



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 20, 2017 – 10:41 AM EDT

PDB ID : 3ZUH
EMDB ID: : EMD-1932
Title : Negative stain EM Map of the AAA protein CbbX, a red-type Rubisco activase from *R. sphaeroides*
Authors : Mueller-Cajar, O.; Stotz, M.; Wendler, P.; Hartl, F.U.; Bracher, A.; Hayer-Hartl, M.
Deposited on : unknown
Resolution : 21.00 Å(reported)
Based on PDB ID : 3SYL

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

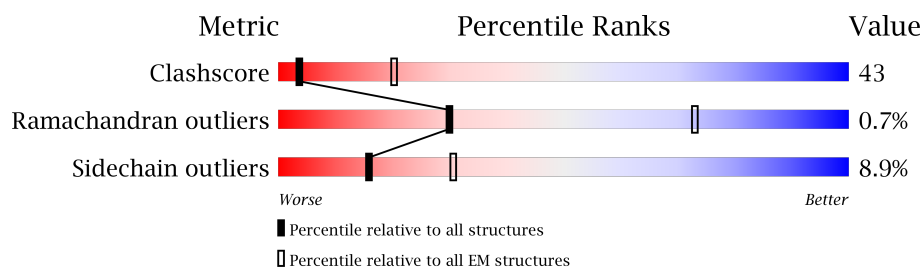
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 21.00 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	289	
1	B	289	
1	C	289	
1	D	289	
1	E	289	
1	F	289	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	RUB	A	1298	X	-	-	-
2	RUB	B	1298	X	-	-	-
2	RUB	C	1298	X	-	-	-
2	RUB	D	1298	X	-	-	-
2	RUB	E	1298	X	-	-	-
2	RUB	F	1298	X	-	-	-
3	ADP	A	1299	-	-	X	-
3	ADP	B	1299	-	-	X	-
3	ADP	C	1299	-	-	X	-
3	ADP	D	1299	-	-	X	-
3	ADP	E	1299	-	-	X	-
3	ADP	F	1299	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13884 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

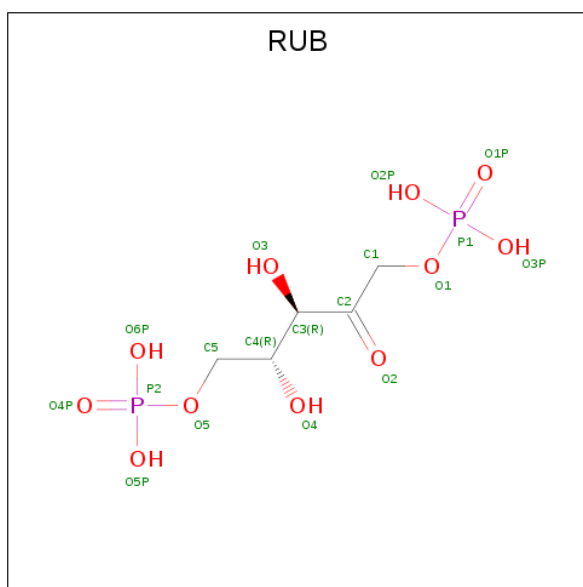
- Molecule 1 is a protein called PROTEIN CBBX.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	286	Total	C	N	O	S	0	0
			2269	1419	417	426	7		
1	B	286	Total	C	N	O	S	0	0
			2269	1419	417	426	7		
1	C	286	Total	C	N	O	S	0	0
			2269	1419	417	426	7		
1	D	286	Total	C	N	O	S	0	0
			2269	1419	417	426	7		
1	E	286	Total	C	N	O	S	0	0
			2269	1419	417	426	7		
1	F	286	Total	C	N	O	S	0	0
			2269	1419	417	426	7		

There are 6 discrepancies between the modelled and reference sequences:

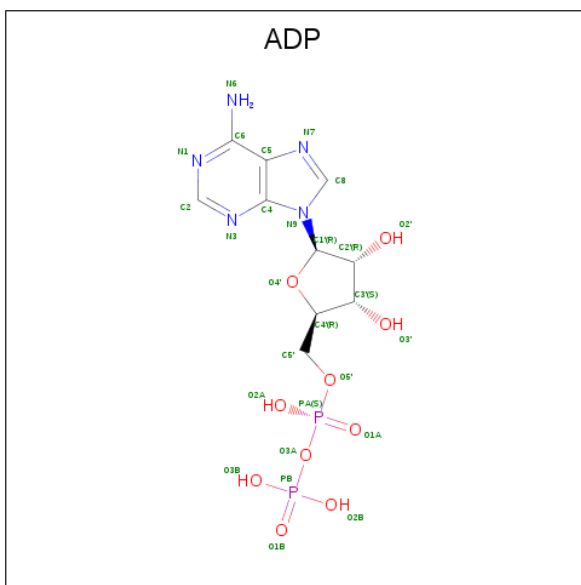
Chain	Residue	Modelled	Actual	Comment	Reference
A	282	ILE	MET	conflict	UNP P95648
B	282	ILE	MET	conflict	UNP P95648
C	282	ILE	MET	conflict	UNP P95648
D	282	ILE	MET	conflict	UNP P95648
E	282	ILE	MET	conflict	UNP P95648
F	282	ILE	MET	conflict	UNP P95648

- Molecule 2 is RIBULOSE-1,5-DIPHOSPHATE (three-letter code: RUB) (formula: $C_5H_{12}O_{11}P_2$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			18	5	11	2	
2	B	1	Total	C	O	P	0
			18	5	11	2	
2	C	1	Total	C	O	P	0
			18	5	11	2	
2	D	1	Total	C	O	P	0
			18	5	11	2	
2	E	1	Total	C	O	P	0
			18	5	11	2	
2	F	1	Total	C	O	P	0
			18	5	11	2	

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

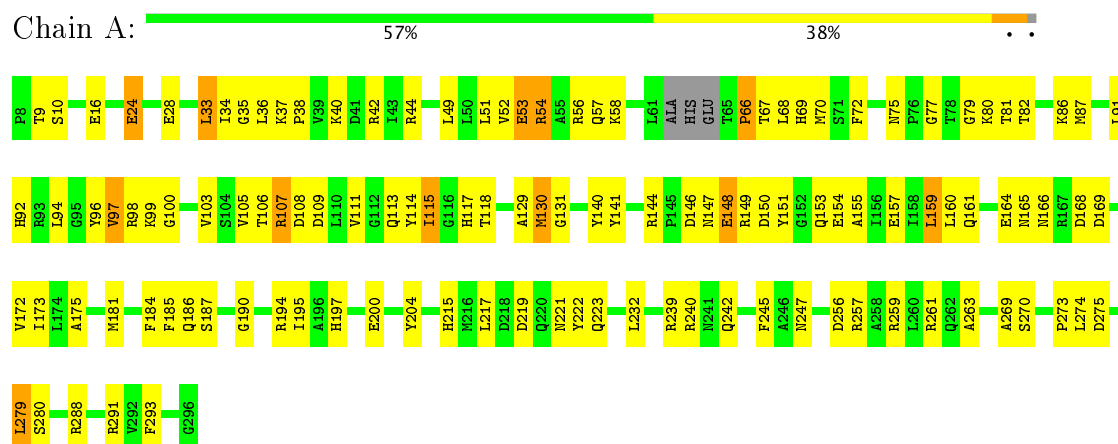


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0

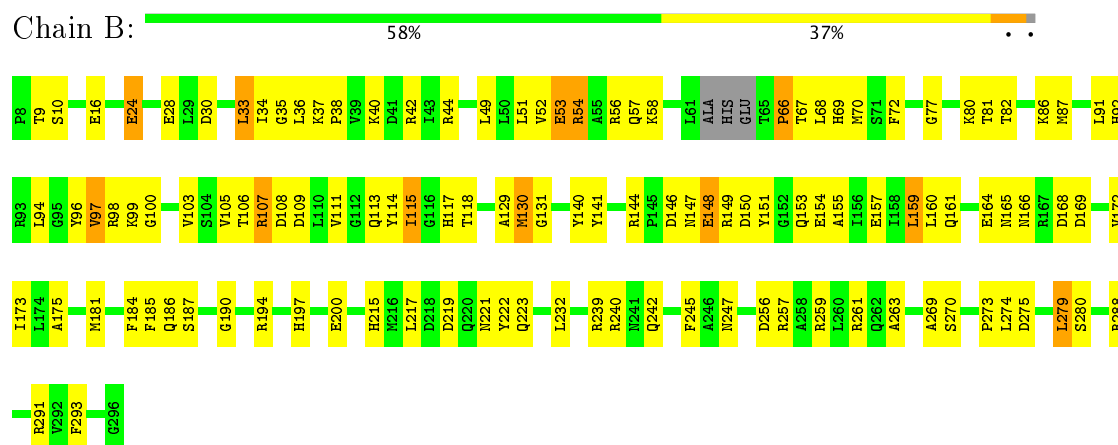
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

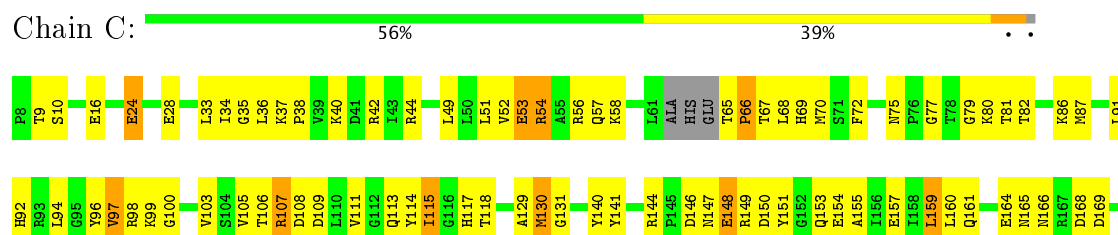
• Molecule 1: PROTEIN CBBX



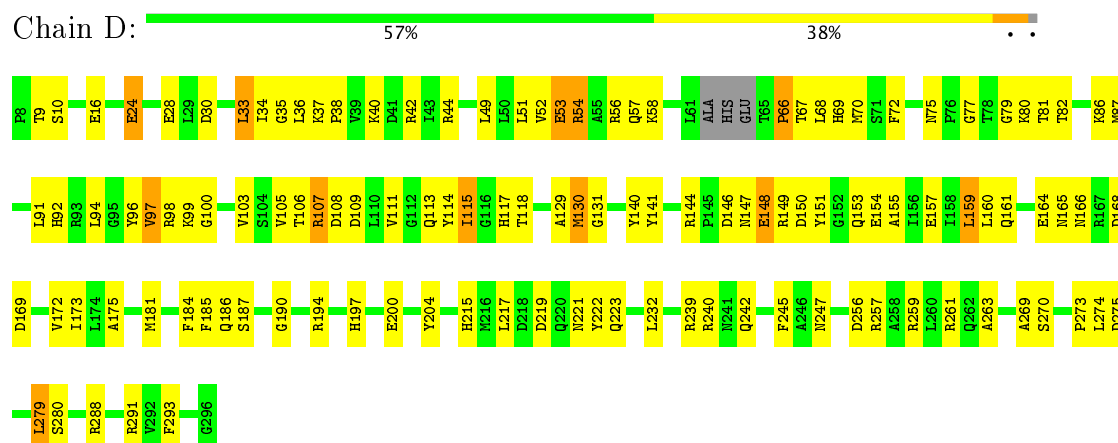
• Molecule 1: PROTEIN CBBX



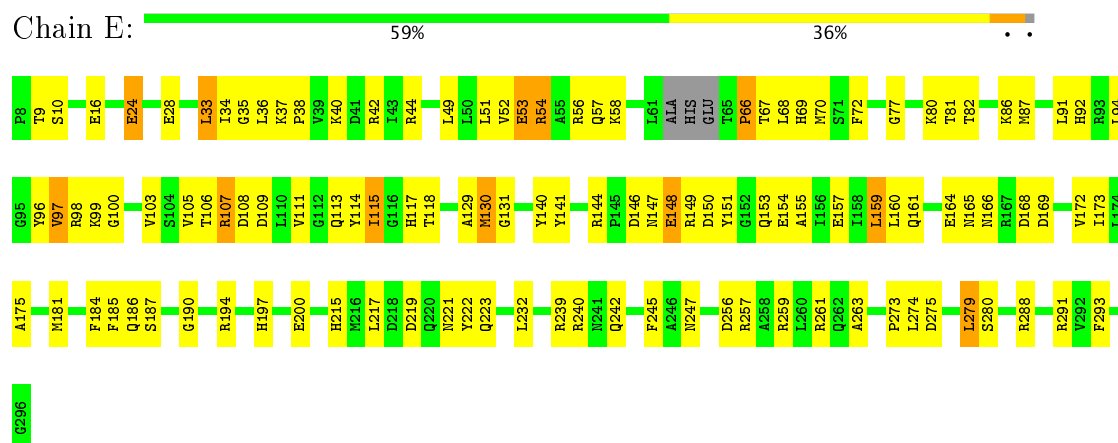
• Molecule 1: PROTEIN CBBX



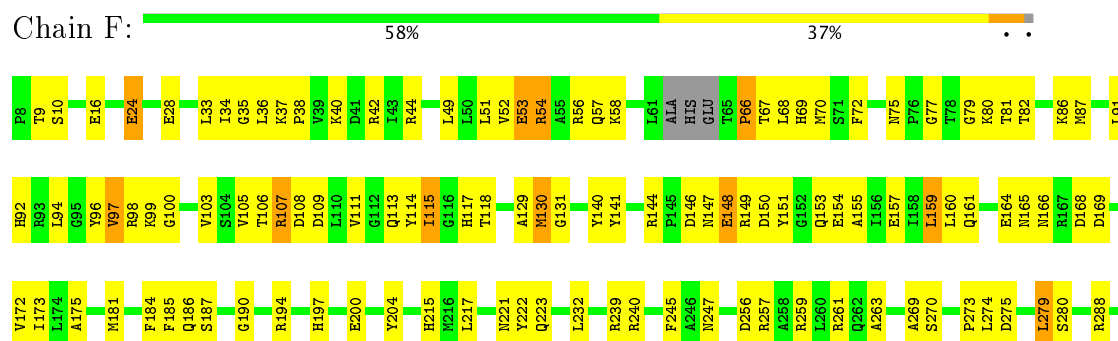
- Molecule 1: PROTEIN CBBX



- Molecule 1: PROTEIN CBBX



- Molecule 1: PROTEIN CBBX





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	245	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE FLIPPING, EACH PARTICLE	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	260	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	90600	Depositor
Image detector	FEI EAGLE (2k x 2k)	Depositor

5 Model quality

5.1 Standard geometry

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

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 >2	RMSZ	# Z >2
1	A	0.39	0/2306	0.65	0/3106
1	B	0.39	0/2306	0.66	0/3106
1	C	0.39	0/2306	0.66	0/3106
1	D	0.39	0/2306	0.65	0/3106
1	E	0.39	0/2306	0.66	0/3106
1	F	0.39	0/2306	0.66	0/3106
All	All	0.39	0/13836	0.66	0/18636

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

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	2269	0	2259	235	0
1	B	2269	0	2256	207	0
1	C	2269	0	2257	223	0
1	D	2269	0	2259	230	0
1	E	2269	0	2256	203	0
1	F	2269	0	2256	218	0
2	A	18	0	8	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	18	0	8	5	0
2	C	18	0	8	5	0
2	D	18	0	8	5	0
2	E	18	0	8	5	0
2	F	18	0	8	5	0
3	A	27	0	12	44	0
3	B	27	0	12	30	0
3	C	27	0	11	27	0
3	D	27	0	12	41	0
3	E	27	0	12	28	0
3	F	27	0	11	28	0
All	All	13884	0	13661	1179	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 43.

The worst 5 of 1179 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:B:34:ILE:CB	1:B:215:HIS:CE1	1.74	1.69
1:E:34:ILE:CB	1:E:215:HIS:CE1	1.74	1.64
1:F:34:ILE:CG2	1:F:215:HIS:HE1	0.99	1.63
1:F:34:ILE:CG2	1:F:215:HIS:CE1	1.79	1.60
1:C:34:ILE:CG2	1:C:215:HIS:CE1	1.79	1.58

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 PDB entries followed by that with respect to all EM entries.

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	280/289 (97%)	263 (94%)	15 (5%)	2 (1%)	25 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	280/289 (97%)	263 (94%)	15 (5%)	2 (1%)	25	68
1	C	280/289 (97%)	263 (94%)	15 (5%)	2 (1%)	25	68
1	D	280/289 (97%)	263 (94%)	15 (5%)	2 (1%)	25	68
1	E	280/289 (97%)	263 (94%)	15 (5%)	2 (1%)	25	68
1	F	280/289 (97%)	263 (94%)	15 (5%)	2 (1%)	25	68
All	All	1680/1734 (97%)	1578 (94%)	90 (5%)	12 (1%)	30	68

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	GLY
1	B	35	GLY
1	C	35	GLY
1	D	35	GLY
1	E	35	GLY

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 PDB entries followed by that with respect to all EM entries.

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	236/238 (99%)	215 (91%)	21 (9%)	11	39
1	B	236/238 (99%)	215 (91%)	21 (9%)	11	39
1	C	236/238 (99%)	215 (91%)	21 (9%)	11	39
1	D	236/238 (99%)	215 (91%)	21 (9%)	11	39
1	E	236/238 (99%)	215 (91%)	21 (9%)	11	39
1	F	236/238 (99%)	215 (91%)	21 (9%)	11	39
All	All	1416/1428 (99%)	1290 (91%)	126 (9%)	16	39

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	160	LEU

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Mol	Chain	Res	Type
1	D	82	THR
1	F	130	MET
1	C	187	SER
1	D	9	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	215	HIS
1	D	165	ASN
1	F	186	GLN
1	C	220	GLN
1	D	69	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 carbohydrates 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	RUB	A	1298	-	16,17,17	0.79	0	18,25,25	1.49	3 (16%)
3	ADP	A	1299	-	25,29,29	1.46	3 (12%)	24,45,45	2.69	3 (12%)
2	RUB	B	1298	-	16,17,17	0.79	0	18,25,25	1.48	3 (16%)
3	ADP	B	1299	-	25,29,29	1.76	5 (20%)	24,45,45	2.89	1 (4%)
2	RUB	C	1298	-	16,17,17	0.80	0	18,25,25	1.49	3 (16%)
3	ADP	C	1299	-	25,29,29	1.65	3 (12%)	24,45,45	2.94	3 (12%)
2	RUB	D	1298	-	16,17,17	0.79	0	18,25,25	1.49	3 (16%)
3	ADP	D	1299	-	25,29,29	1.45	3 (12%)	24,45,45	2.70	3 (12%)
2	RUB	E	1298	-	16,17,17	0.80	0	18,25,25	1.48	3 (16%)
3	ADP	E	1299	-	25,29,29	1.76	5 (20%)	24,45,45	2.89	1 (4%)
2	RUB	F	1298	-	16,17,17	0.79	0	18,25,25	1.49	3 (16%)
3	ADP	F	1299	-	25,29,29	1.66	3 (12%)	24,45,45	2.95	3 (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	RUB	A	1298	-	2/2/5/5	0/20/20/20	0/0/0/0
3	ADP	A	1299	-	-	0/12/32/32	0/3/3/3
2	RUB	B	1298	-	2/2/5/5	0/20/20/20	0/0/0/0
3	ADP	B	1299	-	-	0/12/32/32	0/3/3/3
2	RUB	C	1298	-	2/2/5/5	0/20/20/20	0/0/0/0
3	ADP	C	1299	-	-	0/12/32/32	0/3/3/3
2	RUB	D	1298	-	2/2/5/5	0/20/20/20	0/0/0/0
3	ADP	D	1299	-	-	0/12/32/32	0/3/3/3
2	RUB	E	1298	-	2/2/5/5	0/20/20/20	0/0/0/0
3	ADP	E	1299	-	-	0/12/32/32	0/3/3/3
2	RUB	F	1298	-	2/2/5/5	0/20/20/20	0/0/0/0
3	ADP	F	1299	-	-	0/12/32/32	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1299	ADP	C5-N7	-2.89	1.29	1.39
3	C	1299	ADP	C5-N7	-2.89	1.29	1.39
3	B	1299	ADP	C5-N7	-2.62	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1299	ADP	C5-N7	-2.60	1.30	1.39
3	A	1299	ADP	C5-N7	-2.54	1.30	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1299	ADP	N3-C2-N1	-13.38	117.20	128.86
3	C	1299	ADP	N3-C2-N1	-13.36	117.22	128.86
3	E	1299	ADP	N3-C2-N1	-13.21	117.35	128.86
3	B	1299	ADP	N3-C2-N1	-13.21	117.35	128.86
3	D	1299	ADP	N3-C2-N1	-12.32	118.13	128.86

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1298	RUB	C3
2	B	1298	RUB	C4
2	C	1298	RUB	C3
2	C	1298	RUB	C4
2	A	1298	RUB	C3

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 229 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1298	RUB	6	0
3	A	1299	ADP	44	0
2	B	1298	RUB	5	0
3	B	1299	ADP	30	0
2	C	1298	RUB	5	0
3	C	1299	ADP	27	0
2	D	1298	RUB	5	0
3	D	1299	ADP	41	0
2	E	1298	RUB	5	0
3	E	1299	ADP	28	0
2	F	1298	RUB	5	0
3	F	1299	ADP	28	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1
1	E	1
1	B	1
1	C	1
1	A	1
1	F	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	203:ASP	C	204:TYR	N	9.53
1	D	203:ASP	C	204:TYR	N	9.53
1	C	203:ASP	C	204:TYR	N	8.68
1	F	203:ASP	C	204:TYR	N	8.68
1	B	203:ASP	C	204:TYR	N	7.69