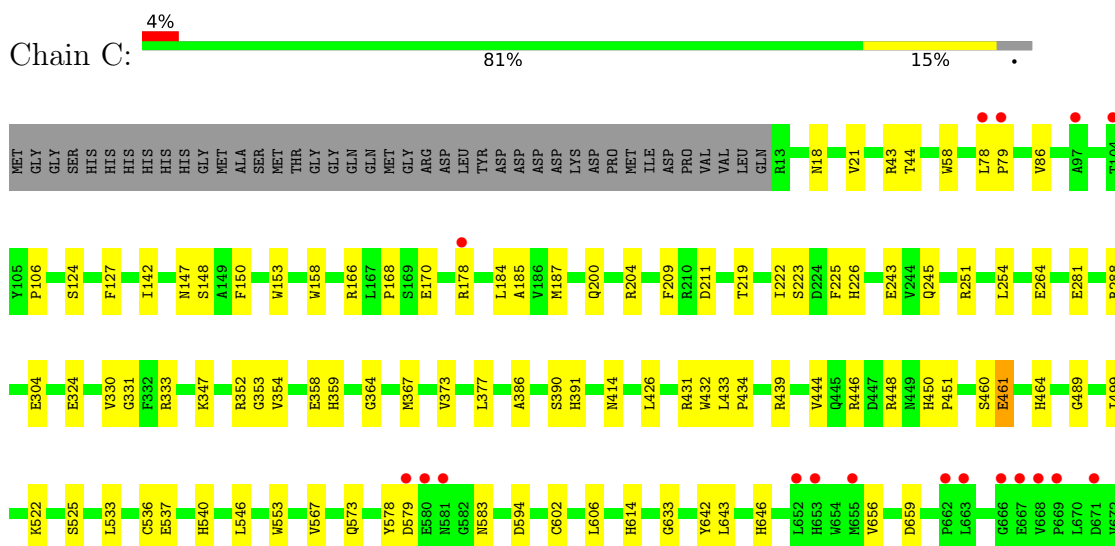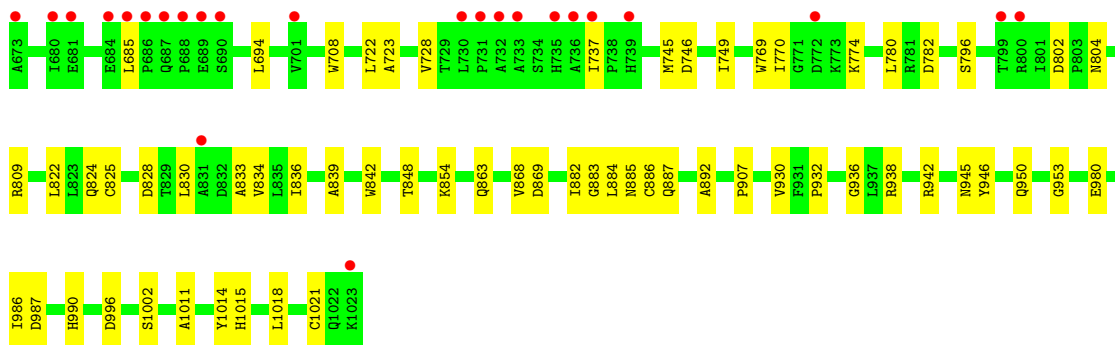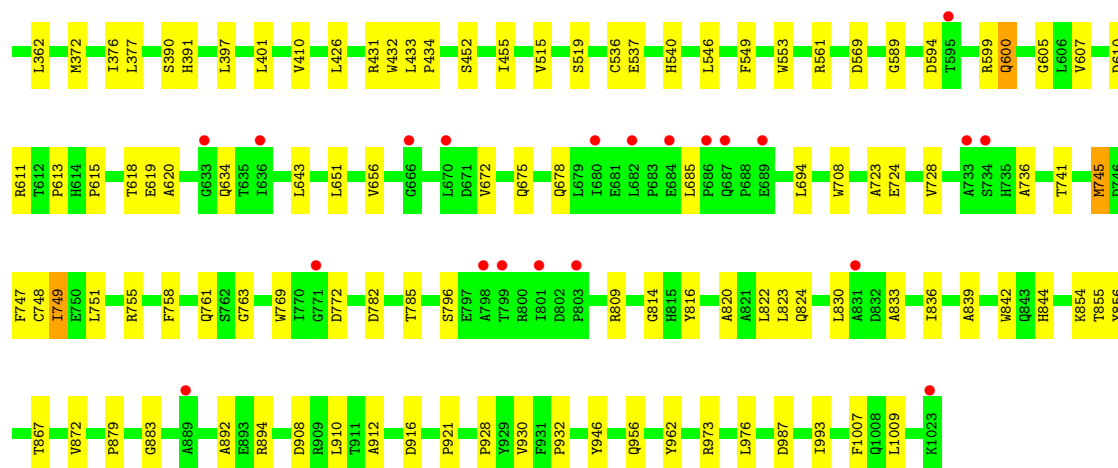
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	126.30Å 150.75Å 131.09Å 90.00° 104.06° 90.00°	Depositor
Resolution (Å)	54.58 – 2.70 54.58 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.58-2.70) 91.0 (54.58-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.203 , 0.276 0.194 , 0.268	Depositor DCC
R_{free} test set	5937 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.1	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	33647	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality (i)

5.1   Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.40	0/8366	0.56	1/11412 (0.0%)
1	B	0.38	0/8366	0.55	0/11412
1	C	0.37	0/8366	0.53	0/11412
1	D	0.39	0/8366	0.55	0/11412
All	All	0.39	0/33464	0.55	1/45648 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	291	LEU	CA-CB-CG	5.33	127.57	115.30

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	8124	0	7715	55	0
1	B	8124	0	7715	75	0
1	C	8124	0	7715	90	0
1	D	8124	0	7715	85	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
4	A	32	0	48	2	0
4	B	16	0	24	0	0
4	C	24	0	36	3	0
4	D	24	0	36	0	0
5	A	314	0	0	1	0
5	B	246	0	0	1	0
5	C	204	0	0	3	0
5	D	272	0	0	4	0
All	All	33647	0	31004	296	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.

The worst 5 of 296 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.48	0.94
1:C:226:HIS:ND1	1:C:448:ARG:HD3	1.85	0.91
1:B:656:VAL:HG21	1:B:685:LEU:HD22	1.56	0.88
1:B:656:VAL:HG21	1:B:685:LEU:CD2	2.12	0.80
1:D:245:GLN:HG3	1:D:288:ARG:HG2	1.67	0.77

There are no symmetry-related clashes.

5.3   Torsion angles (i)

5.3.1   Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1009/1052 (96%)	972 (96%)	37 (4%)	0	100	100
1	B	1009/1052 (96%)	965 (96%)	41 (4%)	3 (0%)	41	66
1	C	1009/1052 (96%)	947 (94%)	56 (6%)	6 (1%)	25	50
1	D	1009/1052 (96%)	935 (93%)	74 (7%)	0	100	100
All	All	4036/4208 (96%)	3819 (95%)	208 (5%)	9 (0%)	47	73

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	461	GLU
1	C	659	ASP
1	C	722	LEU
1	B	916	ASP
1	B	540	HIS

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	864/898 (96%)	844 (98%)	20 (2%)	50	78
1	B	864/898 (96%)	836 (97%)	28 (3%)	39	68
1	C	864/898 (96%)	850 (98%)	14 (2%)	62	85
1	D	864/898 (96%)	842 (98%)	22 (2%)	47	76
All	All	3456/3592 (96%)	3372 (98%)	84 (2%)	49	77

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	124	SER
1	B	634	GLN
1	B	178	ARG
1	B	344	LEU
1	B	745	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	93	HIS
1	B	1015	HIS
1	C	623	GLN
1	C	878	HIS
1	D	418	HIS

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 43 ligands modelled in this entry, 19 are monoatomic - leaving 24 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	B	8002	-	3,3,3	2.65	1 (33%)	3,3,3	0.51	0
4	DMS	A	8002	-	3,3,3	2.55	1 (33%)	3,3,3	0.43	0
4	DMS	A	8004	-	3,3,3	2.61	1 (33%)	3,3,3	0.67	0
4	DMS	B	8001	-	3,3,3	2.69	1 (33%)	3,3,3	0.63	0
4	DMS	C	8003	-	3,3,3	2.67	1 (33%)	3,3,3	0.58	0
4	DMS	A	8008	-	3,3,3	2.67	1 (33%)	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	D	8005	-	3,3,3	2.58	1 (33%)	3,3,3	0.59	0
4	DMS	D	8003	-	3,3,3	2.69	1 (33%)	3,3,3	0.47	0
4	DMS	C	8002	-	3,3,3	2.67	1 (33%)	3,3,3	0.62	0
4	DMS	D	8004	-	3,3,3	2.64	1 (33%)	3,3,3	0.55	0
4	DMS	D	8006	-	3,3,3	2.70	1 (33%)	3,3,3	0.52	0
4	DMS	B	8003	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
4	DMS	D	8002	-	3,3,3	2.61	1 (33%)	3,3,3	0.38	0
4	DMS	C	8004	-	3,3,3	2.62	1 (33%)	3,3,3	0.49	0
4	DMS	A	8005	-	3,3,3	2.70	1 (33%)	3,3,3	0.58	0
4	DMS	A	8006	-	3,3,3	2.72	1 (33%)	3,3,3	0.64	0
4	DMS	A	8001	-	3,3,3	2.62	1 (33%)	3,3,3	0.59	0
4	DMS	B	8004	-	3,3,3	1.66	1 (33%)	3,3,3	0.36	0
4	DMS	A	8007	-	3,3,3	2.73	1 (33%)	3,3,3	0.70	0
4	DMS	C	8005	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
4	DMS	C	8006	-	3,3,3	2.74	1 (33%)	3,3,3	0.66	0
4	DMS	A	8003	-	3,3,3	2.65	1 (33%)	3,3,3	0.70	0
4	DMS	D	8001	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
4	DMS	C	8001	-	3,3,3	2.66	1 (33%)	3,3,3	0.61	0

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	8007	DMS	O-S	4.57	1.81	1.50
4	C	8006	DMS	O-S	4.57	1.81	1.50
4	A	8006	DMS	O-S	4.56	1.81	1.50
4	A	8005	DMS	O-S	4.54	1.80	1.50
4	D	8006	DMS	O-S	4.53	1.80	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	8002	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	8004	DMS	1	0
4	C	8002	DMS	3	0

5.7   Other polymers ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	1011/1052 (96%)	-0.17	22 (2%)	62	63	24, 43, 79, 114	0
1	B	1011/1052 (96%)	-0.04	26 (2%)	56	57	28, 51, 75, 111	0
1	C	1011/1052 (96%)	0.08	42 (4%)	36	35	30, 56, 87, 123	0
1	D	1011/1052 (96%)	0.06	51 (5%)	28	27	27, 48, 94, 127	0
All	All	4044/4208 (96%)	-0.02	141 (3%)	44	44	24, 50, 84, 127	0

The worst 5 of 141 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	689	GLU	6.5
1	D	732	ALA	5.5
1	D	833	ALA	5.5
1	C	685	LEU	5.4
1	D	771	GLY	5.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å²)	Q<0.9
3	NA	D	3101	1/1	0.75	0.18	55,55,55,55	0
3	NA	C	3101	1/1	0.79	0.11	57,57,57,57	0
3	NA	C	3103	1/1	0.80	0.14	62,62,62,62	0
3	NA	B	3101	1/1	0.80	0.12	55,55,55,55	0
2	MG	B	3001	1/1	0.88	0.06	50,50,50,50	0
4	DMS	C	8001	4/4	0.88	0.24	75,77,79,80	0
3	NA	C	3102	1/1	0.90	0.14	41,41,41,41	0
4	DMS	C	8003	4/4	0.91	0.30	83,84,85,86	0
2	MG	C	3002	1/1	0.93	0.10	54,54,54,54	0
3	NA	B	3102	1/1	0.93	0.15	35,35,35,35	0
3	NA	A	3103	1/1	0.93	0.12	59,59,59,59	0
3	NA	D	3102	1/1	0.93	0.15	34,34,34,34	0
2	MG	C	3001	1/1	0.94	0.09	42,42,42,42	0
4	DMS	A	8007	4/4	0.95	0.16	57,58,59,67	0
4	DMS	A	8008	4/4	0.95	0.14	81,82,83,86	0
2	MG	D	3002	1/1	0.95	0.09	42,42,42,42	0
3	NA	B	3103	1/1	0.95	0.23	58,58,58,58	0
4	DMS	C	8005	4/4	0.95	0.21	63,64,64,65	0
4	DMS	C	8006	4/4	0.95	0.27	65,65,66,70	0
4	DMS	D	8006	4/4	0.95	0.15	58,60,62,65	0
4	DMS	B	8003	4/4	0.95	0.15	63,65,67,68	0
4	DMS	B	8004	4/4	0.95	0.15	43,46,46,46	0
2	MG	B	3002	1/1	0.96	0.06	56,56,56,56	0
2	MG	D	3001	1/1	0.96	0.08	39,39,39,39	0
4	DMS	D	8005	4/4	0.96	0.20	53,56,57,61	0
4	DMS	A	8001	4/4	0.96	0.22	71,71,72,74	0
4	DMS	C	8002	4/4	0.96	0.20	49,53,53,55	0
4	DMS	A	8004	4/4	0.96	0.27	60,61,63,64	0
3	NA	A	3101	1/1	0.97	0.10	51,51,51,51	0
4	DMS	C	8004	4/4	0.97	0.18	53,54,55,56	0
4	DMS	B	8001	4/4	0.97	0.14	64,66,67,70	0
4	DMS	B	8002	4/4	0.97	0.18	58,59,61,62	0
4	DMS	D	8003	4/4	0.97	0.15	66,67,68,69	0
4	DMS	D	8004	4/4	0.97	0.19	74,75,76,76	0
4	DMS	A	8006	4/4	0.98	0.14	56,58,59,63	0
3	NA	A	3102	1/1	0.98	0.10	34,34,34,34	0
4	DMS	A	8002	4/4	0.98	0.20	53,53,53,54	0
2	MG	A	3002	1/1	0.98	0.08	43,43,43,43	0
4	DMS	D	8001	4/4	0.98	0.22	56,56,56,58	0
4	DMS	D	8002	4/4	0.98	0.30	58,62,62,63	0
4	DMS	A	8005	4/4	0.98	0.12	56,56,57,60	0
4	DMS	A	8003	4/4	0.99	0.17	44,45,47,47	0
2	MG	A	3001	1/1	0.99	0.05	51,51,51,51	0

6.5 Other polymers ⓘ

There are no such residues in this entry.