Full wwPDB X-ray Structure Validation Report (i)

Jun 14, 2020 – 10:38 pm BST

PDB ID	:	3EGH
Title	:	Crystal structure of a complex between Protein Phosphatase 1 alpha (PP1), the PP1 binding and PDZ domains of Spinophilin and the small natural molecular toxin Nodularin-R
Authors	:	Ragusa, M.J.; Page, R.; Peti, W.
Deposited on	:	2008-09-10
Resolution	:	2.00 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.00 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	Percentile Ranks	Value
Rfree		0.232
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		1.3%
RSRZ outliers		7.4%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
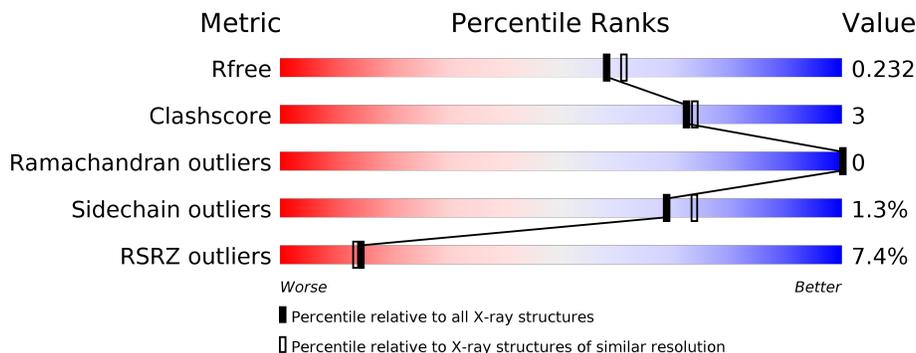
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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% 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	329	81% 7% · 11%
1	B	329	84% 5% 11%
2	C	170	25% 83% 10% · 6%
2	D	170	8% 36% · 61%
3	E	5	20% 80% 20%
3	F	5	80% 20%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6990 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 Serine/threonine-protein phosphatase PP1-alpha catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total 2358	C 1520	N 390	O 429	S 19	0	5	0
1	B	294	Total 2346	C 1509	N 387	O 431	S 19	0	2	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	EXPRESSION TAG	UNP P62136
A	3	HIS	-	EXPRESSION TAG	UNP P62136
A	4	MET	-	EXPRESSION TAG	UNP P62136
A	5	GLY	-	EXPRESSION TAG	UNP P62136
A	6	SER	-	EXPRESSION TAG	UNP P62136
B	2	GLY	-	EXPRESSION TAG	UNP P62136
B	3	HIS	-	EXPRESSION TAG	UNP P62136
B	4	MET	-	EXPRESSION TAG	UNP P62136
B	5	GLY	-	EXPRESSION TAG	UNP P62136
B	6	SER	-	EXPRESSION TAG	UNP P62136

- Molecule 2 is a protein called Spinophilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	160	Total 1172	C 736	N 201	O 231	S 4	0	1	0
2	D	66	Total 496	C 312	N 79	O 104	S 1	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	414	GLY	-	EXPRESSION TAG	UNP O35274

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Chain	Residue	Modelled	Actual	Comment	Reference
C	415	SER	-	EXPRESSION TAG	UNP O35274
C	416	MET	-	EXPRESSION TAG	UNP O35274
D	414	GLY	-	EXPRESSION TAG	UNP O35274
D	415	SER	-	EXPRESSION TAG	UNP O35274
D	416	MET	-	EXPRESSION TAG	UNP O35274

- Molecule 3 is a protein called nodularin R.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total 55	C 40	N 5	O 10	0	0	0
3	F	5	Total 54	C 39	N 5	O 10	0	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
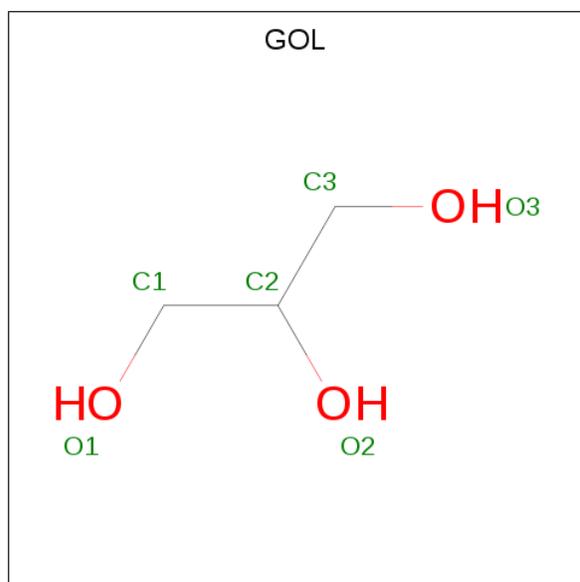
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Mn 2 2	0	0
5	A	2	Total Mn 2 2	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	179	Total O 179 179	0	0
6	B	198	Total O 198 198	0	0
6	C	61	Total O 61 61	0	0
6	D	38	Total O 38 38	0	0
6	E	3	Total O 3 3	0	0
6	F	2	Total O 2 2	0	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 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: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit
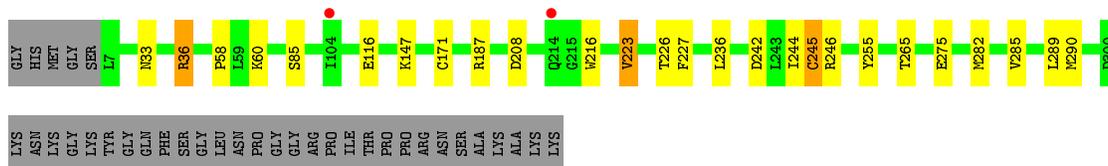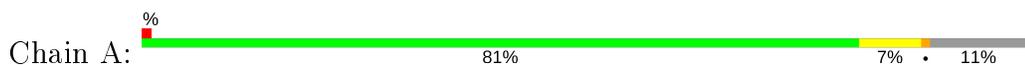
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit
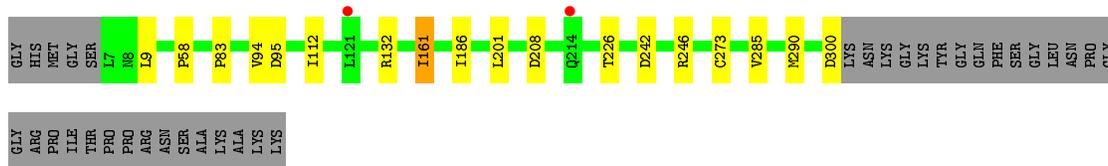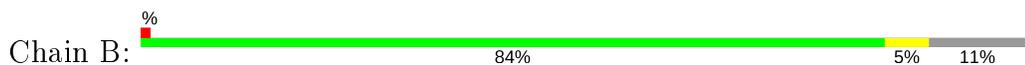
- Molecule 2: Spinophilin
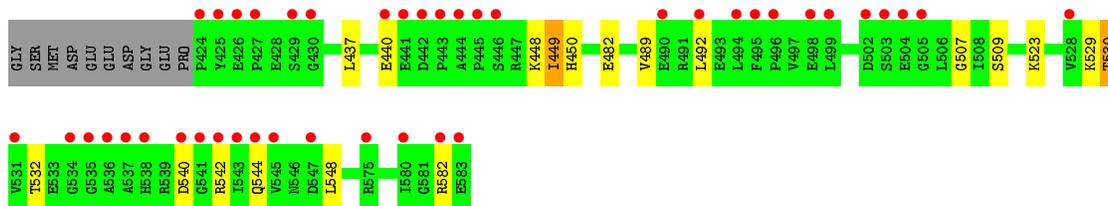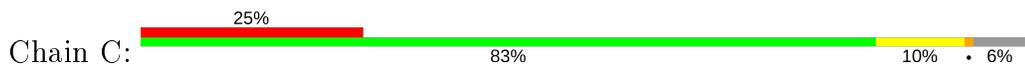
- Molecule 2: Spinophilin
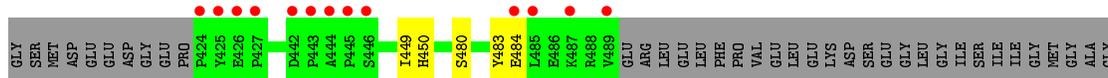
ALA ASP MET GLY LEU GLU LYS LEU GLY ILE PHE VAL LYS THR VAL THR GLU GLY GLY ALA ALA HIS ASP ARG GLY ARG ILE GLN VAL ASN ASP LEU LEU VAL GLU VAL ASP GLY THR SER LEU VAL GLY VAL THR GLN SER PHE ALA ALA SER VAL LEU ARG ASN THR LYS GLY ARG VAL

ARG PHE MET ILE GLY ARG GLU

• Molecule 3: nodularin R

Chain E:

20%

80%　　　　　　　　　　　　20%

D1 R2　X5

• Molecule 3: nodularin R

Chain F:

80%　　　　　　　　　　　　20%

D1　X5
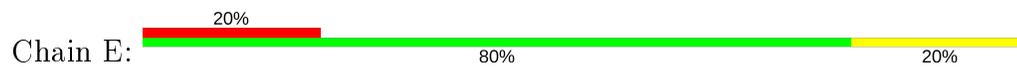
4 Data and refinement statistics (i)

| Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	119.41Å 84.43Å 109.31Å 90.00° 93.58° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 39.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.3 (40.00-2.00) 96.3 (39.37-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.04 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.235 0.191 , 0.232	Depositor DCC
R_{free} test set	3528 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6990	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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 44.52 % 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 1.5088e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: ACB, MDH, GOL, MN, 1ZN, FGA

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	0.74	1/2428 (0.0%)	0.75	1/3285 (0.0%)
1	B	0.79	1/2406 (0.0%)	0.77	1/3256 (0.0%)
2	C	0.61	0/1195	0.67	0/1619
2	D	0.70	0/516	0.66	0/705
3	E	0.39	0/6	0.67	0/6
3	F	0.41	0/5	1.02	0/5
All	All	0.73	2/6556 (0.0%)	0.74	2/8876 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	CYS	CB-SG	-5.83	1.72	1.81
1	B	300	ASP	CA-CB	5.25	1.65	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	300	ASP	N-CA-C	6.11	127.49	111.00
1	A	223	VAL	CB-CA-C	-5.65	100.66	111.40

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	2358	0	2304	20	0
1	B	2346	0	2282	12	0
2	C	1172	0	1126	15	0
2	D	496	0	440	6	0
3	E	55	0	48	1	0
3	F	54	0	46	1	0
4	A	18	0	24	4	0
4	C	6	0	8	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	179	0	0	2	0
6	B	198	0	0	0	0
6	C	61	0	0	0	0
6	D	38	0	0	0	0
6	E	3	0	0	0	0
6	F	2	0	0	0	0
All	All	6990	0	6278	44	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 3.

All (44) 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:290[B]:MET:HE3	2:D:450:HIS:ND1	1.96	0.81
1:A:85:SER:HB3	4:A:402:GOL:H31	1.71	0.73
2:C:509:SER:OG	2:C:530:THR:HB	1.89	0.73
1:B:290[B]:MET:CE	2:D:450:HIS:ND1	2.58	0.67
1:A:290[B]:MET:HE3	2:C:450:HIS:ND1	2.09	0.66
1:B:290[B]:MET:HE3	2:D:450:HIS:CE1	2.41	0.56
1:A:116:GLU:OE1	4:A:403:GOL:H31	2.09	0.53
1:A:290[B]:MET:CE	2:C:450:HIS:ND1	2.72	0.52
1:A:289:LEU:HD12	2:C:448:LYS:HD3	1.90	0.52
1:A:216:TRP:CZ3	1:A:227:PHE:HB3	2.46	0.51
2:C:489:VAL:O	2:C:492:LEU:HB2	2.11	0.51
1:A:242:ASP:HB3	2:C:449:ILE:HG12	1.93	0.50
2:D:480:SER:O	2:D:484:GLU:HG2	2.12	0.50
1:B:208:ASP:O	1:B:226:THR:HA	2.11	0.49
1:B:161:ILE:HD12	1:B:201:LEU:HD13	1.95	0.49
4:A:403:GOL:H12	6:A:597:HOH:O	2.12	0.49
1:B:94:VAL:O	1:B:95:ASP:HB2	2.13	0.49
2:C:544:GLN:OE1	2:C:582:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:482:GLU:CG	2:C:523:LYS:HD2	2.45	0.47
1:A:187:ARG:HG2	6:A:534:HOH:O	2.14	0.47
1:A:36[A]:ARG:HH22	1:A:147:LYS:CG	2.27	0.47
1:B:161:ILE:HD11	1:B:186:ILE:HG23	1.96	0.46
1:B:58:PRO:HA	1:B:285:VAL:O	2.15	0.46
2:C:440:GLU:HG3	2:C:440:GLU:O	2.17	0.45
1:A:36[A]:ARG:HH11	1:A:36[A]:ARG:HG3	1.82	0.45
1:A:289:LEU:CD1	2:C:448:LYS:HD3	2.48	0.44
1:B:9:LEU:HD11	1:B:112:ILE:HG22	2.00	0.43
1:A:85:SER:CB	4:A:402:GOL:H31	2.46	0.43
1:A:255:TYR:HA	1:A:265:THR:O	2.18	0.42
1:A:58:PRO:HA	1:A:285:VAL:O	2.20	0.42
2:C:489:VAL:HG22	2:C:548:LEU:HD21	2.02	0.42
1:A:275:GLU:OE1	3:E:5:MDH:HG1	2.19	0.42
1:B:242:ASP:HB3	2:D:449:ILE:HG12	2.02	0.42
1:A:33:ASN:OD1	1:A:36[B]:ARG:NH1	2.53	0.42
1:A:236:LEU:HD21	1:A:244:ILE:HG13	2.01	0.41
1:A:208:ASP:O	1:A:226:THR:HA	2.20	0.41
2:C:529:LYS:HE2	2:C:529:LYS:HB3	1.84	0.41
2:C:540:ASP:OD2	2:C:542:ARG:HD3	2.20	0.41
1:A:60[B]:LYS:HD3	1:A:282:MET:SD	2.61	0.41
2:C:507:GLY:HA2	2:C:532:THR:OG1	2.21	0.41
1:B:273:CYS:SG	3:F:5:MDH:HG1	2.61	0.40
1:A:171:CYS:HA	1:A:245:CYS:O	2.21	0.40
1:B:132:ARG:HG2	2:D:483:TYR:CG	2.56	0.40
2:C:482:GLU:HG3	2:C:523:LYS:HD2	2.02	0.40

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 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	297/329 (90%)	287 (97%)	10 (3%)	0	100	100
1	B	294/329 (89%)	281 (96%)	13 (4%)	0	100	100
2	C	159/170 (94%)	158 (99%)	1 (1%)	0	100	100
2	D	66/170 (39%)	65 (98%)	1 (2%)	0	100	100
All	All	816/998 (82%)	791 (97%)	25 (3%)	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	253/285 (89%)	249 (98%)	4 (2%)	62	67
1	B	252/285 (88%)	249 (99%)	3 (1%)	71	76
2	C	120/141 (85%)	117 (98%)	3 (2%)	47	49
2	D	52/141 (37%)	52 (100%)	0	100	100
All	All	677/852 (80%)	667 (98%)	10 (2%)	69	69

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36[A]	ARG
1	A	36[B]	ARG
1	A	223	VAL
1	A	246	ARG
1	B	83	PRO
1	B	161	ILE
1	B	246	ARG
2	C	437	LEU
2	C	449	ILE
2	C	530	THR

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

Mol	Chain	Res	Type
1	A	271	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 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	#$\|Z\| > 2$
3	MDH	E	5	3	4,6,7	1.16	1 (25%)	4,6,8	3.64	2 (50%)
3	ACB	E	1	3	5,8,9	0.95	0	4,10,12	0.93	0
3	1ZN	F	3	3	23,23,24	0.86	0	24,29,31	1.20	4 (16%)
3	ACB	F	1	3	5,8,9	1.03	1 (20%)	4,10,12	2.01	1 (25%)
3	MDH	F	5	3	4,6,7	1.87	1 (25%)	4,6,8	2.45	2 (50%)
3	FGA	F	4	3	4,8,9	0.41	0	2,9,11	0.88	0
3	FGA	E	4	3	4,8,9	0.35	0	2,9,11	1.40	0
3	1ZN	E	3	3	23,23,24	0.73	1 (4%)	24,29,31	1.36	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
3	MDH	E	5	3	-	0/2/6/8	-
3	ACB	E	1	3	-	1/5/10/12	-
3	1ZN	F	3	3	-	2/22/25/27	0/1/1/1
3	ACB	F	1	3	-	1/5/10/12	-
3	MDH	F	5	3	-	0/2/6/8	-
3	FGA	F	4	3	-	0/3/8/9	-
3	FGA	E	4	3	-	0/3/8/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1ZN	E	3	3	-	0/22/25/27	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	5	MDH	C-CA	3.45	1.48	1.43
3	E	3	1ZN	C18-C17	-2.16	1.53	1.55
3	E	5	MDH	C-CA	2.15	1.46	1.43
3	F	1	ACB	CB-CA	-2.11	1.53	1.55

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	MDH	O-C-CA	-6.61	116.99	125.39
3	F	5	MDH	O-C-CA	-3.95	120.37	125.39
3	E	3	1ZN	C18-C17-C16	-3.72	107.64	112.98
3	F	1	ACB	C4-CB-CA	3.15	114.29	110.94
3	F	3	1ZN	C4-C3-C2	2.80	117.52	113.42
3	E	3	1ZN	O3-C20-C18	-2.76	117.57	124.91
3	E	3	1ZN	C17-C16-C15	-2.64	119.54	123.59
3	E	5	MDH	CM-N-CA	-2.61	119.48	123.45
3	F	3	1ZN	C11-C10-C12	-2.30	106.22	110.05
3	F	3	1ZN	O3-C20-C18	-2.24	118.96	124.91
3	F	5	MDH	CB-CA-N	-2.09	119.96	122.69
3	F	3	1ZN	C3-C2-C10	-2.06	110.65	115.45

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	ACB	CA-CB-CG-OD1
3	F	3	1ZN	C16-C17-C18-C19
3	F	3	1ZN	C17-C18-C20-O3
3	F	1	ACB	CA-CB-CG-OD1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5	MDH	1	0
3	F	5	MDH	1	0

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5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	GOL	A	401	-	5,5,5	0.40	0	5,5,5	0.55	0
4	GOL	A	403	-	5,5,5	0.21	0	5,5,5	0.78	0
4	GOL	C	601	-	5,5,5	0.23	0	5,5,5	0.27	0
4	GOL	A	402	-	5,5,5	0.39	0	5,5,5	0.39	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
4	GOL	A	401	-	-	0/4/4/4	-
4	GOL	A	403	-	-	2/4/4/4	-
4	GOL	C	601	-	-	2/4/4/4	-
4	GOL	A	402	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	GOL	O1-C1-C2-C3
4	A	402	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	C	601	GOL	O1-C1-C2-C3
4	A	402	GOL	O2-C2-C3-O3
4	A	403	GOL	O1-C1-C2-O2
4	C	601	GOL	O1-C1-C2-O2
4	A	402	GOL	O1-C1-C2-O2
4	A	402	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	GOL	2	0
4	A	402	GOL	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 (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(Å²)	Q<0.9
1	A	294/329 (89%)	0.09	2 (0%)	87	87	23, 29, 36, 40	5 (1%)
1	B	294/329 (89%)	0.09	2 (0%)	87	87	25, 28, 34, 39	7 (2%)
2	C	160/170 (94%)	1.07	42 (26%)	0	0	22, 31, 40, 45	6 (3%)
2	D	66/170 (38%)	0.83	13 (19%)	1	0	23, 30, 43, 47	1 (1%)
3	E	1/5 (20%)	2.62	1 (100%)	0	0	30, 30, 30, 30	1 (100%)
3	F	1/5 (20%)	0.58	0	100	100	30, 30, 30, 30	1 (100%)
All	All	816/1008 (80%)	0.35	60 (7%)	14	13	22, 29, 37, 47	21 (2%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	442	ASP	6.3
2	C	445	PRO	6.0
2	C	543	ILE	5.6
2	C	494	LEU	5.5
2	C	424	PRO	5.3
2	D	426	GLU	5.1
2	C	443	PRO	5.1
2	C	537	ALA	4.9
2	C	536	ALA	4.7
2	D	442	ASP	4.5
2	D	445	PRO	4.4
2	C	444	ALA	4.4
2	C	496	PRO	4.4
2	C	540	ASP	4.3
2	C	547	ASP	4.3
2	C	544	GLN	4.1
2	C	583	GLU	4.1
2	C	425	TYR	3.9
2	C	538	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
2	C	582	ARG	3.8
2	D	485	LEU	3.8
2	D	424	PRO	3.6
2	D	427	PRO	3.6
2	C	541	GLY	3.6
2	C	441	GLU	3.6
2	C	495	PHE	3.5
2	C	575	ARG	3.5
2	C	542	ARG	3.5
2	C	503	SER	3.3
2	C	426	GLU	3.3
2	C	502	ASP	3.3
2	D	489	VAL	3.2
2	C	492	LEU	3.1
2	D	444	ALA	3.1
2	D	443	PRO	3.0
2	C	535	GLY	2.9
2	C	545	VAL	2.8
2	C	490	GLU	2.8
2	C	430	GLY	2.8
2	D	425	TYR	2.8
2	C	499	LEU	2.7
2	C	504	GLU	2.7
2	C	440	GLU	2.7
2	C	427	PRO	2.7
3	E	2	ARG	2.6
2	C	534	GLY	2.6
2	C	531	VAL	2.6
2	C	446	SER	2.5
2	D	446	SER	2.4
1	B	214	GLN	2.4
2	C	580	ILE	2.4
2	D	484	GLU	2.4
2	C	498	GLU	2.3
2	C	429	SER	2.3
2	D	487	LYS	2.1
2	C	528	VAL	2.1
2	C	505	GLY	2.1
1	B	121	LEU	2.1
1	A	104	ILE	2.1
1	A	214	GLN	2.1

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. 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	B-factors($Å^2$)	Q<0.9
3	FGA	E	4	9/10	0.78	0.22	29,31,33,36	9
3	FGA	F	4	9/10	0.85	0.23	28,30,31,31	9
3	ACB	F	1	9/10	0.87	0.26	30,32,34,36	9
3	MDH	E	5	7/8	0.88	0.26	28,29,30,31	7
3	MDH	F	5	7/8	0.88	0.19	30,31,32,33	7
3	ACB	E	1	9/10	0.88	0.24	27,29,30,30	9
3	1ZN	F	3	23/24	0.88	0.17	22,28,30,31	23
3	1ZN	E	3	23/24	0.91	0.19	24,27,28,31	23

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. 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	B-factors($Å^2$)	Q<0.9
4	GOL	A	401	6/6	0.77	0.19	42,43,43,44	6
4	GOL	A	402	6/6	0.85	0.27	25,33,35,40	6
4	GOL	A	403	6/6	0.86	0.15	42,46,48,50	6
4	GOL	C	601	6/6	0.94	0.11	30,32,33,34	6
5	MN	A	404	1/1	0.99	0.05	23,23,23,23	1
5	MN	B	401	1/1	0.99	0.08	21,21,21,21	1
5	MN	A	405	1/1	0.99	0.05	27,27,27,27	0
5	MN	B	402	1/1	1.00	0.06	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.