



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:33 AM UTC

PDB ID : 2CHT / pdb_00002cht
Title : CRYSTAL STRUCTURES OF THE MONOFUNCTIONAL CHORISMATE
MUTASE FROM BACILLUS SUBTILIS AND ITS COMPLEX WITH A
TRANSITION STATE ANALOG
Authors : Chook, Y.M.; Ke, H.; Lipscomb, W.N.
Deposited on : 1994-04-08
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

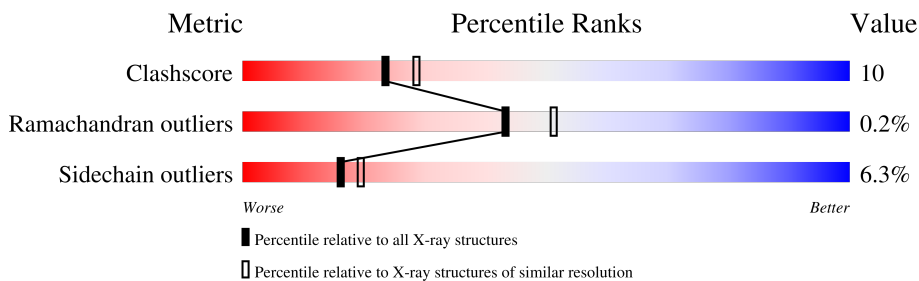
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)





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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	127	
1	B	127	
1	C	127	
1	D	127	
1	E	127	
1	F	127	
1	G	127	
1	H	127	

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Mol	Chain	Length	Quality of chain
1	I	127	 52% 34% 10% 10%
1	J	127	 56% 26% 10% 8%
1	K	127	 61% 25% 8% 10%
1	L	127	 46% 36% 7% 10%

2 Entry composition [i](#)

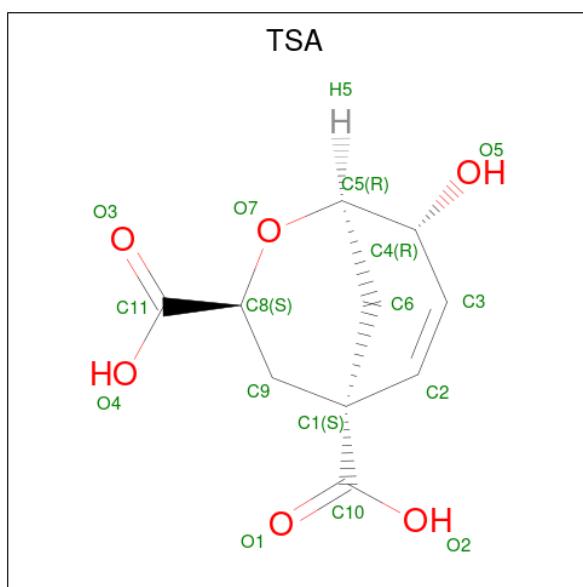
There are 3 unique types of molecules in this entry. The entry contains 15344 atoms, of which 3554 are hydrogens and 0 are deuteriums.

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 CHORISMATE MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	114	1106	570	201	156	171	8	0	0	0
1	B	117	1139	585	208	162	176	8	0	0	0
1	C	118	1148	591	209	163	177	8	0	0	0
1	D	114	1106	570	201	156	171	8	0	0	0
1	E	117	1139	585	208	162	176	8	0	0	0
1	F	118	1148	591	209	163	177	8	0	0	0
1	G	115	1123	576	207	160	172	8	0	0	0
1	H	116	1130	581	207	161	173	8	0	0	0
1	I	114	1106	570	201	156	171	8	0	0	0
1	J	117	1139	585	208	162	176	8	0	0	0
1	K	117	1139	585	208	162	176	8	0	0	0
1	L	114	1106	570	201	156	171	8	0	0	0

- Molecule 2 is 8-HYDROXY-2-OXA-BICYCLO[3.3.1]NON-6-ENE-3,5-DICARBOXYLIC ACID (CCD ID: TSA) (formula: C₁₀H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	H			O
2	A	1	17	10	1	6	0	0
2	B	1	17	10	1	6	0	0
2	C	1	17	10	1	6	0	0
2	D	1	17	10	1	6	0	0
2	E	1	17	10	1	6	0	0
2	F	1	17	10	1	6	0	0
2	G	1	17	10	1	6	0	0
2	H	1	17	10	1	6	0	0
2	I	1	17	10	1	6	0	0
2	J	1	17	10	1	6	0	0
2	K	1	17	10	1	6	0	0
2	L	1	17	10	1	6	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	49	Total	H	O	0	0
			147	98	49		
3	B	37	Total	H	O	0	0
			111	74	37		
3	C	56	Total	H	O	0	0
			168	112	56		
3	D	53	Total	H	O	0	0
			159	106	53		
3	E	50	Total	H	O	0	0
			150	100	50		
3	F	48	Total	H	O	0	0
			144	96	48		
3	G	42	Total	H	O	0	0
			126	84	42		
3	H	36	Total	H	O	0	0
			108	72	36		
3	I	39	Total	H	O	0	0
			117	78	39		
3	J	37	Total	H	O	0	0
			111	74	37		
3	K	45	Total	H	O	0	0
			135	90	45		
3	L	45	Total	H	O	0	0
			135	90	45		

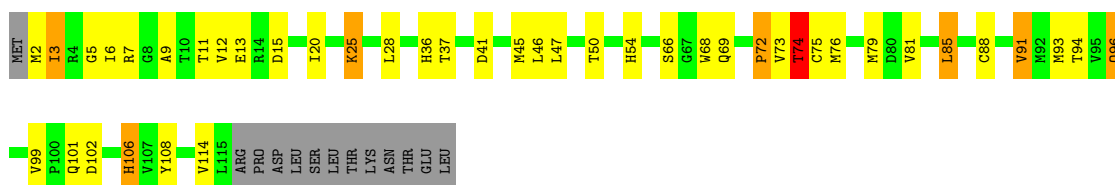
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

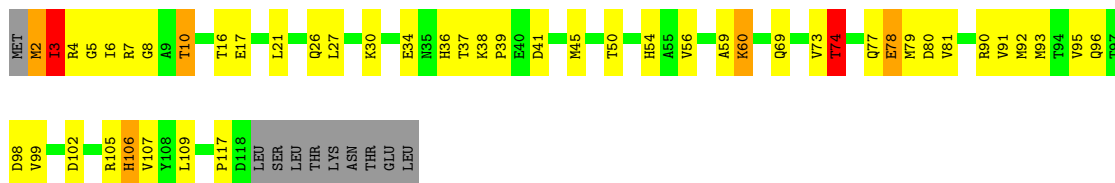
- Molecule 1: CHORISMATE MUTASE

Chain A: 



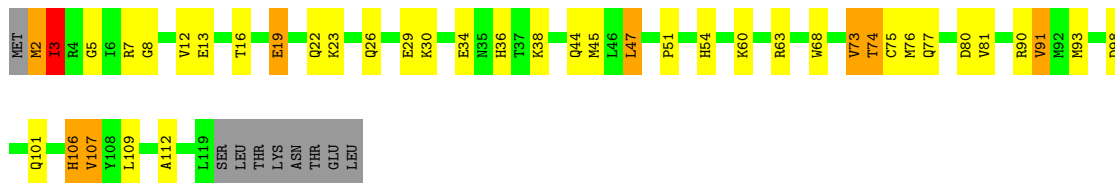
- Molecule 1: CHORISMATE MUTASE

Chain B: 



- Molecule 1: CHORISMATE MUTASE

Chain C: 



- Molecule 1: CHORISMATE MUTASE

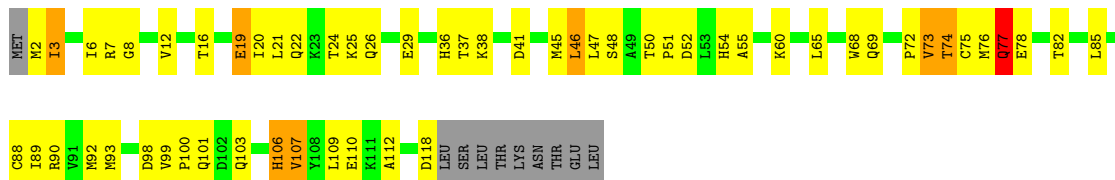
Chain D: 



V114
L115
ARG
PRO
ASP
LEU
SER
LEU
THR
LYS
ASN
THR
GLU
LEU

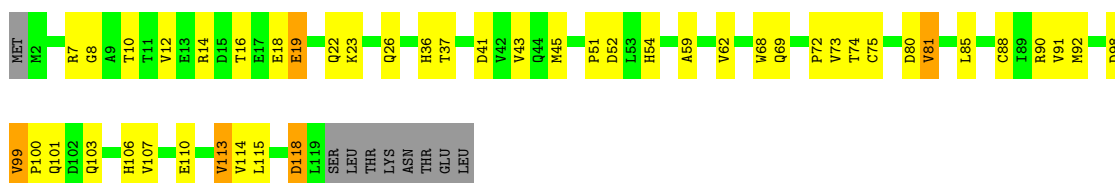
- Molecule 1: CHORISMATE MUTASE

Chain E: 47% 39% 6% • 8%



- Molecule 1: CHORISMATE MUTASE

Chain F: 57% 32% • 7%



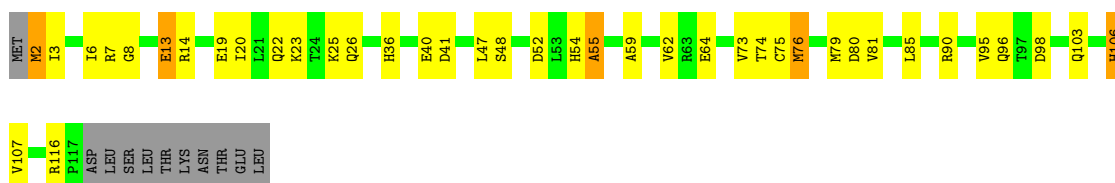
- Molecule 1: CHORISMATE MUTASE

Chain G: 61% 25% • • 9%



- Molecule 1: CHORISMATE MUTASE

Chain H: 60% 28% • 9%



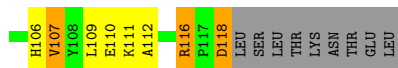
- Molecule 1: CHORISMATE MUTASE

Chain I: 52% 34% • 10%

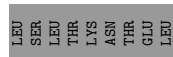




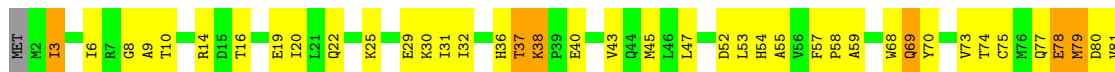
- Molecule 1: CHORISMATE MUTASE



- Molecule 1: CHORISMATE MUTASE



- Molecule 1: CHORISMATE MUTASE



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.40Å 68.30Å 102.80Å 90.00° 105.60° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	15344	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

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: TSA

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	0.99	5/917 (0.5%)	1.81	23/1240 (1.9%)
1	B	1.02	4/944 (0.4%)	1.81	21/1277 (1.6%)
1	C	0.95	4/952 (0.4%)	1.74	17/1288 (1.3%)
1	D	1.00	3/917 (0.3%)	1.75	11/1240 (0.9%)
1	E	0.99	4/944 (0.4%)	1.76	24/1277 (1.9%)
1	F	0.99	4/952 (0.4%)	1.82	19/1288 (1.5%)
1	G	0.92	3/928 (0.3%)	1.74	16/1254 (1.3%)
1	H	0.92	3/936 (0.3%)	1.66	13/1266 (1.0%)
1	I	0.97	4/917 (0.4%)	1.72	17/1240 (1.4%)
1	J	1.01	4/944 (0.4%)	1.73	21/1277 (1.6%)
1	K	0.99	5/944 (0.5%)	1.74	17/1277 (1.3%)
1	L	1.03	4/917 (0.4%)	1.81	22/1240 (1.8%)
All	All	0.98	47/11212 (0.4%)	1.76	221/15164 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
1	J	0	1
All	All	0	2

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	54	HIS	CD2-NE2	-7.14	1.30	1.37
1	K	54	HIS	CD2-NE2	-6.98	1.30	1.37
1	B	106	HIS	CD2-NE2	-6.97	1.30	1.37
1	C	54	HIS	CD2-NE2	-6.94	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	106	HIS	CD2-NE2	-6.91	1.30	1.37

The worst 5 of 221 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	THR	CA-CB-OG1	-12.81	90.39	109.60
1	F	118	ASP	CA-CB-CG	12.17	124.77	112.60
1	B	74	THR	CA-CB-CG2	9.70	126.98	110.50
1	E	98	ASP	CA-CB-CG	9.35	121.95	112.60
1	H	98	ASP	CA-CB-CG	8.84	121.44	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	116	ARG	Peptide
1	J	116	ARG	Peptide

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	905	201	936	19	0
1	B	931	208	960	17	0
1	C	939	209	971	21	0
1	D	905	201	936	20	0
1	E	931	208	960	26	0
1	F	939	209	971	19	0
1	G	916	207	949	20	0
1	H	923	207	956	20	0
1	I	905	201	936	25	0
1	J	931	208	960	28	0
1	K	931	208	960	17	0
1	L	905	201	936	27	2
2	A	16	1	10	0	0
2	B	16	1	10	1	0
2	C	16	1	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	16	1	10	1	0
2	E	16	1	10	1	0
2	F	16	1	10	1	0
2	G	16	1	10	1	0
2	H	16	1	10	1	0
2	I	16	1	10	1	0
2	J	16	1	10	1	0
2	K	16	1	10	1	0
2	L	16	1	10	1	0
3	A	49	98	0	0	0
3	B	37	74	0	0	0
3	C	56	112	0	0	0
3	D	53	106	0	0	1
3	E	50	100	0	0	0
3	F	48	96	0	0	1
3	G	42	84	0	0	0
3	H	36	72	0	0	0
3	I	39	78	0	0	0
3	J	37	74	0	0	0
3	K	45	90	0	0	0
3	L	45	90	0	0	0
All	All	11790	3554	11551	233	2

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 10.

The worst 5 of 233 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:D:74:THR:HA	2:E:204:TSA:H3	1.52	0.89
1:J:45:MET:HB3	1:J:73:VAL:HG12	1.59	0.84
1:G:74:THR:HA	2:H:207:TSA:H3	1.60	0.84
1:J:74:THR:HA	2:K:210:TSA:H3	1.61	0.83
1:K:74:THR:HA	2:L:211:TSA:H3	1.61	0.81

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:86:LYS:HZ2	3:F:228:HOH:H2[1_556]	1.26	0.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:96:GLN:O	3:D:272:HOH:H1[2_746]	1.57	0.03

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	112/127 (88%)	107 (96%)	5 (4%)	0	100	100
1	B	115/127 (91%)	108 (94%)	6 (5%)	1 (1%)	14	14
1	C	116/127 (91%)	108 (93%)	8 (7%)	0	100	100
1	D	112/127 (88%)	104 (93%)	8 (7%)	0	100	100
1	E	115/127 (91%)	108 (94%)	7 (6%)	0	100	100
1	F	116/127 (91%)	108 (93%)	7 (6%)	1 (1%)	14	14
1	G	113/127 (89%)	105 (93%)	8 (7%)	0	100	100
1	H	114/127 (90%)	107 (94%)	7 (6%)	0	100	100
1	I	112/127 (88%)	105 (94%)	7 (6%)	0	100	100
1	J	115/127 (91%)	108 (94%)	7 (6%)	0	100	100
1	K	115/127 (91%)	112 (97%)	3 (3%)	0	100	100
1	L	112/127 (88%)	104 (93%)	7 (6%)	1 (1%)	14	14
All	All	1367/1524 (90%)	1284 (94%)	80 (6%)	3 (0%)	43	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	118	ASP
1	L	101	GLN
1	B	117	PRO

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	103/116 (89%)	93 (90%)	10 (10%)	8	8
1	B	106/116 (91%)	99 (93%)	7 (7%)	15	18
1	C	107/116 (92%)	95 (89%)	12 (11%)	6	5
1	D	103/116 (89%)	99 (96%)	4 (4%)	28	39
1	E	106/116 (91%)	100 (94%)	6 (6%)	18	23
1	F	107/116 (92%)	100 (94%)	7 (6%)	15	18
1	G	104/116 (90%)	97 (93%)	7 (7%)	15	17
1	H	105/116 (90%)	102 (97%)	3 (3%)	37	51
1	I	103/116 (89%)	99 (96%)	4 (4%)	28	39
1	J	106/116 (91%)	99 (93%)	7 (7%)	15	18
1	K	106/116 (91%)	98 (92%)	8 (8%)	12	14
1	L	103/116 (89%)	99 (96%)	4 (4%)	28	39
All	All	1259/1392 (90%)	1180 (94%)	79 (6%)	16	19

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	69	GLN
1	K	63	ARG
1	I	98	ASP
1	J	77	GLN
1	L	37	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	26	GLN
1	J	106	HIS
1	I	44	GLN
1	J	44	GLN

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Mol	Chain	Res	Type
1	K	44	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TSA	H	207	-	16,17,17	1.25	2 (12%)	16,26,26	1.52	3 (18%)
2	TSA	A	203	-	16,17,17	1.30	2 (12%)	16,26,26	1.49	2 (12%)
2	TSA	E	204	-	16,17,17	1.17	2 (12%)	16,26,26	1.62	5 (31%)
2	TSA	I	208	-	16,17,17	1.26	2 (12%)	16,26,26	1.40	3 (18%)
2	TSA	G	209	-	16,17,17	1.18	2 (12%)	16,26,26	1.34	3 (18%)
2	TSA	K	210	-	16,17,17	1.46	3 (18%)	16,26,26	1.73	3 (18%)
2	TSA	B	201	-	16,17,17	1.35	4 (25%)	16,26,26	1.73	5 (31%)
2	TSA	J	212	-	16,17,17	1.24	2 (12%)	16,26,26	1.38	2 (12%)
2	TSA	D	206	-	16,17,17	1.24	3 (18%)	16,26,26	1.62	4 (25%)
2	TSA	F	205	-	16,17,17	1.10	1 (6%)	16,26,26	1.72	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TSA	L	211	-	16,17,17	1.20	2 (12%)	16,26,26	1.71	5 (31%)
2	TSA	C	202	-	16,17,17	1.24	3 (18%)	16,26,26	1.53	2 (12%)

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	TSA	H	207	-	-	6/10/34/34	1/3/2/2
2	TSA	A	203	-	-	6/10/34/34	1/3/2/2
2	TSA	E	204	-	-	3/10/34/34	1/3/2/2
2	TSA	I	208	-	-	6/10/34/34	1/3/2/2
2	TSA	G	209	-	-	5/10/34/34	1/3/2/2
2	TSA	K	210	-	-	6/10/34/34	1/3/2/2
2	TSA	B	201	-	-	4/10/34/34	1/3/2/2
2	TSA	J	212	-	-	6/10/34/34	1/3/2/2
2	TSA	D	206	-	-	5/10/34/34	1/3/2/2
2	TSA	F	205	-	-	5/10/34/34	1/3/2/2
2	TSA	L	211	-	-	5/10/34/34	1/3/2/2
2	TSA	C	202	-	-	5/10/34/34	1/3/2/2

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	210	TSA	C8-C11	3.56	1.56	1.52
2	A	203	TSA	C8-C11	2.75	1.55	1.52
2	K	210	TSA	C3-C2	2.58	1.36	1.32
2	H	207	TSA	C3-C2	2.56	1.36	1.32
2	B	201	TSA	O5-C4	-2.48	1.39	1.43

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	202	TSA	O7-C8-C9	3.63	115.10	109.95
2	K	210	TSA	O7-C8-C11	3.56	114.43	107.72
2	F	205	TSA	O7-C8-C11	3.50	114.33	107.72
2	K	210	TSA	C9-C1-C10	-3.39	101.84	109.84
2	E	204	TSA	C9-C1-C10	-3.16	102.39	109.84

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	203	TSA	C6-C1-C10-O2
2	I	208	TSA	C6-C1-C10-O2
2	J	212	TSA	C6-C1-C10-O2
2	K	210	TSA	C6-C1-C10-O2
2	L	211	TSA	C6-C1-C10-O2

5 of 12 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	211	TSA	C1-C2-C3-C4-C5-C8-C9-O7
2	F	205	TSA	C1-C2-C3-C4-C5-C8-C9-O7
2	I	208	TSA	C1-C2-C3-C4-C5-C8-C9-O7
2	C	202	TSA	C1-C2-C3-C4-C5-C8-C9-O7
2	J	212	TSA	C1-C2-C3-C4-C5-C8-C9-O7

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	207	TSA	1	0
2	E	204	TSA	1	0
2	I	208	TSA	1	0
2	G	209	TSA	1	0
2	K	210	TSA	1	0
2	B	201	TSA	1	0
2	J	212	TSA	1	0
2	D	206	TSA	1	0
2	F	205	TSA	1	0
2	L	211	TSA	1	0
2	C	202	TSA	2	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.