



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 6, 2023 – 07:33 PM EST

PDB ID : 4I5L
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

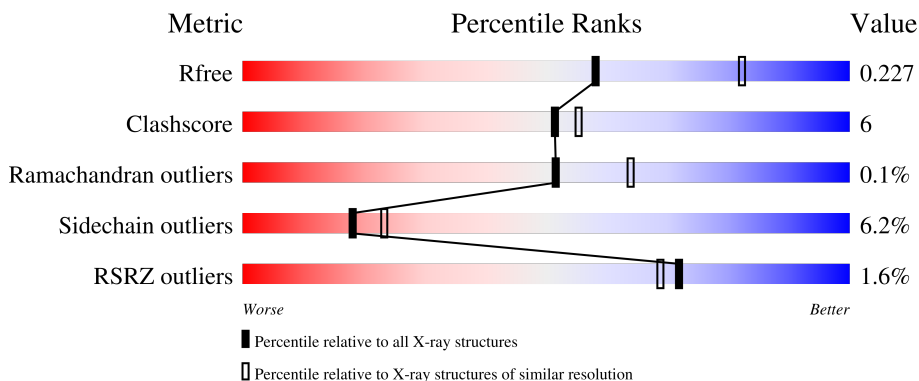
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.




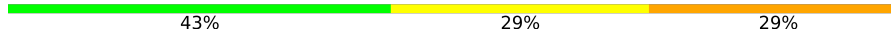

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	 86% 12%
1	D	584	 81% 17%
2	B	413	 70% 13% 14%
2	E	413	 75% 9% 14%
3	C	311	 79% 13% 5%

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Mol	Chain	Length	Quality of chain
3	F	311	 <p>% 81% 10% 5%</p>
4	G	7	 <p>43% 29% 29%</p>
4	H	7	 <p>43% 29% 29%</p>

2 Entry composition i

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
			Total	C	N	O	S			
1	A	582	4534	2882	764	860	28	0	0	0
1	D	582	4534	2882	764	860	28	0	0	0

- 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
			Total	C	N	O	S			
2	B	356	2905	1866	486	533	20	0	0	0
2	E	357	2912	1870	488	534	20	0	0	0

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

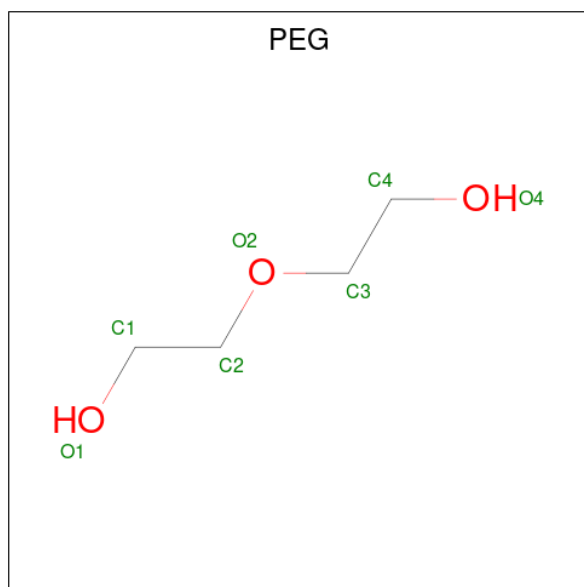
- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform, PP2A-alpha.

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

- 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 (three-letter code: 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		

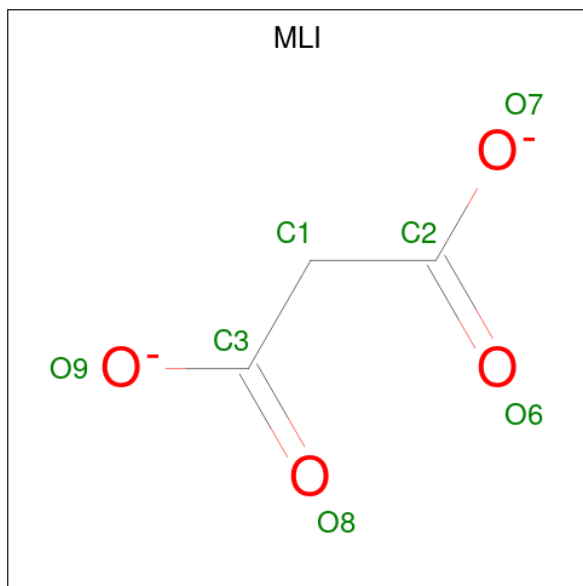
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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 (three-letter code: 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 (three-letter code: 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		

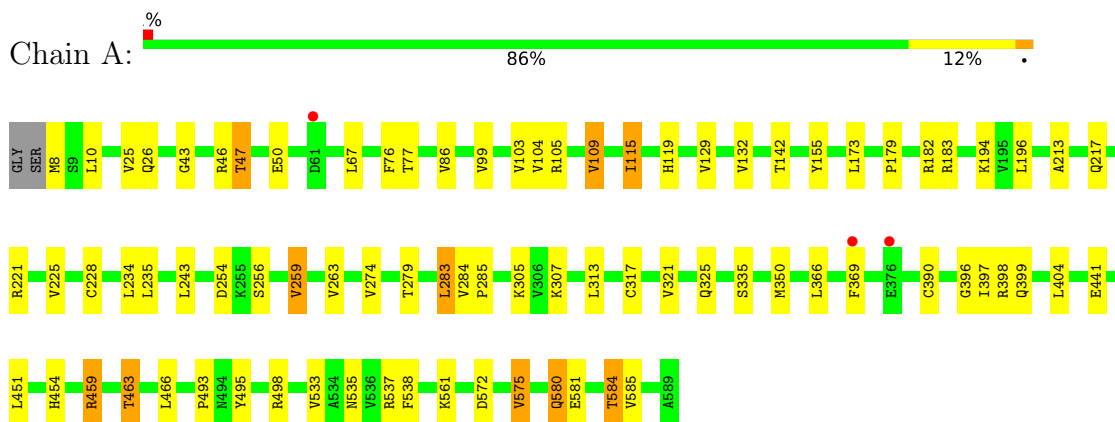
- Molecule 9 is water.

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		

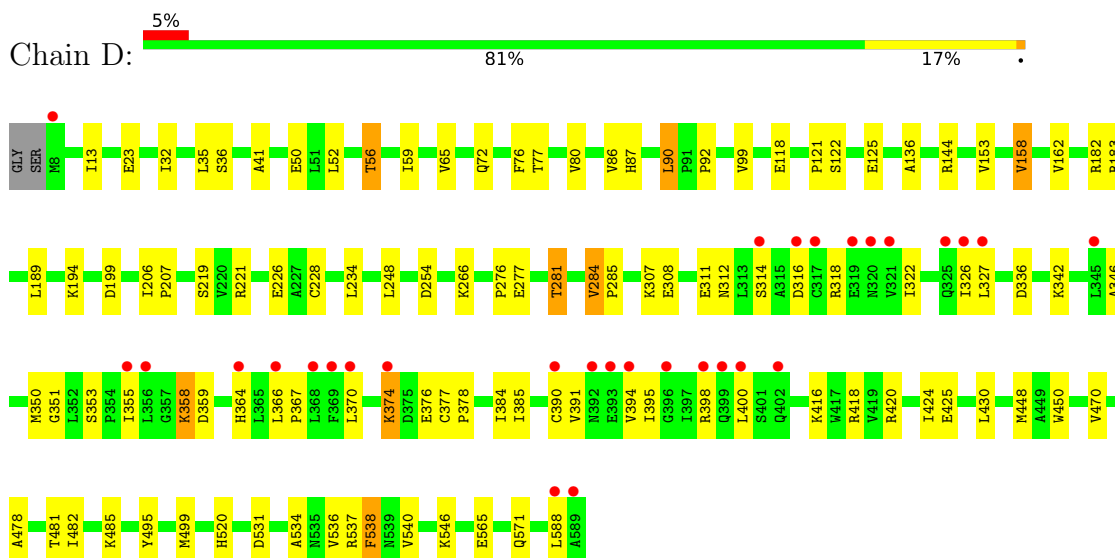
3 Residue-property plots

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 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 2A 65 kDa regulatory subunit A alpha isoform



- Molecule 1: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform



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





- 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 49.80 – 2.43	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.85-2.43) 98.6 (49.80-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.42Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.179 , 0.228 0.178 , 0.227	Depositor DCC
R_{free} test set	6193 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtrriage
Anisotropy	0.067	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1ZN, ACB, CA, PEG, MAA, MN, DAL, FGA, MLI

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	0.45	0/4608	0.69	4/6256 (0.1%)
1	D	0.39	0/4608	0.60	2/6256 (0.0%)
2	B	0.49	0/2979	0.69	1/4025 (0.0%)
2	E	0.44	0/2986	0.62	1/4034 (0.0%)
3	C	0.48	0/2438	0.70	1/3304 (0.0%)
3	F	0.43	0/2438	0.66	1/3304 (0.0%)
4	G	0.34	0/17	0.63	0/19
4	H	0.33	0/17	0.65	0/19
All	All	0.44	0/20091	0.66	10/27217 (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	2
4	H	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	ARG	NE-CZ-NH2	-10.75	114.93	120.30
2	B	412	GLU	OE1-CD-OE2	9.14	134.27	123.30
1	A	537	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	A	182	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	459	ARG	NE-CZ-NH1	6.25	123.42	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	5	1ZN	Mainchain,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	4534	0	4642	39	0
1	D	4534	0	4642	52	0
2	B	2905	0	2816	43	0
2	E	2912	0	2822	39	0
3	C	2381	0	2284	30	0
3	F	2381	0	2284	24	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
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	220	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 220 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%)	41	49
2	E	353/413 (86%)	343 (97%)	10 (3%)	0	100	100
3	C	293/311 (94%)	282 (96%)	10 (3%)	1 (0%)	41	49
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%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	134	ARG

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Mol	Chain	Res	Type
3	C	295	ARG

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	509/510 (100%)	479 (94%)	30 (6%)	19	25
1	D	509/510 (100%)	479 (94%)	30 (6%)	19	25
2	B	316/366 (86%)	292 (92%)	24 (8%)	13	16
2	E	316/366 (86%)	298 (94%)	18 (6%)	20	26
3	C	260/275 (94%)	243 (94%)	17 (6%)	17	21
3	F	260/275 (94%)	245 (94%)	15 (6%)	20	26
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%)	2040 (94%)	134 (6%)	18	23

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	385	GLU
3	F	4	LYS
3	F	275	ILE
2	B	389	THR
2	B	364	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
3	C	122	GLN
2	E	435	GLN
3	F	141	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	ACB	H	3	4	7,8,9	1.90	1 (14%)	6,10,12	3.14	3 (50%)
4	1ZN	G	5	4	23,23,24	2.38	4 (17%)	24,29,31	2.18	4 (16%)
4	MAA	H	7	4,3	4,5,6	0.84	0	1,5,7	0.98	0
4	ACB	G	3	4	7,8,9	1.92	1 (14%)	6,10,12	2.71	1 (16%)
4	1ZN	H	5	4	23,23,24	2.65	5 (21%)	24,29,31	2.19	5 (20%)
4	FGA	H	6	4	7,8,9	1.57	1 (14%)	8,9,11	0.90	0
4	FGA	G	6	4	7,8,9	1.52	1 (14%)	8,9,11	0.86	0
4	MAA	G	7	4,3	4,5,6	0.62	0	1,5,7	0.50	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	H	3	4	-	3/10/10/12	-
4	1ZN	G	5	4	-	3/22/25/27	0/1/1/1
4	MAA	H	7	4,3	-	1/1/4/6	-
4	ACB	G	3	4	-	2/10/10/12	-
4	1ZN	H	5	4	-	2/22/25/27	0/1/1/1
4	FGA	H	6	4	-	2/8/8/9	-
4	FGA	G	6	4	-	2/8/8/9	-
4	MAA	G	7	4,3	-	1/1/4/6	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	5	1ZN	C15-C16	8.67	1.52	1.32
4	G	5	1ZN	C15-C16	7.81	1.50	1.32
4	H	5	1ZN	C12-C13	6.00	1.53	1.34
4	G	5	1ZN	C12-C13	5.63	1.52	1.34
4	H	3	ACB	OD2-CG	-4.47	1.23	1.42

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5	1ZN	CA-C16-C15	-8.53	110.51	123.59
4	H	5	1ZN	CA-C16-C15	-8.51	110.55	123.59
4	H	3	ACB	OD2-CG-CB	6.46	124.53	111.33
4	G	3	ACB	OD2-CG-CB	6.23	124.05	111.33
4	G	5	1ZN	C10-C12-C13	-3.32	116.15	126.67

There are no chirality outliers.

5 of 16 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	H	6	FGA	O-C-CA-N
4	G	6	FGA	OXT-C-CA-N

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	H	6	FGA	2	0
4	G	6	FGA	2	0
4	G	7	MAA	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	A	604	-	6,6,6	0.58	0	5,5,5	0.26	0
5	PEG	A	603	-	6,6,6	0.51	0	5,5,5	0.25	0
5	PEG	B	604	-	6,6,6	0.49	0	5,5,5	0.30	0
5	PEG	B	603	-	6,6,6	0.46	0	5,5,5	0.41	0
5	PEG	A	602	-	6,6,6	0.47	0	5,5,5	0.32	0
8	MLI	C	405	-	6,6,6	1.13	0	7,7,7	1.72	1 (14%)
5	PEG	A	601	-	6,6,6	0.43	0	5,5,5	0.44	0
5	PEG	D	602	-	6,6,6	0.43	0	5,5,5	0.43	0
8	MLI	F	403	-	6,6,6	1.11	0	7,7,7	1.22	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	0.39	0
5	PEG	C	404	-	6,6,6	0.46	0	5,5,5	0.33	0
8	MLI	E	704	-	6,6,6	1.04	0	7,7,7	1.23	0
5	PEG	E	703	-	6,6,6	0.53	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	A	604	-	-	4/4/4/4	-
5	PEG	A	603	-	-	3/4/4/4	-
5	PEG	B	604	-	-	2/4/4/4	-
5	PEG	B	603	-	-	1/4/4/4	-
5	PEG	A	602	-	-	3/4/4/4	-
8	MLI	C	405	-	-	2/4/4/4	-
5	PEG	A	601	-	-	2/4/4/4	-
5	PEG	D	602	-	-	3/4/4/4	-
8	MLI	F	403	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	D	601	-	-	4/4/4/4	-
5	PEG	C	403	-	-	3/4/4/4	-
5	PEG	C	404	-	-	1/4/4/4	-
8	MLI	E	704	-	-	3/4/4/4	-
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	112.87

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	604	PEG	O1-C1-C2-O2
5	B	604	PEG	O2-C3-C4-O4
5	C	403	PEG	O2-C3-C4-O4
5	D	601	PEG	O1-C1-C2-O2
5	E	703	PEG	O2-C3-C4-O4

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
8	C	405	MLI	1	0
5	C	403	PEG	3	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%)	-0.31	3 (0%) 91 91	20, 36, 59, 92	0
1	D	582/584 (99%)	0.03	30 (5%) 27 24	30, 49, 81, 107	0
2	B	356/413 (86%)	-0.25	1 (0%) 94 94	21, 37, 70, 92	0
2	E	357/413 (86%)	-0.20	1 (0%) 94 94	26, 40, 76, 92	0
3	C	295/311 (94%)	-0.39	1 (0%) 94 94	18, 34, 51, 98	0
3	F	295/311 (94%)	-0.30	4 (1%) 75 73	26, 41, 65, 115	0
4	G	2/7 (28%)	0.71	0 100 100	64, 64, 64, 75	0
4	H	2/7 (28%)	0.04	0 100 100	54, 54, 54, 64	0
All	All	2471/2630 (93%)	-0.21	40 (1%) 72 69	18, 40, 73, 115	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	589	ALA	9.7
3	F	2	ASP	4.1
1	D	398	ARG	3.5
1	D	588	LEU	3.3
1	A	61	ASP	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	0.90	0.21	54,54,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAA	G	7	6/7	0.95	0.11	46,48,49,51	0
4	DAL	H	1	5/6	0.95	0.16	50,50,55,56	0
4	1ZN	G	5	23/24	0.95	0.16	38,42,45,51	0
4	1ZN	H	5	23/24	0.95	0.16	34,37,42,44	0
4	FGA	H	6	9/10	0.95	0.11	38,39,43,43	0
4	ACB	H	3	9/10	0.96	0.14	44,46,47,49	0
4	ACB	G	3	9/10	0.96	0.20	52,55,57,60	0
4	FGA	G	6	9/10	0.97	0.15	42,47,50,50	0
4	MAA	H	7	6/7	0.97	0.13	38,44,46,47	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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
5	PEG	A	604	7/7	0.70	0.35	64,66,71,76	0
5	PEG	D	601	7/7	0.72	0.18	65,76,85,87	0
5	PEG	C	404	7/7	0.76	0.25	62,70,75,78	0
8	MLI	C	405	7/7	0.80	0.20	47,53,56,59	0
5	PEG	D	602	7/7	0.81	0.23	72,73,76,78	0
5	PEG	A	602	7/7	0.81	0.24	57,65,79,80	0
5	PEG	E	703	7/7	0.84	0.25	59,64,65,66	0
5	PEG	B	604	7/7	0.86	0.26	62,63,65,68	0
5	PEG	A	601	7/7	0.86	0.20	71,72,76,76	0
5	PEG	C	403	7/7	0.87	0.15	41,45,53,56	0
6	CA	E	702	1/1	0.88	0.06	48,48,48,48	0
8	MLI	E	704	7/7	0.88	0.24	61,63,66,66	0
6	CA	B	602	1/1	0.91	0.07	43,43,43,43	0
8	MLI	F	403	7/7	0.91	0.25	67,69,73,73	0
5	PEG	B	603	7/7	0.92	0.21	67,67,72,72	0
5	PEG	A	603	7/7	0.92	0.13	62,65,67,68	0
6	CA	E	701	1/1	0.97	0.07	27,27,27,27	0
7	MN	F	402	1/1	0.98	0.06	43,43,43,43	0
6	CA	B	601	1/1	0.99	0.06	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MN	C	401	1/1	0.99	0.08	34,34,34,34	0
7	MN	C	402	1/1	0.99	0.05	40,40,40,40	0
7	MN	F	401	1/1	0.99	0.06	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.