wwPDB X-ray Structure Validation Summary Report (i)

Jun 11, 2024 – 11:29 PM EDT

PDB ID	:	1COM
Title	:	THE MONOFUNCTIONAL CHORISMATE MUTASE FROM BACILLUS SUBTILIS: STRUCTURE DETERMINATION OF CHORISMATE MUTASE AND ITS COMPLEXES WITH A TRANSITION STATE ANALOG AND PREPHENATE, AND IMPLICATIONS ON THE MECHANISM OF ENZYMATIC REACTION
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 (i) 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 (i)) were used in the production of this report:

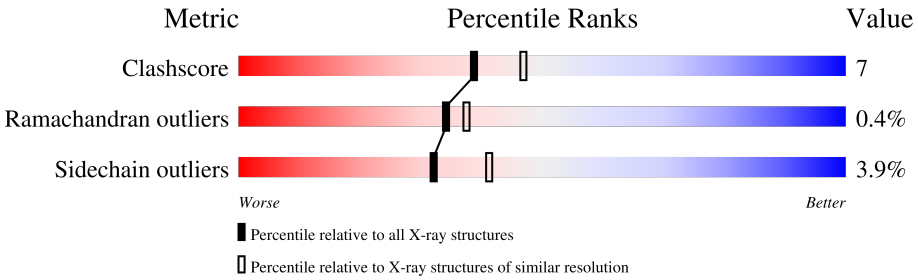
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	127	72% 16% • 10%
1	B	127	70% 20% • 7%
1	C	127	65% 25% • 6%
1	D	127	69% 19% • 10%
1	E	127	71% 17% 5% 7%
1	F	127	64% 24% • 8%
1	G	127	70% 18% • 10%
1	H	127	66% 20% • • 10%

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Mol	Chain	Length	Quality of chain
1	I	127	68% 20% • 10%
1	J	127	72% 16% • 10%
1	K	127	65% 23% • 9%
1	L	127	65% 23% • 10%

2 Entry composition (i)

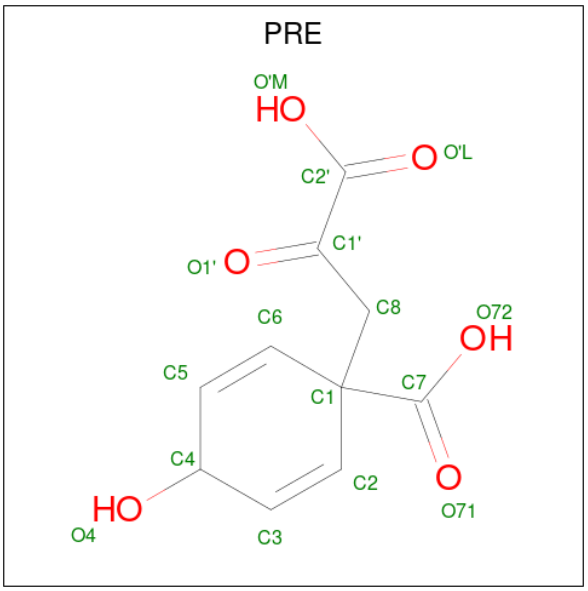
There are 3 unique types of molecules in this entry. The entry contains 15125 atoms, of which 3466 are hydrogens and 0 are deuteriums.

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
1	A	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	B	118	Total	C	H	N	O	S	0	0	0
			1148	591	209	163	177	8			
1	C	119	Total	C	H	N	O	S	0	0	0
			1156	594	211	164	179	8			
1	D	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	E	118	Total	C	H	N	O	S	0	0	0
			1148	591	209	163	177	8			
1	F	117	Total	C	H	N	O	S	0	0	0
			1139	585	208	162	176	8			
1	G	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	H	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	I	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	J	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	K	116	Total	C	H	N	O	S	0	0	0
			1130	581	207	161	173	8			
1	L	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			

- Molecule 2 is PREPHENIC ACID (three-letter code: PRE) (formula: $C_{10}H_{10}O_6$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	36	Total H O 108 72 36	0	0
3	B	42	Total H O 126 84 42	0	0
3	C	44	Total H O 132 88 44	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	37	Total H O 111 74 37	0	0
3	E	45	Total H O 135 90 45	0	0
3	F	57	Total H O 171 114 57	0	0
3	G	33	Total H O 99 66 33	0	0
3	H	16	Total H O 48 32 16	0	0
3	I	49	Total H O 147 98 49	0	0
3	J	36	Total H O 108 72 36	0	0
3	K	38	Total H O 114 76 38	0	0
3	L	70	Total H O 210 140 70	0	0

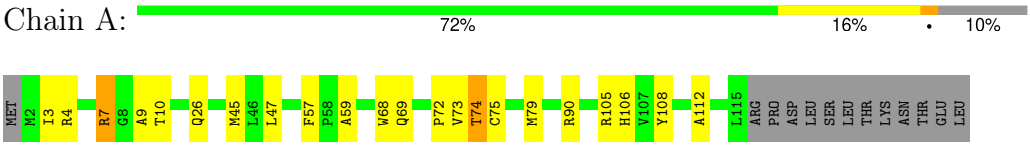
3 Residue-property plots (i)

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. 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.

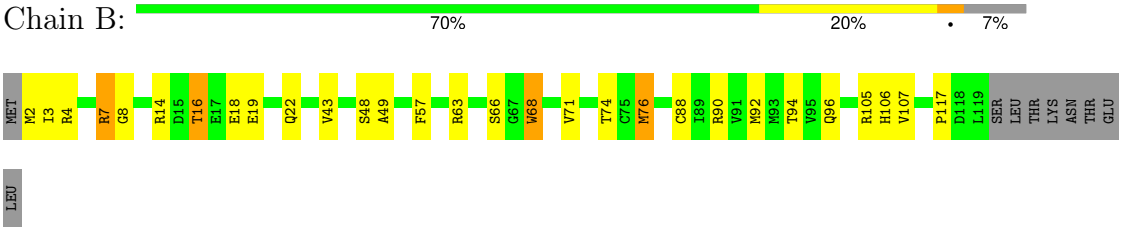
• Molecule 1: CHORISMATE MUTASE

Chain A:



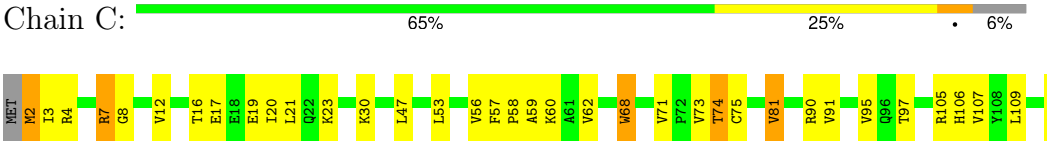
• Molecule 1: CHORISMATE MUTASE

Chain B:



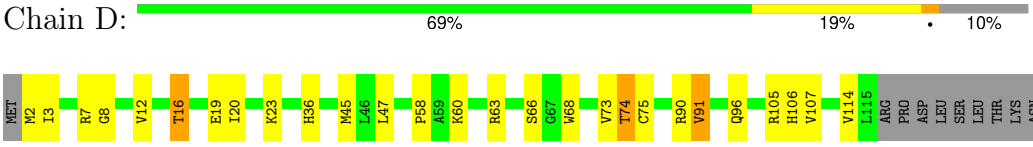
• Molecule 1: CHORISMATE MUTASE

Chain C:



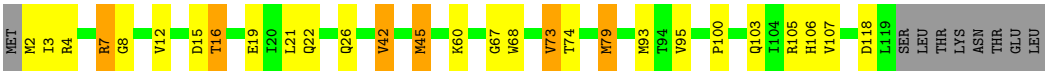
• Molecule 1: CHORISMATE MUTASE

Chain D:



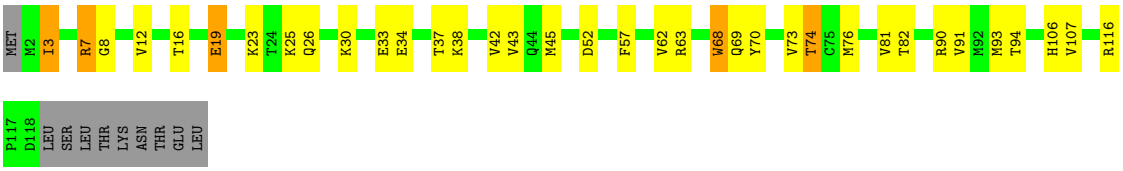
• Molecule 1: CHORISMATE MUTASE

Chain E:



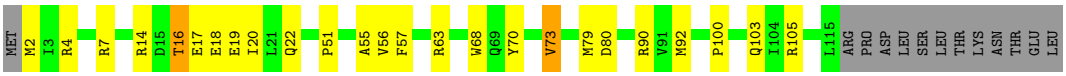
• Molecule 1: CHORISMATE MUTASE

Chain F:



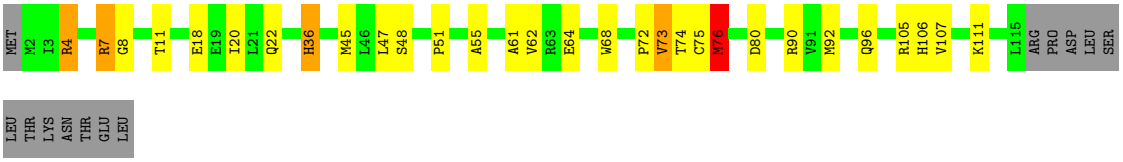
• Molecule 1: CHORISMATE MUTASE

Chain G:



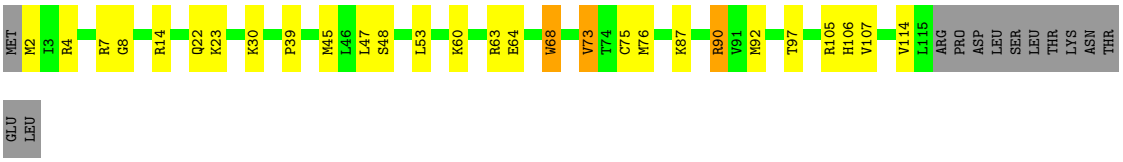
• Molecule 1: CHORISMATE MUTASE

Chain H:



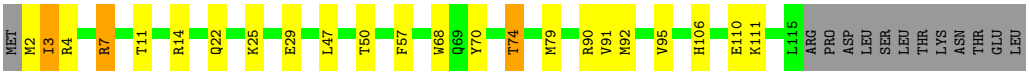
• Molecule 1: CHORISMATE MUTASE

Chain I:



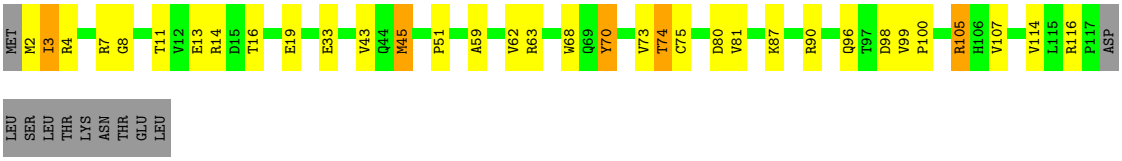
• Molecule 1: CHORISMATE MUTASE

Chain J:



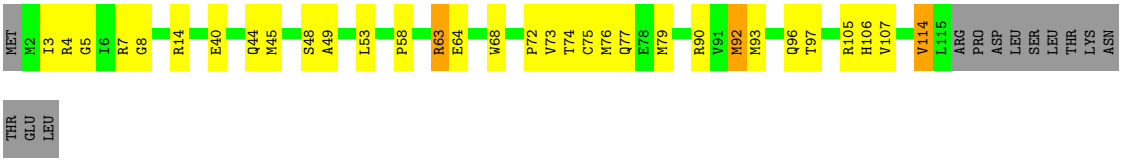
• Molecule 1: CHORISMATE MUTASE

Chain K:



• Molecule 1: CHORISMATE MUTASE

Chain L:



4 Data and refinement statistics (i)

Xtriage (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}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15125	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PRE

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	0.80	0/917	1.46	12/1240 (1.0%)
1	B	0.79	0/952	1.46	14/1288 (1.1%)
1	C	0.76	0/958	1.47	13/1296 (1.0%)
1	D	0.82	0/917	1.47	7/1240 (0.6%)
1	E	0.81	0/952	1.53	14/1288 (1.1%)
1	F	0.79	0/944	1.44	16/1277 (1.3%)
1	G	0.79	0/917	1.47	16/1240 (1.3%)
1	H	0.76	0/917	1.43	12/1240 (1.0%)
1	I	0.81	0/917	1.48	12/1240 (1.0%)
1	J	0.80	0/917	1.51	13/1240 (1.0%)
1	K	0.78	0/936	1.47	17/1266 (1.3%)
1	L	0.82	0/917	1.54	19/1240 (1.5%)
All	All	0.79	0/11161	1.48	165/15095 (1.1%)

There are no bond length outliers.

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	7	ARG	NE-CZ-NH2	-11.68	114.46	120.30
1	D	105	ARG	NE-CZ-NH2	-11.21	114.69	120.30
1	H	4	ARG	NE-CZ-NH1	10.41	125.50	120.30
1	B	4	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	E	4	ARG	NE-CZ-NH1	10.19	125.40	120.30

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	905	201	936	13	0
1	B	939	209	971	18	0
1	C	945	211	976	27	0
1	D	905	201	936	18	2
1	E	939	209	971	19	1
1	F	931	208	960	19	1
1	G	905	201	936	6	0
1	H	905	201	936	15	1
1	I	905	201	936	12	0
1	J	905	201	936	9	0
1	K	923	207	956	15	1
1	L	905	201	936	12	1
2	A	16	1	8	4	0
2	B	16	1	8	2	0
2	C	16	1	8	1	0
2	D	16	1	8	3	0
2	E	16	1	8	1	0
2	F	16	1	8	1	0
2	G	16	1	8	0	0
2	H	16	1	8	1	0
2	K	16	1	8	2	0
3	A	36	72	0	0	0
3	B	42	84	0	0	0
3	C	44	88	0	0	0
3	D	37	74	0	0	1
3	E	45	90	0	0	1
3	F	57	114	0	0	0
3	G	33	66	0	0	0
3	H	16	32	0	0	0
3	I	49	98	0	0	0
3	J	36	72	0	0	0
3	K	38	76	0	1	0
3	L	70	140	0	0	3
All	All	11659	3466	11458	169	6

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 7.

The worst 5 of 169 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:H:45:MET:HB3	1:H:73:VAL:HG12	1.58	0.84
1:G:100:PRO:HG2	1:G:103:GLN:HG3	1.61	0.82
1:B:7:ARG:H	1:B:106:HIS:HD2	1.34	0.76
1:F:7:ARG:H	1:F:106:HIS:HD2	1.31	0.74
1:D:7:ARG:H	1:D:106:HIS:HD2	1.33	0.74

The worst 5 of 6 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:F:38:LYS:HZ2	1:H:36:HIS:HD1[2_656]	1.29	0.31
1:D:96:GLN:O	3:L:797:HOH:H2[2_756]	1.56	0.04
1:E:67:GLY:O	3:E:734:HOH:H2[2_756]	1.56	0.04
1:L:96:GLN:O	3:D:326:HOH:H1[2_746]	1.57	0.03
1:D:36:HIS:O	3:L:495:HOH:H2[2_756]	1.60	0.00

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%)	110 (98%)	2 (2%)	0	100	100
1	B	116/127 (91%)	111 (96%)	4 (3%)	1 (1%)	17	16
1	C	117/127 (92%)	110 (94%)	7 (6%)	0	100	100
1	D	112/127 (88%)	105 (94%)	5 (4%)	2 (2%)	8	5
1	E	116/127 (91%)	112 (97%)	3 (3%)	1 (1%)	17	16
1	F	115/127 (91%)	111 (96%)	4 (4%)	0	100	100
1	G	112/127 (88%)	107 (96%)	5 (4%)	0	100	100
1	H	112/127 (88%)	108 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	112/127 (88%)	107 (96%)	5 (4%)	0	100	100
1	J	112/127 (88%)	110 (98%)	2 (2%)	0	100	100
1	K	114/127 (90%)	112 (98%)	2 (2%)	0	100	100
1	L	112/127 (88%)	108 (96%)	3 (3%)	1 (1%)	17	16
All	All	1362/1524 (89%)	1311 (96%)	46 (3%)	5 (0%)	34	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	118	ASP
1	L	44	GLN
1	B	117	PRO
1	D	66	SER
1	D	114	VAL

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%)	100 (97%)	3 (3%)	42	54
1	B	107/116 (92%)	101 (94%)	6 (6%)	21	25
1	C	108/116 (93%)	105 (97%)	3 (3%)	43	56
1	D	103/116 (89%)	100 (97%)	3 (3%)	42	54
1	E	107/116 (92%)	105 (98%)	2 (2%)	57	71
1	F	106/116 (91%)	99 (93%)	7 (7%)	16	19
1	G	103/116 (89%)	98 (95%)	5 (5%)	25	31
1	H	103/116 (89%)	101 (98%)	2 (2%)	57	71
1	I	103/116 (89%)	100 (97%)	3 (3%)	42	54
1	J	103/116 (89%)	99 (96%)	4 (4%)	32	41
1	K	105/116 (90%)	98 (93%)	7 (7%)	16	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	103/116 (89%)	99 (96%)	4 (4%)	32 41
All	All	1254/1392 (90%)	1205 (96%)	49 (4%)	32 41

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	73	VAL
1	J	22	GLN
1	H	76	MET
1	I	73	VAL
1	J	74	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	44	GLN
1	K	101	GLN
1	L	106	HIS
1	E	44	GLN
1	D	106	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

9 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	PRE	E	224	-	16,16,16	1.52	3 (18%)	14,23,23	1.84	5 (35%)
2	PRE	A	223	-	16,16,16	1.62	3 (18%)	14,23,23	1.75	4 (28%)
2	PRE	G	229	-	16,16,16	1.50	2 (12%)	14,23,23	1.68	2 (14%)
2	PRE	H	227	-	16,16,16	1.65	3 (18%)	14,23,23	2.02	5 (35%)
2	PRE	D	226	-	16,16,16	1.61	3 (18%)	14,23,23	1.64	5 (35%)
2	PRE	B	221	-	16,16,16	1.43	2 (12%)	14,23,23	1.56	2 (14%)
2	PRE	K	230	-	16,16,16	1.59	4 (25%)	14,23,23	1.65	3 (21%)
2	PRE	C	222	-	16,16,16	1.69	5 (31%)	14,23,23	1.63	2 (14%)
2	PRE	F	225	-	16,16,16	1.50	1 (6%)	14,23,23	1.85	4 (28%)

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	PRE	E	224	-	-	0/15/27/27	0/1/1/1
2	PRE	A	223	-	-	0/15/27/27	0/1/1/1
2	PRE	G	229	-	-	3/15/27/27	0/1/1/1
2	PRE	H	227	-	-	4/15/27/27	0/1/1/1
2	PRE	D	226	-	-	2/15/27/27	0/1/1/1
2	PRE	B	221	-	-	5/15/27/27	0/1/1/1
2	PRE	K	230	-	-	2/15/27/27	0/1/1/1
2	PRE	C	222	-	-	1/15/27/27	0/1/1/1
2	PRE	F	225	-	-	5/15/27/27	0/1/1/1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	229	PRE	C8-C1'	2.97	1.54	1.51
2	D	226	PRE	C5-C6	2.92	1.36	1.32
2	A	223	PRE	C5-C6	2.82	1.36	1.32
2	C	222	PRE	C8-C1'	2.73	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	221	PRE	O'M-C2'	-2.72	1.23	1.30

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	227	PRE	C4-C5-C6	-4.76	119.49	123.40
2	F	225	PRE	O'L-C2'-C1'	-3.68	117.23	121.81
2	A	223	PRE	C4-C3-C2	-3.59	120.44	123.40
2	G	229	PRE	C4-C5-C6	-3.32	120.67	123.40
2	F	225	PRE	C4-C3-C2	-3.31	120.67	123.40

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	221	PRE	C2'-C1'-C8-C1
2	B	221	PRE	C8-C1'-C2'-O'L
2	B	221	PRE	C8-C1'-C2'-O'M
2	F	225	PRE	C6-C1-C7-O72
2	F	225	PRE	C8-C1'-C2'-O'M

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	224	PRE	1	0
2	A	223	PRE	4	0
2	H	227	PRE	1	0
2	D	226	PRE	3	0
2	B	221	PRE	2	0
2	K	230	PRE	2	0
2	C	222	PRE	1	0
2	F	225	PRE	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

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.