



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:34 AM UTC

PDB ID : 5TCH / pdb_00005tch
Title : Crystal structure of tryptophan synthase from M. tuberculosis - ligand-free form, TrpA-G66V mutant
Authors : Michalska, K.; Maltseva, N.; Jedrzejczak, R.; Wellington, S.; Nag, P.P.; Fisher, S.L.; Schreiber, S.L.; Hung, D.T.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2016-09-15
Resolution : 2.35 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

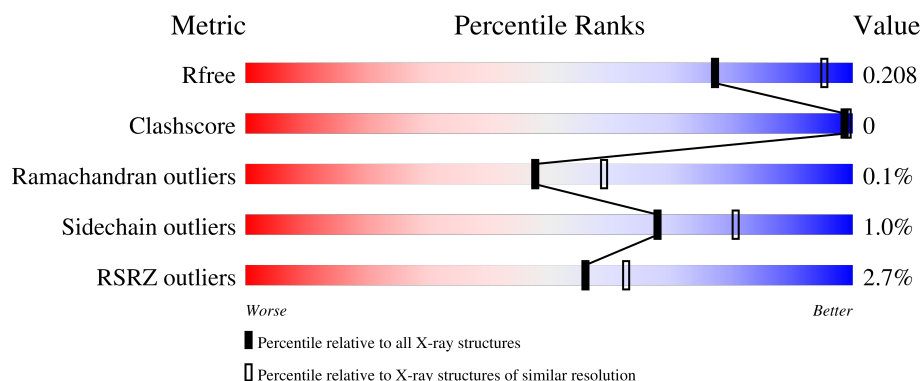
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	276	0% 88% 10%
1	C	276	3% 89% 10%
1	E	276	9% 87% 11%
1	G	276	2% 88% 11%

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Mol	Chain	Length	Quality of chain
2	B	410	2% 96% ..
2	D	410	95% ..
2	F	410	2% 95% ..
2	H	410	2% 96% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20207 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 Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	2	0
			1826	1145	329	347	5			
1	G	247	Total	C	N	O	S	0	2	0
			1815	1139	329	342	5			
1	E	246	Total	C	N	O	S	0	0	0
			1785	1121	320	339	5			
1	C	248	Total	C	N	O	S	0	0	0
			1802	1132	322	343	5			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	VAL	GLY	engineered mutation	UNP P9WFY1
A	271	HIS	-	expression tag	UNP P9WFY1
A	272	HIS	-	expression tag	UNP P9WFY1
A	273	HIS	-	expression tag	UNP P9WFY1
A	274	HIS	-	expression tag	UNP P9WFY1
A	275	HIS	-	expression tag	UNP P9WFY1
A	276	HIS	-	expression tag	UNP P9WFY1
G	66	VAL	GLY	engineered mutation	UNP P9WFY1
G	271	HIS	-	expression tag	UNP P9WFY1
G	272	HIS	-	expression tag	UNP P9WFY1
G	273	HIS	-	expression tag	UNP P9WFY1
G	274	HIS	-	expression tag	UNP P9WFY1
G	275	HIS	-	expression tag	UNP P9WFY1
G	276	HIS	-	expression tag	UNP P9WFY1
E	66	VAL	GLY	engineered mutation	UNP P9WFY1
E	271	HIS	-	expression tag	UNP P9WFY1
E	272	HIS	-	expression tag	UNP P9WFY1
E	273	HIS	-	expression tag	UNP P9WFY1
E	274	HIS	-	expression tag	UNP P9WFY1
E	275	HIS	-	expression tag	UNP P9WFY1
E	276	HIS	-	expression tag	UNP P9WFY1

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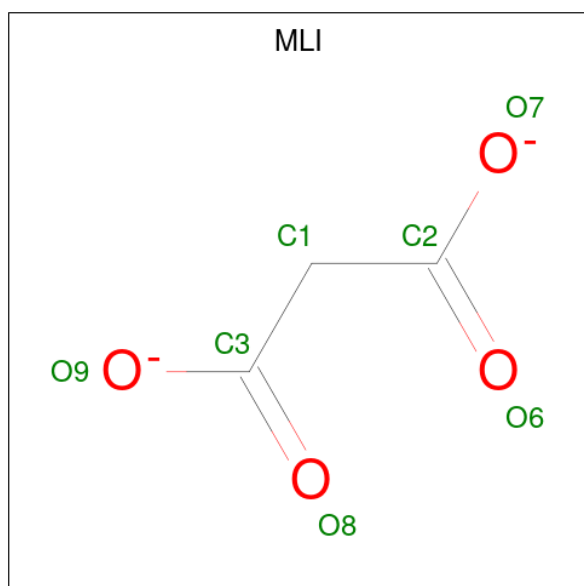
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Chain	Residue	Modelled	Actual	Comment	Reference
C	66	VAL	GLY	engineered mutation	UNP P9WFY1
C	271	HIS	-	expression tag	UNP P9WFY1
C	272	HIS	-	expression tag	UNP P9WFY1
C	273	HIS	-	expression tag	UNP P9WFY1
C	274	HIS	-	expression tag	UNP P9WFY1
C	275	HIS	-	expression tag	UNP P9WFY1
C	276	HIS	-	expression tag	UNP P9WFY1

- Molecule 2 is a protein called Tryptophan synthase beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	P	S	0	2	0
			3047	1901	551	580	1	14			
2	H	406	Total	C	N	O	P	S	0	1	0
			3044	1899	551	580	1	13			
2	F	399	Total	C	N	O	P	S	0	1	0
			2995	1869	540	572	1	13			
2	D	398	Total	C	N	O	P	S	0	0	0
			2980	1861	538	567	1	13			

- Molecule 3 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



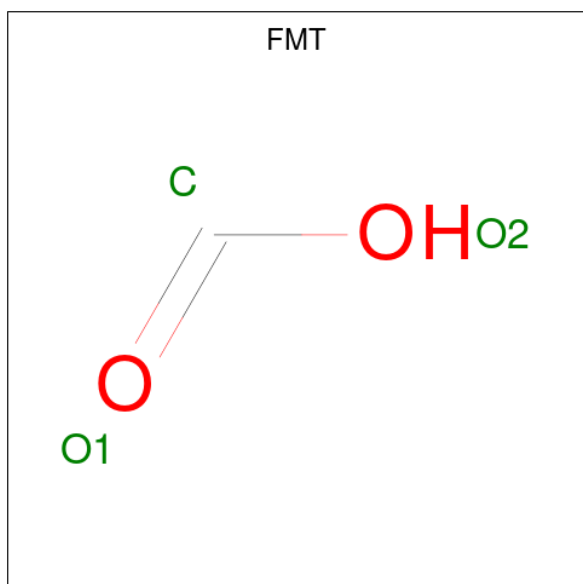
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	3	4		
3	B	1	Total	C	O	0	0
			7	3	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			7	3	4		
3	H	1	Total	C	O	0	0
			7	3	4		
3	E	1	Total	C	O	0	0
			7	3	4		
3	F	1	Total	C	O	0	0
			7	3	4		
3	C	1	Total	C	O	0	0
			7	3	4		
3	D	1	Total	C	O	0	0
			7	3	4		

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	G	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total C O 3 1 2	0	0
4	H	1	Total C O 3 1 2	0	0
4	H	1	Total C O 3 1 2	0	0
4	H	1	Total C O 3 1 2	0	0
4	H	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0
4	F	1	Total C O 3 1 2	0	0
4	F	1	Total C O 3 1 2	0	0
4	C	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	44	Total O 44 44	0	1
5	B	177	Total O 177 177	0	3
5	G	73	Total O 73 73	0	0
5	H	171	Total O 172 172	0	2

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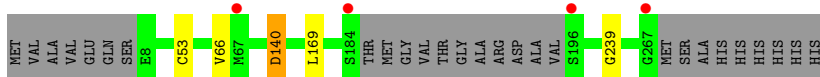
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	9	Total 9	O 9	0	0
5	F	122	Total 123	O 123	0	1
5	C	50	Total 50	O 50	0	0
5	D	149	Total 149	O 149	0	0

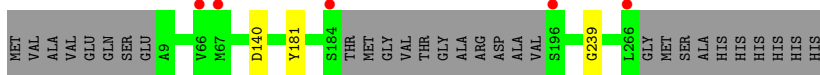
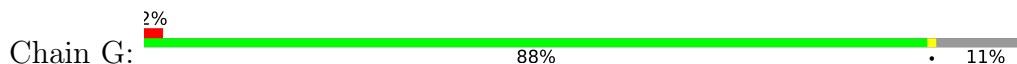
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

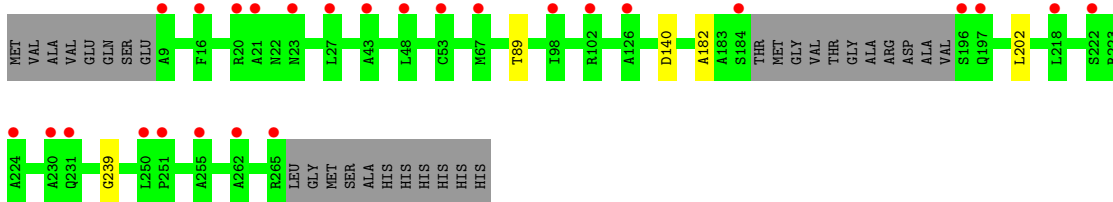
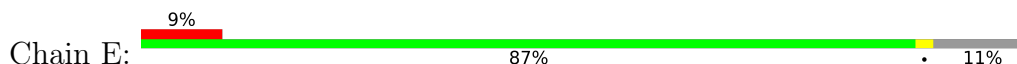
- Molecule 1: Tryptophan synthase alpha chain



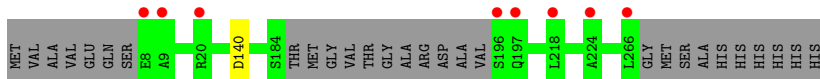
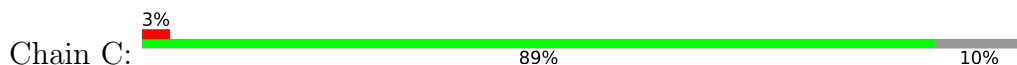
- Molecule 1: Tryptophan synthase alpha chain



- Molecule 1: Tryptophan synthase alpha chain



- Molecule 1: Tryptophan synthase alpha chain



- Molecule 2: Tryptophan synthase beta chain





- Molecule 2: Tryptophan synthase beta chain



- Molecule 2: Tryptophan synthase beta chain



- Molecule 2: Tryptophan synthase beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.32Å 158.81Å 166.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.35 30.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.35) 99.9 (30.00-2.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.175 , 0.206 0.180 , 0.208	Depositor DCC
R_{free} test set	2883 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20207	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MLI, LLP, FMT

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	0.75	0/1855	0.90	0/2531
1	C	0.76	0/1831	0.93	0/2500
1	E	0.75	0/1814	0.94	0/2477
1	G	0.76	0/1844	0.91	0/2516
2	B	0.76	0/3083	0.90	0/4177
2	D	0.82	0/3015	0.91	0/4085
2	F	0.74	0/3030	0.92	0/4106
2	H	0.82	0/3080	0.92	0/4174
All	All	0.77	0/19552	0.92	0/26566

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	1826	0	1847	1	0
1	C	1802	0	1825	0	0
1	E	1785	0	1808	1	0
1	G	1815	0	1843	0	0
2	B	3047	0	2959	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2980	0	2894	2	0
2	F	2995	0	2904	4	0
2	H	3044	0	2956	6	0
3	A	7	0	2	0	0
3	B	7	0	2	0	0
3	C	7	0	2	0	0
3	D	7	0	2	0	0
3	E	7	0	2	0	0
3	F	7	0	2	0	0
3	G	7	0	2	0	0
3	H	7	0	2	0	0
4	A	3	0	1	0	0
4	B	9	0	3	0	0
4	C	3	0	1	0	0
4	D	15	0	5	0	0
4	E	6	0	2	0	0
4	F	6	0	2	0	0
4	G	6	0	2	0	0
4	H	12	0	4	0	0
5	A	44	0	0	0	0
5	B	177	0	0	0	0
5	C	50	0	0	0	0
5	D	149	0	0	0	0
5	E	9	0	0	0	0
5	F	123	0	0	0	0
5	G	73	0	0	0	0
5	H	172	0	0	0	0
All	All	20207	0	19072	19	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 0.

All (19) 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)
2:F:230:ILE:HG21	2:F:238:PRO:HD3	1.87	0.56
2:H:34:LEU:HD11	2:H:188:PHE:HD2	1.76	0.51
2:B:242:VAL:HG12	2:B:267:VAL:HB	1.92	0.50
2:D:129:HIS:CE1	2:D:203:GLY:HA2	2.47	0.49
2:H:207:GLY:HA2	2:H:294:HIS:O	2.12	0.49
2:H:101:LLP:NZ	2:H:101:LLP:O3	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:123:GLU:HG3	2:D:184:ILE:CG1	2.45	0.47
2:B:123:GLU:OE1	2:B:200:TYR:OH	2.30	0.47
2:F:123:GLU:HG3	2:F:184:ILE:HG12	1.97	0.45
2:B:207:GLY:HA2	2:B:294:HIS:O	2.18	0.44
1:E:182:ALA:HB1	1:E:202:LEU:HD23	2.01	0.43
2:F:207:GLY:HA2	2:F:294:HIS:O	2.19	0.43
2:F:41:VAL:HG22	2:F:115:MET:HE1	2.00	0.43
1:A:140:ASP:OD1	1:A:140:ASP:N	2.50	0.42
2:B:129:HIS:CE1	2:B:203:GLY:HA2	2.55	0.42
2:B:5:ILE:HD11	2:H:225:GLU:HG2	2.01	0.42
2:H:230:ILE:HG21	2:H:238:PRO:HD3	2.03	0.41
2:H:129:HIS:CE1	2:H:203:GLY:HA2	2.56	0.40
2:B:402:LYS:HG3	2:B:407:LEU:HD12	2.03	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	247/276 (90%)	244 (99%)	2 (1%)	1 (0%)	30	34
1	C	244/276 (88%)	239 (98%)	5 (2%)	0	100	100
1	E	242/276 (88%)	236 (98%)	5 (2%)	1 (0%)	30	34
1	G	245/276 (89%)	240 (98%)	4 (2%)	1 (0%)	30	34
2	B	404/410 (98%)	399 (99%)	5 (1%)	0	100	100
2	D	395/410 (96%)	387 (98%)	8 (2%)	0	100	100
2	F	397/410 (97%)	388 (98%)	9 (2%)	0	100	100
2	H	404/410 (98%)	397 (98%)	7 (2%)	0	100	100
All	All	2578/2744 (94%)	2530 (98%)	45 (2%)	3 (0%)	48	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLY
1	E	239	GLY
1	G	239	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/201 (90%)	178 (98%)	4 (2%)	45	59
1	C	180/201 (90%)	179 (99%)	1 (1%)	78	87
1	E	178/201 (89%)	176 (99%)	2 (1%)	65	79
1	G	181/201 (90%)	179 (99%)	2 (1%)	65	79
2	B	300/301 (100%)	299 (100%)	1 (0%)	86	92
2	D	293/301 (97%)	291 (99%)	2 (1%)	76	86
2	F	295/301 (98%)	292 (99%)	3 (1%)	68	81
2	H	299/301 (99%)	295 (99%)	4 (1%)	61	76
All	All	1908/2008 (95%)	1889 (99%)	19 (1%)	68	81

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	CYS
1	A	66	VAL
1	A	140	ASP
1	A	169	LEU
2	B	256	HIS
1	G	140	ASP
1	G	181	TYR
2	H	128	GLN
2	H	256	HIS
2	H	300	LEU
2	H	315	SER

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Mol	Chain	Res	Type
1	E	89	THR
1	E	140	ASP
2	F	23	SER
2	F	184	ILE
2	F	256	HIS
1	C	140	ASP
2	D	128	GLN
2	D	256	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	52	GLN
2	B	96	HIS
1	G	143	GLN
1	G	225	GLN
2	H	52	GLN
2	H	80	GLN
2	H	81	HIS
2	F	96	HIS
2	F	108	GLN
2	F	231	GLN
2	D	96	HIS
2	D	104	ASN
2	D	108	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LLP	D	101	2	23,24,25	2.51	7 (30%)	25,32,34	1.68	7 (28%)
2	LLP	H	101	2	23,24,25	2.50	7 (30%)	25,32,34	1.68	6 (24%)
2	LLP	B	101	2	23,24,25	2.56	6 (26%)	25,32,34	1.62	4 (16%)
2	LLP	F	101	2	23,24,25	2.38	7 (30%)	25,32,34	1.47	4 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LLP	D	101	2	-	3/16/17/19	0/1/1/1
2	LLP	H	101	2	-	5/16/17/19	0/1/1/1
2	LLP	B	101	2	-	4/16/17/19	0/1/1/1
2	LLP	F	101	2	-	4/16/17/19	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	101	LLP	C4-C4'	7.91	1.63	1.46
2	D	101	LLP	C4-C4'	7.63	1.62	1.46
2	H	101	LLP	C4-C4'	7.19	1.61	1.46
2	F	101	LLP	C4-C4'	7.11	1.61	1.46
2	B	101	LLP	C4'-NZ	5.37	1.45	1.27
2	F	101	LLP	C4'-NZ	5.20	1.44	1.27
2	D	101	LLP	C4'-NZ	5.13	1.44	1.27
2	H	101	LLP	C4'-NZ	4.91	1.43	1.27
2	H	101	LLP	C4-C5	-4.74	1.35	1.42
2	D	101	LLP	C6-N1	3.29	1.41	1.34
2	B	101	LLP	C4-C5	-3.26	1.37	1.42
2	B	101	LLP	C2'-C2	3.20	1.55	1.50
2	F	101	LLP	C4-C5	-3.15	1.37	1.42
2	D	101	LLP	C4-C5	-3.06	1.37	1.42
2	H	101	LLP	C2'-C2	3.06	1.55	1.50
2	D	101	LLP	C2'-C2	2.97	1.55	1.50
2	F	101	LLP	C6-N1	2.96	1.40	1.34
2	B	101	LLP	C6-N1	2.92	1.40	1.34
2	F	101	LLP	C2'-C2	2.80	1.54	1.50
2	H	101	LLP	C6-N1	2.68	1.39	1.34
2	D	101	LLP	P-OP1	2.40	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	101	LLP	C5'-C5	2.30	1.56	1.50
2	D	101	LLP	C5'-C5	2.26	1.56	1.50
2	F	101	LLP	P-OP4	-2.19	1.53	1.60
2	F	101	LLP	P-OP2	-2.06	1.47	1.54
2	H	101	LLP	CB-CA	-2.03	1.50	1.53
2	B	101	LLP	P-OP2	-2.00	1.47	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	101	LLP	C4-C4'-NZ	-4.90	101.44	124.04
2	B	101	LLP	C4-C4'-NZ	-4.82	101.81	124.04
2	F	101	LLP	C4-C4'-NZ	-4.36	103.93	124.04
2	H	101	LLP	C4-C4'-NZ	-4.20	104.64	124.04
2	H	101	LLP	C3-C4-C5	3.33	120.95	118.28
2	B	101	LLP	OP4-C5'-C5	3.33	115.59	109.36
2	D	101	LLP	C3-C4-C4'	-3.02	114.95	120.40
2	D	101	LLP	OP4-C5'-C5	2.41	113.87	109.36
2	F	101	LLP	C2'-C2-N1	2.38	122.12	117.64
2	B	101	LLP	OP4-P-OP1	2.35	112.80	106.44
2	H	101	LLP	C2'-C2-N1	2.32	122.02	117.64
2	D	101	LLP	C5-C4-C4'	2.27	124.97	121.47
2	H	101	LLP	OP4-C5'-C5	2.22	113.51	109.36
2	F	101	LLP	C2'-C2-C3	-2.21	118.22	120.80
2	D	101	LLP	C3-C4-C5	2.15	120.00	118.28
2	H	101	LLP	C2'-C2-C3	-2.14	118.29	120.80
2	B	101	LLP	C5-C6-N1	-2.11	120.39	123.83
2	D	101	LLP	C2'-C2-C3	-2.10	118.33	120.80
2	D	101	LLP	C2'-C2-N1	2.08	121.56	117.64
2	F	101	LLP	C5-C6-N1	-2.06	120.49	123.83
2	H	101	LLP	CE-NZ-C4'	-2.03	112.20	118.72

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	101	LLP	C4-C4'-NZ-CE
2	H	101	LLP	C5'-OP4-P-OP1
2	F	101	LLP	C4-C4'-NZ-CE
2	H	101	LLP	CG-CD-CE-NZ
2	F	101	LLP	CG-CD-CE-NZ
2	D	101	LLP	C3-C4-C4'-NZ

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Mol	Chain	Res	Type	Atoms
2	B	101	LLP	CD-CE-NZ-C4'
2	H	101	LLP	CD-CE-NZ-C4'
2	F	101	LLP	CD-CE-NZ-C4'
2	D	101	LLP	C5-C4-C4'-NZ
2	F	101	LLP	C3-C4-C4'-NZ
2	D	101	LLP	CD-CE-NZ-C4'
2	B	101	LLP	C3-C4-C4'-NZ
2	H	101	LLP	C3-C4-C4'-NZ
2	B	101	LLP	C5-C4-C4'-NZ
2	B	101	LLP	C4-C4'-NZ-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	101	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MLI	E	301	-	6,6,6	1.09	0	7,7,7	0.98	0
4	FMT	B	502	-	2,2,2	0.69	0	1,1,1	0.67	0
3	MLI	A	301	-	6,6,6	1.12	0	7,7,7	1.15	0
3	MLI	F	501	-	6,6,6	1.19	0	7,7,7	1.26	1 (14%)
3	MLI	G	301	-	6,6,6	1.16	0	7,7,7	0.91	0
3	MLI	D	501	-	6,6,6	1.26	0	7,7,7	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MLI	B	501	-	6,6,6	1.22	0	7,7,7	1.09	0
4	FMT	B	503	-	2,2,2	0.77	0	1,1,1	0.68	0
4	FMT	H	505	-	2,2,2	0.83	0	1,1,1	0.50	0
4	FMT	H	504	-	2,2,2	0.80	0	1,1,1	0.61	0
4	FMT	D	504	-	2,2,2	0.74	0	1,1,1	0.65	0
4	FMT	D	506	-	2,2,2	0.72	0	1,1,1	0.68	0
4	FMT	C	302	-	2,2,2	0.83	0	1,1,1	0.57	0
4	FMT	F	503	-	2,2,2	0.70	0	1,1,1	0.70	0
3	MLI	C	301	-	6,6,6	1.13	0	7,7,7	1.05	0
4	FMT	E	303	-	2,2,2	0.70	0	1,1,1	0.69	0
4	FMT	F	502	-	2,2,2	0.69	0	1,1,1	0.70	0
4	FMT	G	303	-	2,2,2	0.67	0	1,1,1	0.74	0
4	FMT	D	503	-	2,2,2	0.70	0	1,1,1	0.67	0
3	MLI	H	501	-	6,6,6	1.27	0	7,7,7	1.02	0
4	FMT	G	302	-	2,2,2	0.77	0	1,1,1	0.56	0
4	FMT	A	302	-	2,2,2	0.86	0	1,1,1	0.49	0
4	FMT	D	505	-	2,2,2	0.63	0	1,1,1	0.75	0
4	FMT	H	503	-	2,2,2	0.74	0	1,1,1	0.48	0
4	FMT	D	502	-	2,2,2	0.65	0	1,1,1	0.72	0
4	FMT	B	504	-	2,2,2	0.65	0	1,1,1	0.74	0
4	FMT	E	302	-	2,2,2	0.69	0	1,1,1	0.71	0
4	FMT	H	502	-	2,2,2	0.74	0	1,1,1	0.68	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
3	MLI	B	501	-	-	4/4/4/4	-
3	MLI	F	501	-	-	2/4/4/4	-
3	MLI	C	301	-	-	0/4/4/4	-
3	MLI	E	301	-	-	2/4/4/4	-
3	MLI	A	301	-	-	0/4/4/4	-
3	MLI	G	301	-	-	0/4/4/4	-
3	MLI	H	501	-	-	2/4/4/4	-
3	MLI	D	501	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	F	501	MLI	O7-C2-C1	2.10	121.00	114.51

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	501	MLI	C2-C1-C3-O8
3	H	501	MLI	C2-C1-C3-O9
3	B	501	MLI	C3-C1-C2-O7
3	D	501	MLI	C2-C1-C3-O9
3	B	501	MLI	C3-C1-C2-O6
3	D	501	MLI	C3-C1-C2-O6
3	D	501	MLI	C3-C1-C2-O7
3	D	501	MLI	C2-C1-C3-O8
3	B	501	MLI	C2-C1-C3-O9
3	B	501	MLI	C2-C1-C3-O8
3	E	301	MLI	C2-C1-C3-O9
3	F	501	MLI	C2-C1-C3-O8
3	E	301	MLI	C2-C1-C3-O8
3	F	501	MLI	C2-C1-C3-O9

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	249/276 (90%)	-0.12	4 (1%) 70 76	22, 45, 64, 88	2 (0%)
1	C	248/276 (89%)	0.09	8 (3%) 50 57	30, 50, 81, 101	0
1	E	246/276 (89%)	0.96	26 (10%) 11 13	48, 80, 118, 136	0
1	G	247/276 (89%)	-0.22	5 (2%) 65 70	22, 42, 60, 77	2 (0%)
2	B	404/410 (98%)	-0.38	8 (1%) 65 70	15, 32, 52, 80	2 (0%)
2	D	397/410 (96%)	-0.38	2 (0%) 87 90	23, 32, 52, 66	0
2	F	398/410 (97%)	-0.29	8 (2%) 65 70	17, 35, 57, 81	1 (0%)
2	H	405/410 (98%)	-0.36	9 (2%) 62 67	16, 31, 53, 84	1 (0%)
All	All	2594/2744 (94%)	-0.15	70 (2%) 56 63	15, 38, 82, 136	8 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	4	ALA	8.1
1	C	196	SER	5.5
1	E	9	ALA	5.4
1	C	266	LEU	5.3
2	H	408	GLY	4.8
2	F	9	THR	4.8
1	E	184	SER	4.3
2	H	6	ALA	4.2
2	B	6	ALA	3.8
1	E	224	ALA	3.8
1	A	67	MET	3.7
2	B	8	PRO	3.7
1	E	53	CYS	3.3
1	A	184	SER	3.3
2	H	8	PRO	3.3
2	B	9	THR	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	408	GLY	3.1
1	G	184	SER	3.1
2	D	22	PRO	3.0
2	F	176	GLY	3.0
1	C	218	LEU	3.0
1	E	231	GLN	3.0
2	B	5	ILE	3.0
1	E	67	MET	2.9
1	E	20	ARG	2.9
1	E	98	ILE	2.9
1	A	267	GLY	2.9
1	E	251	PRO	2.9
1	G	196	SER	2.8
1	E	218	LEU	2.8
2	H	23	SER	2.7
1	E	265	ARG	2.7
1	E	222	SER	2.7
2	H	5	ILE	2.7
1	E	196	SER	2.7
2	H	22	PRO	2.7
2	H	188	PHE	2.6
1	C	9	ALA	2.6
1	E	126	ALA	2.6
1	E	255	ALA	2.6
2	F	22	PRO	2.6
2	B	202	PHE	2.5
1	G	66	VAL	2.5
1	C	224	ALA	2.4
2	B	7	GLU	2.4
2	H	7	GLU	2.3
1	E	250	LEU	2.2
1	E	21	ALA	2.2
1	E	48	LEU	2.2
1	E	23	ASN	2.2
2	B	409	ASN	2.2
1	E	230	ALA	2.2
1	E	27	LEU	2.2
2	D	180	LEU	2.2
1	G	67	MET	2.2
1	E	102	ARG	2.1
1	E	262	ALA	2.1
1	E	197	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	175	THR	2.1
2	F	21	GLY	2.1
1	C	20	ARG	2.1
1	E	16	PHE	2.1
1	A	196	SER	2.0
1	C	197	GLN	2.0
1	G	266	LEU	2.0
2	F	319	ASP	2.0
1	C	8	GLU	2.0
2	F	179	THR	2.0
1	E	43	ALA	2.0
2	F	309	ILE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LLP	H	101	24/25	0.98	0.06	22,24,26,27	0
2	LLP	F	101	24/25	0.98	0.05	24,27,29,29	0
2	LLP	D	101	24/25	0.98	0.06	23,24,26,27	0
2	LLP	B	101	24/25	0.99	0.05	25,27,28,29	0

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
4	FMT	B	503	3/3	0.70	0.22	64,64,67,68	0
4	FMT	H	503	3/3	0.74	0.20	56,56,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FMT	C	302	3/3	0.80	0.18	52,52,56,57	0
3	MLI	E	301	7/7	0.81	0.14	75,79,81,87	0
4	FMT	H	505	3/3	0.84	0.23	54,54,55,60	0
3	MLI	F	501	7/7	0.85	0.18	58,64,71,74	0
4	FMT	F	503	3/3	0.85	0.20	70,70,74,74	0
3	MLI	C	301	7/7	0.85	0.11	59,63,65,66	0
4	FMT	E	303	3/3	0.87	0.13	80,80,81,82	0
3	MLI	D	501	7/7	0.87	0.15	57,63,69,69	0
4	FMT	E	302	3/3	0.87	0.14	59,59,60,61	0
4	FMT	H	504	3/3	0.88	0.13	52,52,54,56	0
4	FMT	G	302	3/3	0.88	0.14	45,45,52,53	0
3	MLI	B	501	7/7	0.89	0.13	53,59,67,68	0
4	FMT	A	302	3/3	0.90	0.12	43,43,46,47	0
3	MLI	H	501	7/7	0.91	0.12	51,54,56,58	0
4	FMT	B	504	3/3	0.91	0.13	61,61,62,62	0
3	MLI	A	301	7/7	0.92	0.10	44,47,49,51	0
3	MLI	G	301	7/7	0.92	0.11	51,54,56,56	0
4	FMT	D	504	3/3	0.92	0.13	62,62,62,65	0
4	FMT	F	502	3/3	0.93	0.09	60,60,61,62	0
4	FMT	D	502	3/3	0.93	0.14	65,65,68,68	0
4	FMT	G	303	3/3	0.93	0.10	53,53,54,54	0
4	FMT	D	506	3/3	0.93	0.12	57,57,58,60	0
4	FMT	H	502	3/3	0.94	0.10	53,53,54,54	0
4	FMT	D	505	3/3	0.94	0.10	53,53,53,54	0
4	FMT	B	502	3/3	0.94	0.08	47,47,48,49	0
4	FMT	D	503	3/3	0.95	0.08	50,50,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.