



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 5, 2023 – 06:46 AM EST

PDB ID : 2NYL
Title : Crystal structure of Protein Phosphatase 2A (PP2A) holoenzyme with the catalytic subunit carboxyl terminus truncated
Authors : Xing, Y.; Xu, Y.; Chen, Y.; Chao, Y.; Lin, Z.; Shi, Y.
Deposited on : 2006-11-20
Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

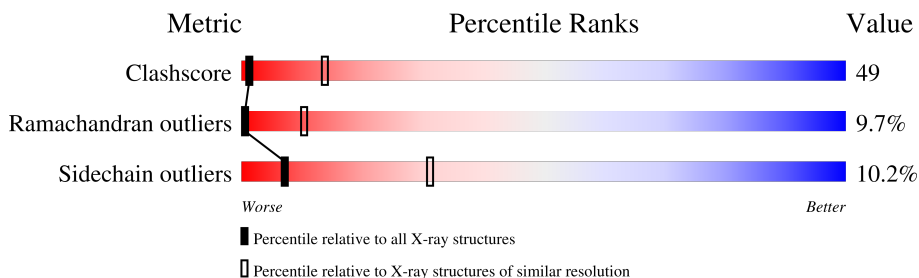
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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))
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	582	34% 54% 11% .
1	D	582	37% 49% 13% .
2	B	388	30% 56% 13% .
2	E	388	28% 55% 14% .
3	C	293	32% 58% 10%
3	F	293	38% 53% 9% .
4	G	7	43% 14% 43%
4	H	7	14% 71% 14%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 20212 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 Protein phosphatase 2, regulatory subunit A (PR 65), alpha isoform.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	582	Total 4535	C 2881	N 764	O 863	S 14	Se 13	0	0	0
1	D	582	Total 4535	C 2881	N 764	O 863	S 14	Se 13	0	0	0

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	388	Total 3131	C 2043	N 513	O 561	S 3	Se 11	0	0	0
2	E	388	Total 3131	C 2043	N 513	O 561	S 3	Se 11	0	0	0

- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	293	Total 2367	C 1497	N 405	O 450	S 15	0	0	0
3	F	293	Total 2367	C 1497	N 405	O 450	S 15	0	0	0

- Molecule 4 is a protein called microcystin LR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	7	Total 71	C 49	N 10	O 12	0	0	0
4	H	7	Total 71	C 49	N 10	O 12	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total 2	Mn 2	0	0
5	F	2	Total 2	Mn 2	0	0

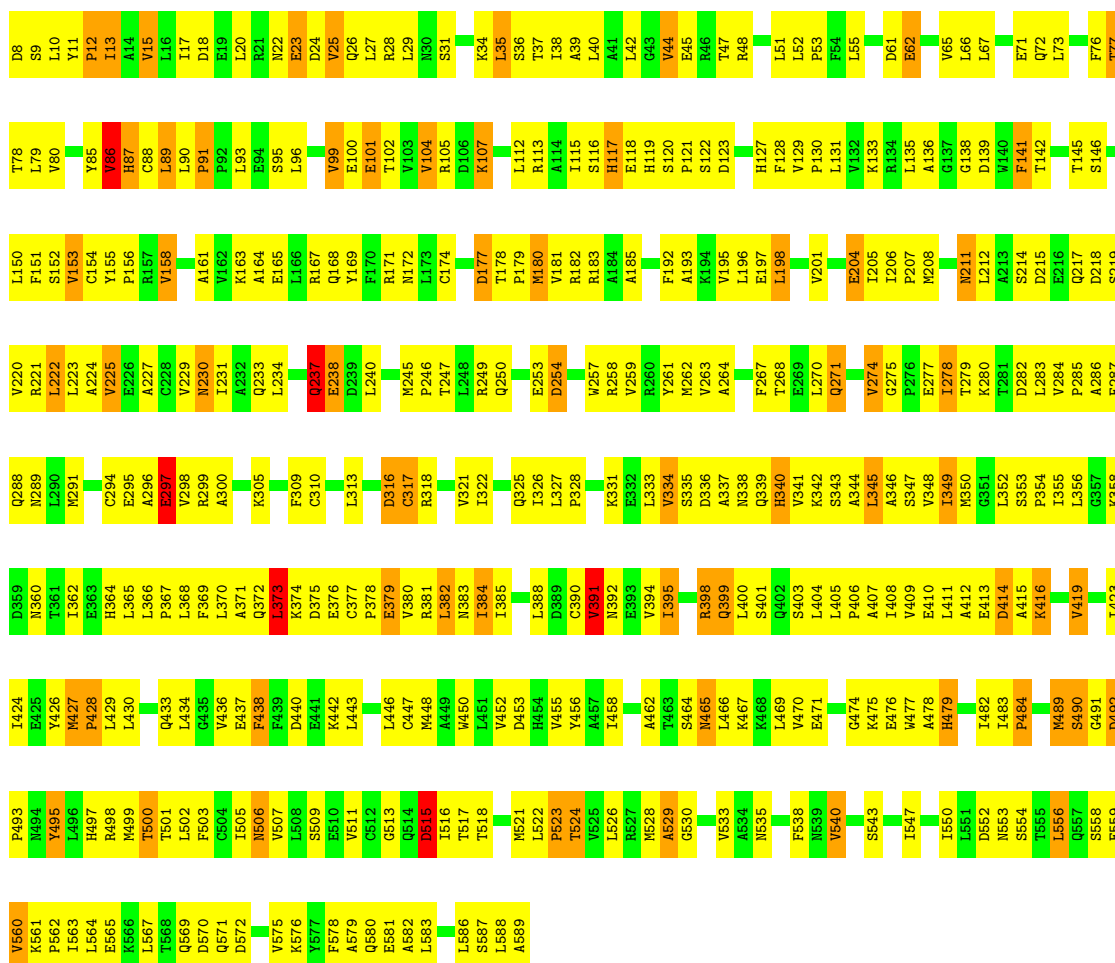
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

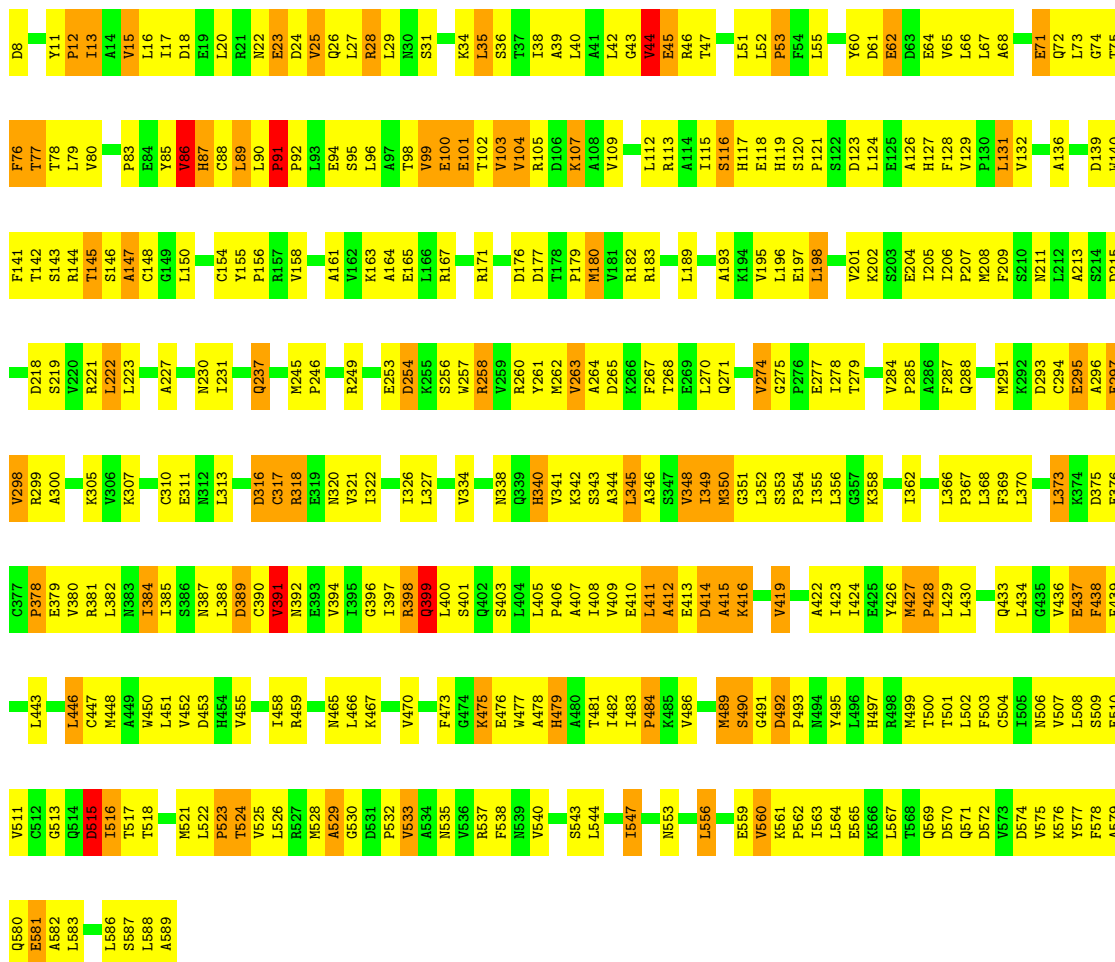
- Molecule 1: Protein phosphatase 2, regulatory subunit A (PR 65), alpha isoform

Chain A: 

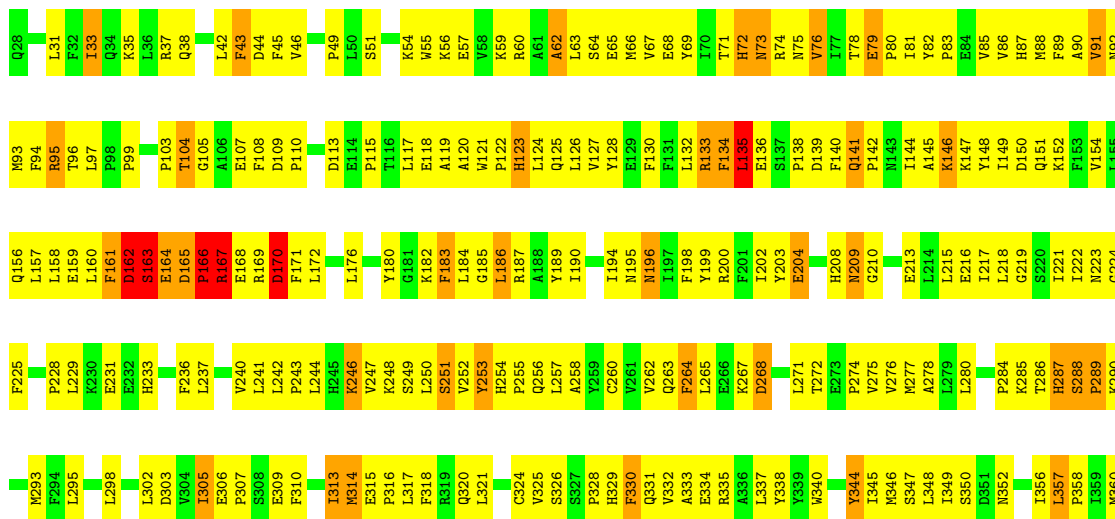
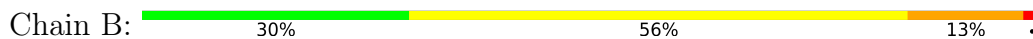


- Molecule 1: Protein phosphatase 2, regulatory subunit A (PR 65), alpha isoform

Chain D: 



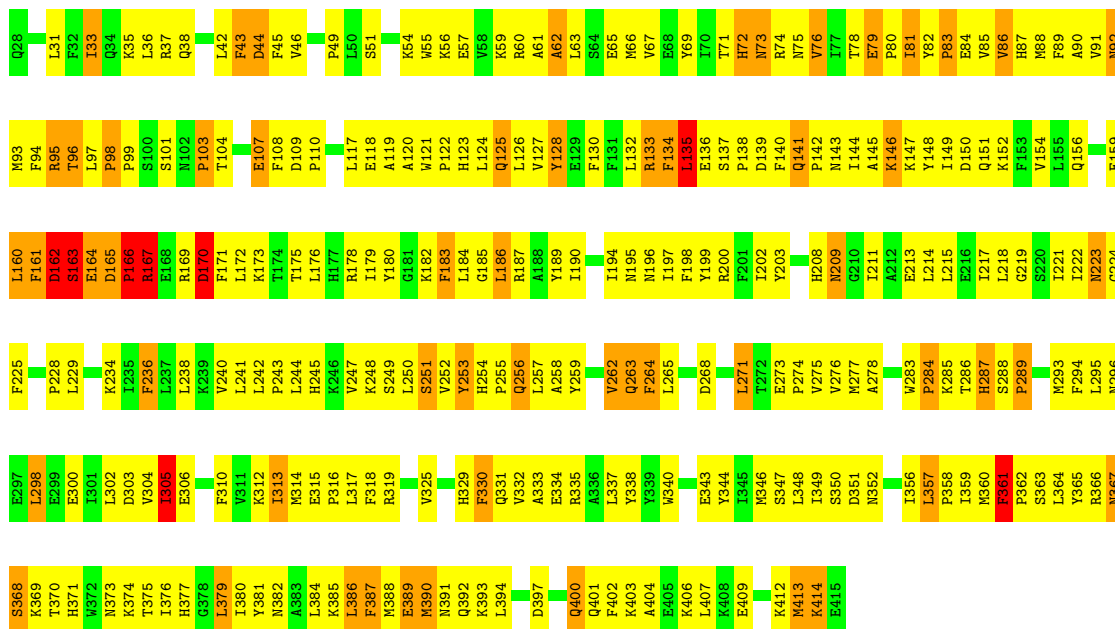
• Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform





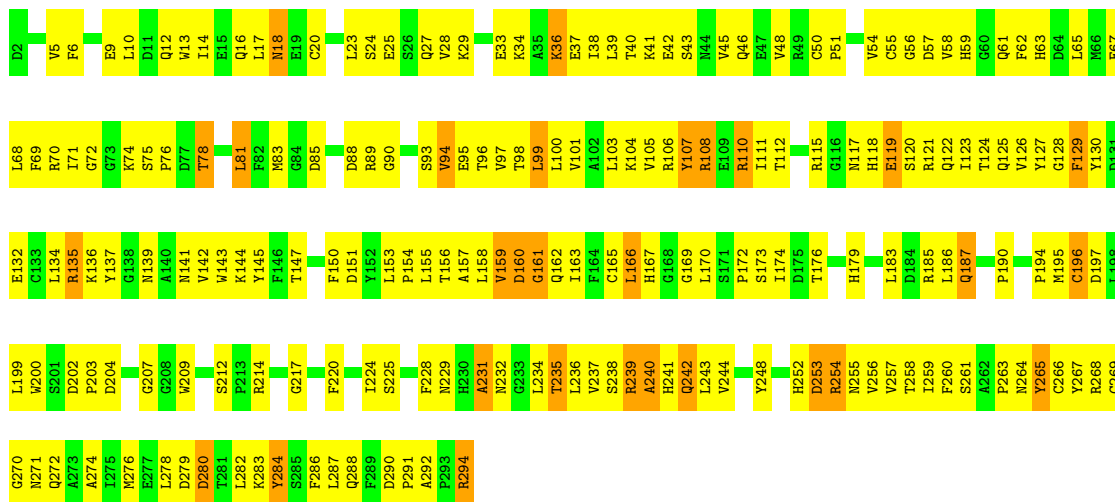
- Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform

Chain E: 28% 55% 14%



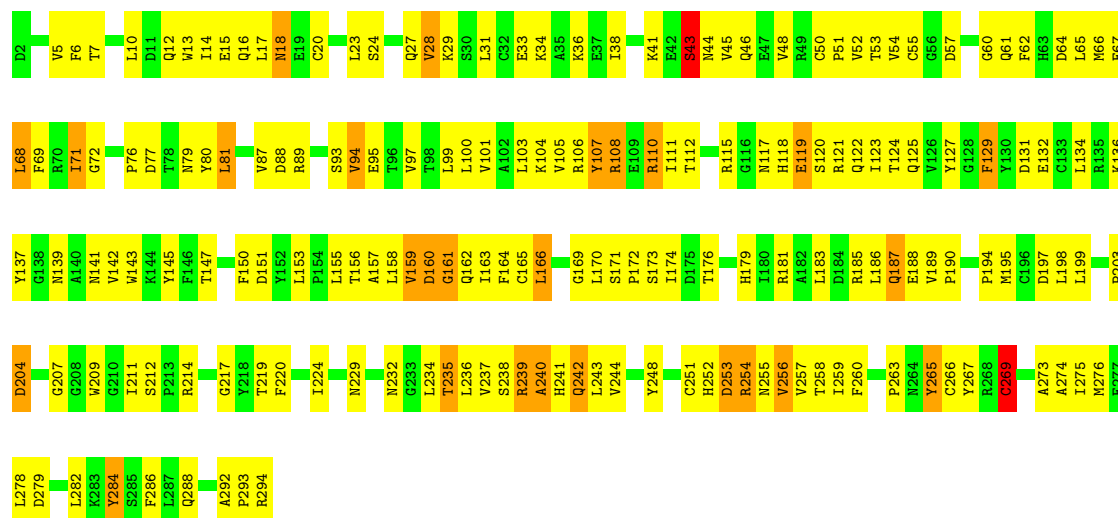
- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain C: 32% 58% 10%



- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

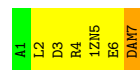
Chain F: 38% 53% 9%



- Molecule 4: microcystin LR



- Molecule 4: microcystin LR



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.48Å 159.85Å 270.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.80	Depositor
% Data completeness (in resolution range)	99.6 (100.00-3.80)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.282 , 0.335	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	20212	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

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: 1ZN, ACB, DAL, DAM, MN, 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	0.50	0/4596	0.72	0/6218
1	D	0.58	0/4596	0.75	0/6218
2	B	0.51	0/3202	0.74	3/4326 (0.1%)
2	E	0.53	0/3202	0.75	4/4326 (0.1%)
3	C	0.49	0/2424	0.73	0/3285
3	F	0.51	0/2424	0.74	1/3285 (0.0%)
4	G	0.36	0/17	0.80	0/19
4	H	0.38	0/17	0.89	0/19
All	All	0.53	0/20478	0.74	8/27696 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	G	0	3
4	H	0	3
All	All	0	6

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	162	ASP	N-CA-C	6.79	129.35	111.00
2	E	162	ASP	N-CA-C	6.71	129.12	111.00
2	E	163	SER	N-CA-C	6.21	127.77	111.00
2	B	163	SER	N-CA-C	5.95	127.06	111.00
2	E	219	GLY	N-CA-C	-5.95	98.24	113.10

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	4	ARG	Peptide
4	G	5	1ZN	Mainchain,Peptide
4	H	4	ARG	Peptide
4	H	5	1ZN	Mainchain,Peptide

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	4535	0	4637	449	0
1	D	4535	0	4637	431	0
2	B	3131	0	3050	330	0
2	E	3131	0	3050	359	0
3	C	2367	0	2268	221	0
3	F	2367	0	2268	215	0
4	G	71	0	61	1	0
4	H	71	0	61	3	0
5	C	2	0	0	0	0
5	F	2	0	0	0	0
All	All	20212	0	20032	1982	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 49.

The worst 5 of 1982 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:D:278:ILE:H	1:D:278:ILE:HD12	1.10	1.12
2:E:325:VAL:HG13	2:E:337:LEU:HD11	1.29	1.11
1:D:350:MSE:HE1	1:D:391:VAL:HG13	1.24	1.10
2:B:277:MSE:HE1	2:B:316:PRO:HG3	1.35	1.08
2:E:340:TRP:HA	2:E:346:MSE:HE3	1.34	1.06

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	580/582 (100%)	411 (71%)	124 (21%)	45 (8%)	1	15
1	D	580/582 (100%)	411 (71%)	119 (20%)	50 (9%)	1	12
2	B	386/388 (100%)	234 (61%)	97 (25%)	55 (14%)	0	4
2	E	386/388 (100%)	234 (61%)	95 (25%)	57 (15%)	0	4
3	C	291/293 (99%)	203 (70%)	69 (24%)	19 (6%)	1	19
3	F	291/293 (99%)	210 (72%)	63 (22%)	18 (6%)	1	20
4	G	1/7 (14%)	1 (100%)	0	0	100	100
4	H	1/7 (14%)	1 (100%)	0	0	100	100
All	All	2516/2540 (99%)	1705 (68%)	567 (22%)	244 (10%)	0	10

5 of 244 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	35	LEU
1	A	44	VAL
1	A	317	CYS
1	A	391	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	509/496 (103%)	450 (88%)	59 (12%)	5	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	509/496 (103%)	450 (88%)	59 (12%)	5	27
2	B	331/351 (94%)	299 (90%)	32 (10%)	8	33
2	E	331/351 (94%)	295 (89%)	36 (11%)	6	29
3	C	259/259 (100%)	239 (92%)	20 (8%)	13	43
3	F	259/259 (100%)	241 (93%)	18 (7%)	15	46
4	G	2/2 (100%)	2 (100%)	0	100	100
4	H	2/2 (100%)	2 (100%)	0	100	100
All	All	2202/2216 (99%)	1978 (90%)	224 (10%)	7	31

5 of 224 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	53	PRO
3	F	256	VAL
1	D	340	HIS
3	F	239	ARG
2	E	338	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	392	GLN
3	F	27	GLN
2	B	373	ASN
2	B	329	HIS
3	F	44	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](#)

10 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
4	1ZN	H	5	4	23,23,24	0.99	0	24,29,31	0.83	0
4	FGA	H	6	4	7,8,9	2.45	2 (28%)	7,9,11	1.74	2 (28%)
4	FGA	G	6	4	7,8,9	2.33	2 (28%)	7,9,11	1.93	2 (28%)
4	1ZN	G	5	4	23,23,24	1.19	1 (4%)	24,29,31	0.92	1 (4%)
4	ACB	H	3	-	7,8,9	1.74	2 (28%)	8,10,12	0.73	0
4	DAM	G	7	4,3	4,5,6	1.92	1 (25%)	3,5,7	3.89	3 (100%)
4	DAM	H	7	4,3	4,5,6	1.96	1 (25%)	3,5,7	4.23	3 (100%)
4	ACB	G	3	-	7,8,9	1.34	0	8,10,12	0.58	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	1ZN	H	5	4	-	3/22/25/27	0/1/1/1
4	FGA	H	6	4	-	2/7/8/9	-
4	FGA	G	6	4	-	3/7/8/9	-
4	1ZN	G	5	4	-	3/22/25/27	0/1/1/1
4	ACB	H	3	-	-	1/9/10/12	-
4	DAM	G	7	4,3	-	0/0/4/6	-
4	DAM	H	7	4,3	-	0/0/4/6	-
4	ACB	G	3	-	-	1/9/10/12	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	6	FGA	O-C	5.27	1.38	1.22
4	G	6	FGA	O-C	5.15	1.37	1.22
4	G	7	DAM	C-CA	3.47	1.50	1.45
4	H	7	DAM	C-CA	3.45	1.50	1.45
4	H	3	ACB	CB-CG	2.86	1.55	1.50

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	7	DAM	O-C-CA	-4.96	118.85	125.22
4	H	7	DAM	CM-N-CA	-4.89	116.01	123.45
4	G	7	DAM	CM-N-CA	-4.83	116.11	123.45
4	G	7	DAM	O-C-CA	-4.19	119.85	125.22
4	G	6	FGA	O-C-CA	-3.44	110.01	122.14

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	3	ACB	CA-CB-CG-OD1
4	G	5	1ZN	C12-C13-C15-C16
4	G	5	1ZN	C14-C13-C15-C16
4	H	5	1ZN	C12-C13-C15-C16
4	H	5	1ZN	C14-C13-C15-C16

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	6	FGA	1	0
4	G	7	DAM	1	0
4	H	7	DAM	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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.

5.7 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](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.