



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:05 PM UTC

PDB ID : 4I5L / pdb_00004i5l
Title : Structural mechanism of trimeric PP2A holoenzyme involving PR70: insight for Cdc6 dephosphorylation
Authors : Wlodarchak, N.; Satyshur, K.A.; Guo, F.; Xing, Y.
Deposited on : 2012-11-28
Resolution : 2.43 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:

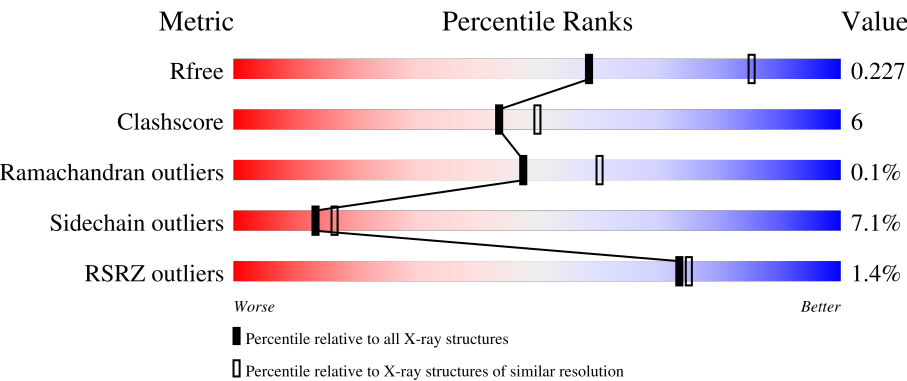
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.43 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}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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 $\leq 5\%$. 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	584	% 84%13%.
1	D	584	% 79%19%.
2	B	413	2% 70%13%.14%
2	E	413	2% 73%11%.14%
3	C	311	% 78%13%.5%

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Mol	Chain	Length	Quality of chain
3	F	311	% 80% 12% 5%
4	G	7	43% 29% 29%
4	H	7	43% 29% 29%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 20426 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 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4534	2882	764	860	28			
1	D	582	Total	C	N	O	S	0	0	0
			4534	2882	764	860	28			

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A regulatory subunit B'' subunit beta - Cell division control protein 6 homolog chimeric construct.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	356	Total	C	N	O	S	0	0	0
			2905	1866	486	533	20			
2	E	357	Total	C	N	O	S	0	0	0
			2912	1870	488	534	20			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	491	SER	-	linker	UNP Q9Y5P8
B	492	THR	-	linker	UNP Q9Y5P8
B	493	GLY	-	linker	UNP Q9Y5P8
B	494	ASN	-	linker	UNP Q9Y5P8
B	495	ALA	-	linker	UNP Q9Y5P8
B	496	SER	-	linker	UNP Q9Y5P8
B	497	ASP	-	linker	UNP Q9Y5P8
B	498	SER	-	linker	UNP Q9Y5P8
B	499	SER	-	linker	UNP Q9Y5P8
B	500	SER	-	linker	UNP Q9Y5P8
B	501	ASP	-	linker	UNP Q9Y5P8
B	502	SER	-	linker	UNP Q9Y5P8
B	503	SER	-	linker	UNP Q9Y5P8
B	504	SER	-	linker	UNP Q9Y5P8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	505	SER	-	linker	UNP Q9Y5P8
B	506	GLU	-	linker	UNP Q9Y5P8
B	507	GLY	-	linker	UNP Q9Y5P8
B	508	ASP	-	linker	UNP Q9Y5P8
B	509	GLY	-	linker	UNP Q9Y5P8
B	510	THR	-	linker	UNP Q9Y5P8
B	511	VAL	-	linker	UNP Q9Y5P8
E	491	SER	-	linker	UNP Q99741
E	492	THR	-	linker	UNP Q99741
E	493	GLY	-	linker	UNP Q99741
E	494	ASN	-	linker	UNP Q99741
E	495	ALA	-	linker	UNP Q99741
E	496	SER	-	linker	UNP Q99741
E	497	ASP	-	linker	UNP Q99741
E	498	SER	-	linker	UNP Q99741
E	499	SER	-	linker	UNP Q99741
E	500	SER	-	linker	UNP Q99741
E	501	ASP	-	linker	UNP Q99741
E	502	SER	-	linker	UNP Q99741
E	503	SER	-	linker	UNP Q99741
E	504	SER	-	linker	UNP Q99741
E	505	SER	-	linker	UNP Q99741
E	506	GLU	-	linker	UNP Q99741
E	507	GLY	-	linker	UNP Q99741
E	508	ASP	-	linker	UNP Q99741
E	509	GLY	-	linker	UNP Q99741
E	510	THR	-	linker	UNP Q99741
E	511	VAL	-	linker	UNP Q99741

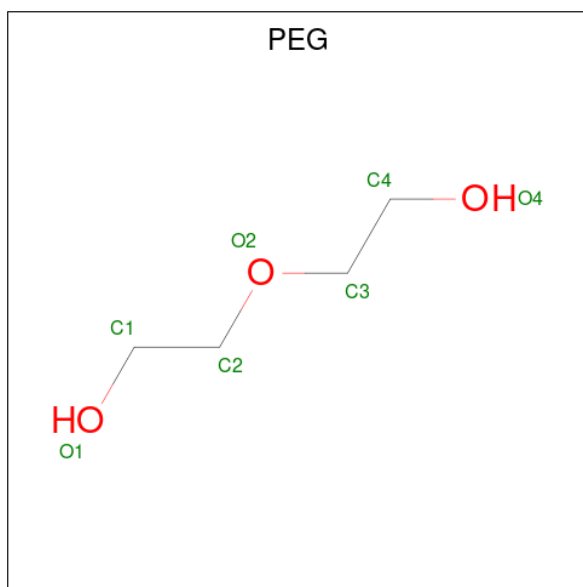
- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform, PP2A-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	295	Total	C	N	O	S	0	0	0
			2381	1505	410	451	15			
3	F	295	Total	C	N	O	S	0	0	0
			2381	1505	410	451	15			

- Molecule 4 is a protein called Microcystin-LR (MCLR) bound form.

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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			7	4	3		

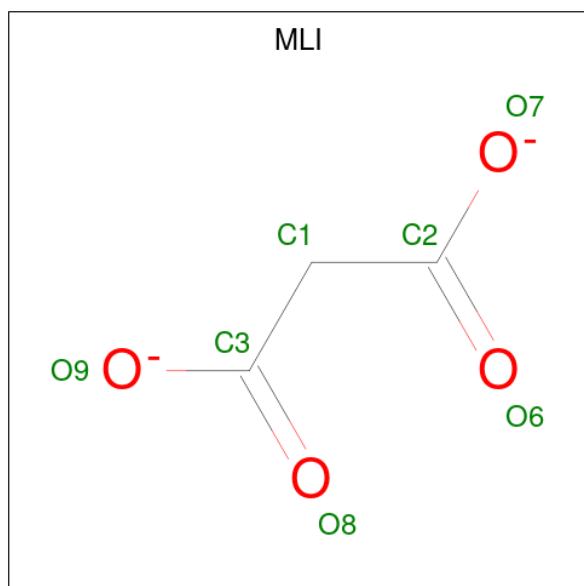
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	2	Total	Ca		0	0
			2	2			
6	E	2	Total	Ca		0	0
			2	2			

- Molecule 7 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 8 is MALONATE ION (CCD ID: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			7	3	4		
8	E	1	Total	C	O	0	0
			7	3	4		

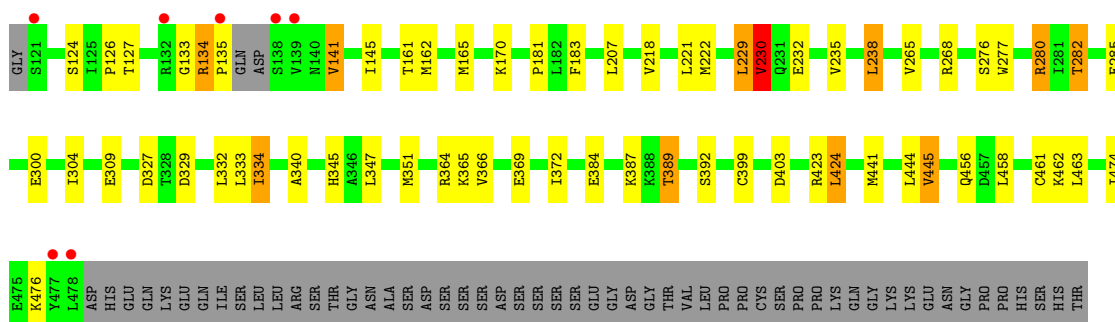
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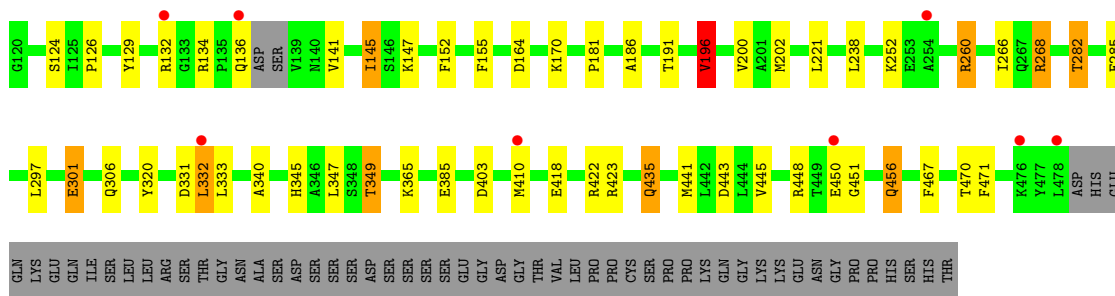
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	C	O	0	0
			7	3	4		

- Molecule 9 is water.

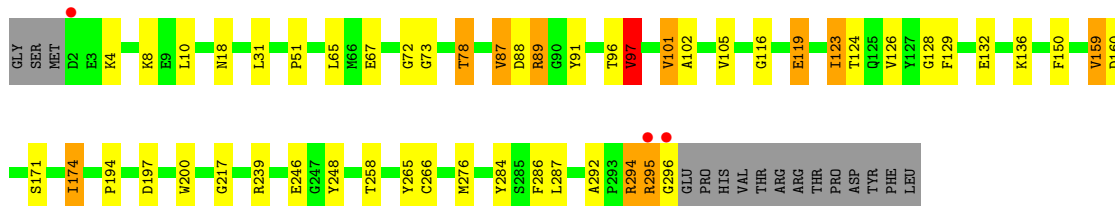
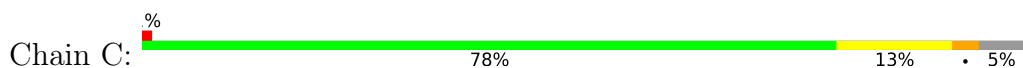
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	152	Total	O	0	0
			152	152		
9	B	82	Total	O	0	0
			82	82		
9	C	79	Total	O	0	0
			79	79		
9	D	70	Total	O	0	0
			70	70		
9	E	73	Total	O	0	0
			73	73		
9	F	71	Total	O	0	0
			71	71		
9	H	4	Total	O	0	0
			4	4		



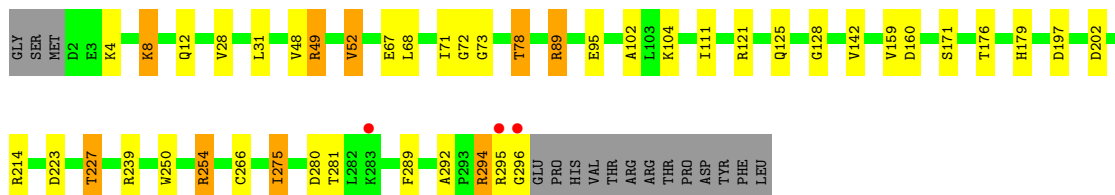
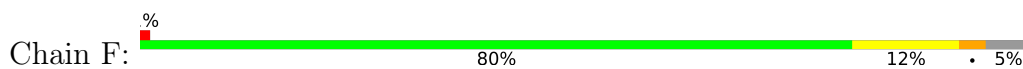
- Molecule 2: Serine/threonine-protein phosphatase 2A regulatory subunit B'' subunit beta - Cell division control protein 6 homolog chimeric construct



- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform, PP2A-alpha

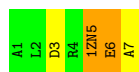


- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform, PP2A-alpha



- Molecule 4: Microcystin-LR (MCLR) bound form

Chain G:  43% 29% 29%



- Molecule 4: Microcystin-LR (MCLR) bound form

Chain H:  43% 29% 29%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.23Å 101.07Å 343.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 2.43 49.85 – 2.43	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.85-2.43) 98.8 (49.85-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.179 , 0.228 0.178 , 0.227	Depositor DCC
R_{free} test set	6266 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20426	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1ZN, MLI, PEG, MAA, ACB, CA, MN, DAL, 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	0.63	0/4608	0.96	2/6256 (0.0%)
1	D	0.55	0/4608	0.92	3/6256 (0.0%)
2	B	0.60	1/2979 (0.0%)	0.90	1/4025 (0.0%)
2	E	0.56	0/2986	0.89	5/4034 (0.1%)
3	C	0.61	0/2438	0.93	4/3304 (0.1%)
3	F	0.55	0/2438	0.86	2/3304 (0.1%)
4	G	0.36	0/17	0.54	0/19
4	H	0.36	0/17	0.51	0/19
All	All	0.58	1/20091 (0.0%)	0.91	17/27217 (0.1%)

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	2
4	H	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	235	VAL	CA-CB	6.21	1.57	1.54

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	196	VAL	CB-CA-C	-8.19	101.39	111.88
3	C	97	VAL	CB-CA-C	-7.30	102.14	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	82	GLY	CA-C-N	6.60	126.85	119.32
1	D	82	GLY	C-N-CA	6.60	126.85	119.32
2	E	134	ARG	CA-C-N	6.54	128.01	119.84

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

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	4534	0	4642	44	0
1	D	4534	0	4642	57	0
2	B	2905	0	2816	45	0
2	E	2912	0	2822	42	0
3	C	2381	0	2284	35	0
3	F	2381	0	2284	25	0
4	G	71	0	62	2	0
4	H	71	0	63	2	0
5	A	28	0	40	0	0
5	B	14	0	20	1	0
5	C	14	0	20	3	0
5	D	14	0	20	0	0
5	E	7	0	10	0	0
6	B	2	0	0	0	0
6	E	2	0	0	0	0
7	C	2	0	0	0	0
7	F	2	0	0	0	0
8	C	7	0	2	1	0
8	E	7	0	2	0	0
8	F	7	0	2	0	0
9	A	152	0	0	1	0
9	B	82	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	79	0	0	0	0
9	D	70	0	0	1	0
9	E	73	0	0	1	0
9	F	71	0	0	1	0
9	H	4	0	0	0	0
All	All	20426	0	19731	240	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 6.

The worst 5 of 240 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:353:SER:HB3	1:D:394:VAL:HG11	1.52	0.90
2:E:268:ARG:HH11	2:E:268:ARG:HG2	1.36	0.90
2:B:389:THR:HG22	2:B:392:SER:H	1.37	0.88
1:D:77:THR:HG21	1:D:118:GLU:HG2	1.57	0.85
1:D:358:LYS:HD2	1:D:359:ASP:H	1.42	0.83

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	580/584 (99%)	571 (98%)	9 (2%)	0	100	100
1	D	580/584 (99%)	571 (98%)	9 (2%)	0	100	100
2	B	352/413 (85%)	344 (98%)	7 (2%)	1 (0%)	36	44
2	E	353/413 (86%)	343 (97%)	10 (3%)	0	100	100
3	C	293/311 (94%)	282 (96%)	10 (3%)	1 (0%)	36	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	293/311 (94%)	281 (96%)	12 (4%)	0	100	100
4	G	1/7 (14%)	1 (100%)	0	0	100	100
4	H	1/7 (14%)	1 (100%)	0	0	100	100
All	All	2453/2630 (93%)	2394 (98%)	57 (2%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	134	ARG
3	C	295	ARG

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	509/510 (100%)	471 (92%)	38 (8%)	12	15
1	D	509/510 (100%)	469 (92%)	40 (8%)	11	13
2	B	316/366 (86%)	293 (93%)	23 (7%)	13	15
2	E	316/366 (86%)	294 (93%)	22 (7%)	14	17
3	C	260/275 (94%)	243 (94%)	17 (6%)	15	20
3	F	260/275 (94%)	245 (94%)	15 (6%)	18	25
4	G	2/2 (100%)	2 (100%)	0	100	100
4	H	2/2 (100%)	2 (100%)	0	100	100
All	All	2174/2306 (94%)	2019 (93%)	155 (7%)	13	16

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	565	GLU
3	F	49	ARG
2	E	136	GLN
2	E	301	GLU

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Mol	Chain	Res	Type
3	F	239	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	433	GLN
2	E	435	GLN
3	F	141	ASN
2	E	136	GLN
2	B	420	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	ACB	G	3	4	8,8,9	1.86	1 (12%)	8,10,12	2.35	1 (12%)
4	MAA	H	7	4,3	4,5,6	0.86	0	2,5,7	0.99	0
4	FGA	G	6	4	7,8,9	1.54	1 (14%)	6,9,11	0.67	0
4	MAA	G	7	4,3	4,5,6	0.64	0	2,5,7	0.86	0
4	ACB	H	3	4	8,8,9	1.81	1 (12%)	8,10,12	2.83	4 (50%)
4	1ZN	G	5	4	21,23,24	2.66	4 (19%)	25,29,31	2.30	5 (20%)
4	1ZN	H	5	4	21,23,24	2.91	4 (19%)	25,29,31	2.16	6 (24%)
4	FGA	H	6	4	7,8,9	1.59	1 (14%)	6,9,11	0.61	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	ACB	G	3	4	-	2/10/10/12	-
4	MAA	H	7	4,3	-	1/2/4/6	-
4	FGA	G	6	4	-	2/8/8/9	-
4	MAA	G	7	4,3	-	1/2/4/6	-
4	ACB	H	3	4	-	2/10/10/12	-
4	1ZN	G	5	4	-	5/23/25/27	0/1/1/1
4	1ZN	H	5	4	-	3/23/25/27	0/1/1/1
4	FGA	H	6	4	-	2/8/8/9	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	5	1ZN	C15-C16	9.11	1.52	1.32
4	G	5	1ZN	C15-C16	8.20	1.50	1.32
4	H	5	1ZN	C12-C13	7.11	1.53	1.34
4	G	5	1ZN	C12-C13	6.67	1.52	1.34
4	H	3	ACB	OD2-CG	-4.50	1.23	1.42

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5	1ZN	CA-C16-C15	-8.04	110.51	123.62
4	H	5	1ZN	CA-C16-C15	-8.02	110.55	123.62
4	H	3	ACB	OD2-CG-CB	6.34	124.53	111.51
4	G	3	ACB	OD2-CG-CB	6.10	124.05	111.51
4	G	5	1ZN	C16-C15-C13	-5.26	115.02	126.32

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	7	MAA	CB-CA-N-CM
4	G	3	ACB	C4-CB-CG-OD2
4	H	3	ACB	C4-CB-CG-OD2
4	G	5	1ZN	O-C-C18-C19
4	H	5	1ZN	O-C-C18-C19

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 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	$\# Z > 2$
5	PEG	C	404	-	6,6,6	0.46	0	5,5,5	0.33	0
5	PEG	A	604	-	6,6,6	0.59	0	5,5,5	0.26	0
5	PEG	D	602	-	6,6,6	0.44	0	5,5,5	0.42	0
5	PEG	A	601	-	6,6,6	0.44	0	5,5,5	0.43	0
5	PEG	A	602	-	6,6,6	0.48	0	5,5,5	0.32	0
5	PEG	A	603	-	6,6,6	0.51	0	5,5,5	0.25	0
5	PEG	B	604	-	6,6,6	0.50	0	5,5,5	0.30	0
5	PEG	D	601	-	6,6,6	0.47	0	5,5,5	0.29	0
5	PEG	C	403	-	6,6,6	0.58	0	5,5,5	0.38	0
8	MLI	E	704	-	6,6,6	1.07	0	7,7,7	1.27	0
5	PEG	B	603	-	6,6,6	0.47	0	5,5,5	0.41	0
8	MLI	F	403	-	6,6,6	1.14	0	7,7,7	1.25	0
8	MLI	C	405	-	6,6,6	1.16	0	7,7,7	1.75	1 (14%)
5	PEG	E	703	-	6,6,6	0.54	0	5,5,5	0.32	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
5	PEG	C	404	-	-	1/4/4/4	-
5	PEG	A	604	-	-	4/4/4/4	-
5	PEG	D	602	-	-	3/4/4/4	-
5	PEG	A	601	-	-	2/4/4/4	-
5	PEG	A	602	-	-	3/4/4/4	-
5	PEG	A	603	-	-	3/4/4/4	-
5	PEG	B	604	-	-	2/4/4/4	-
5	PEG	D	601	-	-	4/4/4/4	-
5	PEG	C	403	-	-	3/4/4/4	-
8	MLI	E	704	-	-	2/4/4/4	-
5	PEG	B	603	-	-	1/4/4/4	-
8	MLI	F	403	-	-	2/4/4/4	-
8	MLI	C	405	-	-	2/4/4/4	-
5	PEG	E	703	-	-	3/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	405	MLI	C3-C1-C2	-3.13	101.90	112.95

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	403	PEG	O2-C3-C4-O4
5	D	601	PEG	O1-C1-C2-O2
5	B	604	PEG	O1-C1-C2-O2
5	B	604	PEG	O2-C3-C4-O4
5	D	602	PEG	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	604	PEG	1	0
5	C	403	PEG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	405	MLI	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	582/584 (99%)	-0.45	5 (0%) 81 82	20, 36, 59, 92	0
1	D	582/584 (99%)	-0.05	8 (1%) 73 75	30, 49, 81, 107	0
2	B	356/413 (86%)	-0.30	7 (1%) 65 66	21, 37, 70, 92	0
2	E	357/413 (86%)	-0.20	8 (2%) 62 63	26, 40, 76, 92	0
3	C	295/311 (94%)	-0.51	3 (1%) 79 81	18, 34, 51, 98	0
3	F	295/311 (94%)	-0.32	3 (1%) 79 81	26, 41, 65, 115	0
4	G	2/7 (28%)	0.60	0 100 100	64, 64, 64, 75	0
4	H	2/7 (28%)	0.58	0 100 100	54, 54, 54, 64	0
All	All	2471/2630 (93%)	-0.29	34 (1%) 73 75	18, 40, 73, 115	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	296	GLY	6.7
2	B	135	PRO	4.8
2	E	478	LEU	3.8
1	D	589	ALA	3.3
2	B	121	SER	3.3

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
4	DAL	G	1	5/6	0.89	0.12	54,54,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DAL	H	1	5/6	0.89	0.12	50,50,55,56	0
4	MAA	G	7	6/7	0.92	0.10	46,48,49,51	0
4	MAA	H	7	6/7	0.92	0.10	38,44,46,47	0
4	ACB	G	3	9/10	0.93	0.10	52,55,57,60	0
4	ACB	H	3	9/10	0.93	0.08	44,46,47,49	0
4	1ZN	G	5	23/24	0.93	0.09	38,42,45,51	0
4	1ZN	H	5	23/24	0.93	0.09	34,37,42,44	0
4	FGA	H	6	9/10	0.93	0.08	38,39,43,43	0
4	FGA	G	6	9/10	0.94	0.08	42,47,50,50	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	PEG	A	604	7/7	0.76	0.28	64,66,71,76	0
8	MLI	C	405	7/7	0.78	0.16	47,53,56,59	0
5	PEG	C	404	7/7	0.79	0.23	62,70,75,78	0
5	PEG	D	601	7/7	0.80	0.20	65,76,85,87	0
5	PEG	B	604	7/7	0.81	0.19	62,63,65,68	0
5	PEG	E	703	7/7	0.82	0.22	59,64,65,66	0
8	MLI	F	403	7/7	0.83	0.15	67,69,73,73	0
5	PEG	C	403	7/7	0.84	0.17	41,45,53,56	0
5	PEG	A	603	7/7	0.85	0.14	62,65,67,68	0
5	PEG	A	602	7/7	0.85	0.17	57,65,79,80	0
5	PEG	D	602	7/7	0.85	0.18	72,73,76,78	0
5	PEG	A	601	7/7	0.88	0.16	71,72,76,76	0
8	MLI	E	704	7/7	0.89	0.15	61,63,66,66	0
5	PEG	B	603	7/7	0.91	0.16	67,67,72,72	0
6	CA	E	702	1/1	0.95	0.09	48,48,48,48	0
6	CA	E	701	1/1	0.98	0.07	27,27,27,27	0
6	CA	B	602	1/1	0.98	0.07	43,43,43,43	0
7	MN	F	402	1/1	0.98	0.12	43,43,43,43	0
6	CA	B	601	1/1	0.99	0.07	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MN	F	401	1/1	0.99	0.10	34,34,34,34	0
7	MN	C	402	1/1	1.00	0.07	40,40,40,40	0
7	MN	C	401	1/1	1.00	0.04	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.