Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:19 PM GMT

PDB ID	:	4LAC
Title	:	Crystal Structure of Protein Phosphatase 2A (PP2A) and PP2A phosphatase activator (PTPA) complex with ATPgammaS
Authors	:	Guo, F.; Stanevich, V.; Wlodarchak, N.; Satyshur, K.A.; Xing, Y.
Deposited on	:	2013-06-19
Resolution	:	2.82 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

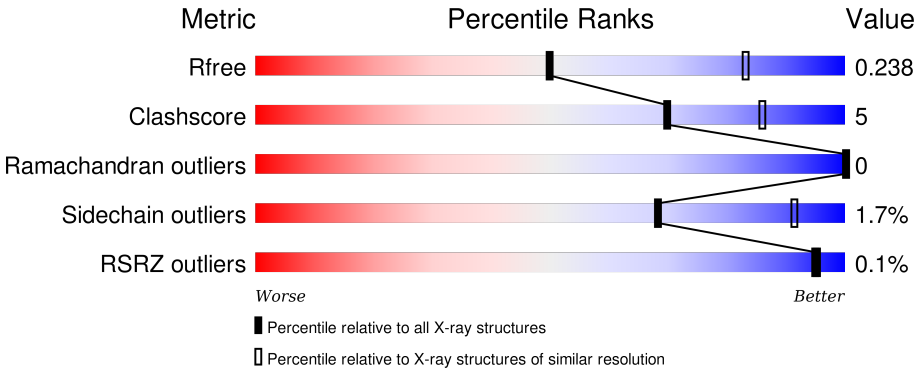
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.82 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	308	88% 10% •
2	A	258	77% 12% 11%
3	C	311	80% 12% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	A	601	-	-	X	-
7	MES	C	504	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6813 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 activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	301	Total	C	N	O	S	0	0	0
			2441	1588	407	435	11			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	GLY	-	EXPRESSION TAG	UNP Q15257
B	17	SER	-	EXPRESSION TAG	UNP Q15257
B	18	MET	-	EXPRESSION TAG	UNP Q15257
B	?	-	SER	DELETION	UNP Q15257
B	?	-	GLU	DELETION	UNP Q15257
B	?	-	MET	DELETION	UNP Q15257
B	?	-	TRP	DELETION	UNP Q15257
B	?	-	ASN	DELETION	UNP Q15257
B	?	-	GLU	DELETION	UNP Q15257
B	?	-	VAL	DELETION	UNP Q15257
B	?	-	HIS	DELETION	UNP Q15257
B	?	-	GLU	DELETION	UNP Q15257
B	?	-	GLU	DELETION	UNP Q15257
B	?	-	LYS	DELETION	UNP Q15257
B	?	-	GLU	DELETION	UNP Q15257
B	?	-	GLN	DELETION	UNP Q15257
B	?	-	ALA	DELETION	UNP Q15257
B	?	-	ALA	DELETION	UNP Q15257
B	?	-	LYS	DELETION	UNP Q15257
B	?	-	GLN	DELETION	UNP Q15257
B	?	-	SER	DELETION	UNP Q15257
B	?	-	VAL	DELETION	UNP Q15257
B	?	-	SER	DELETION	UNP Q15257
B	?	-	CYS	DELETION	UNP Q15257
B	?	-	ASP	DELETION	UNP Q15257
B	?	-	GLU	DELETION	UNP Q15257
B	?	-	CYS	DELETION	UNP Q15257

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ILE	DELETION	UNP Q15257
B	?	-	PRO	DELETION	UNP Q15257
B	?	-	LEU	DELETION	UNP Q15257
B	?	-	PRO	DELETION	UNP Q15257
B	?	-	ARG	DELETION	UNP Q15257
B	?	-	ALA	DELETION	UNP Q15257
B	?	-	GLY	DELETION	UNP Q15257
B	?	-	HIS	DELETION	UNP Q15257
B	?	-	CYS	DELETION	UNP Q15257
B	?	-	ALA	DELETION	UNP Q15257
B	?	-	PRO	DELETION	UNP Q15257

- Molecule 2 is a protein called PP2A Scaffold Subunit A, Truncated, an internal deletion of PP2A A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	229	Total	C	N	O	S	0	0	0
			1807	1162	302	333	10			

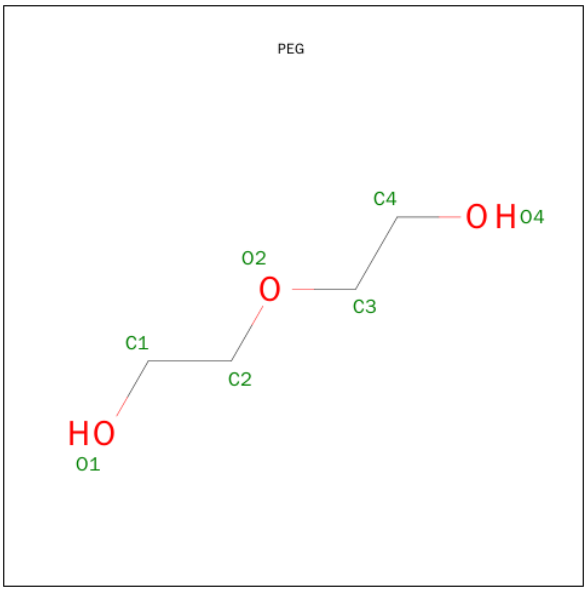
- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	290	Total	C	N	O	S	0	0	0
			2338	1482	399	442	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	EXPRESSION TAG	UNP P67775
C	0	SER	-	EXPRESSION TAG	UNP P67775

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

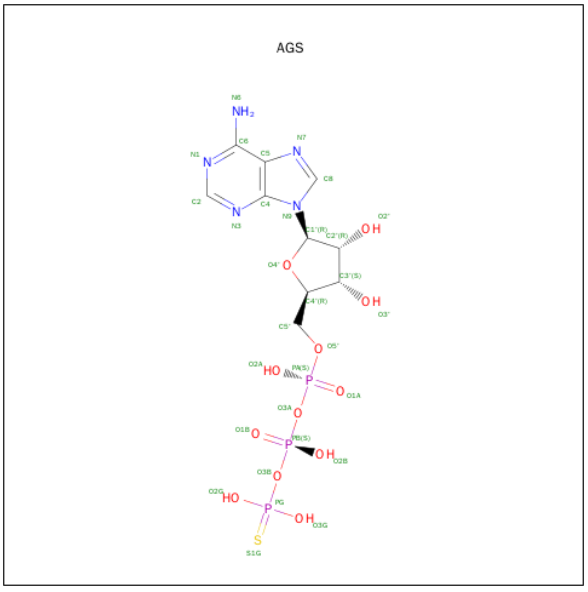


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0

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

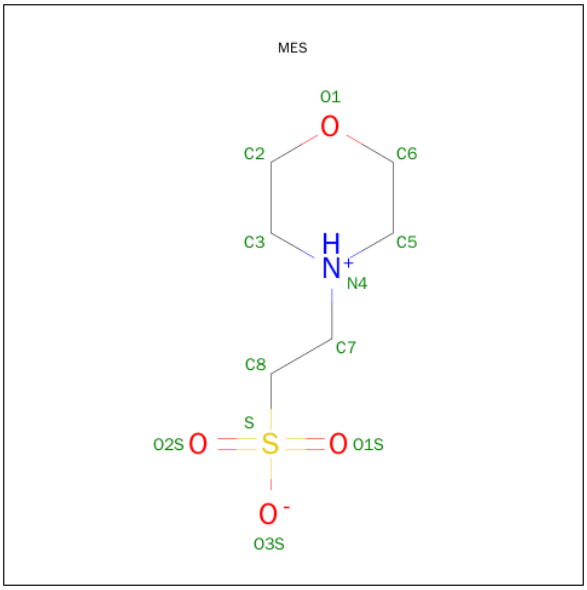
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	2	Total Mn 2 2	0	0

- Molecule 6 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 8 is water.

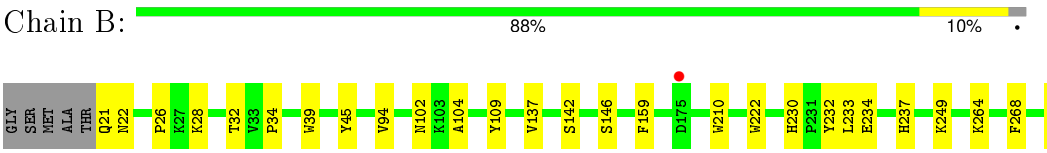
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	64	Total	O	0	0
			64	64		
8	A	33	Total	O	0	0
			33	33		
8	C	78	Total	O	0	0
			78	78		

3 Residue-property plots (i)

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

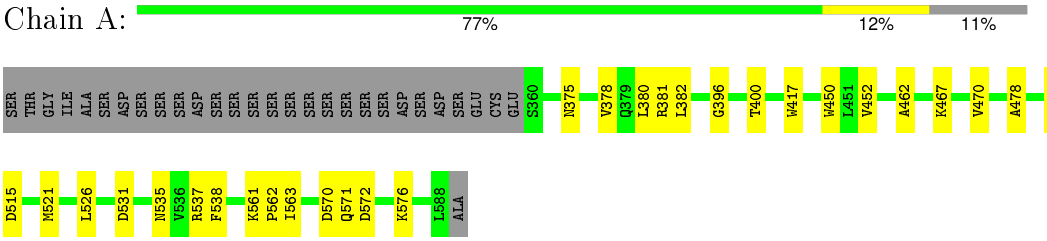
- Molecule 1: Serine/threonine-protein phosphatase 2A activator

Chain B:



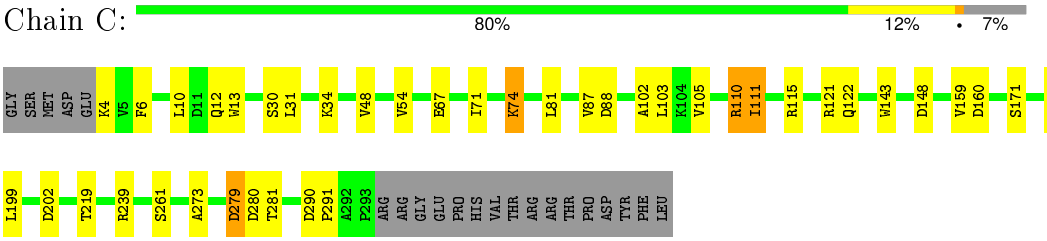
- Molecule 2: PP2A Scaffold Subunit A, Truncated, an internal deletion of PP2A A

Chain A:



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

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.07Å 100.19Å 167.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.82 48.76 – 2.82	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-2.82) 99.0 (48.76-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.188 , 0.242 0.184 , 0.238	Depositor DCC
R_{free} test set	1221 reflections (5.45%)	DCC
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 26.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 23601 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6813	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, AGS, MES, MN

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	B	0.51	3/2509 (0.1%)	0.50	0/3405
2	A	0.44	0/1837	0.52	0/2492
3	C	0.49	2/2395 (0.1%)	0.56	0/3248
All	All	0.48	5/6741 (0.1%)	0.53	0/9145

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	222	TRP	CD2-CE2	5.32	1.47	1.41
1	B	210	TRP	CD2-CE2	5.17	1.47	1.41
3	C	143	TRP	CD2-CE2	5.12	1.47	1.41
1	B	276	TRP	CD2-CE2	5.06	1.47	1.41
3	C	13	TRP	CD2-CE2	5.06	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2441	0	2426	20	0
2	A	1807	0	1880	20	0
3	C	2338	0	2246	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	7	0	10	4	0
5	C	2	0	0	0	0
6	C	31	0	12	0	0
7	C	12	0	13	0	0
8	A	33	0	0	0	0
8	B	64	0	0	1	0
8	C	78	0	0	1	0
All	All	6813	0	6587	60	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 5.

All (60) 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)
2:A:417:TRP:HD1	4:A:601:PEG:H31	1.16	1.10
1:B:234:GLU:H	1:B:237:HIS:HD2	1.10	0.98
2:A:417:TRP:CD1	4:A:601:PEG:H31	2.06	0.89
3:C:74:LYS:HE3	8:C:645:HOH:O	1.80	0.81
3:C:103:LEU:HB3	3:C:111:ILE:HD11	1.65	0.77
1:B:230:HIS:HD2	1:B:233:LEU:H	1.33	0.76
1:B:230:HIS:CD2	1:B:233:LEU:H	2.04	0.74
2:A:417:TRP:H	4:A:601:PEG:H42	1.52	0.72
3:C:290:ASP:HB3	3:C:291:PRO:HD2	1.76	0.66
2:A:505:ILE:HG23	2:A:521:MET:HE2	1.76	0.66
2:A:417:TRP:N	4:A:601:PEG:H42	2.12	0.64
3:C:4:LYS:HG3	3:C:6:PHE:H	1.63	0.64
1:B:102:ASN:HD22	1:B:104:ALA:H	1.48	0.61
3:C:103:LEU:HB3	3:C:111:ILE:CD1	2.31	0.59
3:C:171:SER:HB2	3:C:197:ASP:HB2	1.84	0.59
1:B:234:GLU:H	1:B:237:HIS:CD2	2.03	0.56
3:C:31:LEU:HD11	3:C:102:ALA:HA	1.87	0.55
2:A:570:ASP:O	2:A:576:LYS:HE3	2.06	0.55
1:B:264:LYS:HD3	1:B:271:HIS:HB2	1.90	0.54
3:C:6:PHE:CZ	3:C:34:LYS:HD3	2.42	0.54
2:A:396:GLY:O	2:A:400:THR:HG23	2.07	0.54
3:C:87:VAL:O	3:C:88:ASP:HB2	2.08	0.52
1:B:94:VAL:H	1:B:102:ASN:HD21	1.58	0.52
1:B:300:LEU:HA	1:B:306:ILE:HD11	1.93	0.51
3:C:202:ASP:O	3:C:219:THR:HA	2.10	0.51
3:C:67:GLU:O	3:C:71:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LYS:HE2	1:B:308:HIS:HA	1.92	0.50
3:C:48:VAL:O	3:C:159:VAL:HA	2.13	0.49
1:B:102:ASN:ND2	1:B:104:ALA:H	2.09	0.49
2:A:378:VAL:HA	2:A:381:ARG:HD2	1.94	0.49
1:B:32:THR:HB	1:B:34:PRO:HD2	1.94	0.49
1:B:230:HIS:HD2	1:B:232:TYR:H	1.59	0.49
2:A:572:ASP:OD1	3:C:110:ARG:NH1	2.47	0.47
2:A:531:ASP:O	2:A:537:ARG:HD3	2.14	0.47
2:A:452:VAL:CG1	2:A:452:VAL:O	2.63	0.47
1:B:109:TYR:CD2	1:B:146:SER:HB2	2.50	0.46
2:A:375:ASN:ND2	2:A:380:LEU:HD12	2.30	0.46
1:B:26:PRO:HD2	1:B:137:VAL:HG21	1.97	0.46
2:A:467:LYS:HB2	2:A:507:VAL:CG1	2.46	0.46
3:C:279:ASP:HB3	3:C:281:THR:H	1.81	0.45
1:B:21:GLN:HB2	1:B:22:ASN:H	1.61	0.45
3:C:54:VAL:HG22	3:C:81:LEU:HD23	1.99	0.44
2:A:535:ASN:HA	2:A:538:PHE:CE2	2.52	0.44
3:C:115:ARG:O	3:C:199:LEU:HD22	2.18	0.44
2:A:450:TRP:HB3	2:A:462:ALA:HB2	2.01	0.43
1:B:268:PHE:HA	1:B:271:HIS:CE1	2.53	0.43
2:A:526:LEU:HD22	2:A:563:ILE:HG13	2.00	0.43
3:C:261:SER:HA	3:C:273:ALA:HB1	2.00	0.43
1:B:39:TRP:CZ2	1:B:45:TYR:HD1	2.36	0.43
2:A:521:MET:HE2	2:A:521:MET:HB3	1.98	0.42
1:B:142:SER:HB2	1:B:159:PHE:HB2	2.01	0.42
3:C:121:ARG:NH2	3:C:148:ASP:OD1	2.46	0.42
2:A:561:LYS:N	2:A:562:PRO:HD2	2.35	0.41
1:B:230:HIS:CD2	1:B:232:TYR:H	2.36	0.41
2:A:470:VAL:HG22	2:A:478:ALA:HB2	2.03	0.41
1:B:249:LYS:HD3	8:B:453:HOH:O	2.21	0.41
3:C:10:LEU:HD11	3:C:105:VAL:HG12	2.03	0.41
3:C:122:GLN:HG2	3:C:188:GLU:OE2	2.21	0.40
3:C:103:LEU:CB	3:C:111:ILE:CD1	3.00	0.40
2:A:375:ASN:HD22	2:A:380:LEU:HB2	1.86	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	B	299/308 (97%)	286 (96%)	13 (4%)	0	100	100
2	A	227/258 (88%)	225 (99%)	2 (1%)	0	100	100
3	C	288/311 (93%)	275 (96%)	13 (4%)	0	100	100
All	All	814/877 (93%)	786 (97%)	28 (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	B	263/267 (98%)	263 (100%)	0	100	100
2	A	202/228 (89%)	199 (98%)	3 (2%)	72	93
3	C	256/275 (93%)	247 (96%)	9 (4%)	43	76
All	All	721/770 (94%)	709 (98%)	12 (2%)	68	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	382	LEU
2	A	515	ASP
2	A	571	GLN
3	C	12	GLN
3	C	30	SER

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Mol	Chain	Res	Type
3	C	74	LYS
3	C	110	ARG
3	C	111	ILE
3	C	160	ASP
3	C	239	ARG
3	C	279	ASP
3	C	280	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	102	ASN
1	B	230	HIS
1	B	237	HIS
1	B	274	GLN
2	A	444	ASN
2	A	514	GLN
3	C	122	GLN
3	C	179	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	PEG	A	601	-	6,6,6	0.54	0	5,5,5	0.26	0
6	AGS	C	503	5	24,33,33	2.01	3 (12%)	28,52,52	1.99	4 (14%)
7	MES	C	504	-	11,12,12	0.90	0	14,16,16	7.22	7 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	601	-	-	0/4/4/4	0/0/0/0
6	AGS	C	503	5	-	0/15/38/38	0/3/3/3
7	MES	C	504	-	-	0/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	503	AGS	O4'-C1'	2.03	1.43	1.41
6	C	503	AGS	C5-C4	3.17	1.47	1.40
6	C	503	AGS	PG-S1G	8.39	2.06	1.90

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	504	MES	O3S-S-O2S	-11.70	84.38	111.61
7	C	504	MES	O3S-S-O1S	-11.42	85.04	111.61
6	C	503	AGS	N3-C2-N1	-7.82	122.90	128.89
6	C	503	AGS	PA-O3A-PB	-3.39	123.22	132.73
6	C	503	AGS	C4-C5-N7	-3.38	106.37	109.48
6	C	503	AGS	PB-O3B-PG	-2.80	123.27	132.67
7	C	504	MES	C6-C5-N4	2.56	114.00	110.12
7	C	504	MES	C2-C3-N4	3.07	114.77	110.12
7	C	504	MES	C5-N4-C3	3.19	115.80	108.90
7	C	504	MES	O2S-S-C8	14.42	119.21	106.91
7	C	504	MES	O1S-S-C8	15.01	119.72	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	PEG	4	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	B	301/308 (97%)	-0.39	1 (0%) 94 92	27, 38, 54, 66	0
2	A	229/258 (88%)	-0.28	0 100 100	25, 41, 58, 75	0
3	C	290/311 (93%)	-0.46	0 100 100	23, 31, 41, 63	0
All	All	820/877 (93%)	-0.39	1 (0%) 95 95	23, 35, 54, 75	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	MES	C	504	12/12	0.95	0.28	7.22	46,48,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	PEG	A	601	7/7	0.79	0.18	0.16	38,40,44,44	0
6	AGS	C	503	31/31	0.97	0.13	-0.99	29,31,35,36	0
5	MN	C	501	1/1	0.99	0.10	-1.99	25,25,25,25	0
5	MN	C	502	1/1	0.99	0.07	-3.23	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.