



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:40 am GMT

PDB ID : 5EZV
Title : X-ray crystal structure of AMP-activated protein kinase alpha-2/alpha-1 RIM chimaera (alpha-2(1-347)/alpha-1(349-401)/alpha-2(397-end) beta-1 gamma-1) co-crystallized with C2 (5-(5-hydroxyl-isoxazol-3-yl)-furan-2-phosphonic acid)
Authors : Langendorf, C.G.; Kemp, B.E.
Deposited on : 2015-11-26
Resolution : 2.99 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

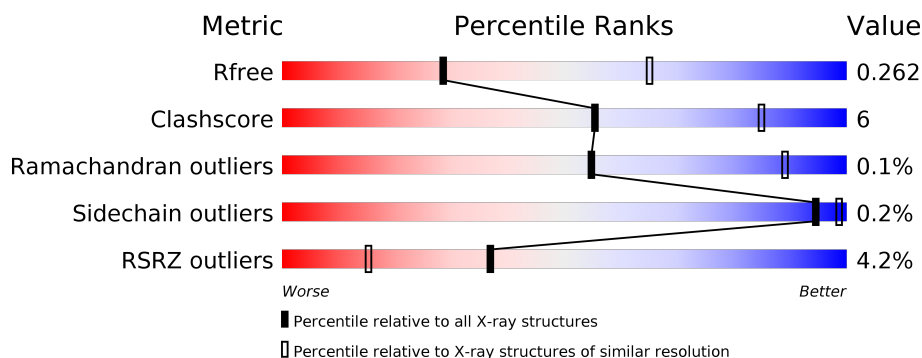
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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 on the lower 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 $\leq 5\%$. 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	560	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>7%</div> <div>21%</div> </div> </div>
1	C	560	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>7%</div> <div>21%</div> </div> </div>
2	B	270	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>13%</div> <div>31%</div> </div> </div>
2	D	270	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>9%</div> <div>31%</div> </div> </div>
3	E	336	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>10%</div> </div> </div>
3	F	336	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>11%</div> </div> </div>

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
1	TPO	A	172	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14682 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 5'-AMP-activated protein kinase catalytic subunit alpha-2/alpha-1 RIM SWAP chimera.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	P	S	0	0	0
			3462	2214	589	634	1	24			
1	C	441	Total	C	N	O	P	S	0	0	0
			3419	2186	588	621	1	23			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP P54646
A	-12	GLY	-	expression tag	UNP P54646
A	-11	SER	-	expression tag	UNP P54646
A	-10	SER	-	expression tag	UNP P54646
A	-9	HIS	-	expression tag	UNP P54646
A	-8	HIS	-	expression tag	UNP P54646
A	-7	HIS	-	expression tag	UNP P54646
A	-6	HIS	-	expression tag	UNP P54646
A	-5	HIS	-	expression tag	UNP P54646
A	-4	HIS	-	expression tag	UNP P54646
A	-3	HIS	-	expression tag	UNP P54646
A	-2	SER	-	expression tag	UNP P54646
A	-1	GLN	-	expression tag	UNP P54646
A	0	ASP	-	expression tag	UNP P54646
A	1	PRO	-	expression tag	UNP P54646
C	-13	MET	-	initiating methionine	UNP P54646
C	-12	GLY	-	expression tag	UNP P54646
C	-11	SER	-	expression tag	UNP P54646
C	-10	SER	-	expression tag	UNP P54646
C	-9	HIS	-	expression tag	UNP P54646
C	-8	HIS	-	expression tag	UNP P54646
C	-7	HIS	-	expression tag	UNP P54646
C	-6	HIS	-	expression tag	UNP P54646
C	-5	HIS	-	expression tag	UNP P54646

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP P54646
C	-3	HIS	-	expression tag	UNP P54646
C	-2	SER	-	expression tag	UNP P54646
C	-1	GLN	-	expression tag	UNP P54646
C	0	ASP	-	expression tag	UNP P54646
C	1	PRO	-	expression tag	UNP P54646

- Molecule 2 is a protein called 5'-AMP-activated protein kinase subunit beta-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	185	Total	C	N	O	P	S	0	0	0
			1400	904	233	257	1	5			
2	D	186	Total	C	N	O	P	S	0	0	0
			1422	914	234	267	1	6			

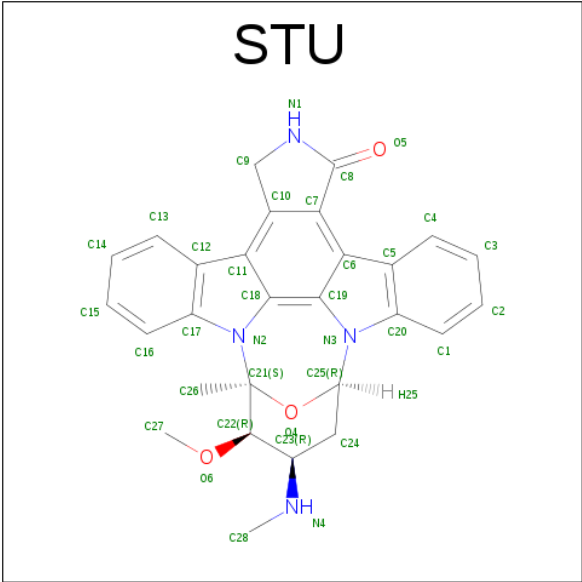
- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	302	Total	C	N	O	S		0	0	0
			2362	1538	391	426	7				
3	F	300	Total	C	N	O	S		0	1	0
			2351	1529	393	422	7				

There are 12 discrepancies between the modelled and reference sequences:

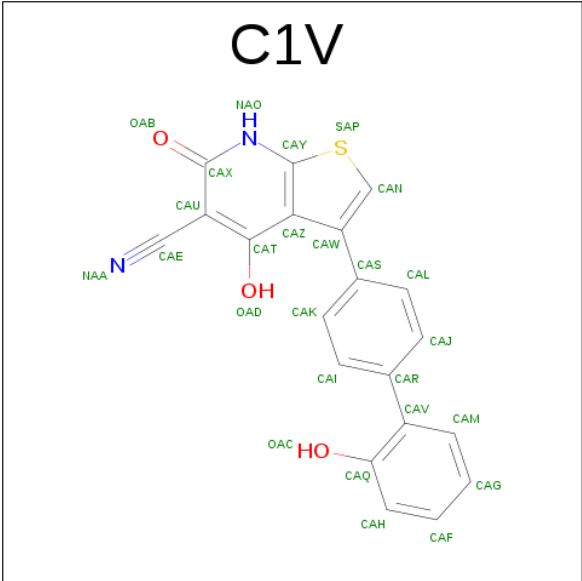
Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	MET	-	initiating methionine	UNP P54619
E	-3	ALA	-	expression tag	UNP P54619
E	-2	ASP	-	expression tag	UNP P54619
E	-1	LEU	-	expression tag	UNP P54619
E	0	ASN	-	expression tag	UNP P54619
E	1	TRP	-	expression tag	UNP P54619
F	-4	MET	-	initiating methionine	UNP P54619
F	-3	ALA	-	expression tag	UNP P54619
F	-2	ASP	-	expression tag	UNP P54619
F	-1	LEU	-	expression tag	UNP P54619
F	0	ASN	-	expression tag	UNP P54619
F	1	TRP	-	expression tag	UNP P54619

- Molecule 4 is STAUROSPORINE (three-letter code: STU) (formula: C₂₈H₂₆N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			35	28	4	3		
4	C	1	Total	C	N	O	0	0
			35	28	4	3		

- Molecule 5 is 3-[4-(2-hydroxyphenyl)phenyl]-4-oxidanyl-6-oxidanylidene-7H-thieno[2,3-b]pyridine-5-carbonitrile (three-letter code: C1V) (formula: C₂₀H₁₂N₂O₃S).



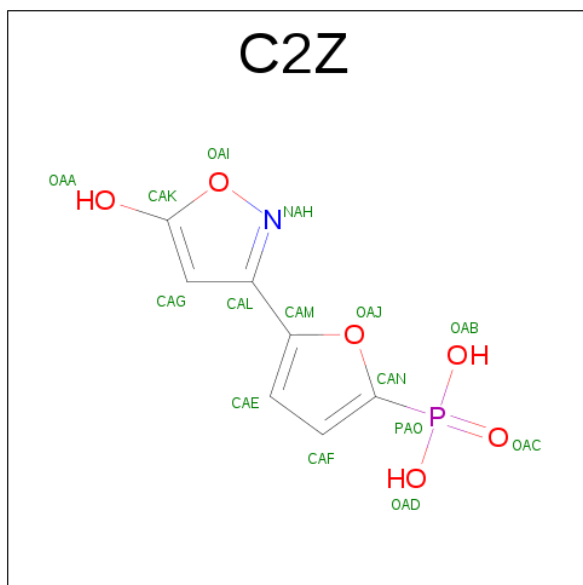
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			26	20	2	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	S	0	0
			26	20	2	3	1		

- Molecule 6 is 5-(5-hydroxyl-isoxazol-3-yl)-furan-2-phosphonic acid (three-letter code: C2Z) (formula: C₇H₆NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			15	7	1	6	1		
6	E	1	Total	C	N	O	P	0	0
			15	7	1	6	1		
6	F	1	Total	C	N	O	P	0	0
			15	7	1	6	1		
6	F	1	Total	C	N	O	P	0	0
			15	7	1	6	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	32	Total	O	0	0
			32	32		
7	B	8	Total	O	0	0
			8	8		
7	C	25	Total	O	0	0
			25	25		
7	D	7	Total	O	0	0
			7	7		

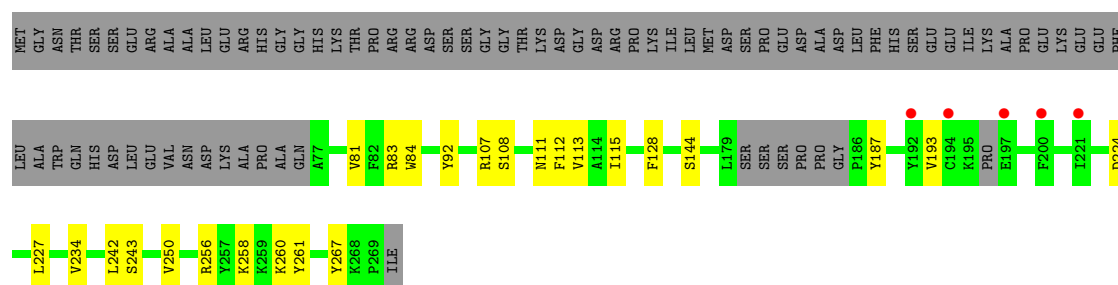
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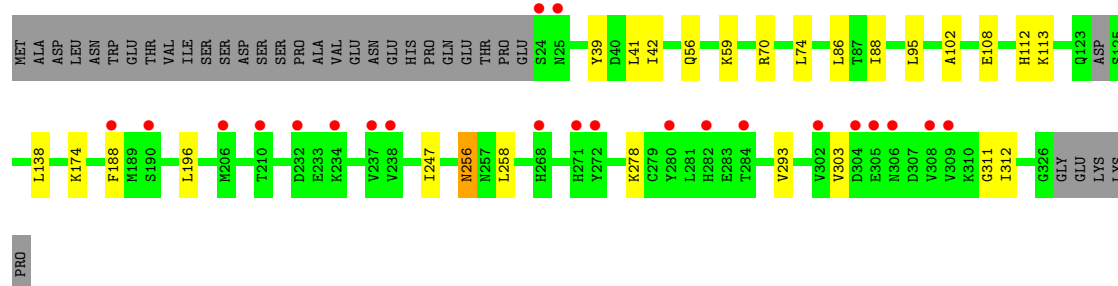
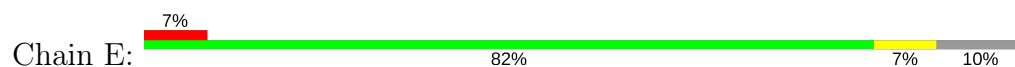
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	7	Total	O	0	0
			7	7		
7	F	5	Total	O	0	0
			5	5		



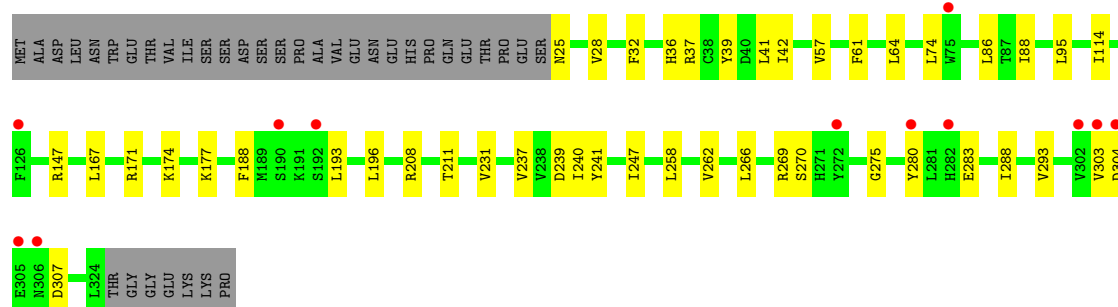
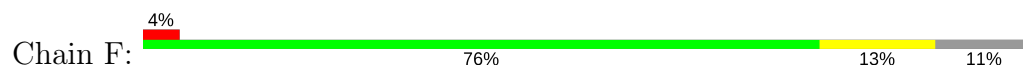
- Molecule 2: 5'-AMP-activated protein kinase subunit beta-1



- Molecule 3: 5'-AMP-activated protein kinase subunit gamma-1



- Molecule 3: 5'-AMP-activated protein kinase subunit gamma-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.61Å 134.11Å 141.29Å 90.00° 93.16° 90.00°	Depositor
Resolution (Å)	49.30 – 2.99 49.31 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.30-2.99) 99.3 (49.31-2.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 3.01Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.224 , 0.245 0.241 , 0.262	Depositor DCC
R_{free} test set	2867 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14682	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: TPO, STU, C2Z, C1V, SEP

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	0.38	0/3528	0.56	0/4778
1	C	0.38	0/3485	0.57	0/4724
2	B	0.38	0/1431	0.58	0/1964
2	D	0.38	0/1452	0.55	0/1989
3	E	0.38	0/2411	0.58	0/3281
3	F	0.38	0/2402	0.58	0/3269
All	All	0.38	0/14709	0.57	0/20005

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	3462	0	3311	33	0
1	C	3419	0	3255	42	1
2	B	1400	0	1308	29	0
2	D	1422	0	1317	22	1
3	E	2362	0	2379	18	0
3	F	2351	0	2368	38	0
4	A	35	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	35	0	26	3	0
5	A	26	0	12	0	0
5	C	26	0	12	1	0
6	E	30	0	0	0	0
6	F	30	0	0	0	0
7	A	32	0	0	0	0
7	B	8	0	0	0	0
7	C	25	0	0	0	0
7	D	7	0	0	0	0
7	E	7	0	0	0	0
7	F	5	0	0	0	0
All	All	14682	0	14014	169	1

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 6.

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:C:292:ALA:O	1:C:296:VAL:HG23	1.55	1.06
1:A:138:ARG:NH2	1:A:172:TPO:O2P	1.89	1.05
3:E:256:ASN:O	3:E:256:ASN:ND2	1.92	1.03
3:F:262:VAL:O	3:F:266:LEU:HD13	1.60	1.00
1:C:296:VAL:CG1	1:C:303:THR:HA	1.94	0.97

All (1) 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:C:285:ALA:O	2:D:144:SER:OG[2_946]	2.16	0.04

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	433/560 (77%)	422 (98%)	11 (2%)	0	100	100
1	C	430/560 (77%)	413 (96%)	17 (4%)	0	100	100
2	B	180/270 (67%)	177 (98%)	3 (2%)	0	100	100
2	D	179/270 (66%)	174 (97%)	4 (2%)	1 (1%)	28	70
3	E	298/336 (89%)	293 (98%)	5 (2%)	0	100	100
3	F	299/336 (89%)	293 (98%)	6 (2%)	0	100	100
All	All	1819/2332 (78%)	1772 (97%)	46 (2%)	1 (0%)	55	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	193	VAL

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	358/497 (72%)	358 (100%)	0	100	100
1	C	349/497 (70%)	349 (100%)	0	100	100
2	B	145/239 (61%)	145 (100%)	0	100	100
2	D	149/239 (62%)	149 (100%)	0	100	100
3	E	259/308 (84%)	258 (100%)	1 (0%)	93	98
3	F	255/308 (83%)	253 (99%)	2 (1%)	85	95
All	All	1515/2088 (73%)	1512 (100%)	3 (0%)	94	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	256	ASN
3	F	147	ARG

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Mol	Chain	Res	Type
3	F	269	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	124	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	$\# Z > 2$
1	TPO	A	172	1	9,10,11	0.82	0	10,14,16	1.26	1 (10%)
2	SEP	B	108	2	9,9,10	0.82	0	9,12,14	1.47	1 (11%)
1	TPO	C	172	1	9,10,11	0.81	0	10,14,16	1.29	1 (10%)
2	SEP	D	108	2	9,9,10	0.86	0	9,12,14	1.45	1 (11%)

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
1	TPO	A	172	1	-	0/8/11/13	0/0/0/0
2	SEP	B	108	2	-	0/5/8/10	0/0/0/0
1	TPO	C	172	1	-	0/8/11/13	0/0/0/0
2	SEP	D	108	2	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	108	SEP	O-C-CA	-2.85	117.14	125.02
1	C	172	TPO	O-C-CA	-2.47	119.39	125.15
1	A	172	TPO	O-C-CA	-2.28	119.82	125.15
2	B	108	SEP	OG-CB-CA	2.83	110.96	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	172	TPO	6	0
2	B	108	SEP	1	0
1	C	172	TPO	3	0
2	D	108	SEP	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
4	STU	A	601	-	29,42,42	2.77	10 (34%)	27,68,68	2.57	6 (22%)
5	C1V	A	602	-	28,29,29	3.39	9 (32%)	29,42,42	6.56	6 (20%)
4	STU	C	601	-	29,42,42	2.75	10 (34%)	27,68,68	2.63	8 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	C1V	C	602	-	28,29,29	3.42	9 (32%)	29,42,42	6.61	6 (20%)
6	C2Z	E	401	-	8,16,16	3.59	5 (62%)	8,24,24	2.15	2 (25%)
6	C2Z	E	402	-	8,16,16	3.12	4 (50%)	8,24,24	2.23	2 (25%)
6	C2Z	F	401	-	8,16,16	3.58	5 (62%)	8,24,24	2.13	2 (25%)
6	C2Z	F	402	-	8,16,16	3.57	5 (62%)	8,24,24	1.78	2 (25%)

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
4	STU	A	601	-	-	0/4/42/42	0/0/8/8
5	C1V	A	602	-	-	0/9/10/10	0/4/4/4
4	STU	C	601	-	-	0/4/42/42	0/0/8/8
5	C1V	C	602	-	-	0/9/10/10	0/4/4/4
6	C2Z	E	401	-	-	0/0/10/10	0/0/2/2
6	C2Z	E	402	-	-	0/0/10/10	0/0/2/2
6	C2Z	F	401	-	-	0/0/10/10	0/0/2/2
6	C2Z	F	402	-	-	0/0/10/10	0/0/2/2

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	401	C2Z	CAM-CAL	-6.58	1.33	1.49
6	F	401	C2Z	CAM-CAL	-6.54	1.34	1.49
6	F	402	C2Z	CAM-CAL	-6.47	1.34	1.49
4	C	601	STU	C9-C10	-6.46	1.45	1.50
6	E	402	C2Z	CAM-CAL	-6.45	1.34	1.49

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	602	C1V	CAU-CAE-NAA	-28.35	120.06	177.22
5	A	602	C1V	CAU-CAE-NAA	-27.71	121.36	177.22
5	A	602	C1V	CAW-CAN-SAP	-19.14	107.19	112.53
5	C	602	C1V	CAW-CAN-SAP	-18.66	107.32	112.53
4	C	601	STU	O5-C8-N1	-10.50	111.60	125.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	STU	2	0
4	C	601	STU	3	0
5	C	602	C1V	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	441/560 (78%)	0.23	14 (3%)	48 21	40, 63, 98, 142	0
1	C	440/560 (78%)	0.25	14 (3%)	48 21	38, 67, 105, 126	0
2	B	184/270 (68%)	0.41	11 (5%)	23 9	42, 71, 109, 131	0
2	D	185/270 (68%)	0.37	5 (2%)	55 26	51, 71, 115, 146	0
3	E	302/336 (89%)	0.44	22 (7%)	16 6	40, 65, 93, 113	0
3	F	300/336 (89%)	0.30	12 (4%)	39 16	43, 68, 93, 109	0
All	All	1852/2332 (79%)	0.31	78 (4%)	37 15	38, 67, 103, 146	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	314	GLY	6.7
1	A	361	PRO	4.4
3	F	304	ASP	4.3
1	A	300	PHE	4.2
2	B	120	GLU	4.2

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	TPO	A	172	11/12	0.92	0.12	-	56,57,60,61	1
2	SEP	D	108	10/11	0.92	0.13	-	65,65,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SEP	B	108	10/11	0.94	0.12	-	64,64,67,67	0
1	TPO	C	172	11/12	0.94	0.14	-	69,69,73,73	2

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
5	C1V	A	602	26/26	0.94	0.24	1.14	44,45,47,48	0
6	C2Z	E	401	15/15	0.83	0.24	0.68	100,100,101,101	0
4	STU	C	601	35/35	0.96	0.21	0.18	39,40,42,43	0
5	C1V	C	602	26/26	0.96	0.21	-0.28	42,44,45,45	0
4	STU	A	601	35/35	0.96	0.18	-0.44	38,39,40,40	0
6	C2Z	E	402	15/15	0.87	0.22	-0.53	92,92,93,93	0
6	C2Z	F	402	15/15	0.91	0.20	-0.98	88,88,88,88	0
6	C2Z	F	401	15/15	0.92	0.18	-1.14	92,93,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.