Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:22 PM GMT

PDB ID	:	4Y3B
Title	:	Crystal structure of C-terminal modified Tau peptide-hybrid 201D with 14-3-3sigma
Authors	:	Bartel, M.; Milroy, L.G.; Brunsveld, L.; Ottmann, C.
Deposited on	:	2015-02-10
Resolution	:	1.80 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
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:

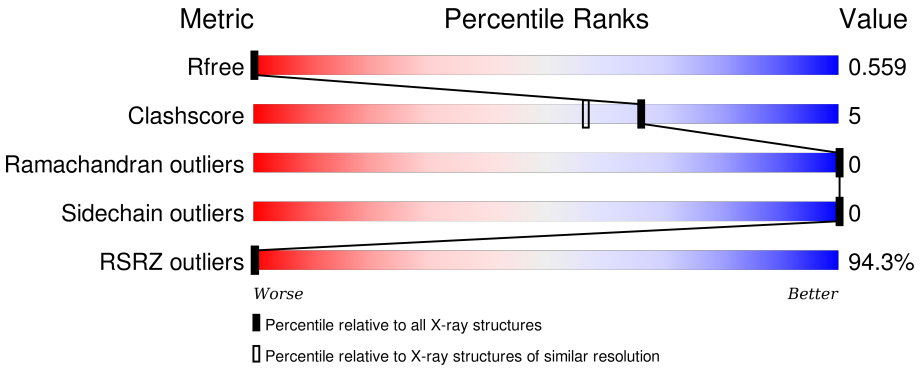
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 <=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	236	90% 89% 8% ·
1	B	236	94% 91% 8% ·
2	C	7	86% 71% 29%
2	D	7	71% 71% 14% 14%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	49F	C	301	-	-	X	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4572 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 14-3-3 protein sigma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	26	0
			1926	1220	316	378	12			
1	B	234	Total	C	N	O	S	0	2	0
			1847	1152	312	372	11			

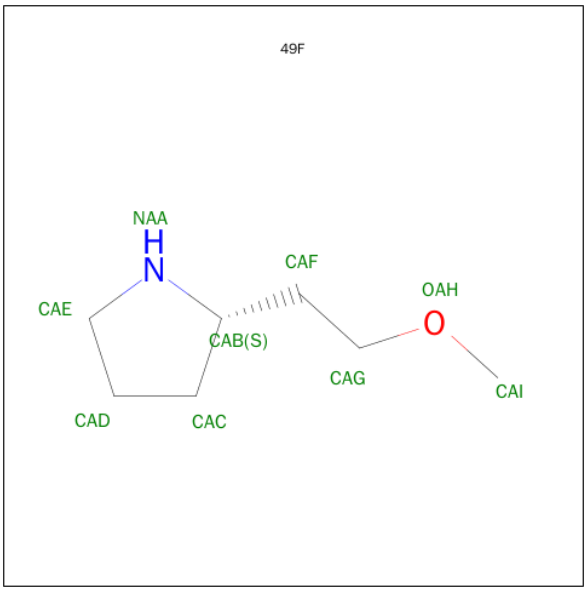
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P31947
A	-3	ALA	-	expression tag	UNP P31947
A	-2	MET	-	expression tag	UNP P31947
A	-1	GLY	-	expression tag	UNP P31947
A	0	SER	-	expression tag	UNP P31947
B	-4	GLY	-	expression tag	UNP P31947
B	-3	ALA	-	expression tag	UNP P31947
B	-2	MET	-	expression tag	UNP P31947
B	-1	GLY	-	expression tag	UNP P31947
B	0	SER	-	expression tag	UNP P31947

- Molecule 2 is a protein called ARG-THR-PRO-SEP-LEU-PRO-THR-[H][C@@]1(C(C2=CC=CC=C2)C3=CC=CC=C3)CCCN1C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	P	0	0	0
			57	33	10	13	1			
2	D	6	Total	C	N	O	P	0	0	0
			46	27	6	12	1			

- Molecule 3 is (2S)-2-(2-methoxyethyl)pyrrolidine (three-letter code: 49F) (formula: $C_7H_{15}NO$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C N O 9 7 1 1	0	0

- Molecule 4 is water.

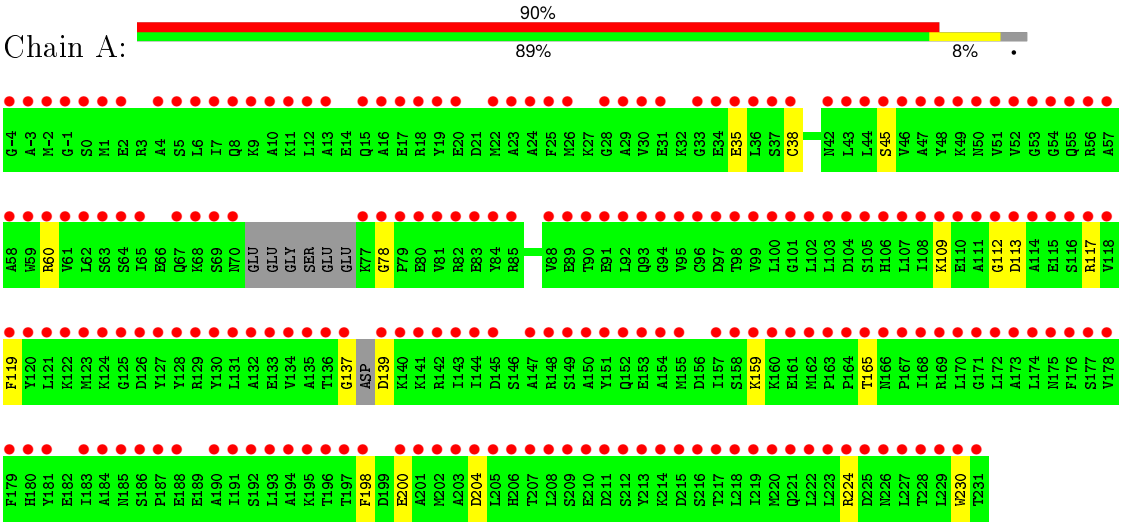
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	330	Total O 330 330	0	0
4	B	334	Total O 334 334	0	0
4	C	15	Total O 15 15	0	0
4	D	8	Total O 8 8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

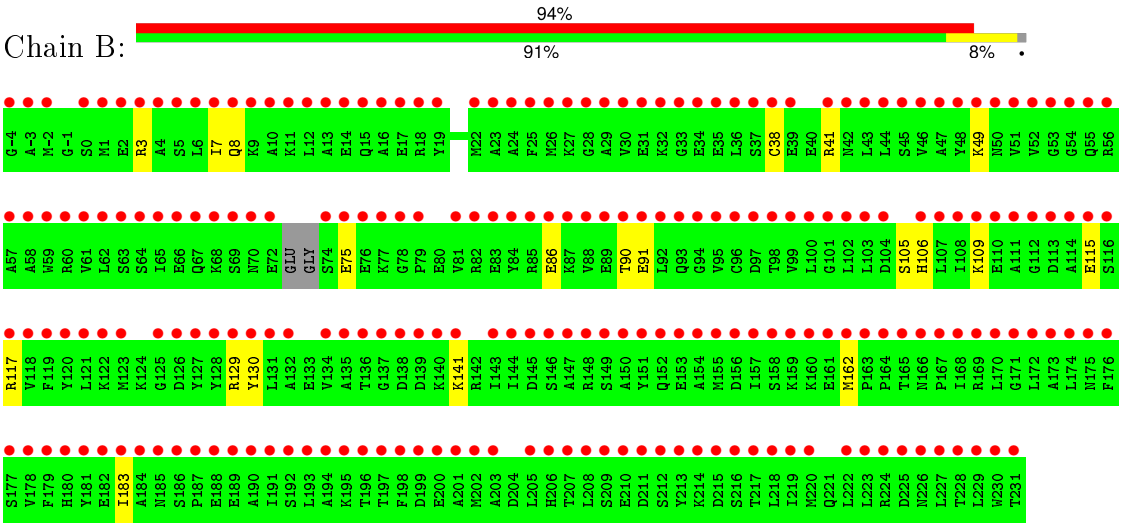
• Molecule 1: 14-3-3 protein sigma

Chain A:



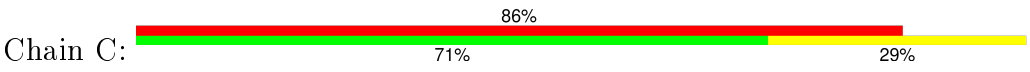
• Molecule 1: 14-3-3 protein sigma

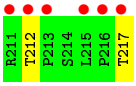
Chain B:



• Molecule 2: ARG-THR-PRO-SEP-LEU-PRO-THR-[H][C@@]1(C(C2=CC=CC=C2)C3=CC=CC=C3)CCCN1C

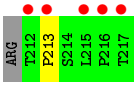
Chain C:





• Molecule 2: ARG-THR-PRO-SEP-LEU-PRO-THR-[H][C@@]1(C(C2=CC=CC=C2)C3=CC=CC=C3)CCCN1C

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.06Å 70.28Å 128.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.49 – 1.80 64.39 – 1.14	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.49-1.80) 12.3 (64.39-1.14)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 1.14Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.165 , 0.193 0.564 , 0.559	Depositor DCC
R_{free} test set	1157 reflections (4.48%)	DCC
Wilson B-factor (Å^2)	0.4	Xtriage
Anisotropy	2.743	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.48 , 602.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 26917 reflections	Xtriage
F_o,F_c correlation	0.19	EDS
Total number of atoms	4572	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 97.61 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2474e-10.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 49F, 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	0.35	0/2029	0.49	0/2722
1	B	0.32	0/1881	0.46	0/2527
2	C	0.39	0/47	0.69	0/63
2	D	0.34	0/36	0.90	0/49
All	All	0.34	0/3993	0.49	0/5361

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	1926	0	1990	18	0
1	B	1847	0	1827	15	0
2	C	57	0	54	5	0
2	D	46	0	41	1	0
3	C	9	0	12	6	0
4	A	330	0	0	10	7
4	B	334	0	0	9	5
4	C	15	0	0	0	0
4	D	8	0	0	1	0
All	All	4572	0	3924	38	7

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 5.

All (38) 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)
3:C:301:49F:CAD	3:C:301:49F:CAC	1.81	1.37
1:A:38:CYS:SG	4:A:546:HOH:O	2.24	0.94
1:A:139:ASP:N	4:A:302:HOH:O	2.01	0.92
1:A:198:PHE:HZ	1:A:224:ARG:HH21	1.25	0.83
1:B:38:CYS:SG	4:B:544:HOH:O	2.38	0.81
1:A:35:GLU:OE2	4:A:301:HOH:O	2.01	0.78
2:C:217:THR:C	3:C:301:49F:H9	1.93	0.71
2:C:217:THR:HA	3:C:301:49F:H18	1.74	0.69
1:B:75:GLU:OE2	4:B:301:HOH:O	2.13	0.66
1:B:8:GLN:OE1	4:B:302:HOH:O	2.14	0.66
1:A:109:LYS:HD2	4:A:536:HOH:O	1.95	0.66
1:A:113:ASP:OD2	4:A:304:HOH:O	2.15	0.64
2:D:213:PRO:HA	4:D:307:HOH:O	2.02	0.59
1:A:117:ARG:NH1	4:A:305:HOH:O	2.22	0.59
2:C:217:THR:C	3:C:301:49F:NAA	2.57	0.57
1:B:86:GLU:O	1:B:90:THR:HG23	2.04	0.57
1:B:41:ARG:NH2	4:B:311:HOH:O	2.39	0.55
1:A:230:TRP:CZ2	2:C:212:THR:HG21	2.44	0.52
1:B:117:ARG:NH1	4:B:305:HOH:O	2.28	0.52
1:A:119:PHE:HE2	3:C:301:49F:H6	1.74	0.52
1:B:141:LYS:NZ	4:B:315:HOH:O	2.43	0.51
1:A:60[B]:ARG:NE	4:A:303:HOH:O	2.14	0.49
1:B:105:SER:HA	1:B:106:HIS:CG	2.48	0.49
1:B:41:ARG:HD3	4:B:371:HOH:O	2.12	0.48
1:B:91:GLU:OE2	4:B:303:HOH:O	2.20	0.48
1:B:109:LYS:HG3	4:B:563:HOH:O	2.14	0.47
1:A:230:TRP:HZ2	2:C:212:THR:HG21	1.80	0.46
1:A:78:GLY:N	4:A:312:HOH:O	2.33	0.45
1:B:3:ARG:NH1	1:B:7:ILE:HD11	2.31	0.45
1:A:137:GLY:HA3	1:A:139:ASP:HB3	1.98	0.44
1:A:45:SER:HB3	3:C:301:49F:H2	2.00	0.44
1:A:112:GLY:O	1:A:117:ARG:NE	2.49	0.44
1:B:129:ARG:HG3	1:B:183:ILE:HG13	1.99	0.44
1:B:115:GLU:HA	1:B:162:MET:HE3	2.00	0.42
1:A:200:GLU:HG3	4:A:322:HOH:O	2.20	0.42
1:A:165:THR:HG23	1:A:204[B]:ASP:HB3	2.03	0.41
1:B:49:LYS:HE3	1:B:130:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159[A]:LYS:NZ	4:A:311:HOH:O	2.33	0.40

All (7) 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)
4:A:472:HOH:O	4:B:301:HOH:O[1_565]	1.90	0.30
4:A:573:HOH:O	4:A:597:HOH:O[4_555]	2.05	0.15
4:A:556:HOH:O	4:B:302:HOH:O[4_445]	2.06	0.14
4:A:355:HOH:O	4:B:611:HOH:O[2_555]	2.11	0.09
4:A:408:HOH:O	4:A:536:HOH:O[4_555]	2.16	0.04
4:A:559:HOH:O	4:B:531:HOH:O[4_445]	2.17	0.03
4:A:608:HOH:O	4:B:596:HOH:O[4_455]	2.19	0.01

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	248/236 (105%)	246 (99%)	2 (1%)	0	100	100
1	B	231/236 (98%)	228 (99%)	3 (1%)	0	100	100
2	C	4/7 (57%)	4 (100%)	0	0	100	100
2	D	3/7 (43%)	3 (100%)	0	0	100	100
All	All	486/486 (100%)	481 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	217/198 (110%)	217 (100%)	0	100	100
1	B	199/198 (100%)	199 (100%)	0	100	100
2	C	6/6 (100%)	6 (100%)	0	100	100
2	D	5/6 (83%)	5 (100%)	0	100	100
All	All	427/408 (105%)	427 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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	SEP	C	214	2	7,9,10	1.51	1 (14%)	8,12,14	1.16	0
2	SEP	D	214	2	7,9,10	1.69	1 (14%)	8,12,14	1.09	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
2	SEP	C	214	2	-	0/5/8/10	0/0/0/0
2	SEP	D	214	2	-	0/5/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	214	SEP	P-O1P	2.92	1.60	1.50
2	D	214	SEP	P-O1P	3.31	1.61	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	49F	C	301	-	8,9,9	3.31	2 (25%)	6,10,10	9.99	3 (50%)

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	49F	C	301	-	-	0/4/11/11	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	49F	CAD-CAE	-5.69	1.22	1.50
3	C	301	49F	CAD-CAC	6.90	1.81	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	301	49F	CAC-CAD-CAE	-5.83	80.05	104.72
3	C	301	49F	CAD-CAE-NAA	2.56	111.78	105.34
3	C	301	49F	CAF-CAB-CAC	23.52	151.52	113.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	49F	6	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	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	70:ASN	C	72:GLU	N	4.38

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, 95^{th} 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	229/236 (97%)	3.93	213 (93%)	0	0	13, 19, 38, 69	0
1	B	234/236 (99%)	4.24	223 (95%)	0	0	15, 22, 41, 93	0
2	C	6/7 (85%)	5.00	6 (100%)	0	0	18, 26, 28, 66	0
2	D	5/7 (71%)	7.16	5 (100%)	0	0	26, 37, 45, 59	0
All	All	474/486 (97%)	4.13	447 (94%)	0	0	13, 21, 42, 93	0

All (447) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	SER	15.8
1	B	231	THR	15.2
1	B	70	ASN	14.0
1	B	69	SER	13.4
1	B	72	GLU	12.6
1	A	77	LYS	12.4
1	A	111	ALA	12.0
1	B	229	LEU	11.4
1	B	208	LEU	9.9
2	D	212	THR	9.6
1	A	70	ASN	9.1
1	A	69	SER	9.0
2	C	211	ARG	8.8
2	D	217	THR	8.6
2	D	213	PRO	8.5
1	A	67	GLN	8.3
1	A	68	LYS	8.2
1	B	38	CYS	8.2
1	B	185	ASN	7.8
1	A	136	THR	7.5
1	A	110	GLU	7.4

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Mol	Chain	Res	Type	RSRZ
1	B	76	GLU	7.3
1	B	228	THR	7.2
1	A	208	LEU	7.1
1	B	75	GLU	7.1
1	A	230	TRP	7.0
1	B	68	LYS	6.8
1	B	13	ALA	6.6
1	B	67	GLN	6.6
1	B	183	ILE	6.6
1	B	230	TRP	6.6
1	B	111	ALA	6.6
1	B	65	ILE	6.5
1	B	77	LYS	6.3
1	B	-3	ALA	6.3
1	A	168[A]	ILE	6.3
1	A	61	VAL	6.2
1	A	7[A]	ILE	6.2
1	A	59	TRP	6.2
1	A	114	ALA	6.2
1	B	207	THR	6.1
1	B	136	THR	6.0
1	B	210	GLU	6.0
1	B	12	LEU	6.0
1	B	147	ALA	6.0
1	B	179	PHE	5.9
1	B	181	TYR	5.9
1	B	187	PRO	5.9
1	A	78	GLY	5.9
1	A	134	VAL	5.9
2	C	217	THR	5.8
1	B	163	PRO	5.8
1	A	231	THR	5.8
1	B	143	ILE	5.8
1	A	95	VAL	5.7
1	A	218	LEU	5.7
1	B	211	ASP	5.6
1	B	212	SER	5.6
1	B	127	TYR	5.6
1	A	170	LEU	5.6
1	B	223	LEU	5.6
1	B	4	ALA	5.6
1	B	7	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	190	ALA	5.5
1	A	52[A]	VAL	5.5
1	B	227	LEU	5.5
1	A	13	ALA	5.5
1	B	144	ILE	5.5
1	A	118	VAL	5.4
1	B	186	SER	5.4
1	B	25	PHE	5.4
1	B	209	SER	5.4
1	A	103	LEU	5.3
1	B	137	GLY	5.3
1	B	34	GLU	5.3
1	B	165	THR	5.3
1	B	128	TYR	5.3
1	A	161[A]	GLU	5.3
1	B	218	LEU	5.3
1	A	43	LEU	5.3
1	B	114	ALA	5.2
1	A	181	TYR	5.2
1	B	191	ILE	5.2
1	B	203	ALA	5.2
1	A	155[A]	MET	5.2
1	A	109	LYS	5.1
1	A	191	ILE	5.1
1	A	204[A]	ASP	5.1
1	A	176	PHE	5.1
1	A	213	TYR	5.1
1	A	163	PRO	5.1
1	A	84	TYR	5.1
1	B	103	LEU	5.1
1	A	159[A]	LYS	5.0
1	B	192	SER	5.0
1	A	92[A]	LEU	5.0
1	B	81	VAL	5.0
1	B	10	ALA	5.0
1	A	79	PRO	5.0
1	B	189	GLU	5.0
1	B	115	GLU	5.0
1	A	139	ASP	4.9
1	A	112	GLY	4.9
1	B	84	TYR	4.9
1	B	62	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	213	TYR	4.9
1	B	164	PRO	4.9
1	B	44	LEU	4.9
1	A	128	TYR	4.9
1	B	108	ILE	4.9
1	B	168	ILE	4.9
1	A	12	LEU	4.9
1	A	107	LEU	4.9
1	B	58	ALA	4.8
1	B	196	THR	4.8
1	B	95	VAL	4.8
1	A	167	PRO	4.8
1	B	113	ASP	4.8
1	B	119	PHE	4.8
1	B	17	GLU	4.8
2	D	215	LEU	4.8
1	A	46	VAL	4.8
1	A	96	CYS	4.8
1	B	162	MET	4.8
1	A	202	MET	4.7
1	A	119	PHE	4.7
1	A	4	ALA	4.7
1	A	121	LEU	4.7
1	A	127	TYR	4.7
1	A	216	SER	4.7
1	B	41	ARG	4.7
1	A	164	PRO	4.7
1	A	212	SER	4.7
1	B	222	LEU	4.6
1	B	160	LYS	4.6
1	B	79	PRO	4.6
1	B	96	CYS	4.6
1	B	104	ASP	4.6
1	A	187	PRO	4.6
1	B	6	LEU	4.6
1	B	59	TRP	4.6
1	B	150	ALA	4.6
1	A	227	LEU	4.6
1	A	151	TYR	4.5
1	A	194	ALA	4.5
1	B	100	LEU	4.5
1	A	130	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	166[A]	ASN	4.5
1	B	61	VAL	4.5
1	B	24	ALA	4.5
1	A	120	TYR	4.5
1	B	188	GLU	4.5
1	A	60[A]	ARG	4.5
1	B	46	VAL	4.5
1	A	10	ALA	4.5
1	A	193[A]	LEU	4.4
1	A	171	GLY	4.4
1	A	206	HIS	4.4
1	B	131	LEU	4.4
1	B	155	MET	4.4
1	A	145[A]	ASP	4.4
1	A	6	LEU	4.4
1	B	205	LEU	4.4
2	D	216	PRO	4.4
1	A	174	LEU	4.4
1	A	142	ARG	4.4
1	A	54	GLY	4.3
1	A	157	ILE	4.3
1	B	16	ALA	4.3
1	B	47	ALA	4.3
1	B	206	HIS	4.3
1	A	36	LEU	4.3
1	B	43	LEU	4.3
1	A	88	VAL	4.3
1	B	57	ALA	4.3
1	B	180	HIS	4.3
1	B	64	SER	4.3
1	A	38	CYS	4.3
1	B	153	GLU	4.3
1	A	154	ALA	4.3
1	A	201	ALA	4.3
1	B	107	LEU	4.3
1	A	179	PHE	4.3
1	A	162	MET	4.3
1	A	131	LEU	4.2
1	A	172	LEU	4.2
1	A	229	LEU	4.2
1	B	92	LEU	4.2
1	B	134	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	53	GLY	4.2
1	B	219	ILE	4.2
1	B	88	VAL	4.2
1	B	36	LEU	4.2
1	A	48	TYR	4.2
1	B	176	PHE	4.2
1	B	23	ALA	4.2
1	B	99	VAL	4.2
1	A	144	ILE	4.2
1	A	100	LEU	4.2
1	A	143	ILE	4.2
1	A	173	ALA	4.2
1	A	184	ALA	4.2
1	A	62	LEU	4.1
2	C	216	PRO	4.1
1	A	150	ALA	4.1
1	B	19	TYR	4.1
1	A	223	LEU	4.1
1	A	153[A]	GLU	4.1
1	A	99	VAL	4.1
1	A	178	VAL	4.1
1	A	47	ALA	4.1
1	A	58	ALA	4.1
1	A	158[A]	SER	4.0
1	A	192	SER	4.0
1	B	51	VAL	4.0
1	B	201	ALA	4.0
1	A	63[A]	SER	4.0
1	A	222	LEU	4.0
1	B	199	ASP	4.0
1	A	196	THR	4.0
1	B	184	ALA	4.0
1	B	198	PHE	4.0
1	A	219	ILE	4.0
1	B	225	ASP	4.0
1	B	193	LEU	4.0
1	B	45	SER	3.9
1	A	115[A]	GLU	3.9
1	A	125	GLY	3.9
2	C	213	PRO	3.9
1	A	90	THR	3.9
2	C	212	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	82	ARG	3.9
1	B	194	ALA	3.9
1	B	97	ASP	3.9
1	A	24	ALA	3.9
1	A	44	LEU	3.9
1	A	210	GLU	3.9
1	A	25	PHE	3.8
1	B	-2	MET	3.8
1	A	228	THR	3.8
1	B	90	THR	3.8
1	B	178	VAL	3.8
1	B	173	ALA	3.8
1	A	-2	MET	3.8
1	A	15[A]	GLN	3.8
1	B	48	TYR	3.8
1	B	130	TYR	3.8
1	B	37	SER	3.8
1	B	174	LEU	3.8
1	A	19	TYR	3.8
1	B	151	TYR	3.8
1	B	102	LEU	3.8
1	B	123	MET	3.7
1	B	217	THR	3.7
1	A	190	ALA	3.7
1	B	140	LYS	3.7
1	A	165	THR	3.7
1	B	26	MET	3.7
1	B	135	ALA	3.7
1	A	108	ILE	3.7
1	A	123	MET	3.7
1	A	205	LEU	3.7
1	B	172	LEU	3.7
1	B	182	GLU	3.7
1	A	101	GLY	3.7
1	A	1	MET	3.6
1	A	102	LEU	3.6
1	A	221	GLN	3.6
1	B	167	PRO	3.6
1	A	-3	ALA	3.6
1	B	63	SER	3.6
1	B	216	SER	3.6
1	B	226	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	145	ASP	3.6
1	B	118	VAL	3.6
1	B	139	ASP	3.6
1	B	98	THR	3.6
1	A	105	SER	3.6
1	A	-1	GLY	3.6
1	B	60	ARG	3.6
1	B	141	LYS	3.6
1	A	177[A]	SER	3.5
1	B	116	SER	3.5
1	A	65	ILE	3.5
1	A	183	ILE	3.5
1	A	117	ARG	3.5
1	A	94	GLY	3.5
1	B	52	VAL	3.5
1	A	195[A]	LYS	3.5
1	B	53	GLY	3.5
1	A	148	ARG	3.5
1	B	39	GLU	3.5
2	C	215	LEU	3.5
1	A	180	HIS	3.5
1	B	157	ILE	3.5
1	A	29	ALA	3.5
1	A	57	ALA	3.5
1	A	135	ALA	3.5
1	A	0[A]	SER	3.5
1	A	132	ALA	3.4
1	B	215	ASP	3.4
1	B	202	MET	3.4
1	B	28	GLY	3.4
1	B	132	ALA	3.4
1	B	91	GLU	3.4
1	A	224	ARG	3.3
1	A	-4	GLY	3.3
1	A	140[A]	LYS	3.3
1	B	117	ARG	3.3
1	A	217	THR	3.3
1	B	1	MET	3.3
1	B	177	SER	3.3
1	A	51	VAL	3.3
1	B	148	ARG	3.3
1	A	45	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	22	MET	3.3
1	A	23	ALA	3.3
1	A	20[A]	GLU	3.3
1	B	125	GLY	3.3
1	B	170	LEU	3.3
1	A	147	ALA	3.3
1	A	226	ASN	3.2
1	A	198	PHE	3.2
1	B	120	TYR	3.2
1	B	15	GLN	3.2
1	A	207	THR	3.2
1	A	22	MET	3.2
1	A	152	GLN	3.2
1	A	30	VAL	3.2
1	B	126	ASP	3.2
1	A	49	LYS	3.2
1	B	156	ASP	3.2
1	B	30	VAL	3.2
1	B	197	THR	3.2
1	A	37	SER	3.2
1	A	9	LYS	3.1
1	A	141[A]	LYS	3.1
1	A	5	SER	3.1
1	A	209	SER	3.1
1	A	215	ASP	3.1
1	A	26	MET	3.1
1	A	81	VAL	3.1
1	B	121	LEU	3.1
1	A	98	THR	3.1
1	A	220	MET	3.1
1	B	5	SER	3.1
1	B	224	ARG	3.1
1	A	97	ASP	3.1
1	A	211	ASP	3.1
1	B	158	SER	3.1
1	A	200	GLU	3.1
1	A	16	ALA	3.0
1	B	55	GLN	3.0
1	A	106	HIS	3.0
1	B	175	ASN	3.0
1	A	50	ASN	2.9
1	A	104	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	220	MET	2.9
1	B	112	GLY	2.9
1	B	32	LYS	2.9
1	A	186[A]	SER	2.9
1	A	17	GLU	2.9
1	A	113	ASP	2.9
1	A	42	ASN	2.9
1	B	171	GLY	2.9
1	B	200	GLU	2.9
1	A	185	ASN	2.8
1	A	116	SER	2.8
1	B	195	LYS	2.8
1	A	166[A]	ASN	2.8
1	A	203	ALA	2.8
1	A	8	GLN	2.8
1	A	64	SER	2.8
1	B	93	GLN	2.8
1	B	54	GLY	2.8
1	A	55[A]	GLN	2.8
1	B	169	ARG	2.7
1	B	149	SER	2.7
1	B	42	ASN	2.7
1	A	214	LYS	2.7
1	B	161	GLU	2.7
1	A	28	GLY	2.7
1	A	33	GLY	2.7
1	B	138	ASP	2.7
1	B	33	GLY	2.7
1	B	94	GLY	2.7
1	B	2	GLU	2.7
1	B	66	GLU	2.7
1	B	159	LYS	2.7
1	A	149	SER	2.7
1	B	152	GLN	2.7
1	A	160	LYS	2.7
1	B	3	ARG	2.7
1	A	126	ASP	2.7
1	B	8	GLN	2.7
1	B	89	GLU	2.7
1	B	29	ALA	2.6
1	A	18	ARG	2.6
1	A	225	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	-4	GLY	2.6
1	B	101	GLY	2.6
1	B	18	ARG	2.6
1	A	175	ASN	2.6
1	A	137	GLY	2.5
1	A	197	THR	2.5
1	B	27	LYS	2.5
1	B	87	LYS	2.5
1	B	214	LYS	2.5
1	B	122	LYS	2.5
1	B	56	ARG	2.5
1	A	80	GLU	2.4
1	A	129	ARG	2.4
1	B	11	LYS	2.4
1	A	34	GLU	2.4
1	B	154	ALA	2.4
1	A	91[A]	GLU	2.4
1	A	133	GLU	2.4
1	B	14	GLU	2.4
1	B	0[A]	SER	2.4
1	A	169	ARG	2.4
1	A	188	GLU	2.4
1	B	78	GLY	2.4
1	B	110	GLU	2.4
1	A	85	ARG	2.3
1	B	85	ARG	2.3
1	B	129	ARG	2.3
1	A	122	LYS	2.3
1	A	89	GLU	2.3
1	A	35	GLU	2.3
1	B	31	GLU	2.3
1	A	124	LYS	2.2
1	B	146	SER	2.2
1	A	31	GLU	2.2
1	B	35	GLU	2.1
1	A	11	LYS	2.1
1	B	49	LYS	2.1
1	B	9	LYS	2.1
1	A	93	GLN	2.1
1	A	56	ARG	2.1
1	A	83	GLU	2.1
1	B	86	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	109	LYS	2.1
1	B	50	ASN	2.0
1	B	106	HIS	2.0
1	B	82	ARG	2.0
1	A	2	GLU	2.0
1	B	83	GLU	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. 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, 95^{th} 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
2	SEP	D	214	10/11	0.83	0.26	-	21,23,26,27	0
2	SEP	C	214	10/11	0.87	0.27	-	16,16,19,19	0

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, 95^{th} 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
3	49F	C	301	9/9	0.27	0.74	9.76	27,42,49,49	1

6.5 Other polymers (i)

There are no such residues in this entry.